

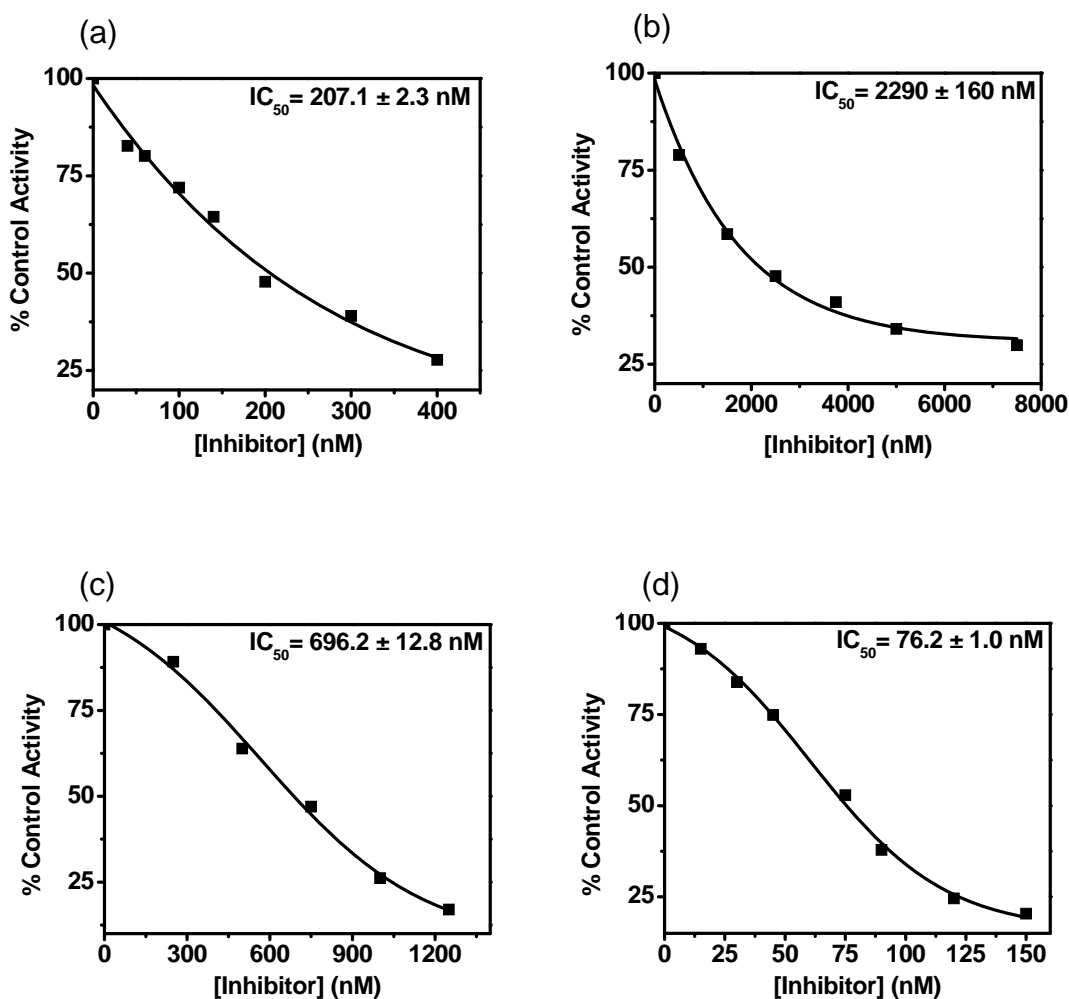
Supporting Information for

Effect of Peptide-based Captopril Analogues on Angiotensin Converting Enzyme Activity and Peroxynitrite-mediated Tyrosine Nitration

by

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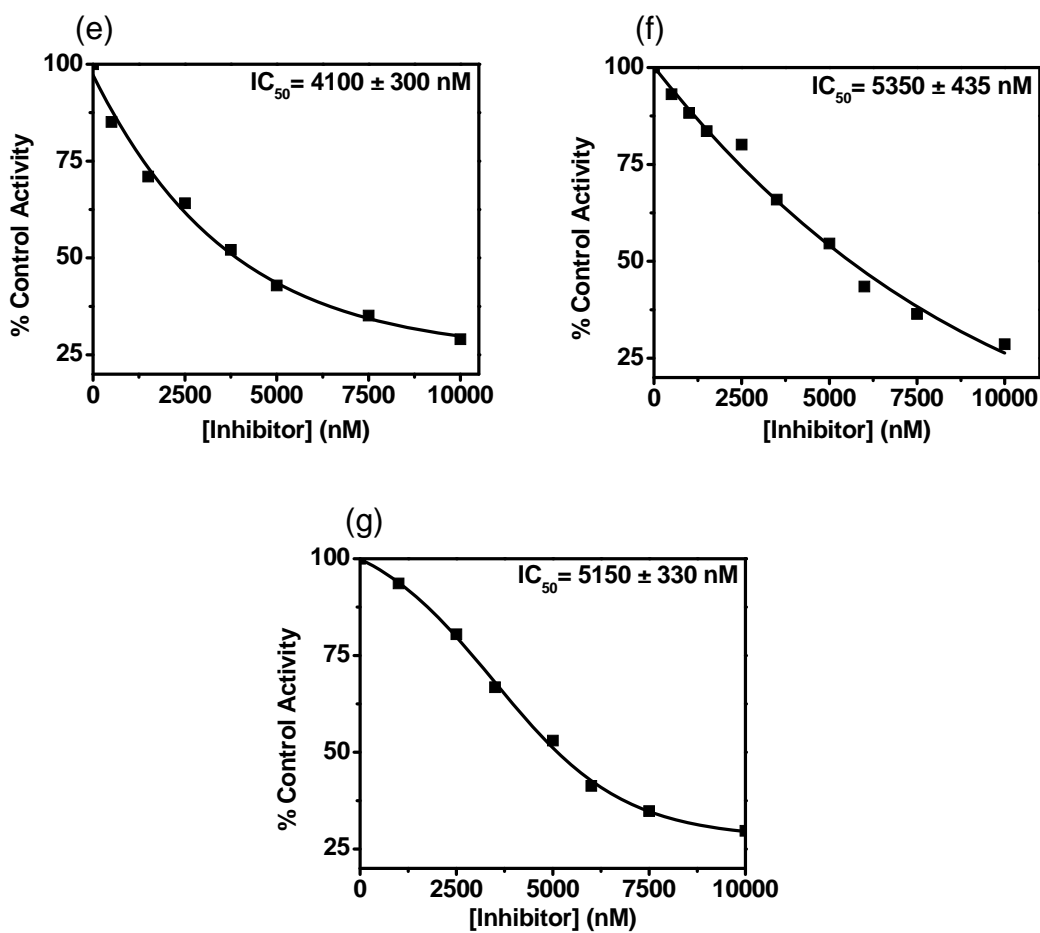
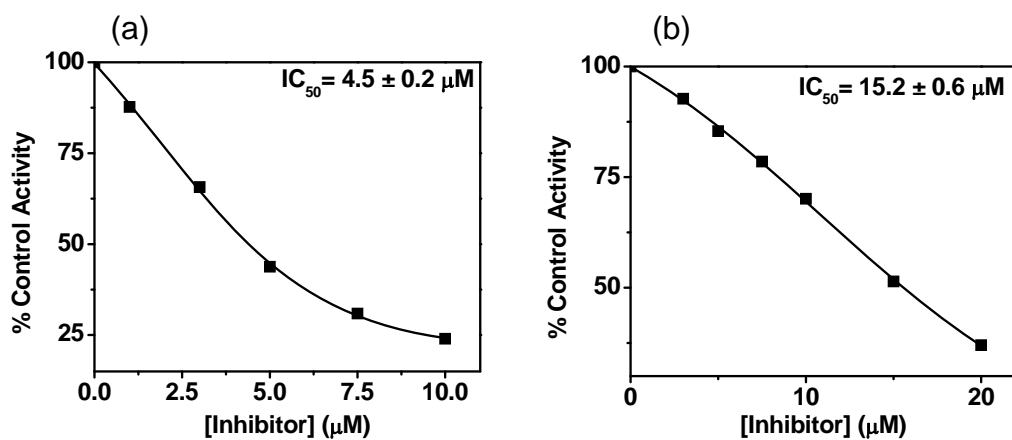
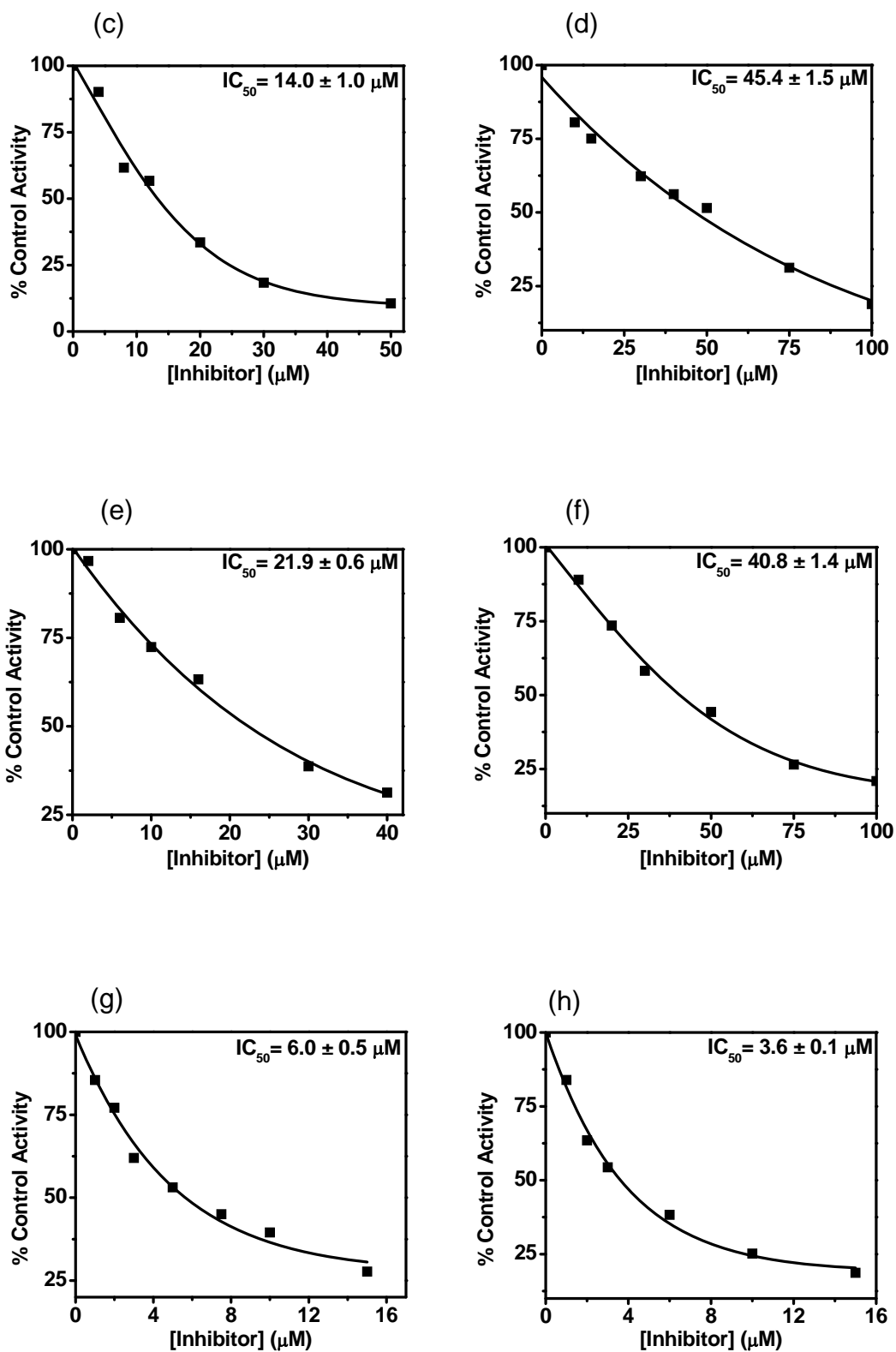
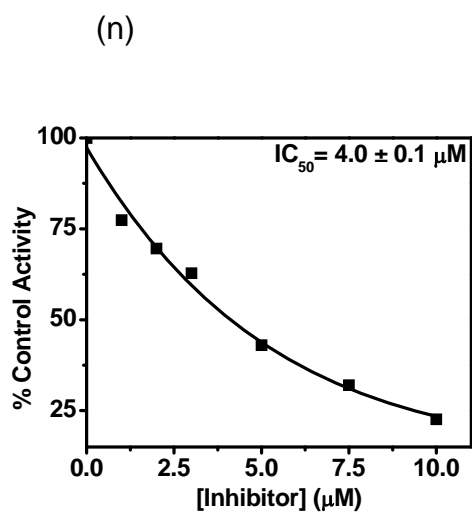
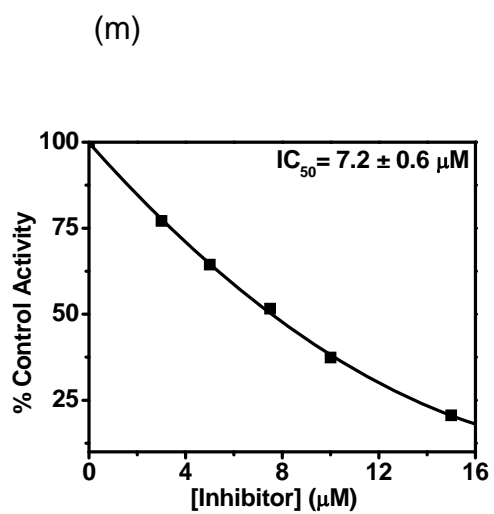
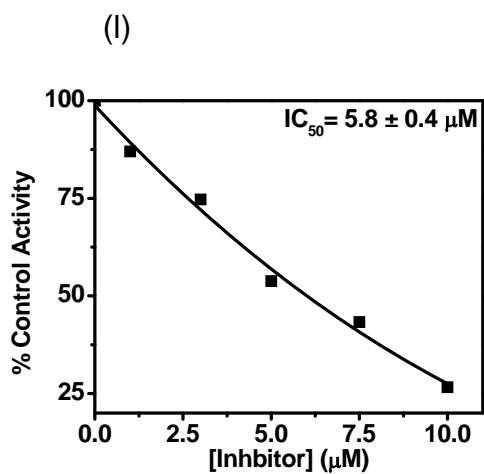
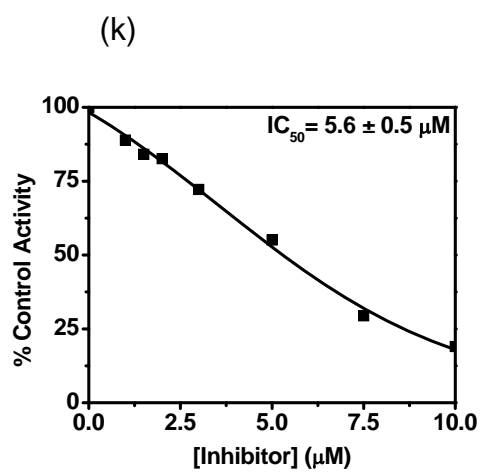
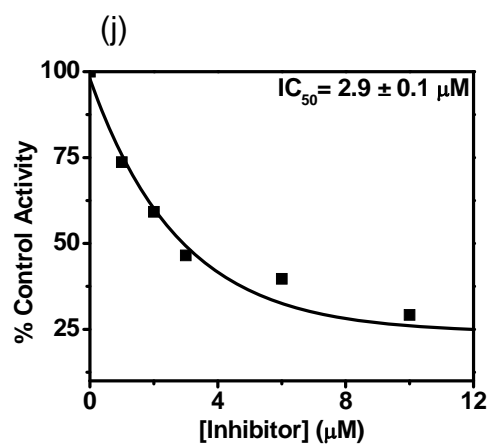
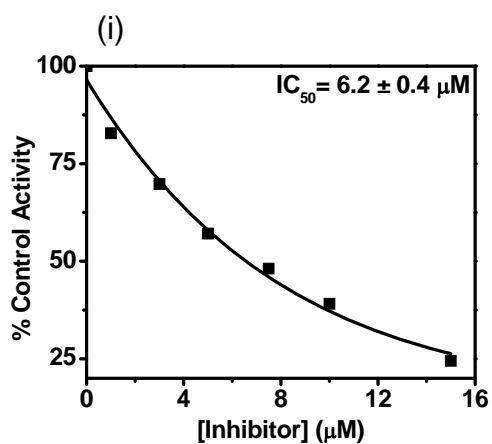


Figure S1. Inhibition plots for ACE-catalyzed hydrolysis of Ang I to Ang II by compounds a) **5**, b) **6**, c) **7**, d) **9**, e) **10**, f) **11** and g) **13**.







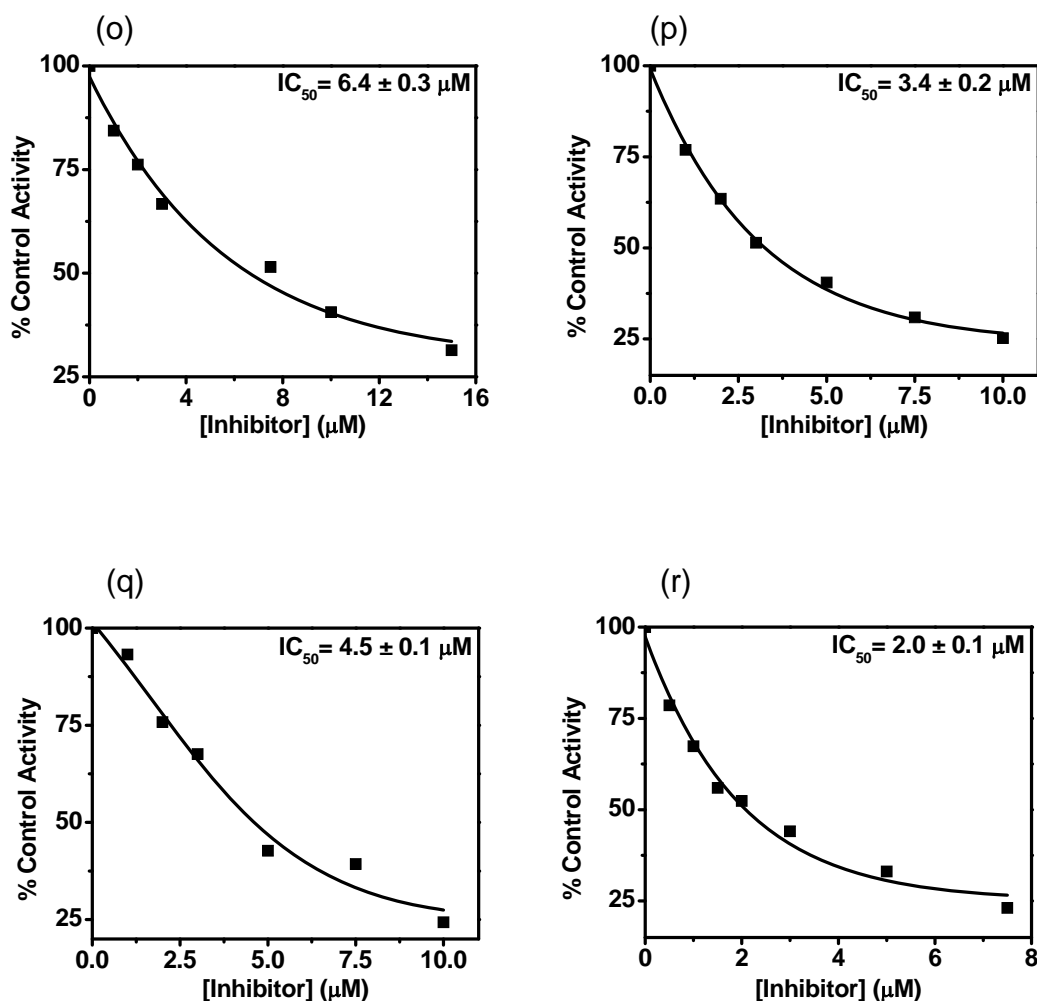


Figure S2. Inhibition plots for PN-mediated nitration of Ang II by compounds a) **5**, b) **6**, c) **7**, d) **23**, e) **8**, f) **22**, g) **9**, h) **31**, i) **10**, j) **28**, k) **11**, l) **32**, m) **12**, n) **29**, o) **13**, p) **33**, q) **14** and r) **30**. Assay condition: Reactions were carried out in sodium phosphate buffer (100 mM, pH 7.5) at 22 °C with a final concentration of 20 μM Ang II, 300 μM PN and different concentrations of the inhibitors.

Table S1. Inhibition of ACE activity by disulfide (**22** and **23**) and diselenides (**28-33**) at 50 μM concentration.

Compound	% Inhibition	Compound	% Inhibition
19	25.1	20	22.9
22	13.1	23	26.3
28	30.0	29	7.6
30	10.0	31	28.9
32	9.7	33	12.9

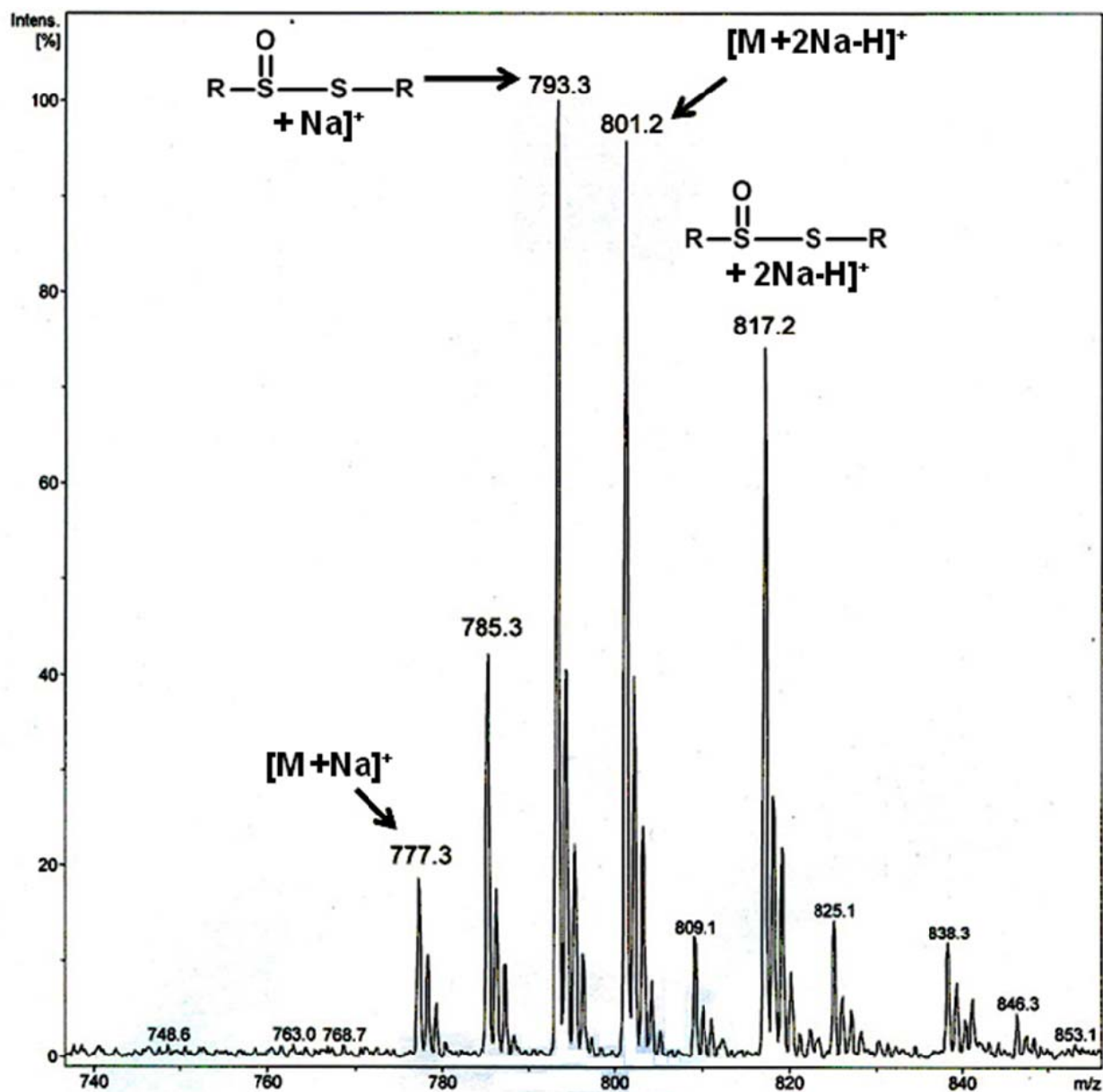


Figure S3. ESI mass spectrum of the reaction mixture of compound 22 with PN.

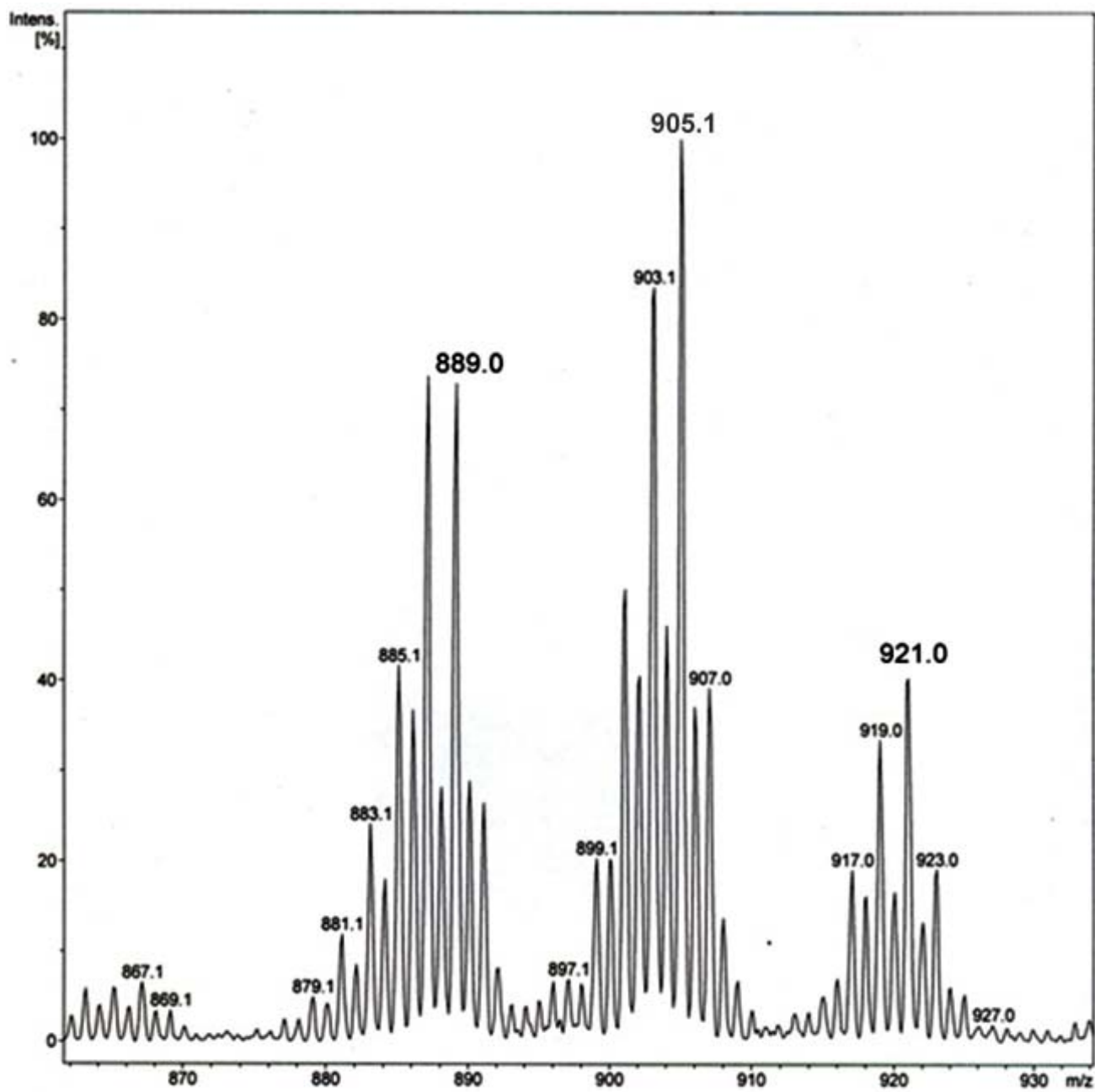


Figure S4. ESI mass spectrum of the reaction mixture of compound **28** with PN.

Figure S5. ^1H NMR Spectrum of Compound **19** in D_2O

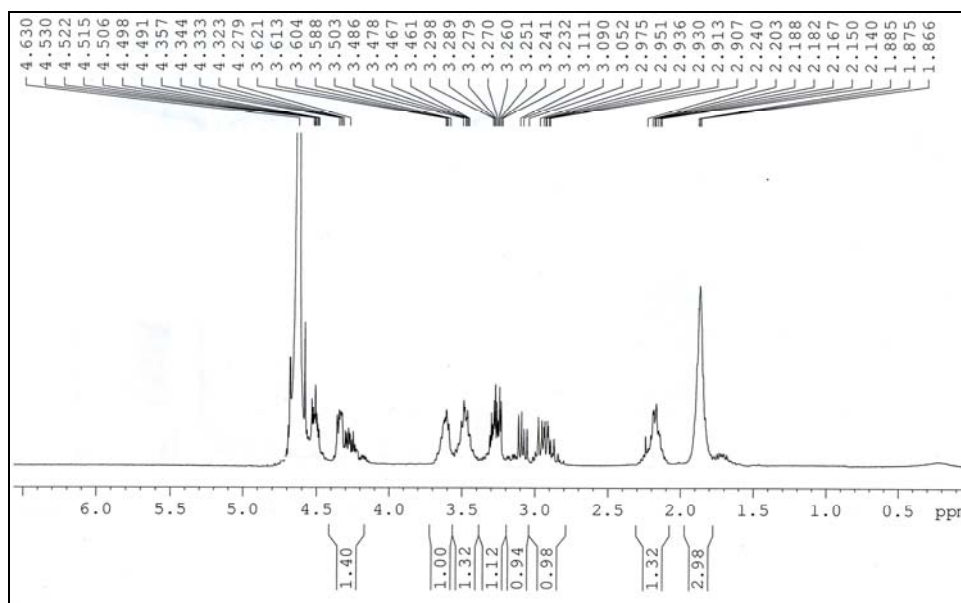


Figure S6. ^{13}C NMR Spectrum of Compound **19** in D_2O

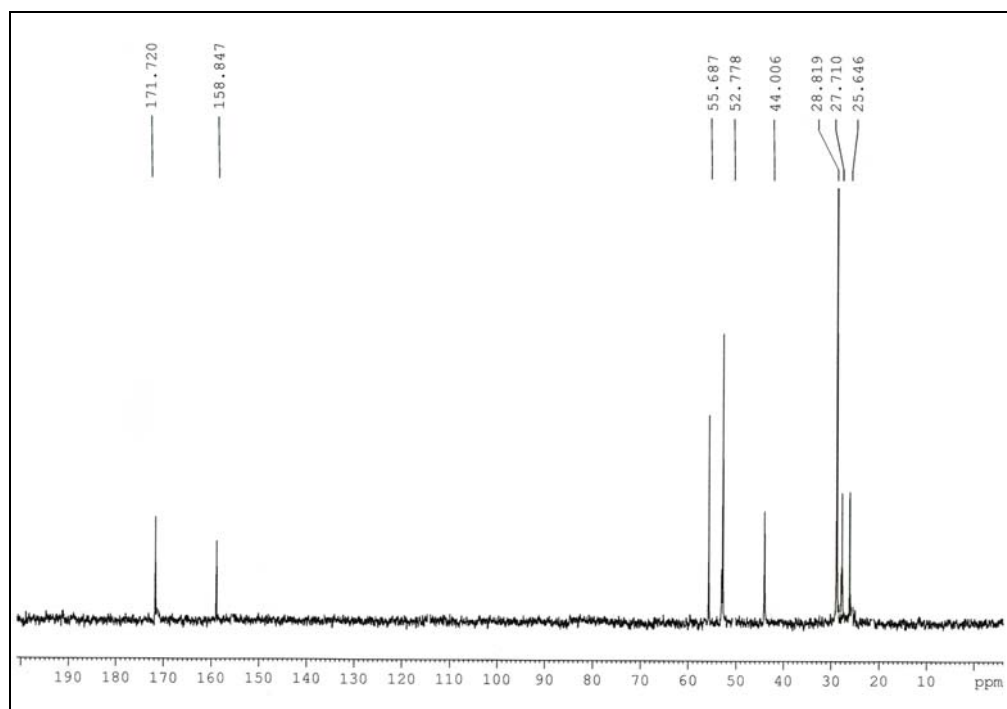


Figure S7. ^{77}Se NMR Spectrum of Compound **19** in D_2O

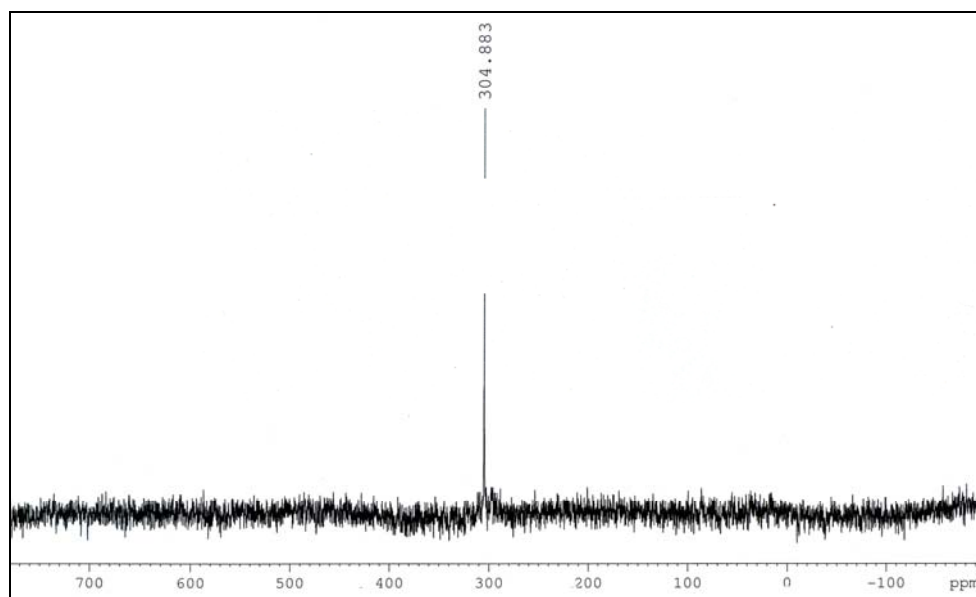


Figure S8. ESI mass Spectrum of the compound **19**. Calculated Mass: 531.0261, found 530.8870.

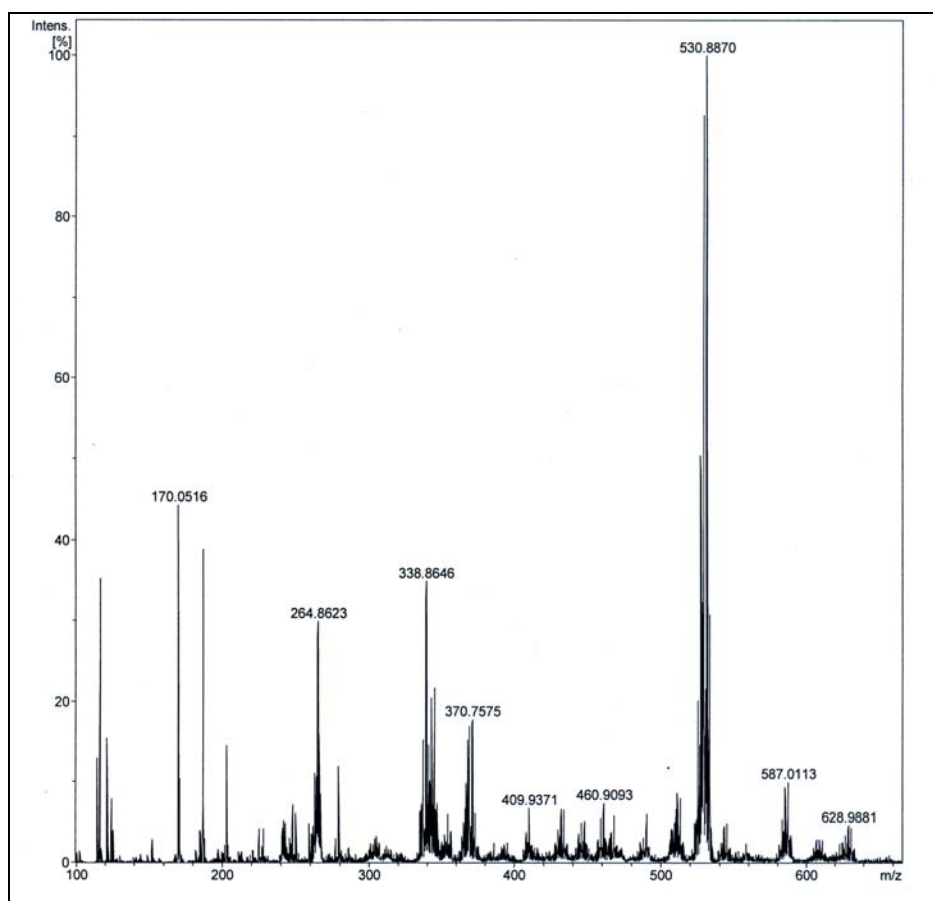


Figure S9. ^1H NMR Spectrum of Compound **20** in D_2O .

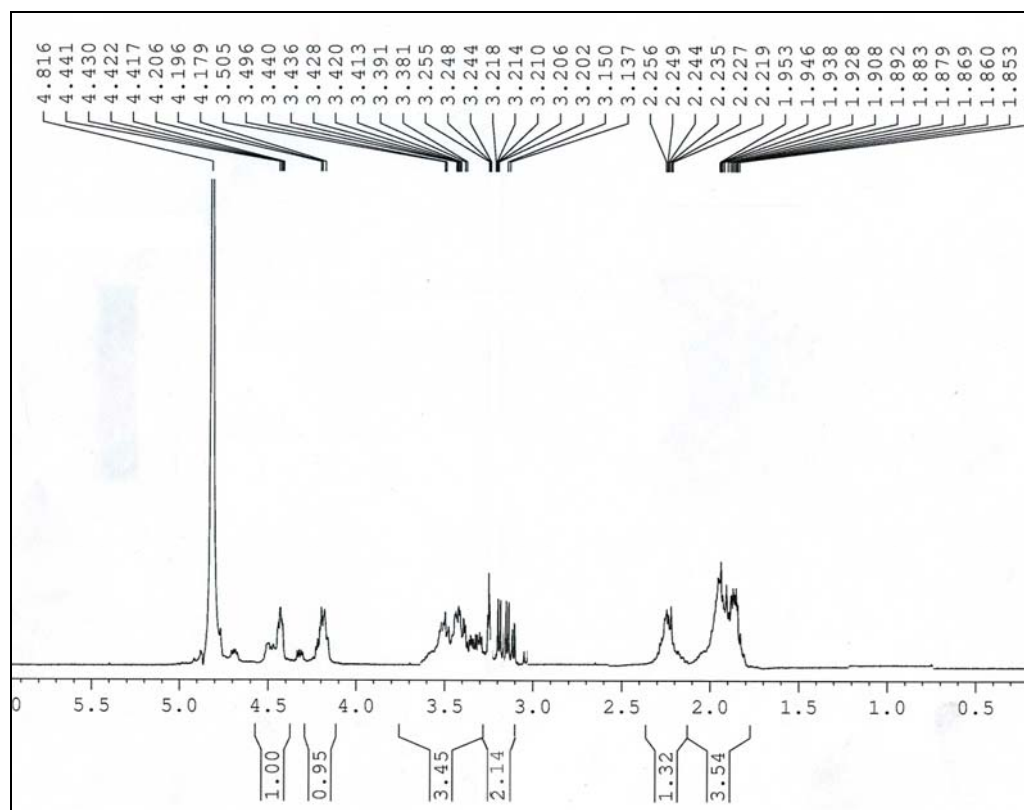


Figure S10. ^{13}C NMR Spectrum of Compound **20** in D_2O

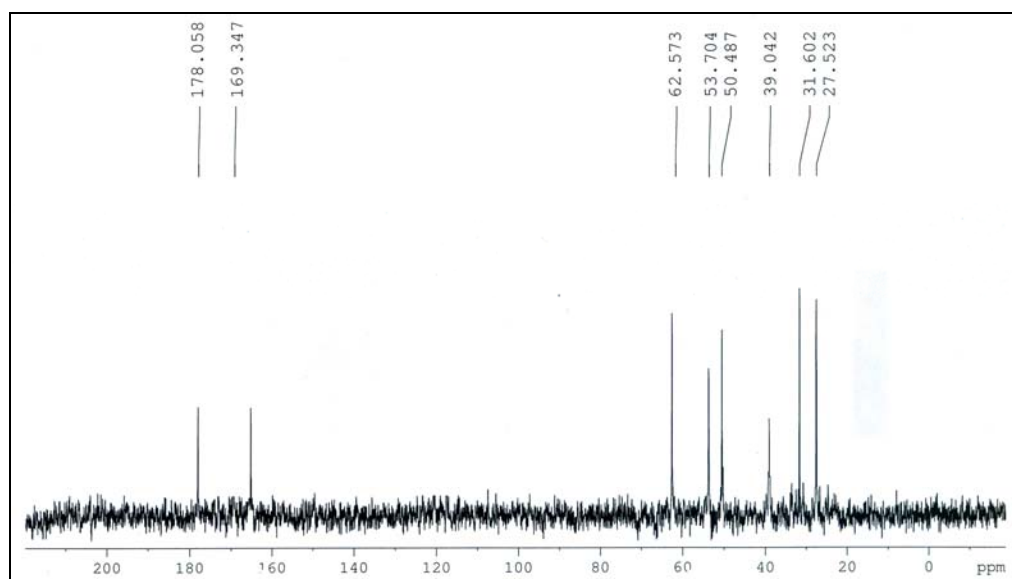


Figure S11. ESI mass Spectrum of the compound **20**. Calculated Mass: 435.1372, found 434.9422.

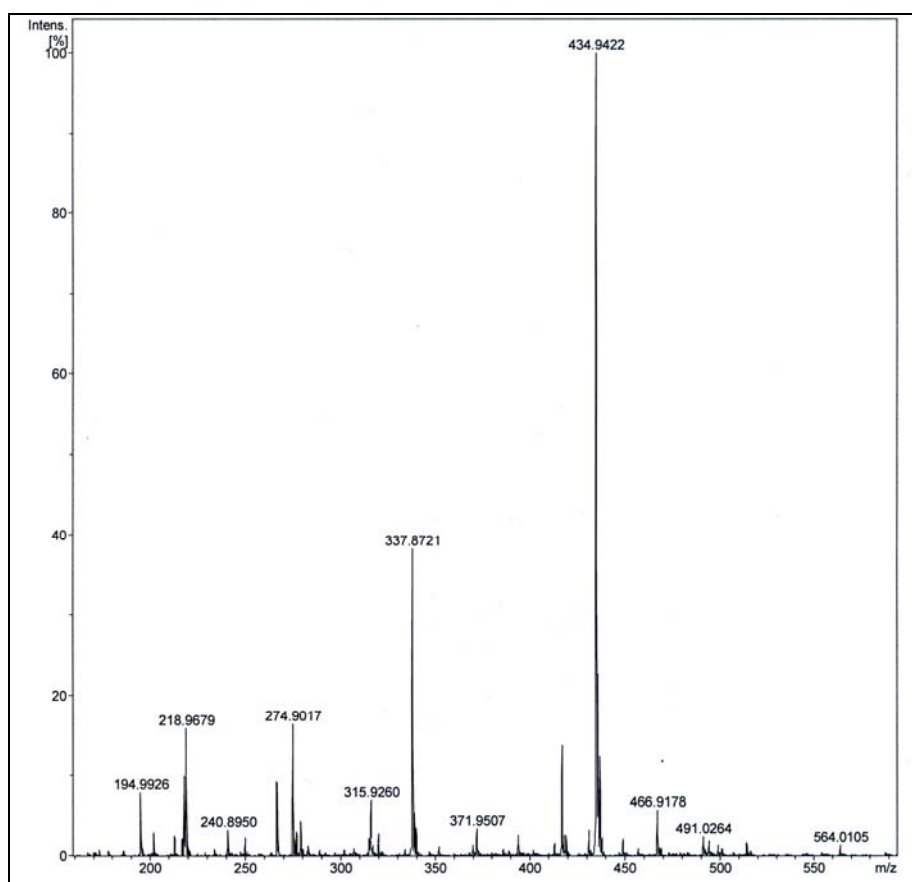


Figure S12. ^1H NMR Spectrum of Compound **22** in CDCl_3

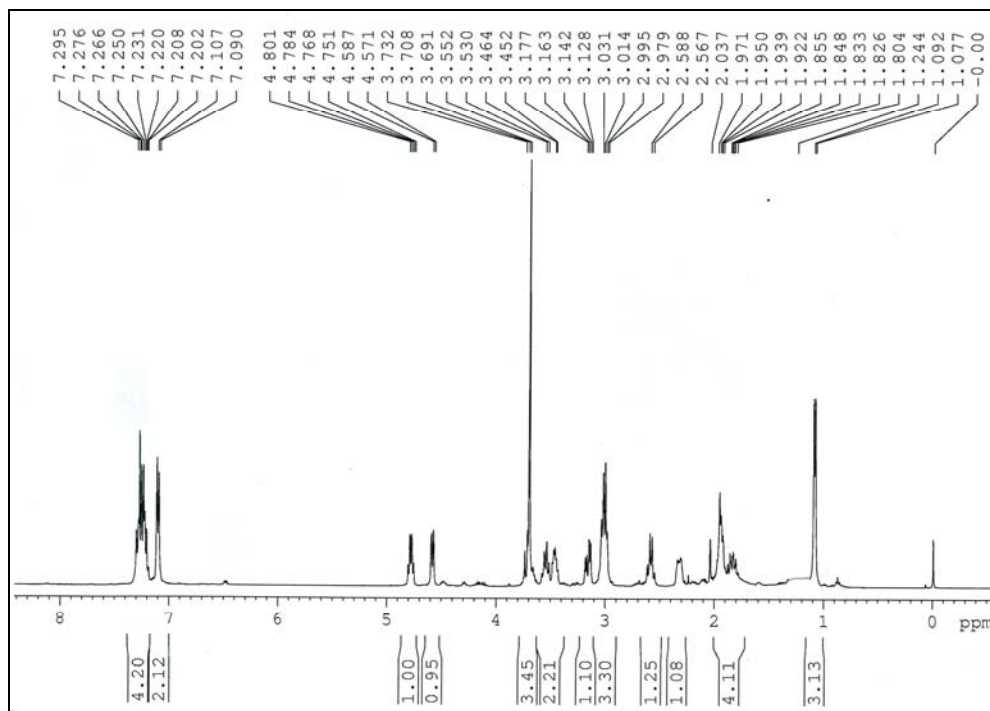


Figure S13. ^{13}C NMR Spectrum of Compound **22** in CDCl_3

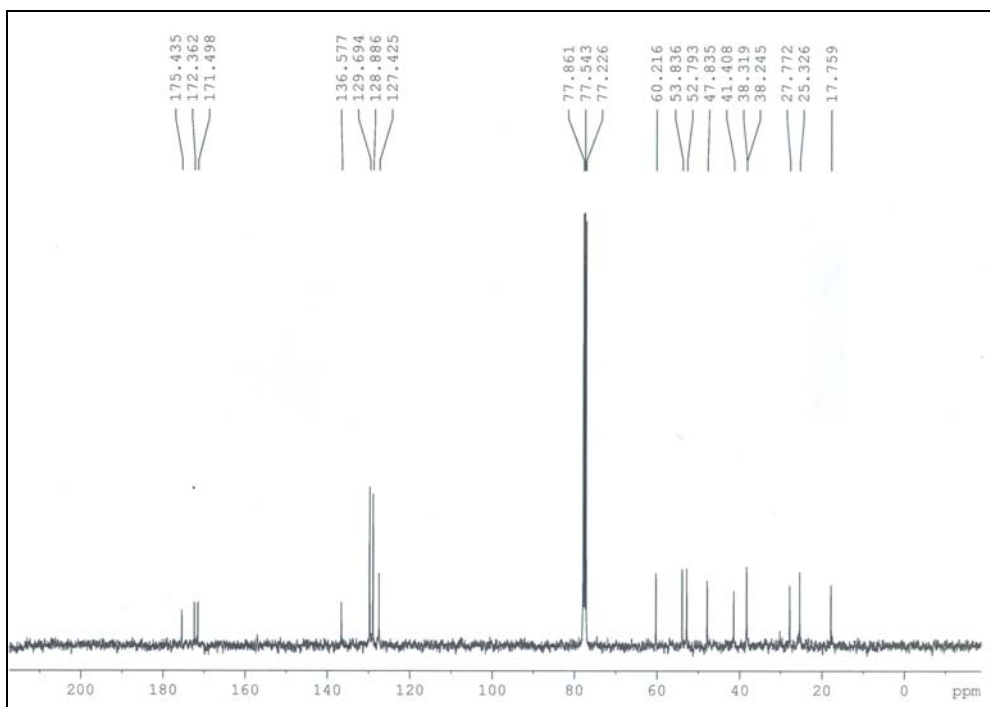


Figure S14. ESI mass Spectrum of the compound **22**. Calculated Mass: 777.2968, found 777.2960

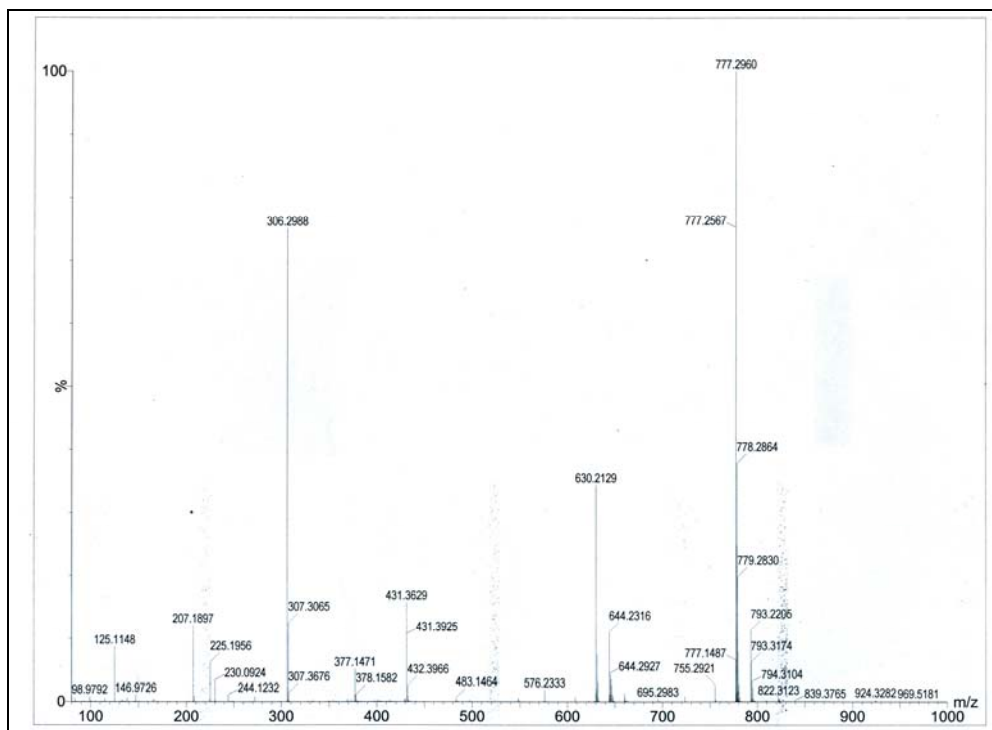


Figure S15. ^1H NMR Spectrum of Compound **23** in CDCl_3

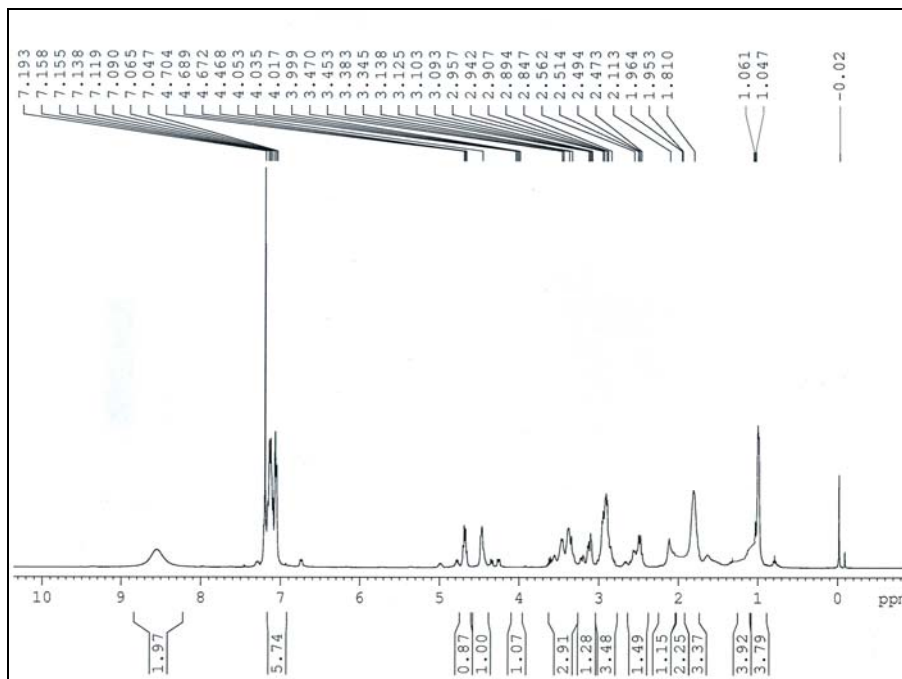


Figure S16. ^{13}C NMR Spectrum of Compound **23** in CDCl_3

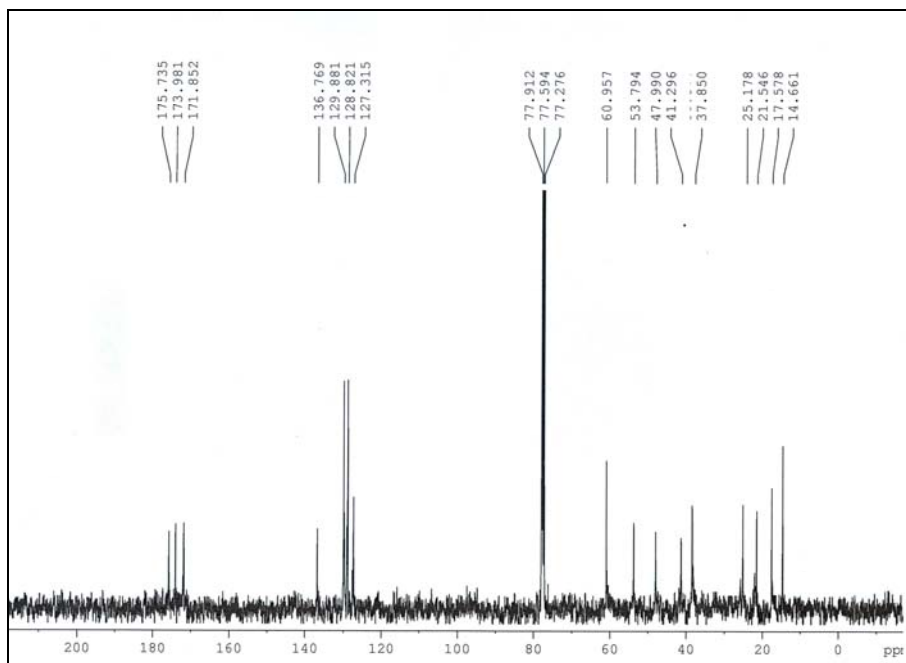
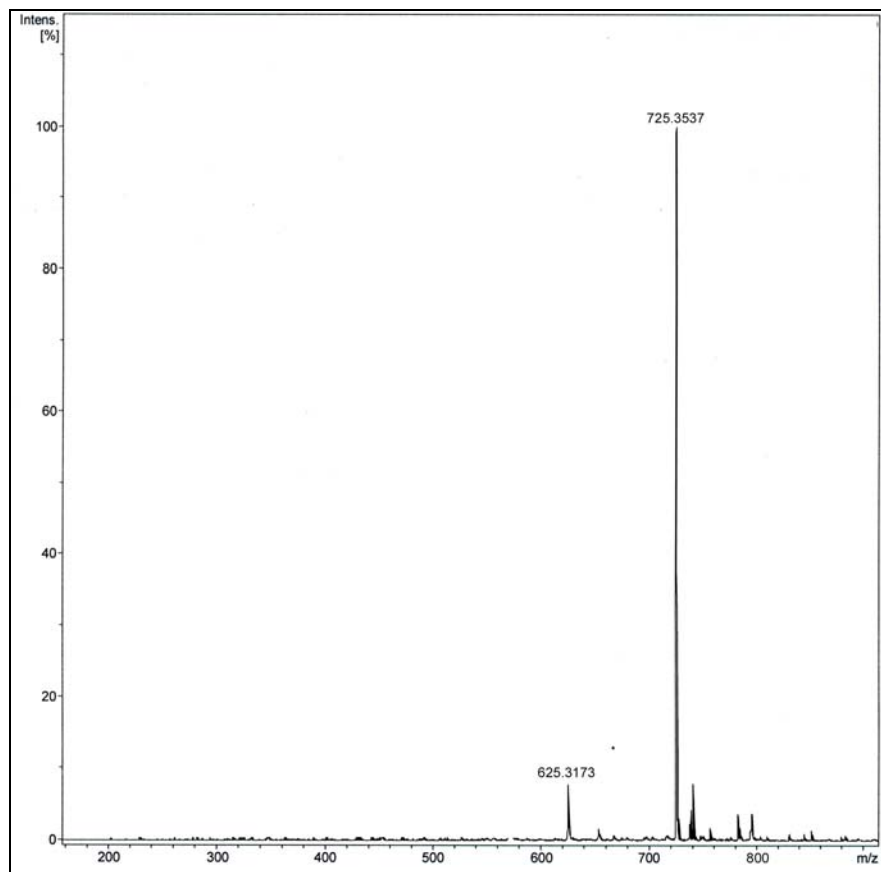


Figure S17. ESI mass Spectrum of the compound **23**. Calculated Mass: 725.2679, found 725.3537



[S14]

Figure S18. ^1H NMR Spectrum of Compound **25** in CDCl_3

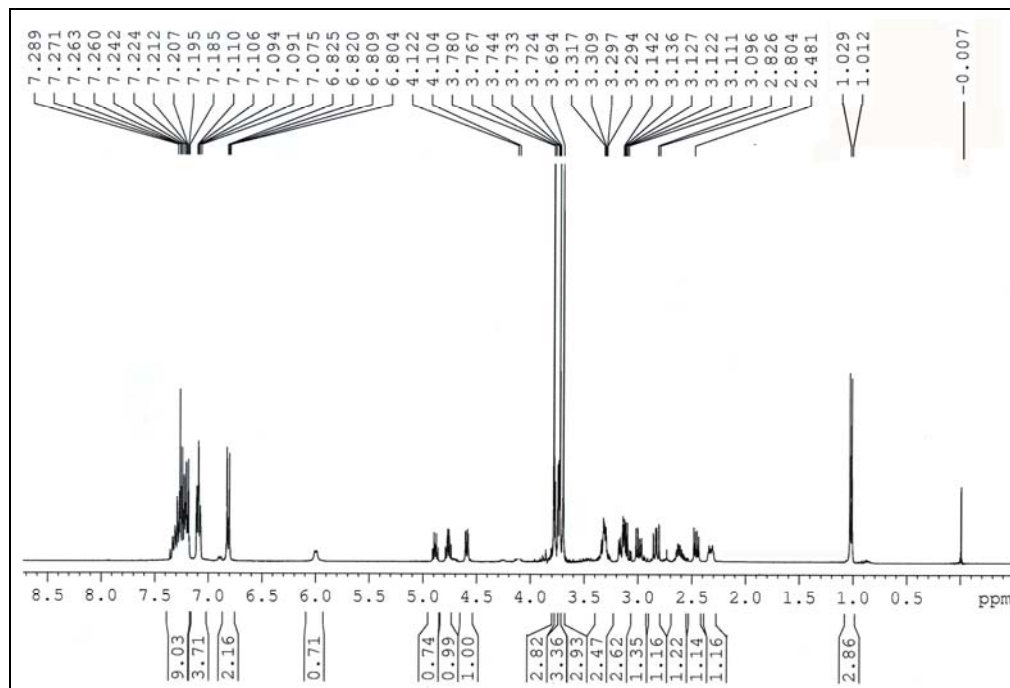


Figure S19. ^{77}Se NMR Spectrum of Compound **25** in CDCl_3

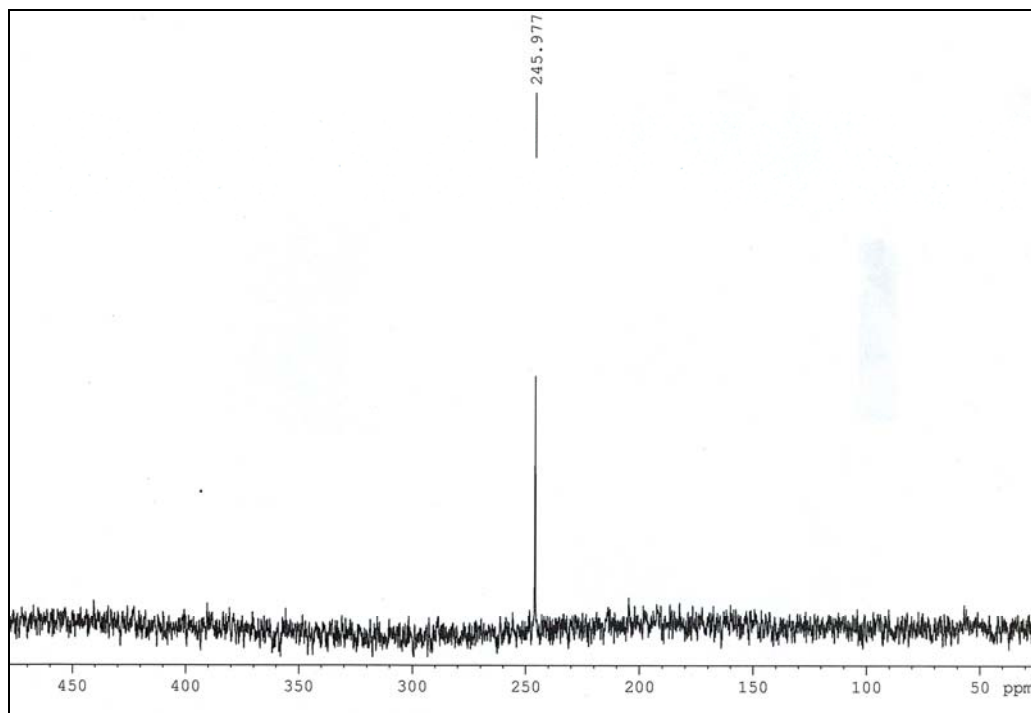


Figure S20. ESI mass Spectrum of the compound **25**. Calculated Mass: 545.1555, found 545.0529.

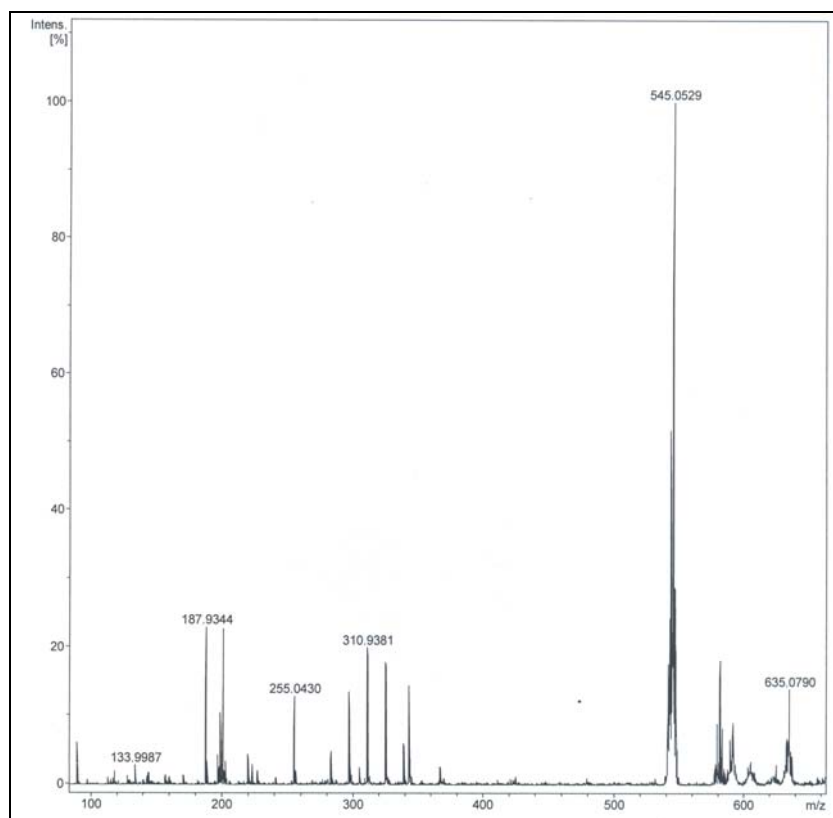


Figure S21. ^1H NMR Spectrum of Compound **26** in CDCl_3

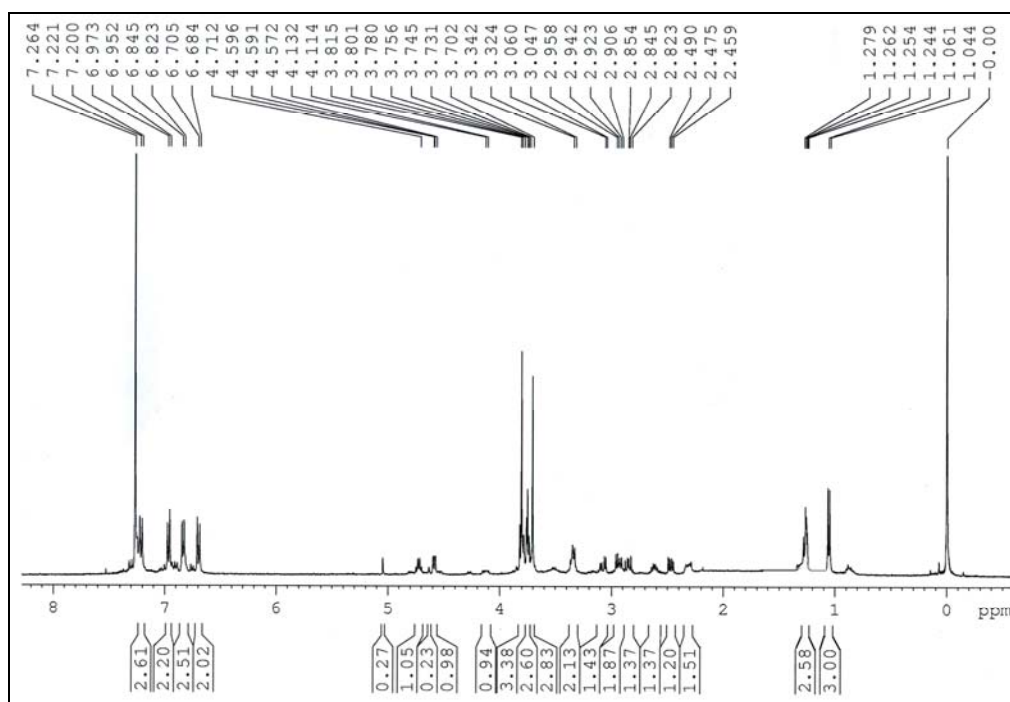


Figure S22. ^{13}C NMR Spectrum of Compound **26** in CDCl_3

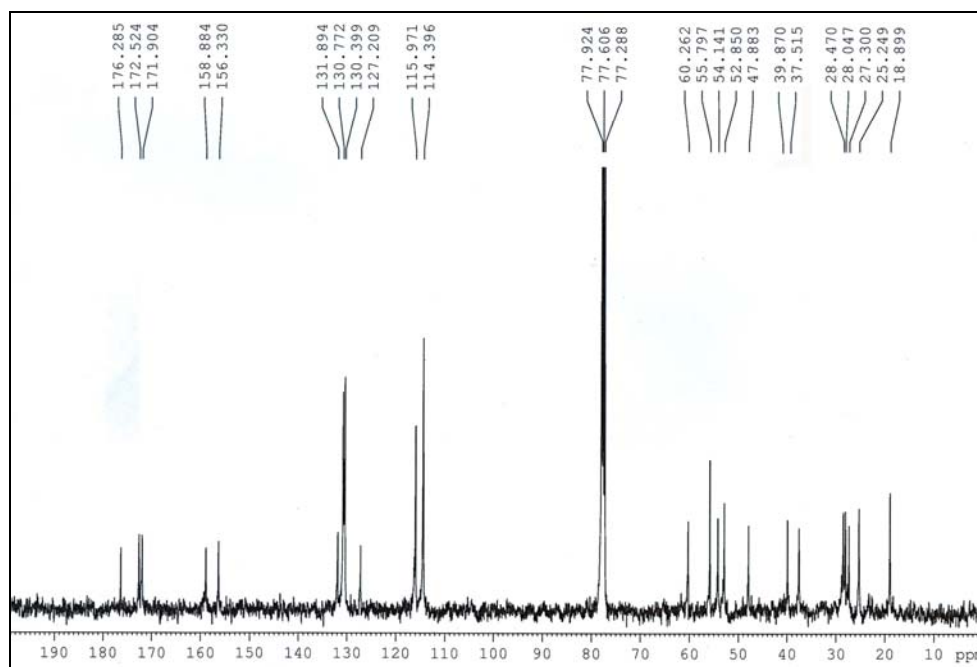


Figure S23. ^{77}Se NMR Spectrum of Compound **26** in CDCl_3

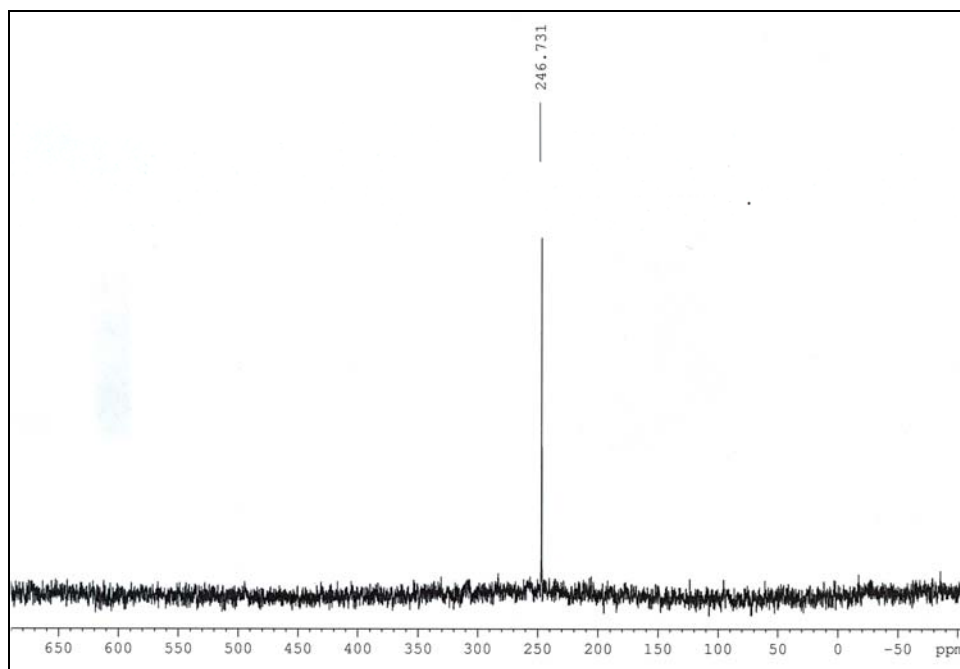


Figure S24. ESI mass Spectrum of the compound **26**. Calculated Mass: 585.1480, found 585.2116.

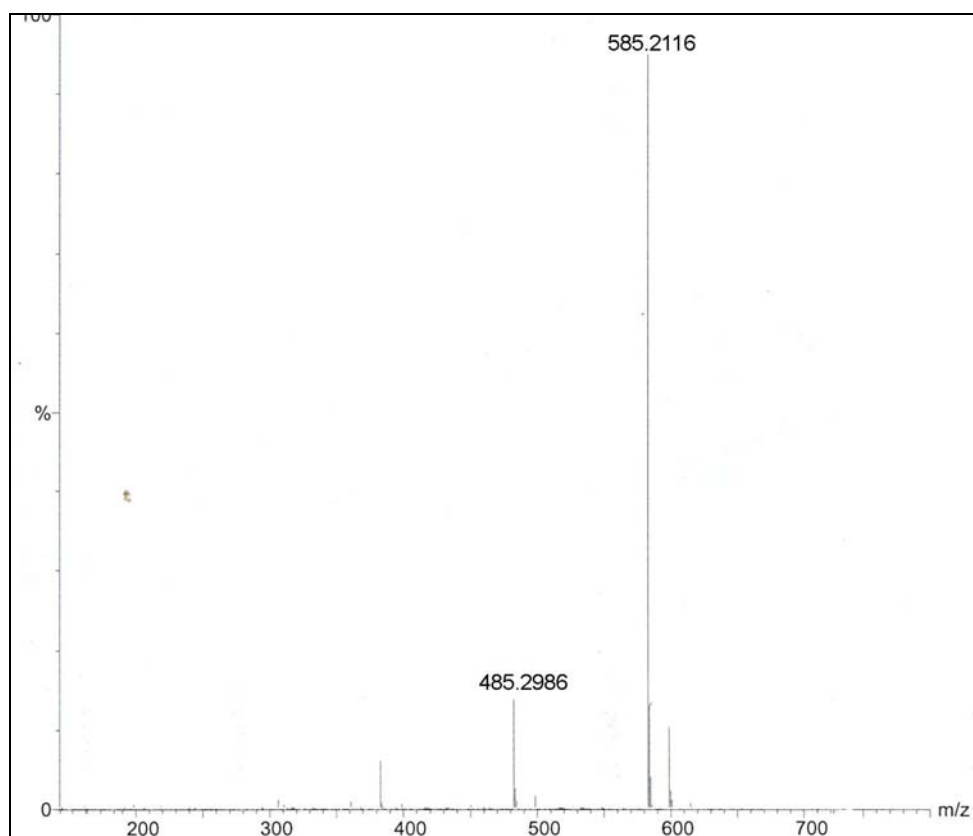


Figure S25. ^1H NMR Spectrum of Compound **27** in CDCl_3

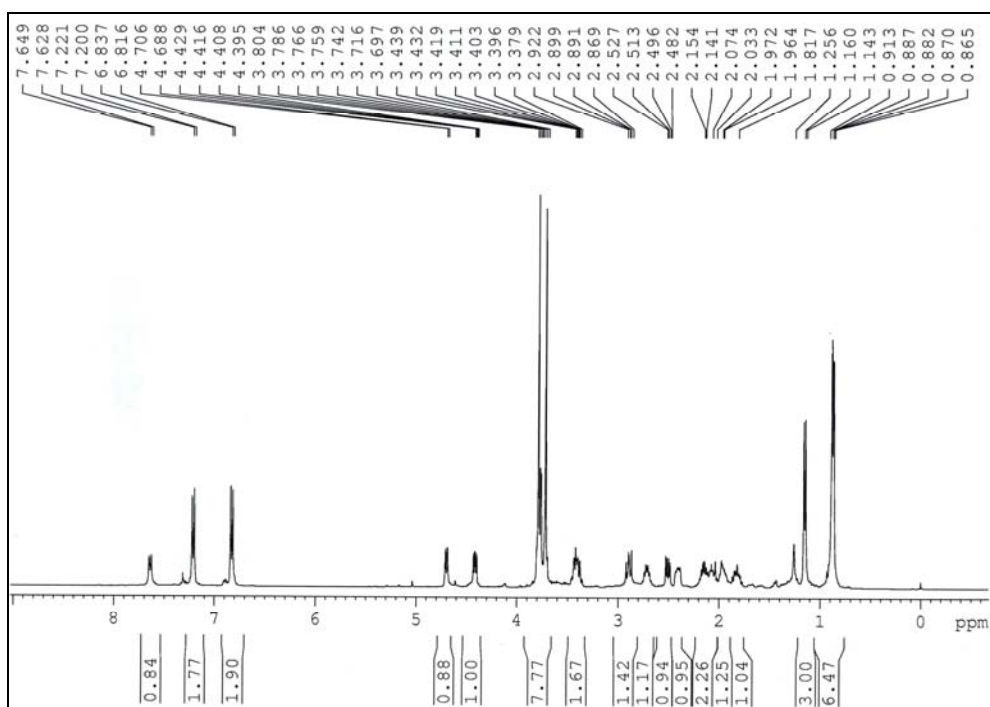


Figure S26. ^{13}C NMR Spectrum of Compound **27** in CDCl_3

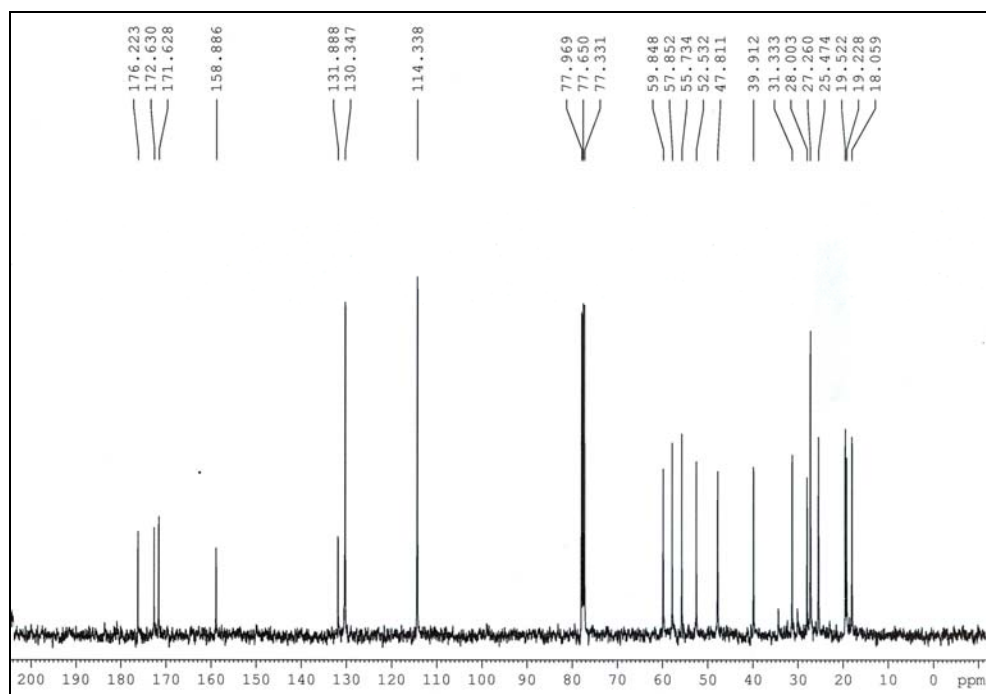


Figure S27. ^{77}Se NMR Spectrum of Compound **27** in CDCl_3

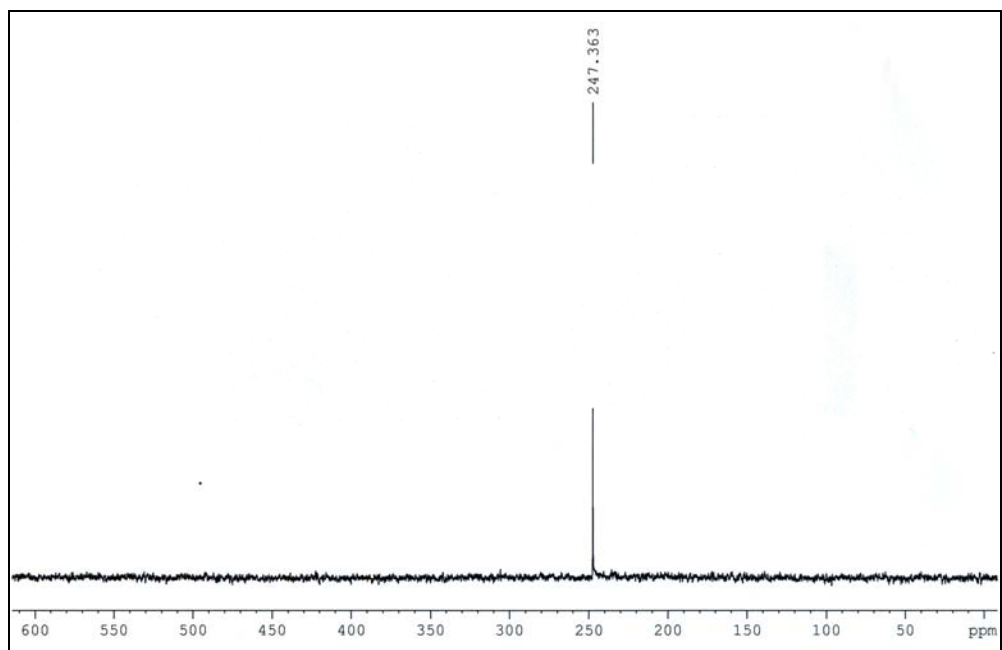


Figure S28. ESI mass Spectrum of the compound **27**. Calculated Mass: 521.1531, found 521.1171.

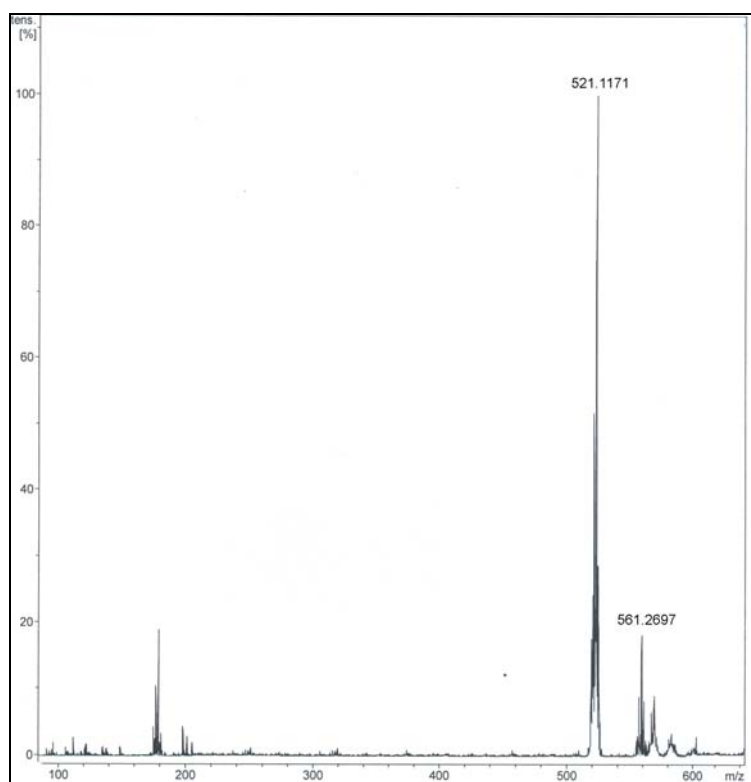


Figure S29. ^1H NMR Spectrum of Compound **28** in CDCl_3

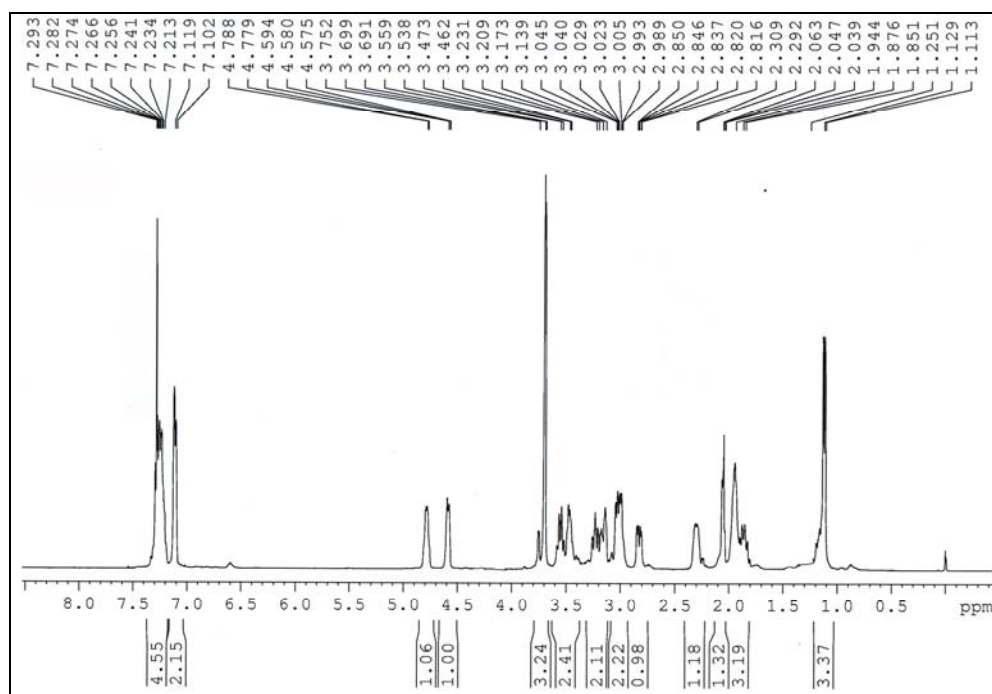


Figure S30. ^{13}C NMR Spectrum of Compound **28** in CDCl_3

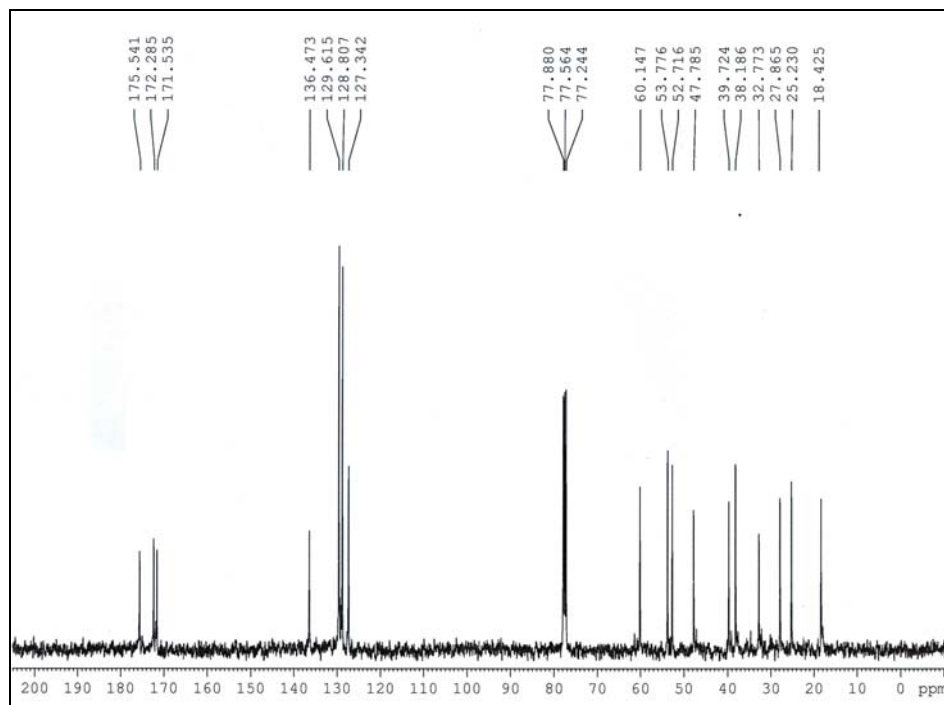


Figure S31. ^{77}Se NMR Spectrum of Compound **28** in CDCl_3

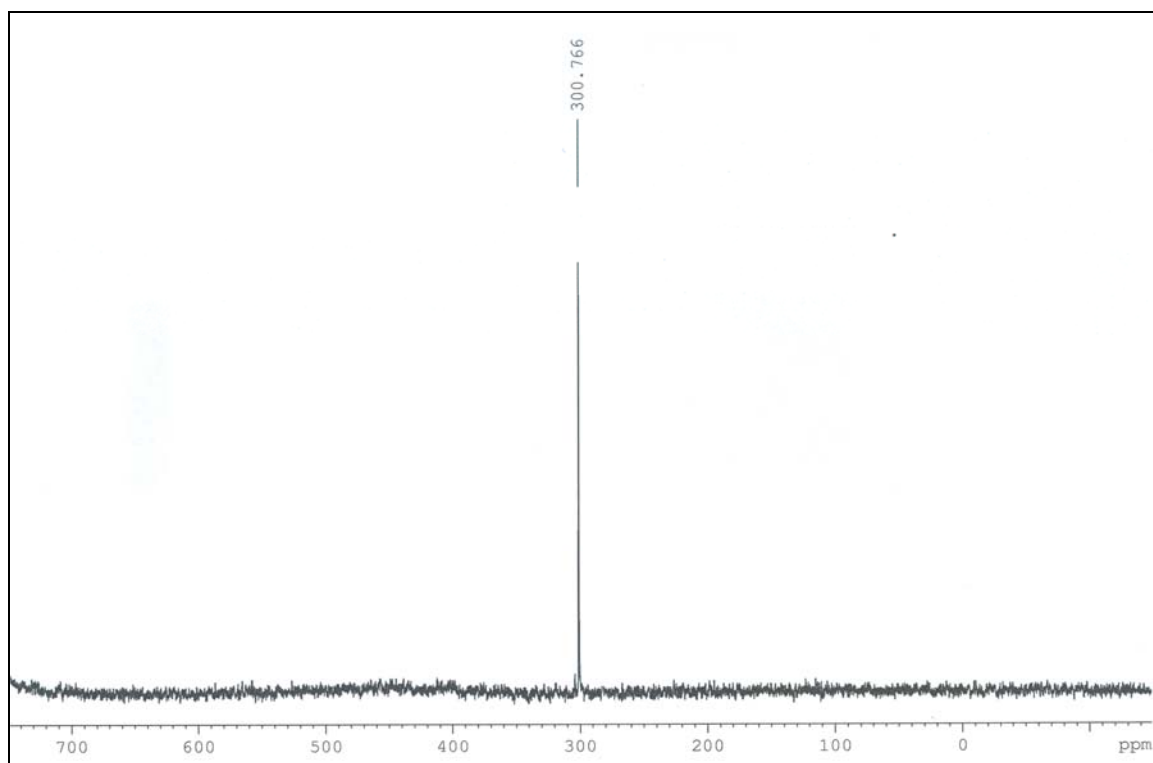


Figure S32. ESI mass Spectrum of the compound **28**. Calculated Mass: 873.1857, found 873.1855

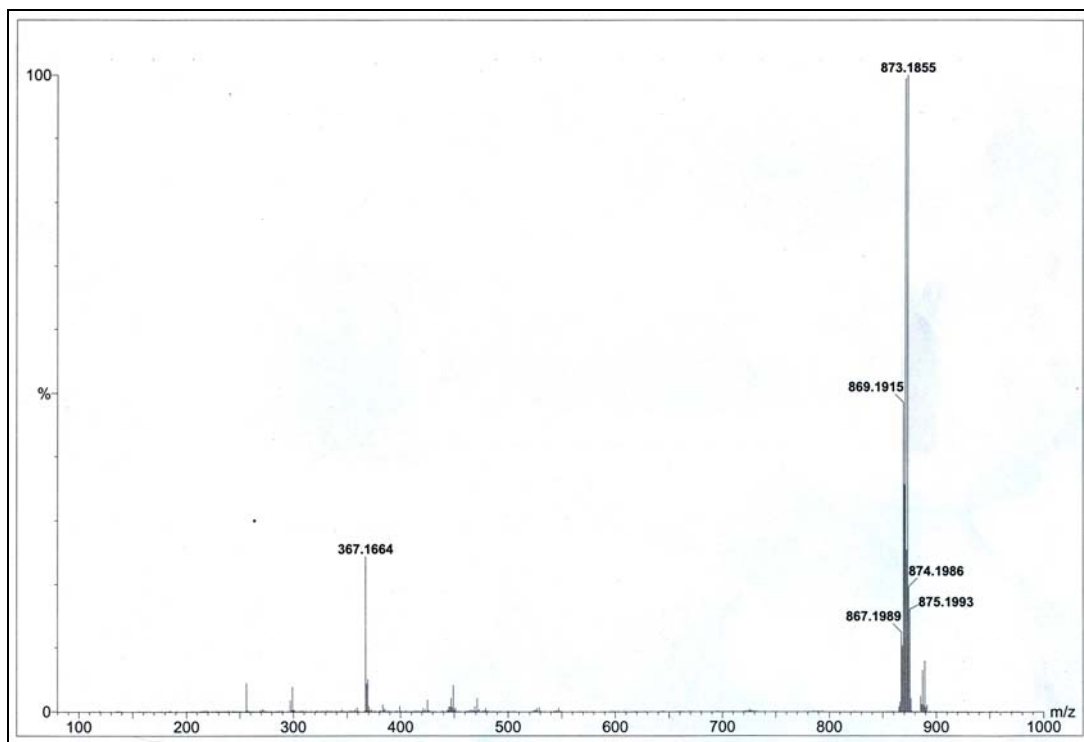


Figure S33. ^1H NMR Spectrum of Compound **29** in CDCl_3

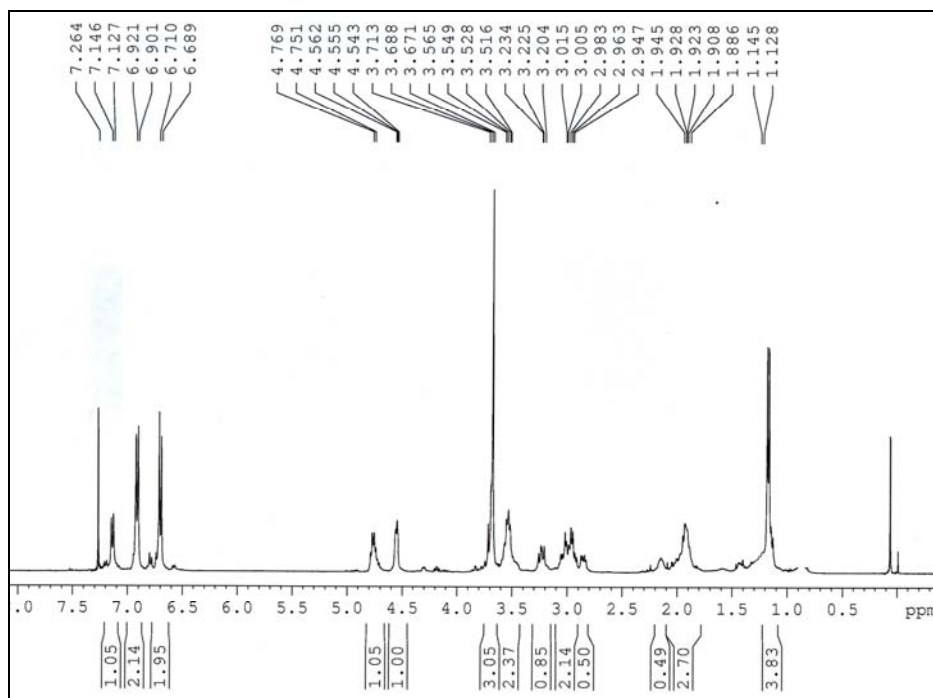


Figure S34. ^{13}C NMR Spectrum of Compound **29** in CDCl_3

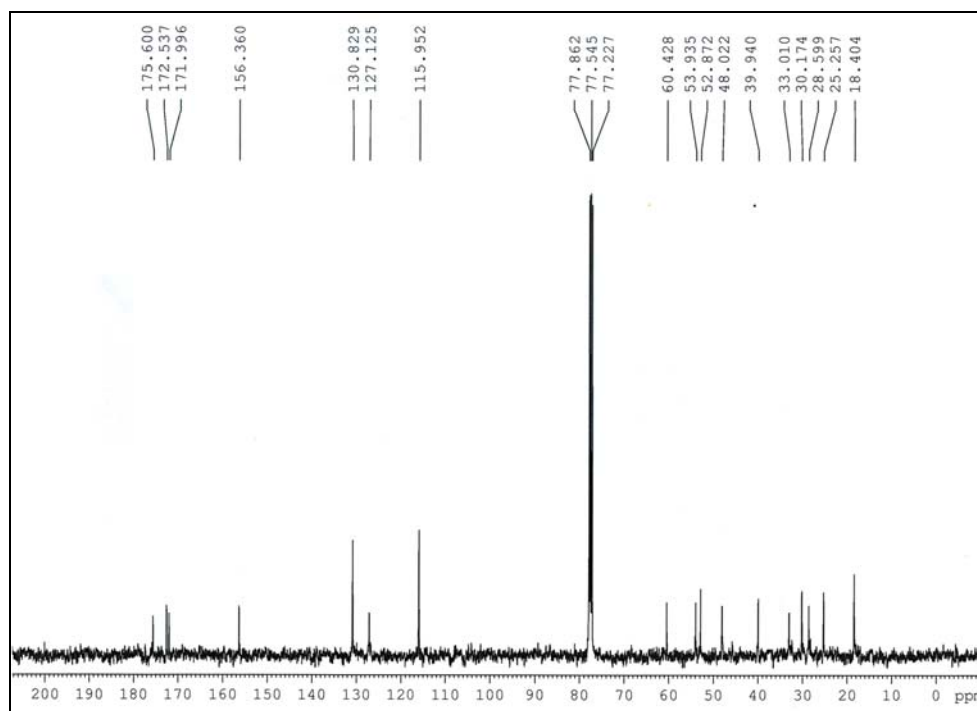


Figure S35. ^{77}Se NMR Spectrum of Compound **29** in CDCl_3

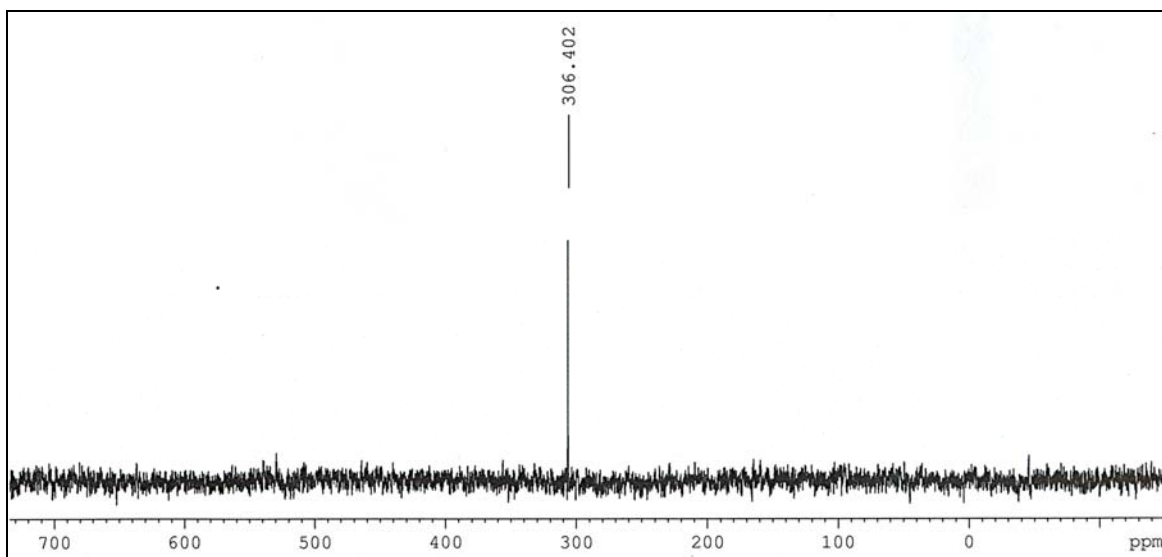


Figure S36. ESI mass Spectrum of the compound **29**. Calculated Mass: 905.1755, found 905.3151.

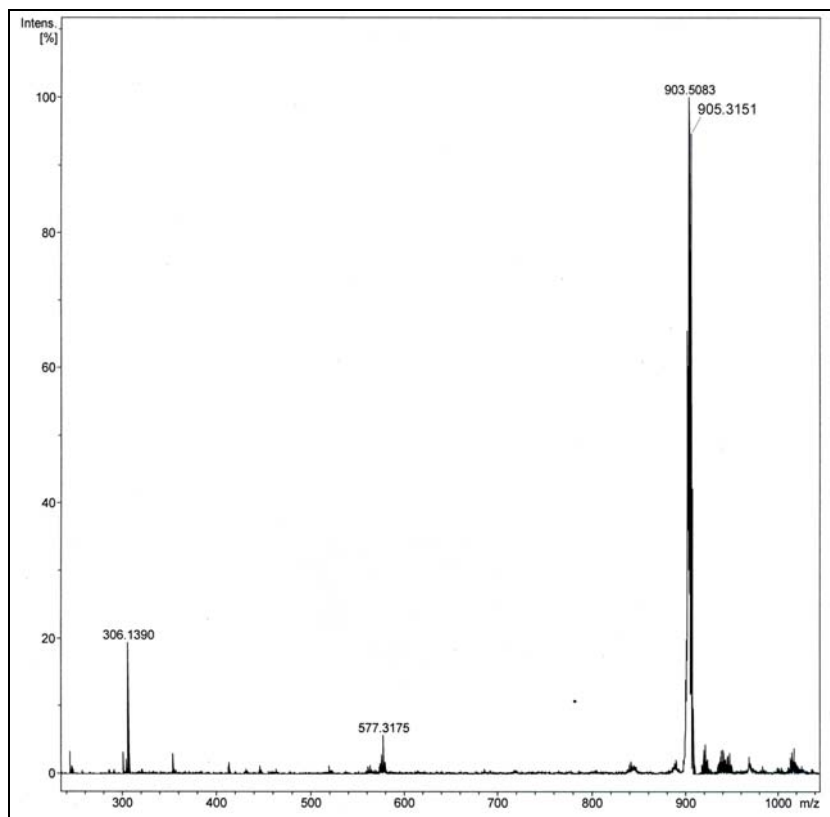


Figure S37. ^1H NMR Spectrum of Compound **30** in CDCl_3

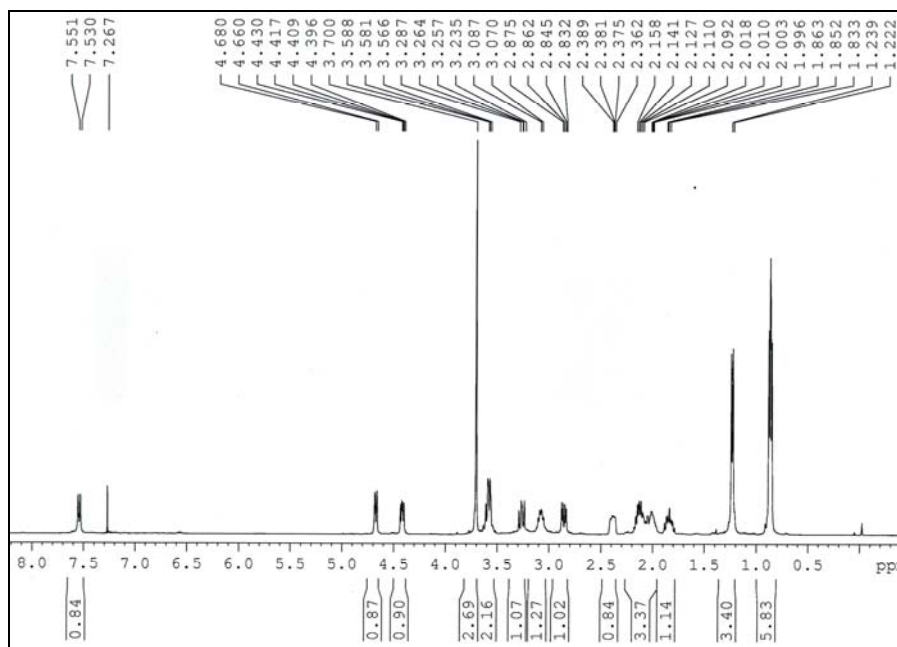


Figure S38. ^{13}C NMR Spectrum of Compound **30** in CDCl_3

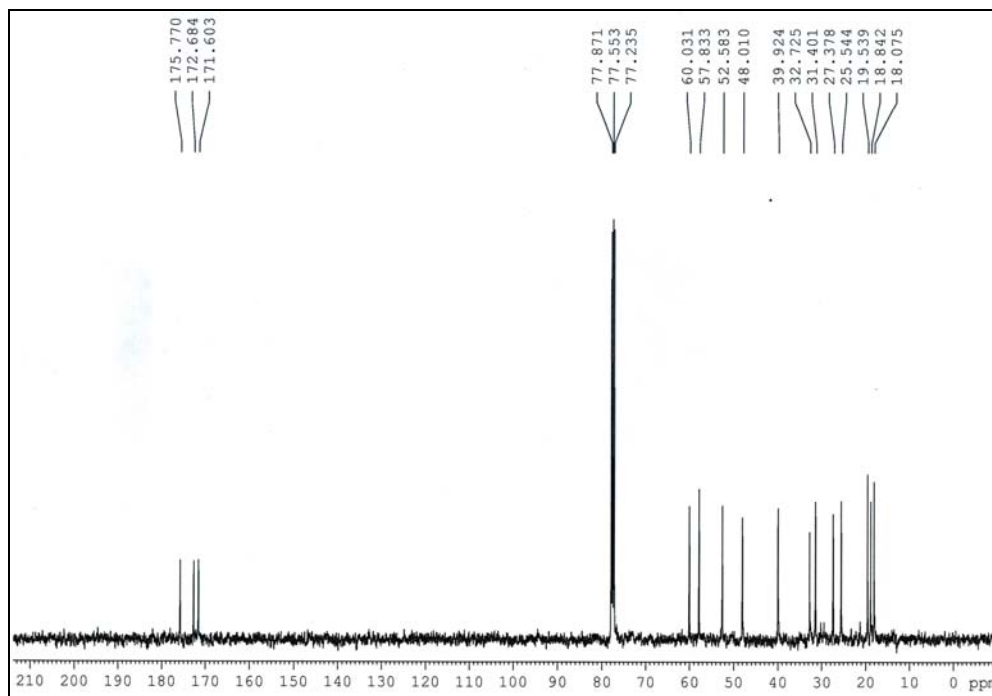


Figure S39. ^{77}Se NMR Spectrum of Compound **30** in CDCl_3

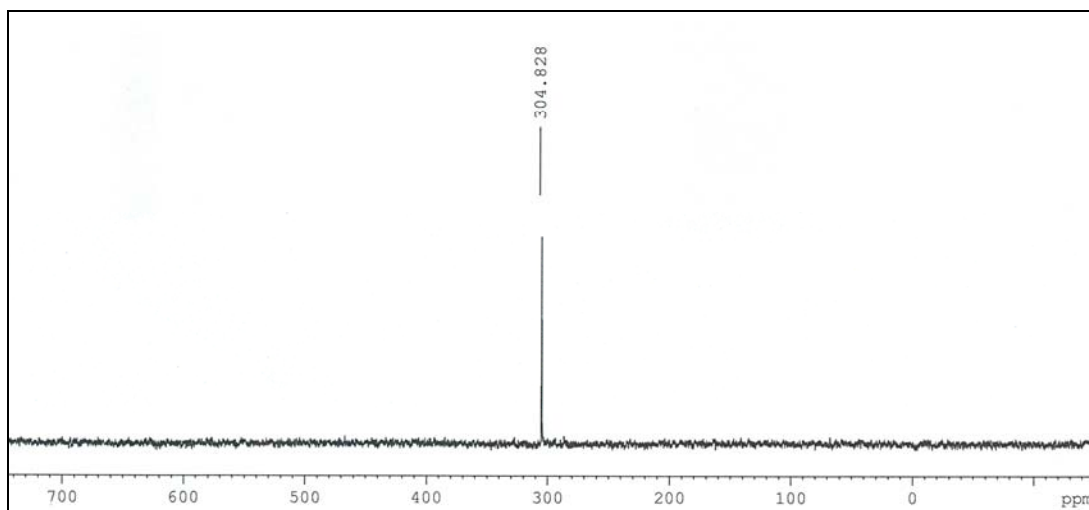


Figure S40. ESI mass Spectrum of the compound **30**. Calculated Mass: 777.1857, found 777.2000

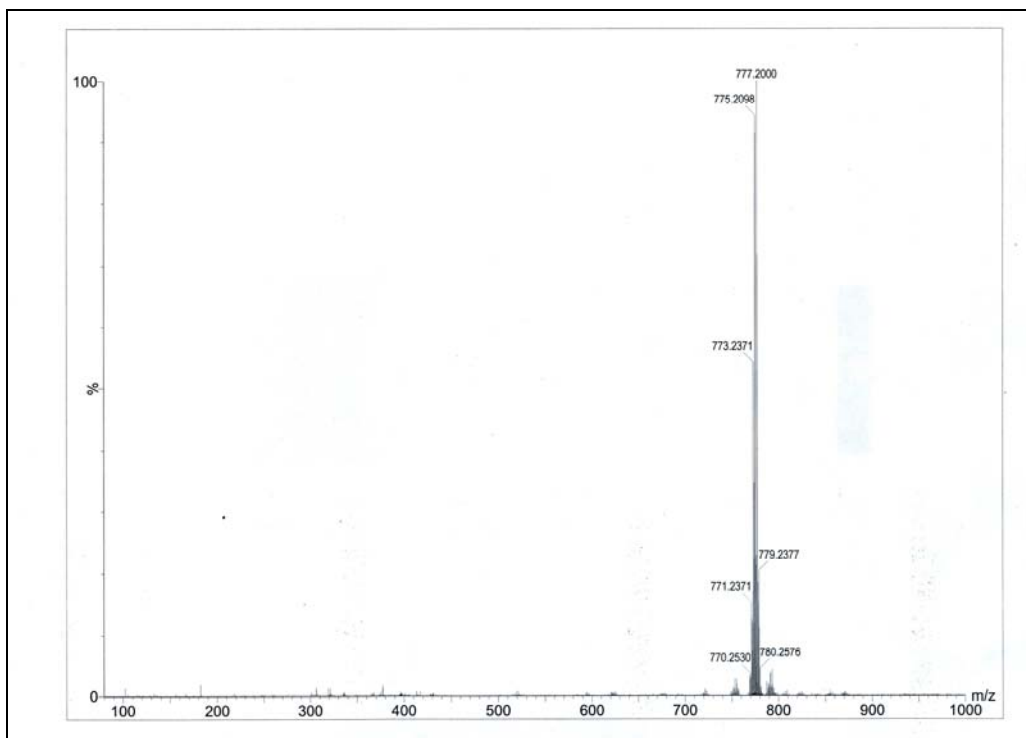


Figure S41. ^1H NMR Spectrum of Compound **31** in CDCl_3

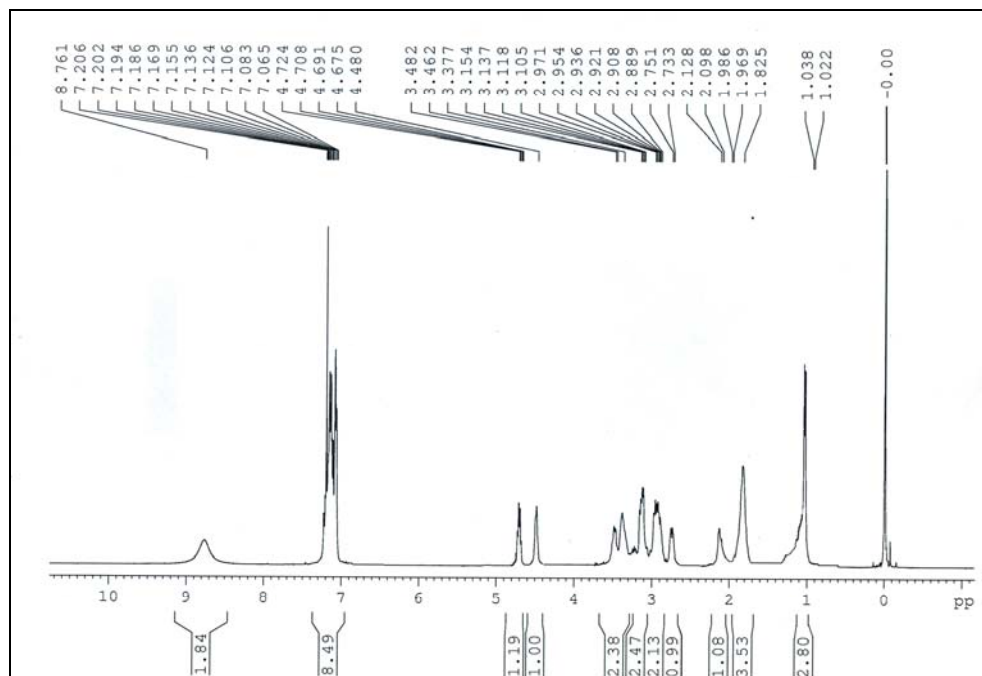


Figure S42. ^{13}C NMR Spectrum of Compound **31** in CDCl_3

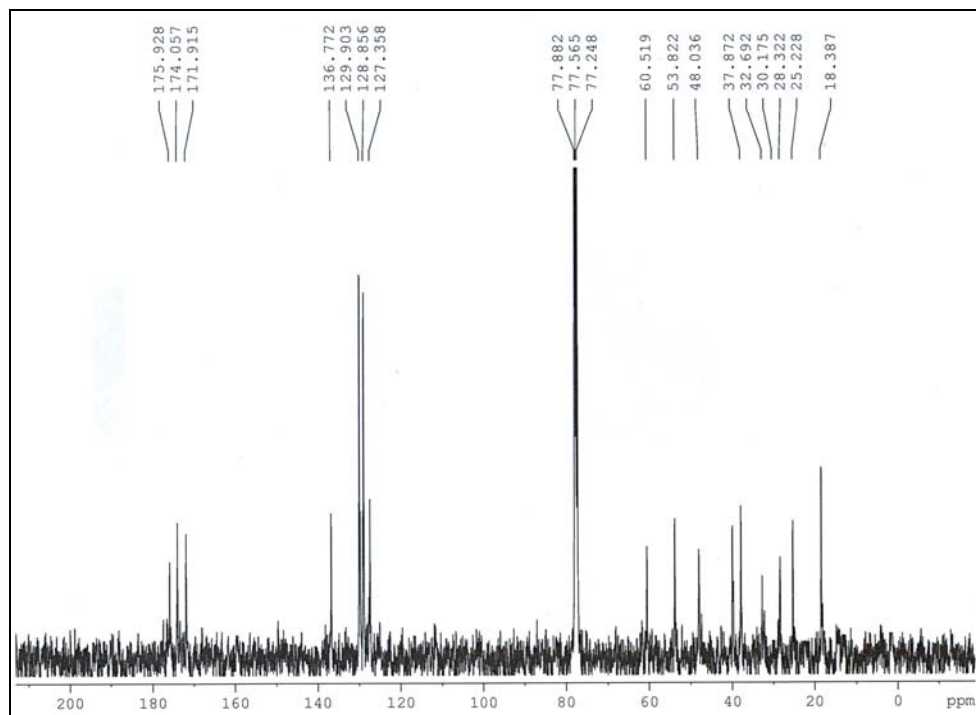


Figure S43. ^{77}Se NMR Spectrum of Compound **31** in CDCl_3

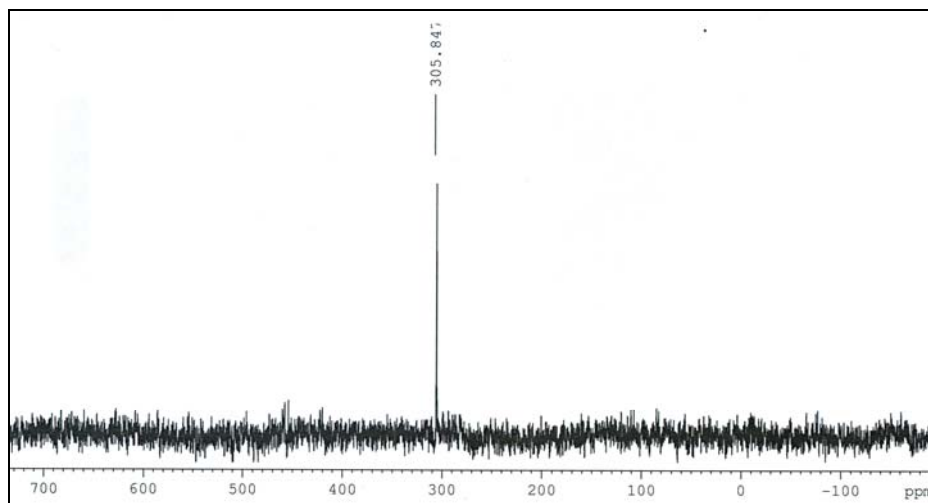


Figure S44. ESI mass Spectrum of the compound **31**. Calculated Mass: 845.1544, found 845.1724

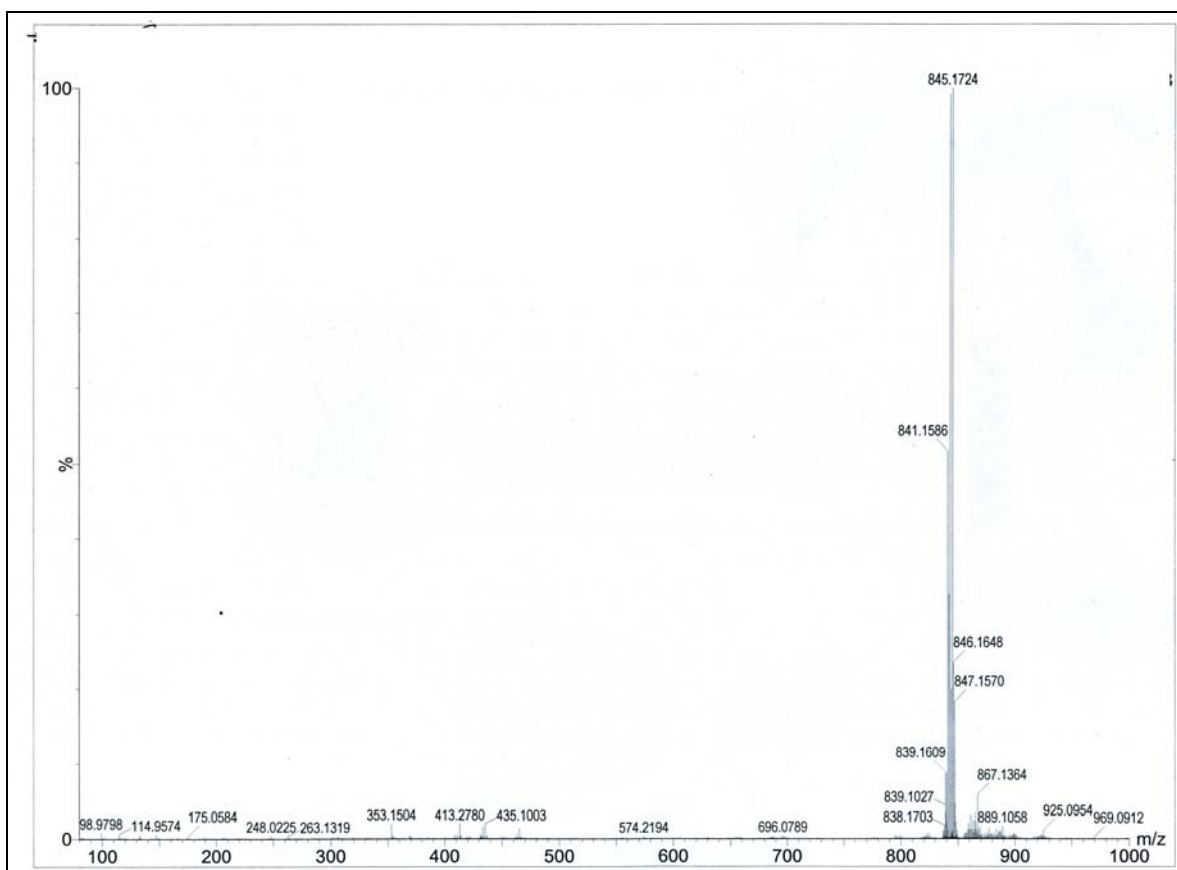


Figure S45. ^1H NMR Spectrum of Compound **32** in MeOH-d_4

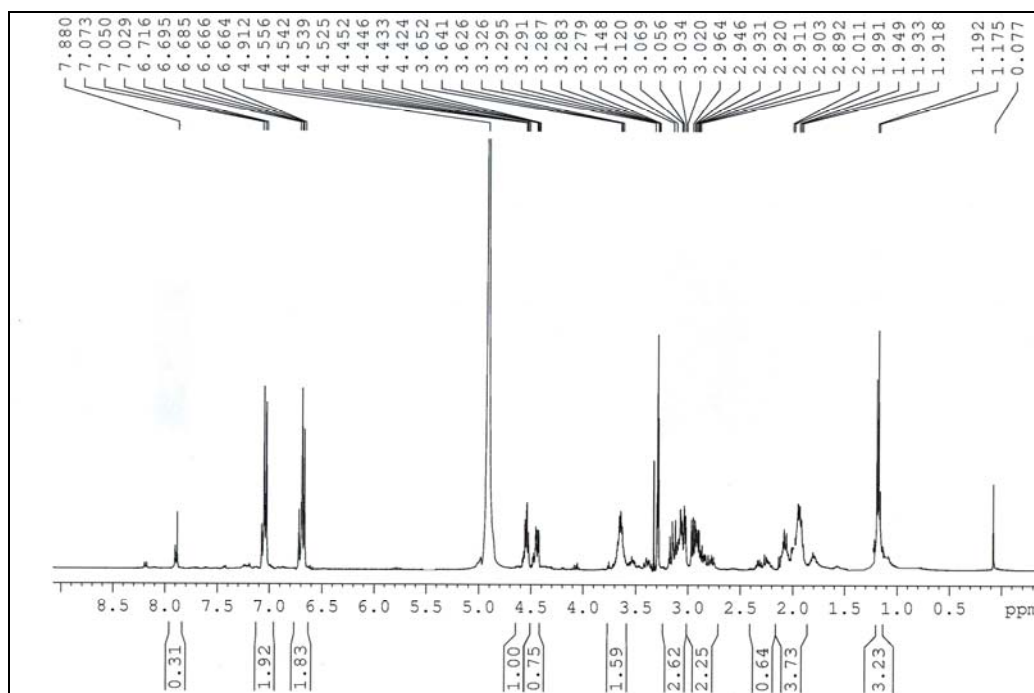


Figure S46. ^{13}C NMR Spectrum of Compound **32** in MeOH-d_4

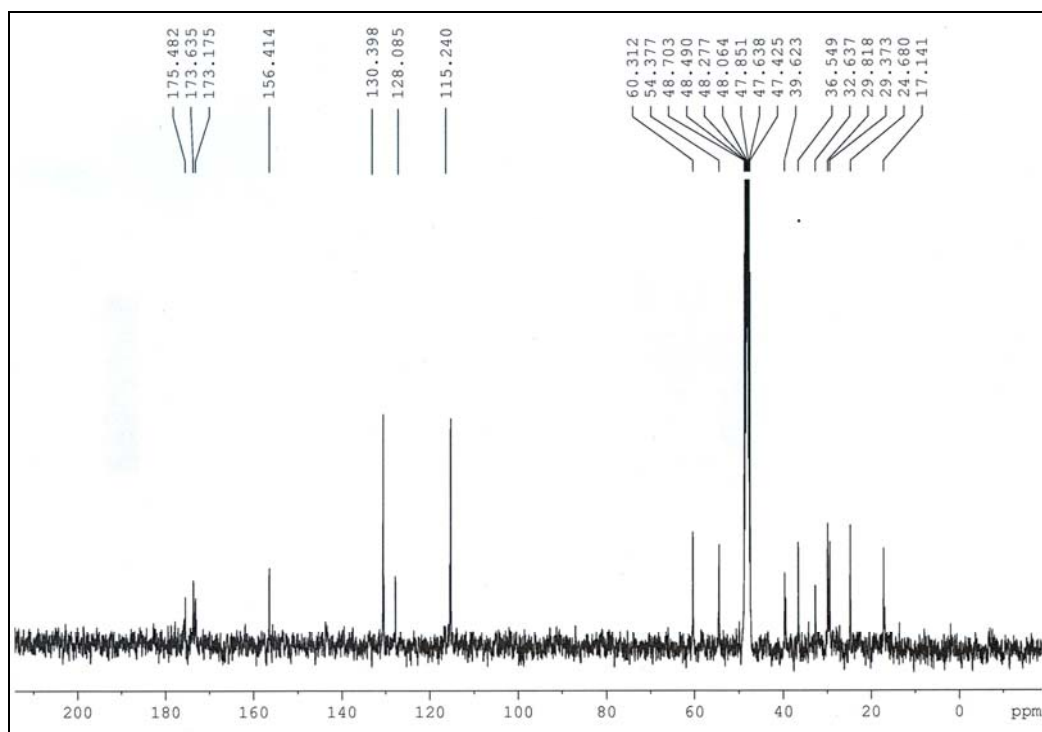


Figure S47. ^{77}Se NMR Spectrum of Compound **32** in MeOH-d_4

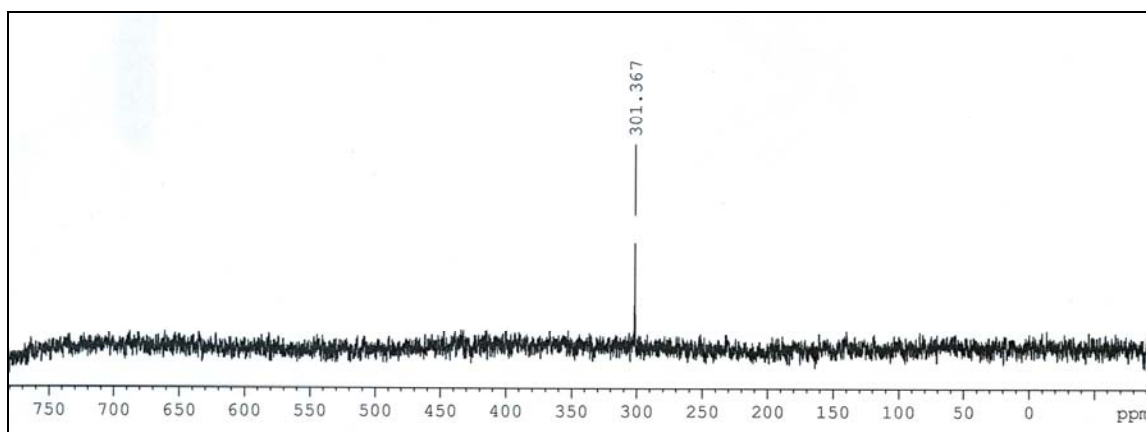


Figure S48. ESI mass Spectrum of the compound **32**. Calculated Mass: 877.1442, found 877.2111

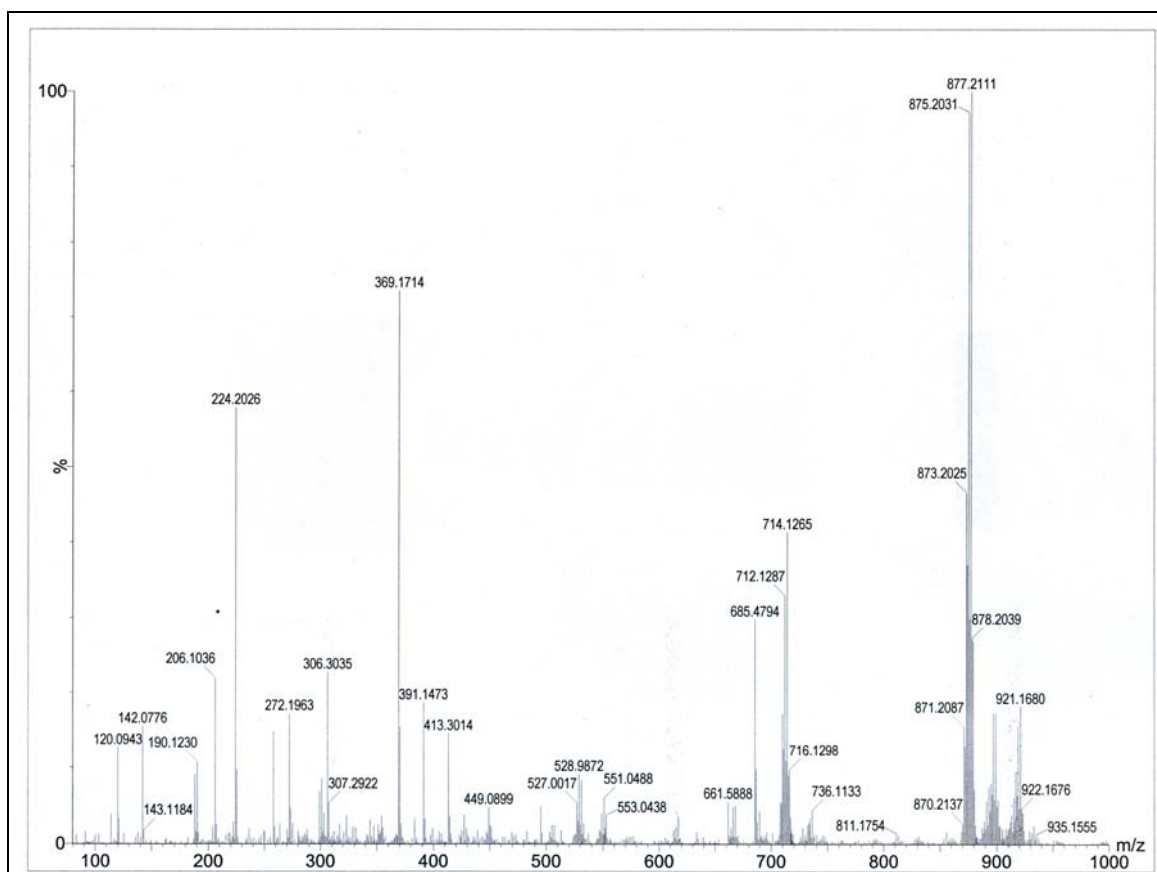


Figure S49. ^{77}Se NMR Spectrum of Compound **33** in CDCl_3

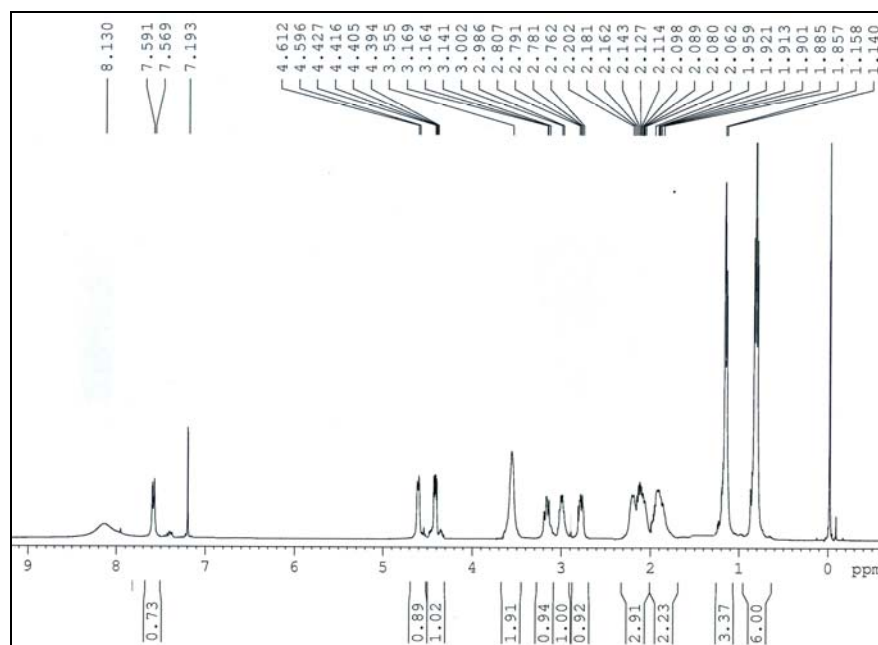


Figure S50. ^{13}C NMR Spectrum of Compound **33** in CDCl_3

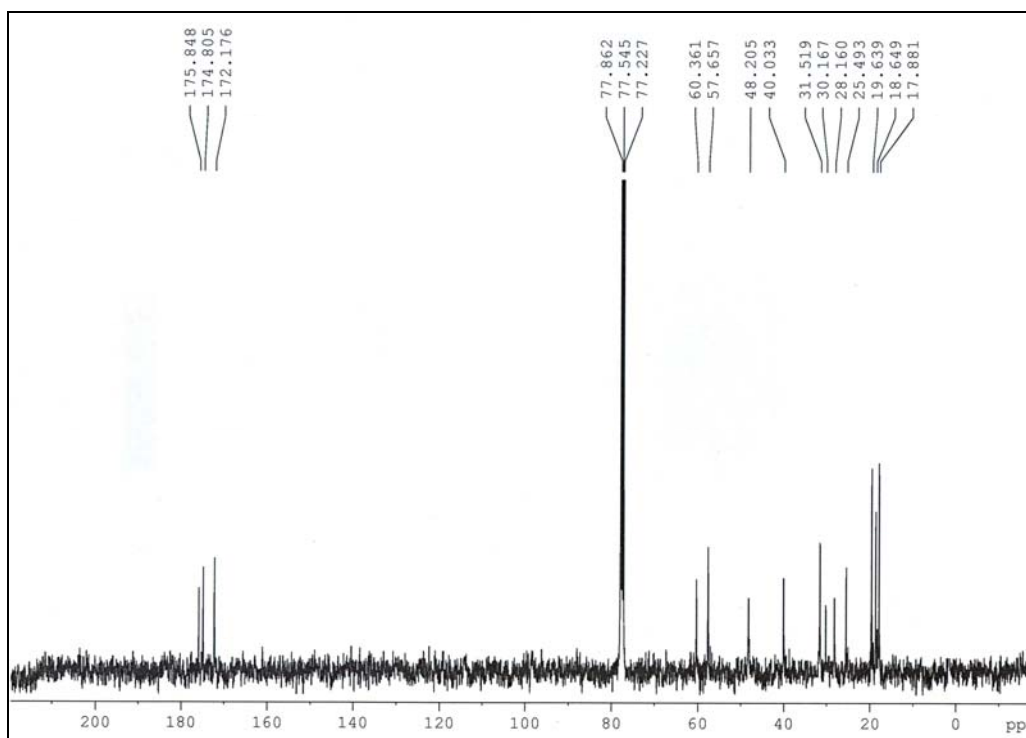


Figure S51. ^{77}Se NMR Spectrum of Compound **33** in CDCl_3

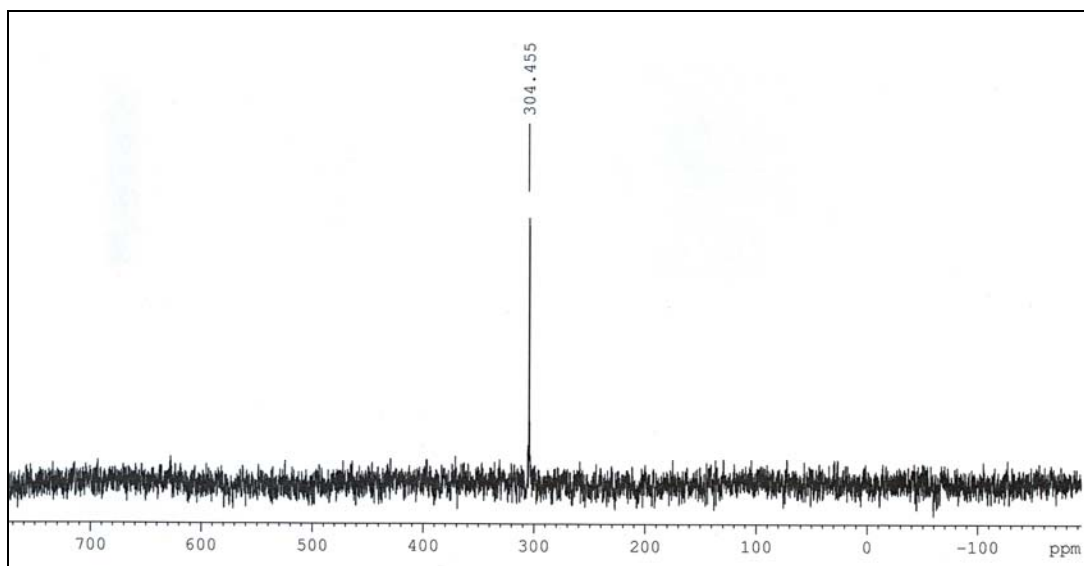


Figure S52. ESI mass Spectrum of the compound **33**. Calculated Mass: 749.1544, found 749.1534

