Supporting Information

Catalytic chalcogenylation under greener conditions: A solvent-free sulfur- and seleno-functionalyzation of olefins via I_2/DMSO oxidant system

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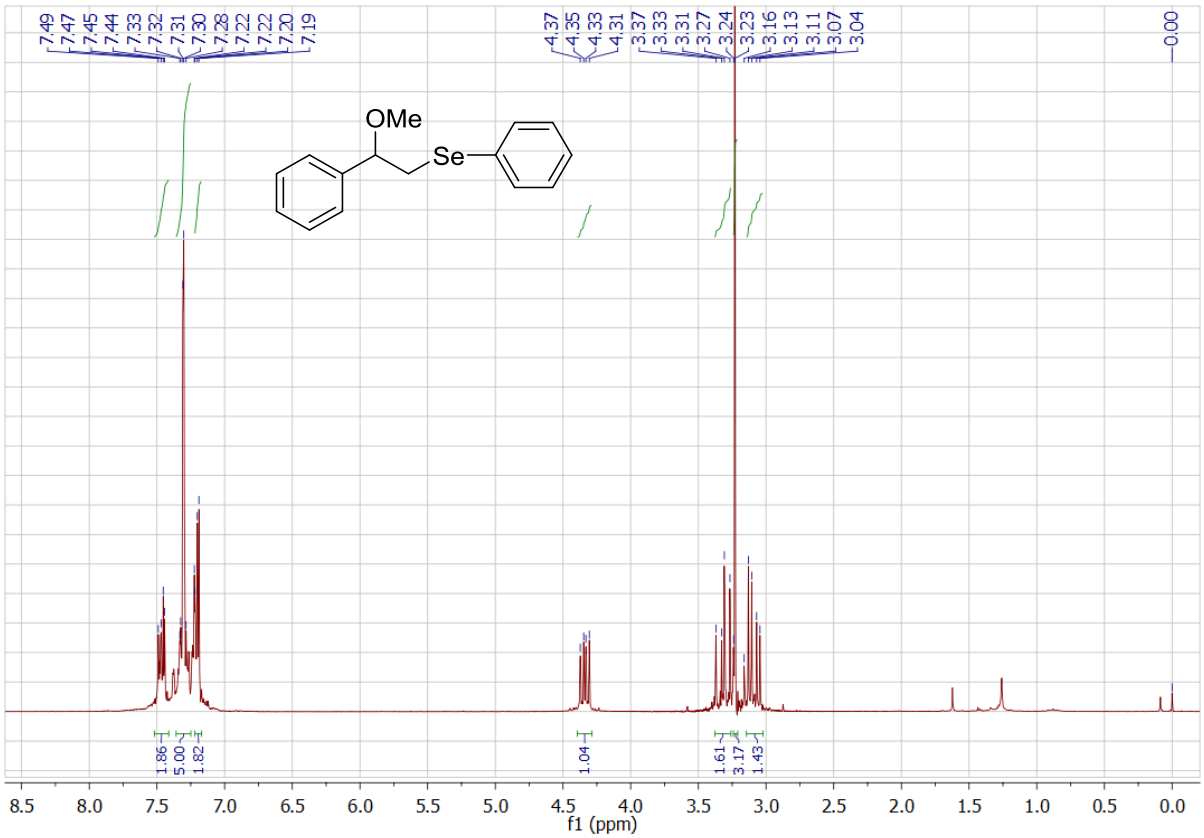
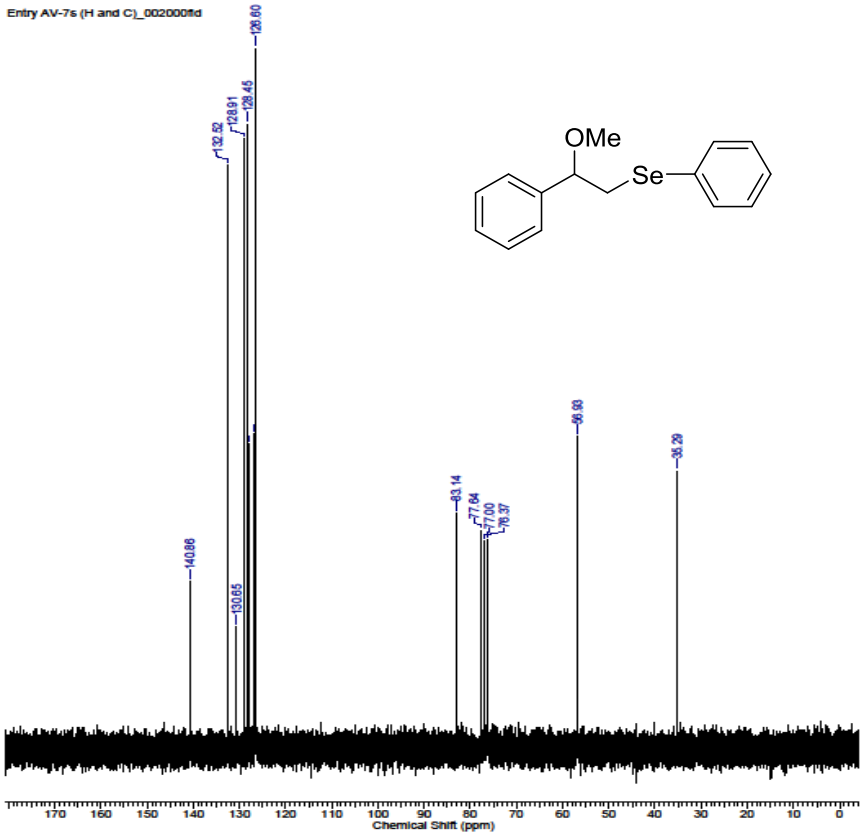
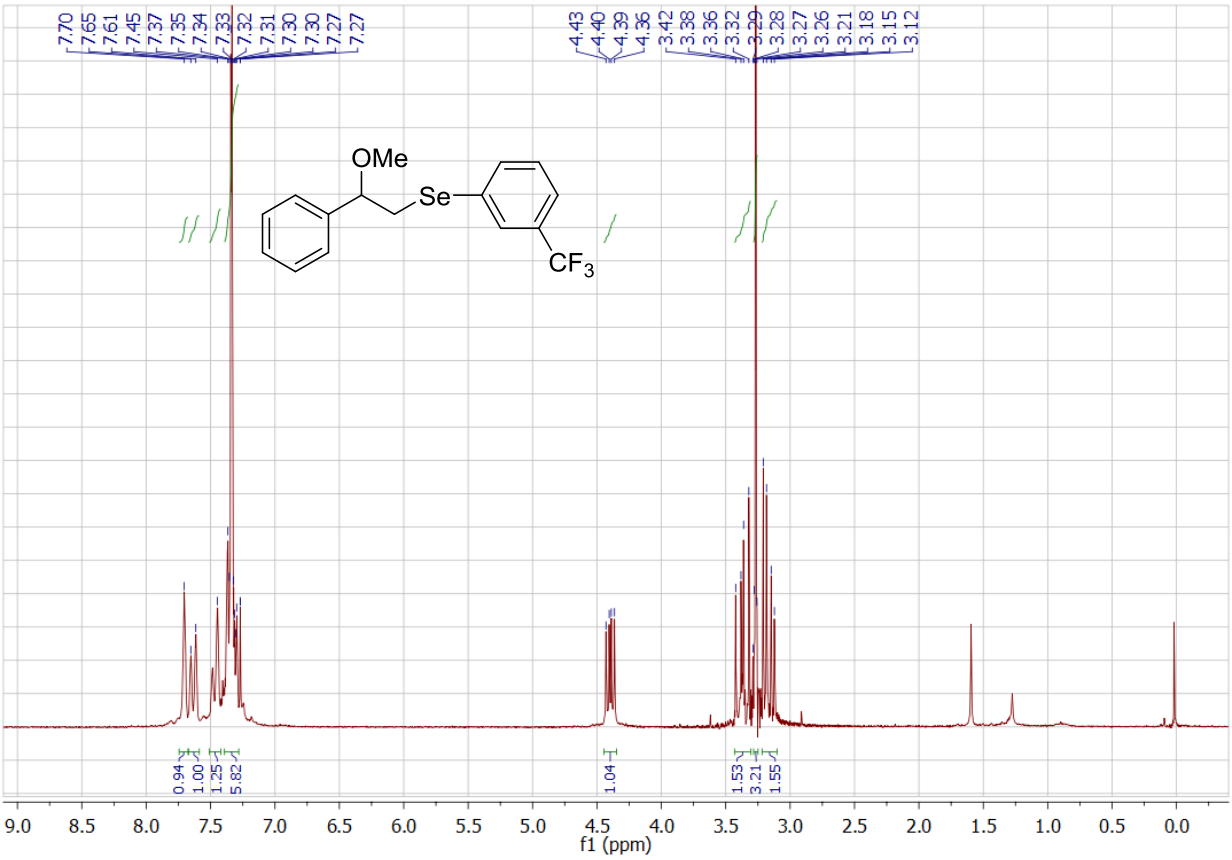
1.1. NMR spectra



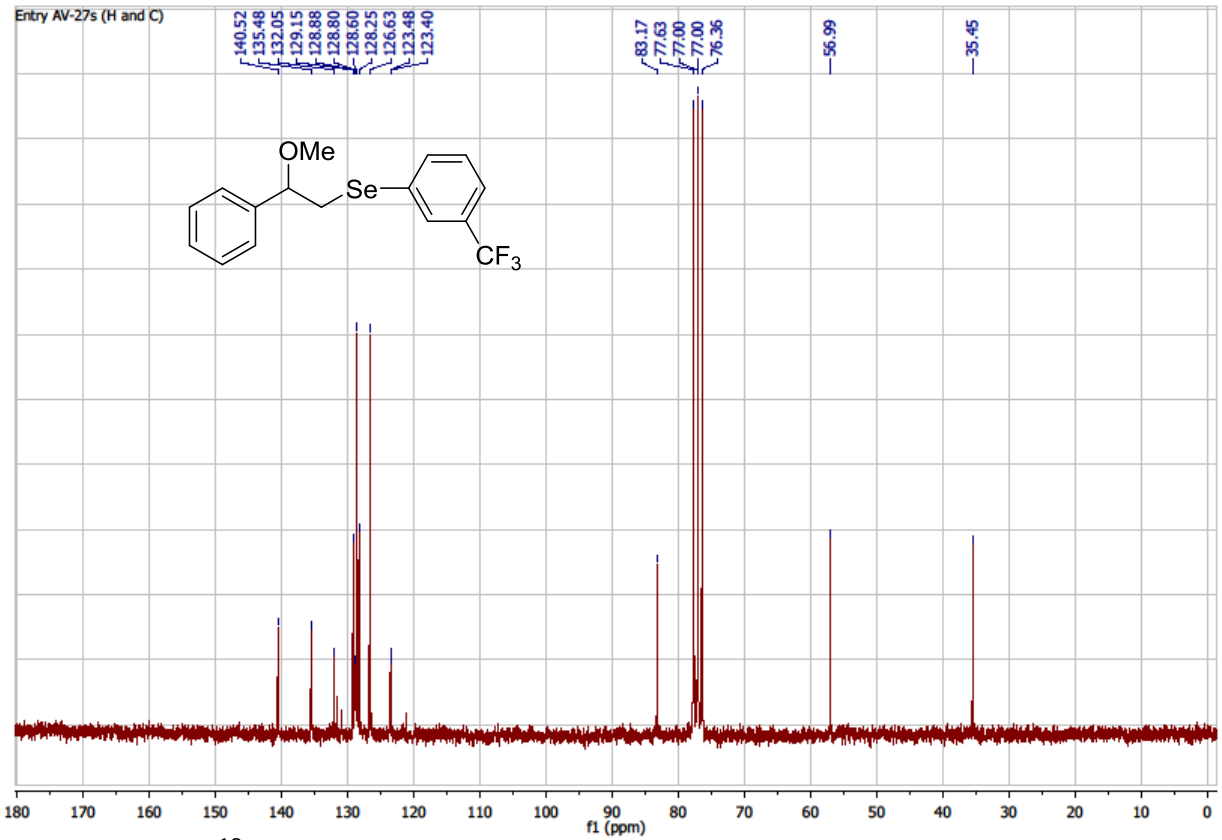
S1. ^{1}H NMR spectrum of compound **3a** in $CDCl_3$ (200 MHz).



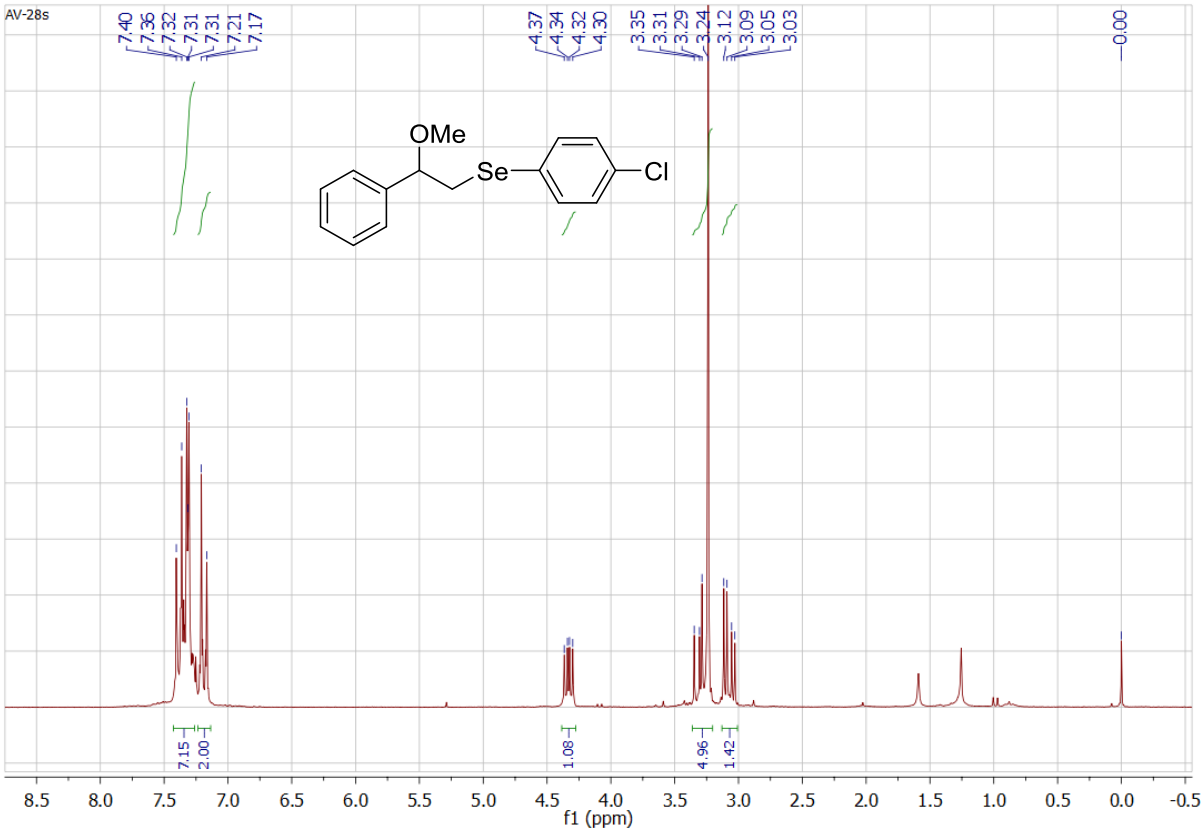
S2. ^{13}C NMR spectrum of compound **3a** in $CDCl_3$ (50 MHz).



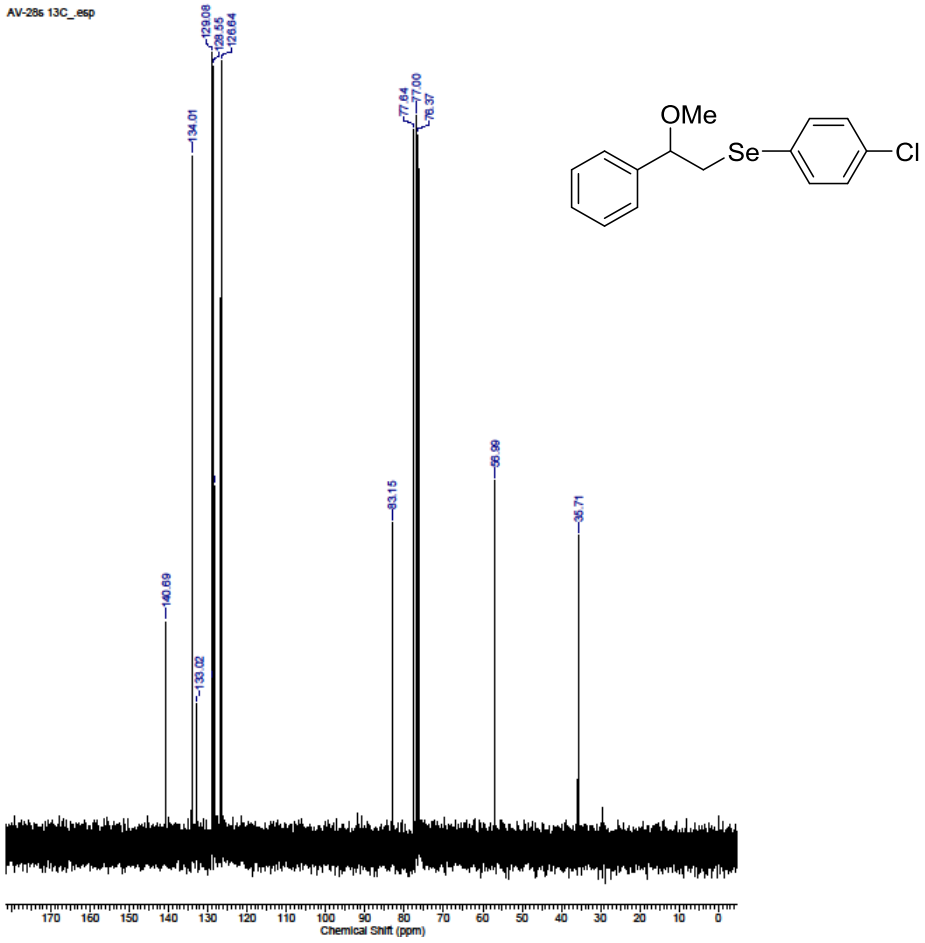
S3. ^{1}H NMR spectrum of compound **3b** in $CDCl_3$ (200 MHz).



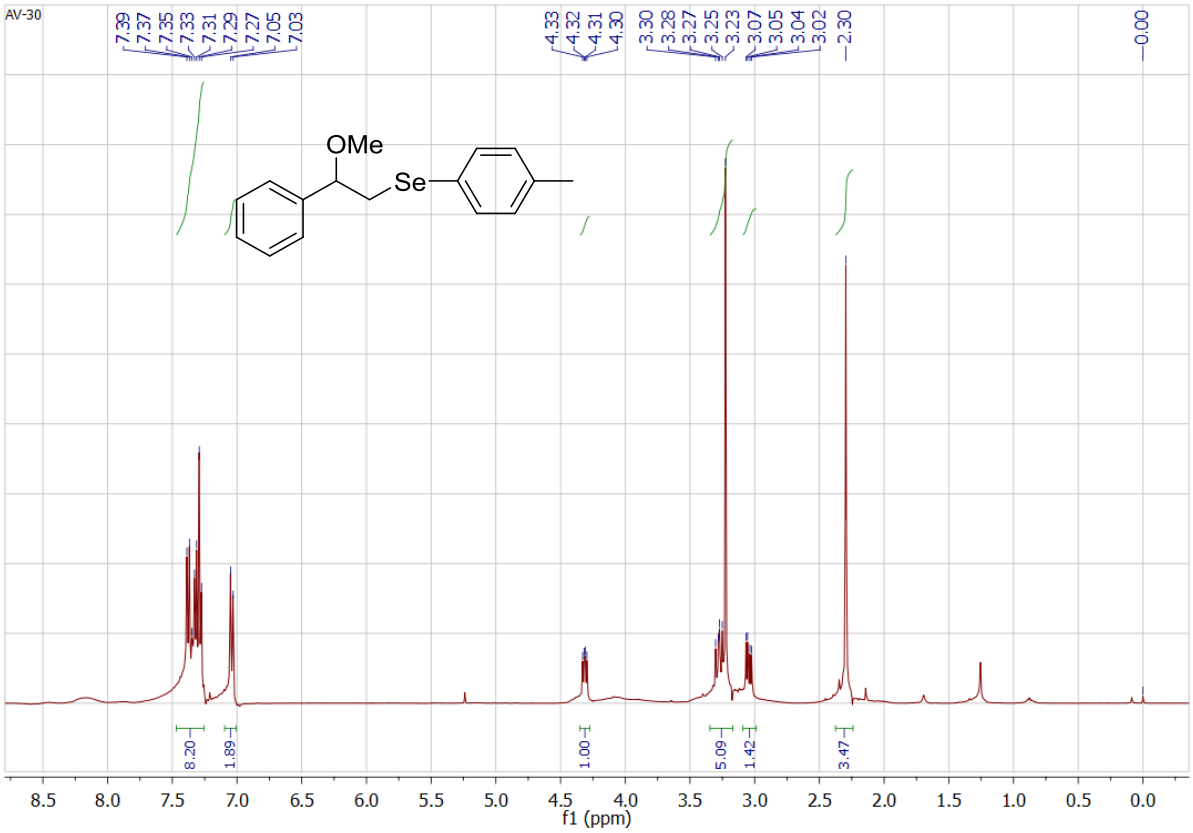
S4. ^{13}C NMR spectrum of compound **3b** in $CDCl_3$ (50 MHz).



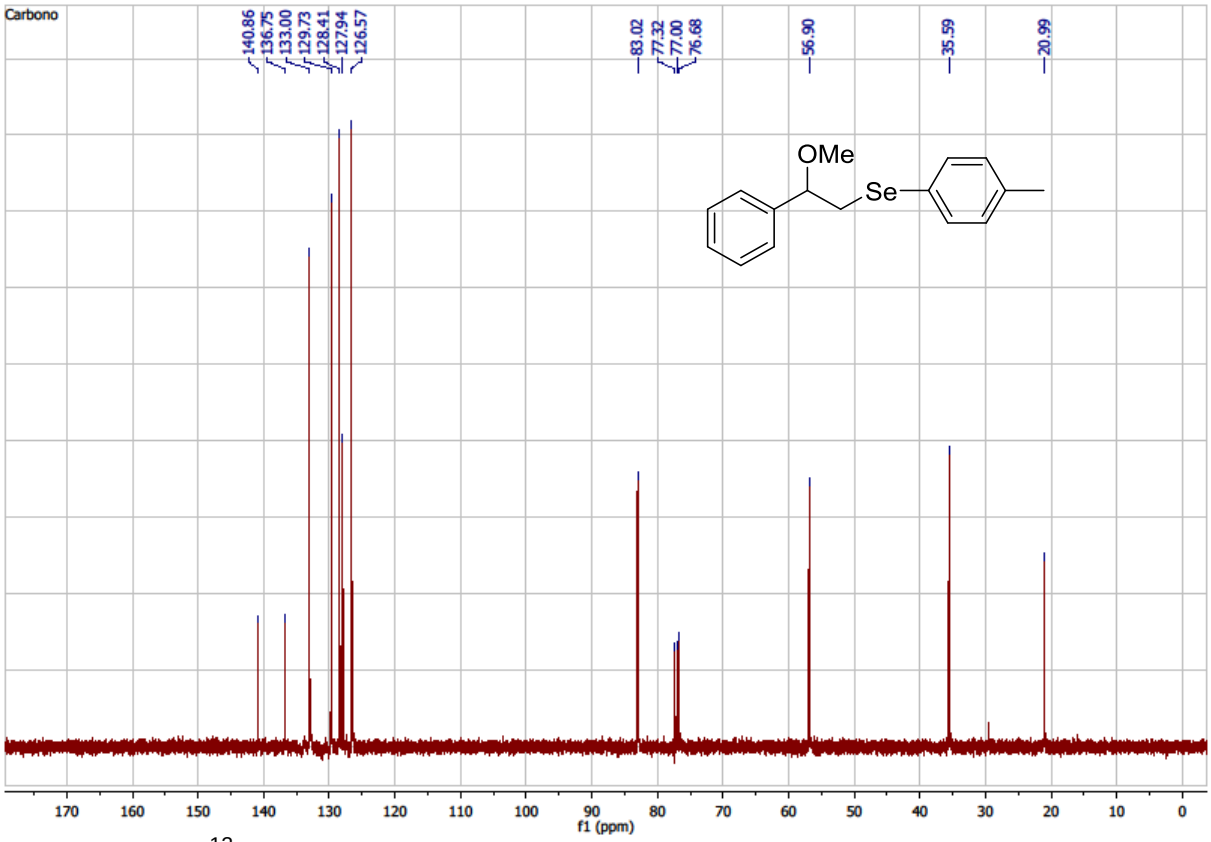
S5. ^{1}H NMR spectrum of compound **3d** in $CDCl_3$ (200 MHz).



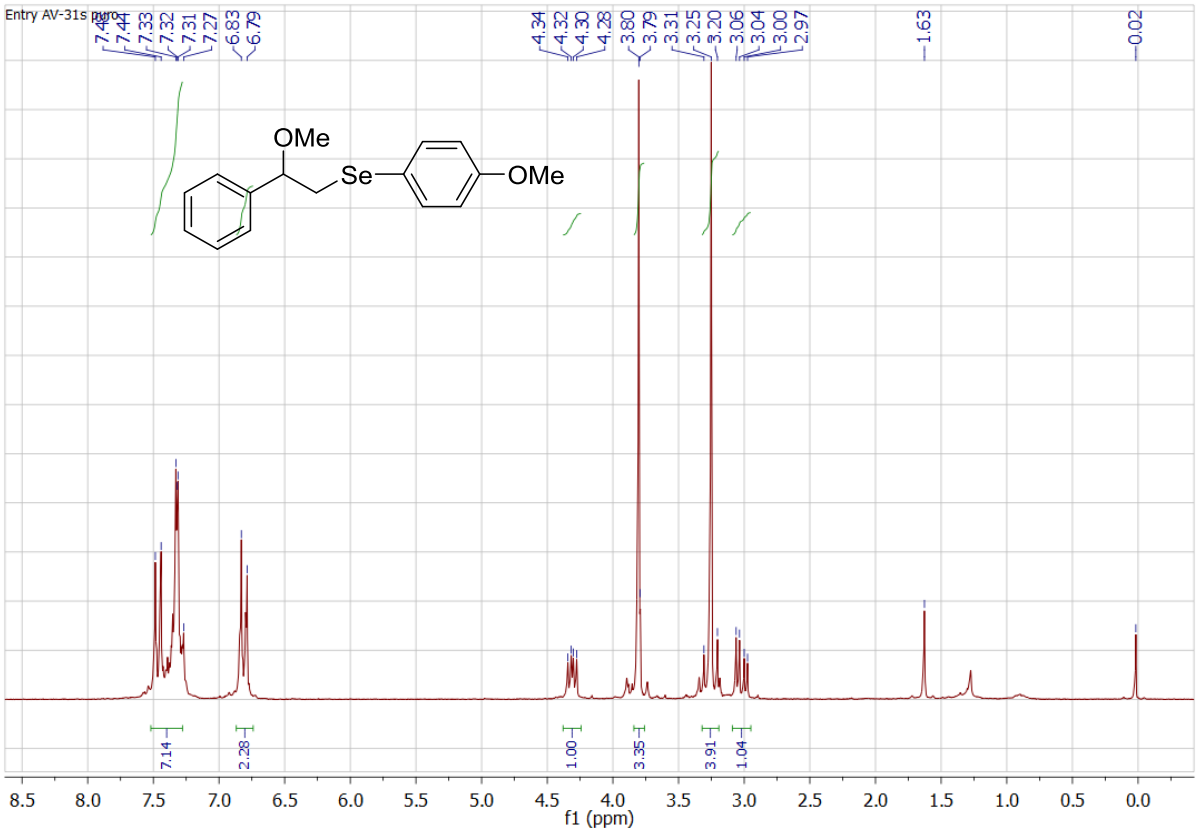
S6. ^{13}C NMR spectrum of compound **3d** in $CDCl_3$ (50 MHz).



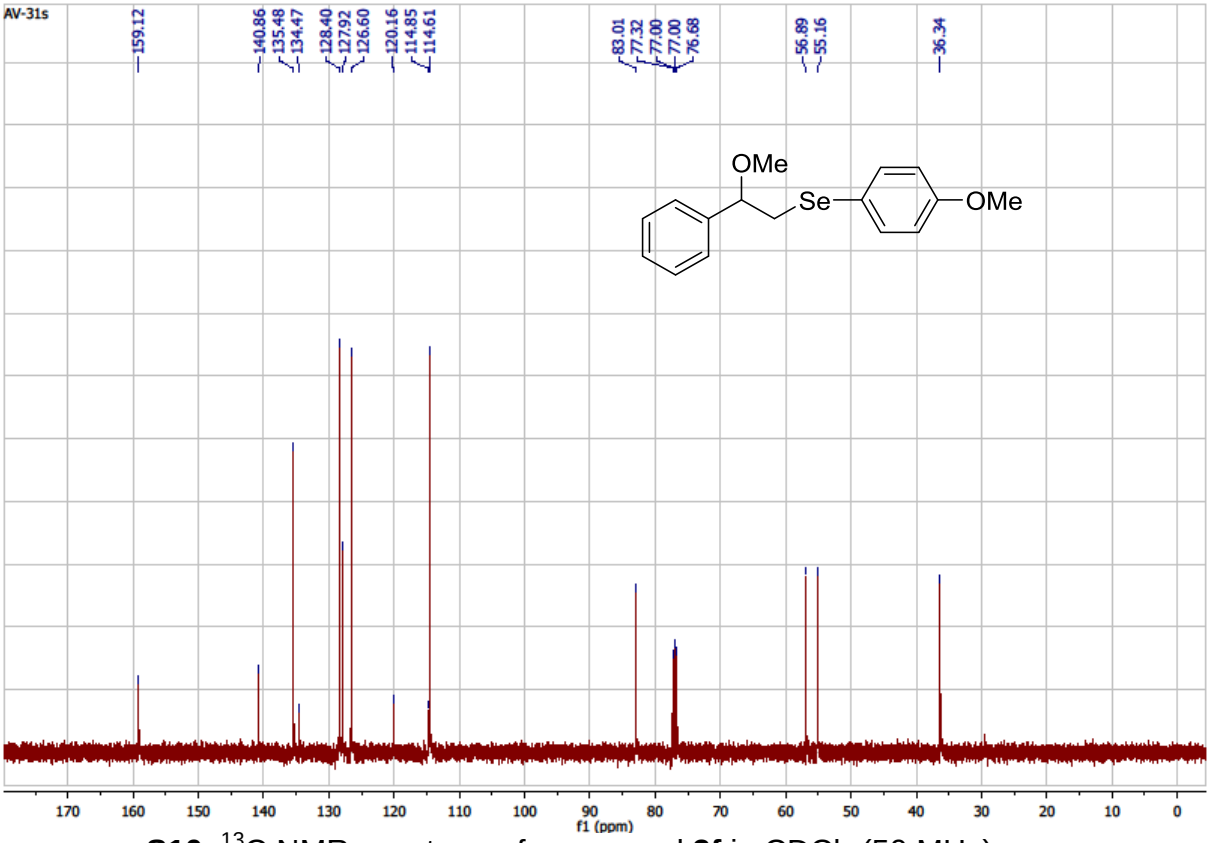
S7. ^{1}H NMR spectrum of compound **3e** in $CDCl_3$ (200 MHz).



S8. ^{13}C NMR spectrum of compound **3e** in $CDCl_3$ (50 MHz).



S9. ^{1}H NMR spectrum of compound **3f** in $CDCl_3$ (200 MHz).



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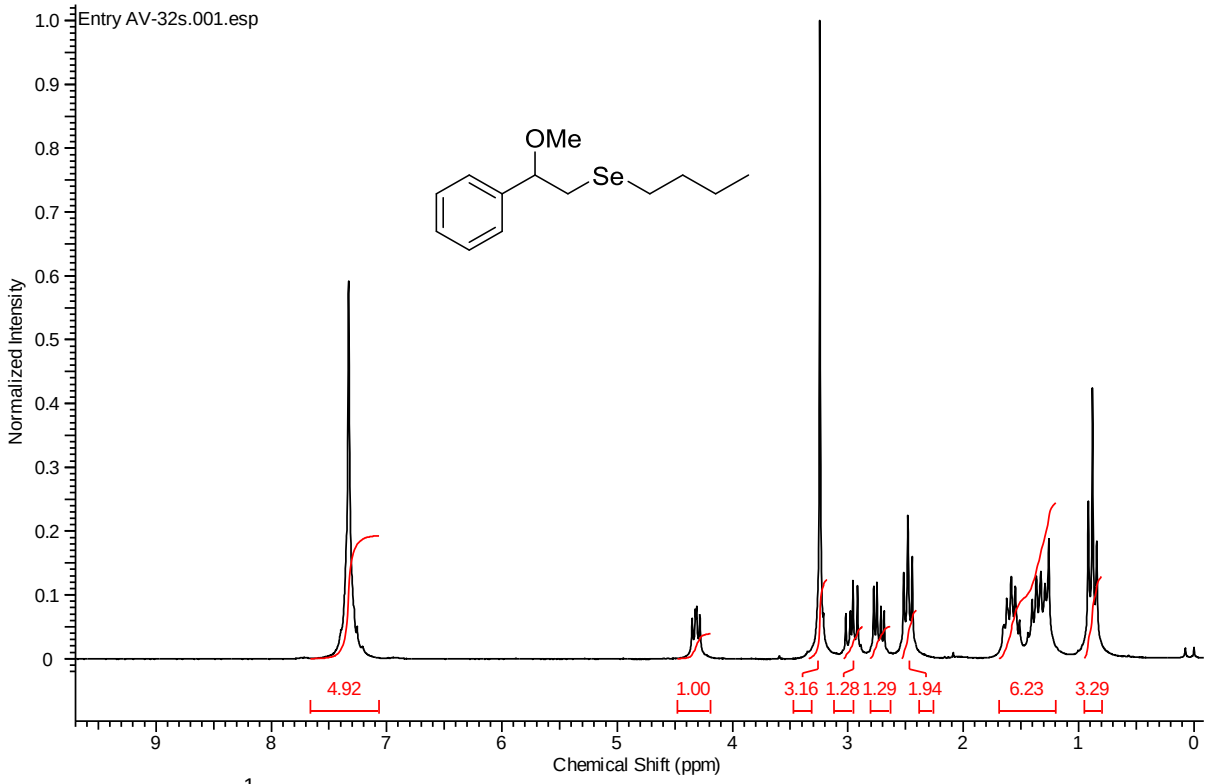

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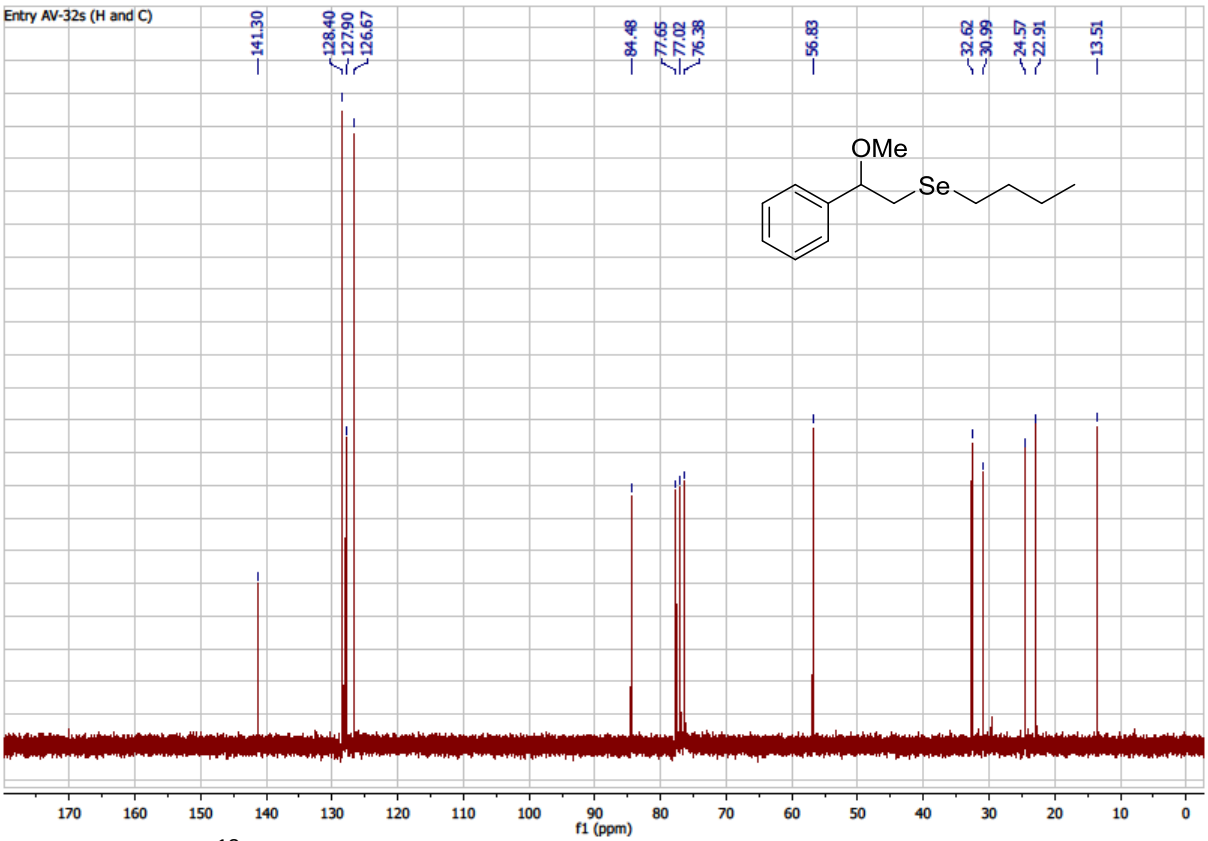
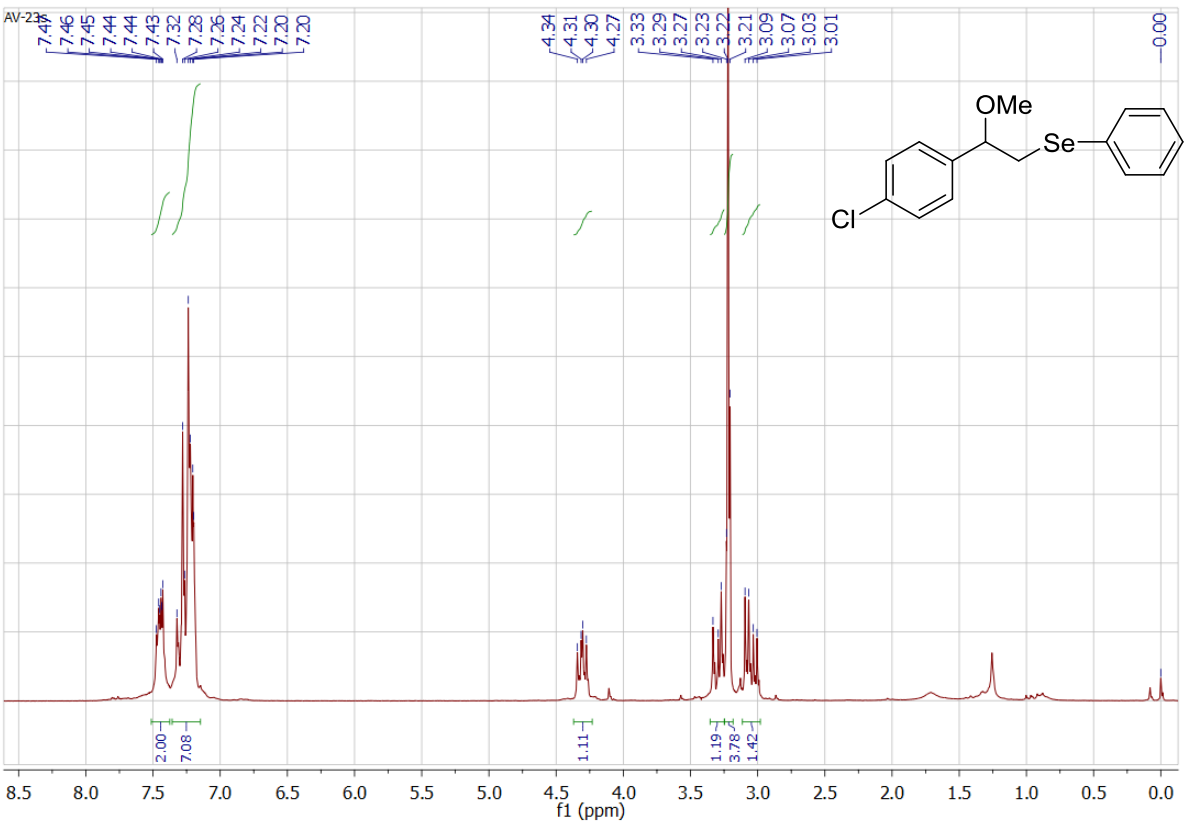
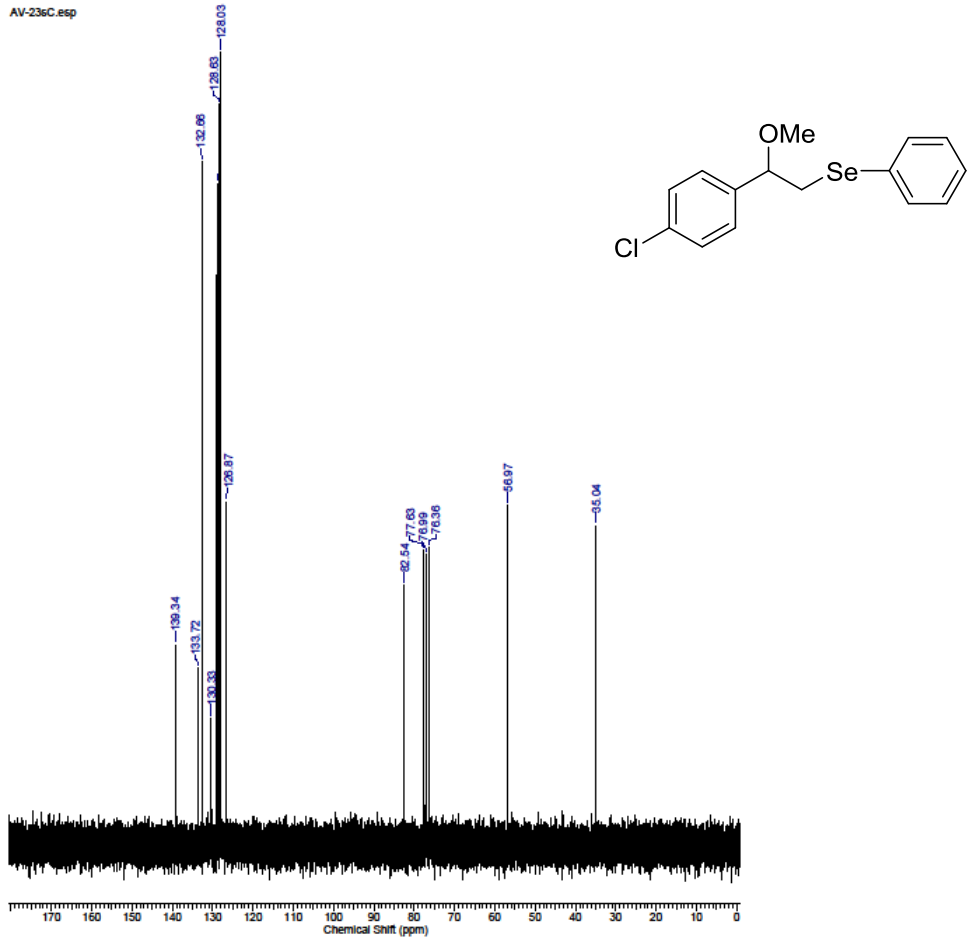


S12. ^{13}C NMR spectrum of compound **3g** in $CDCl_3$ (50 MHz).



S13. ^{1}H NMR spectrum of compound **3h** in $CDCl_3$ (200 MHz).



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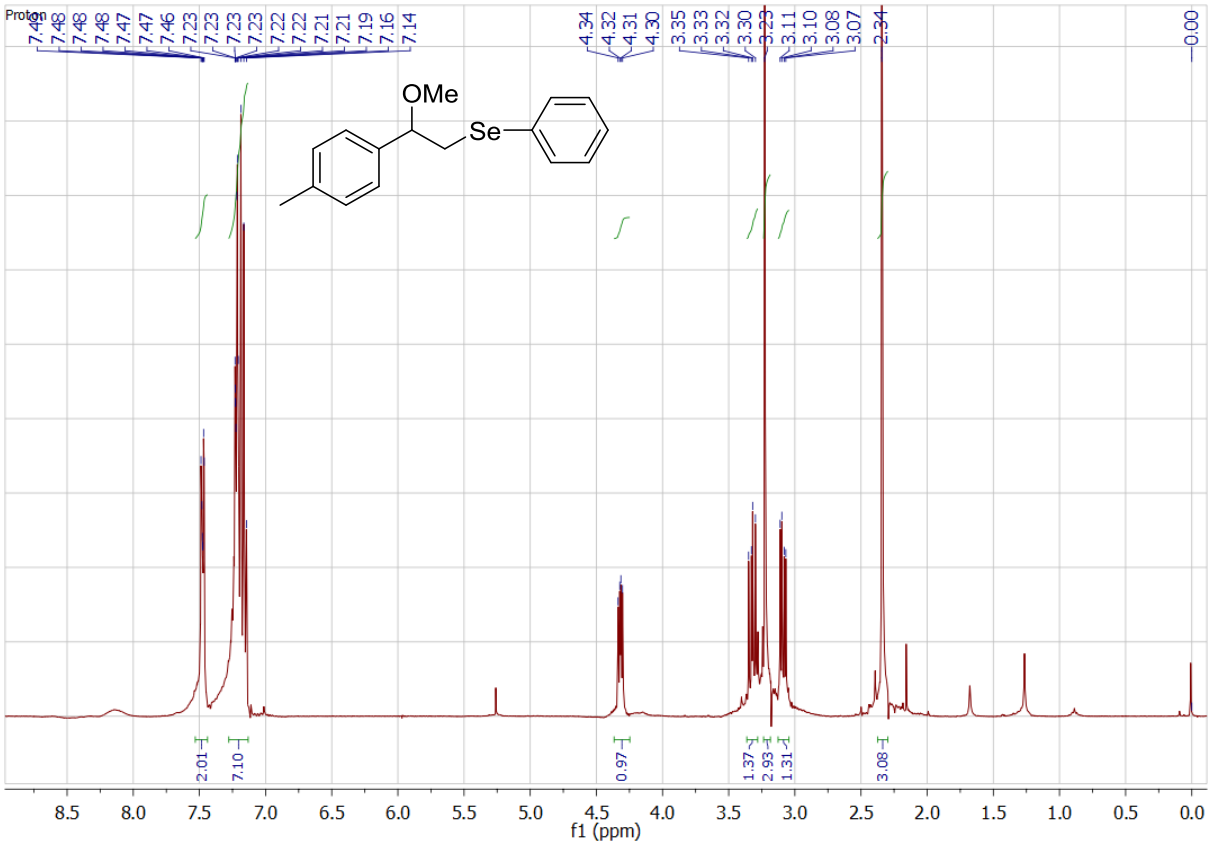
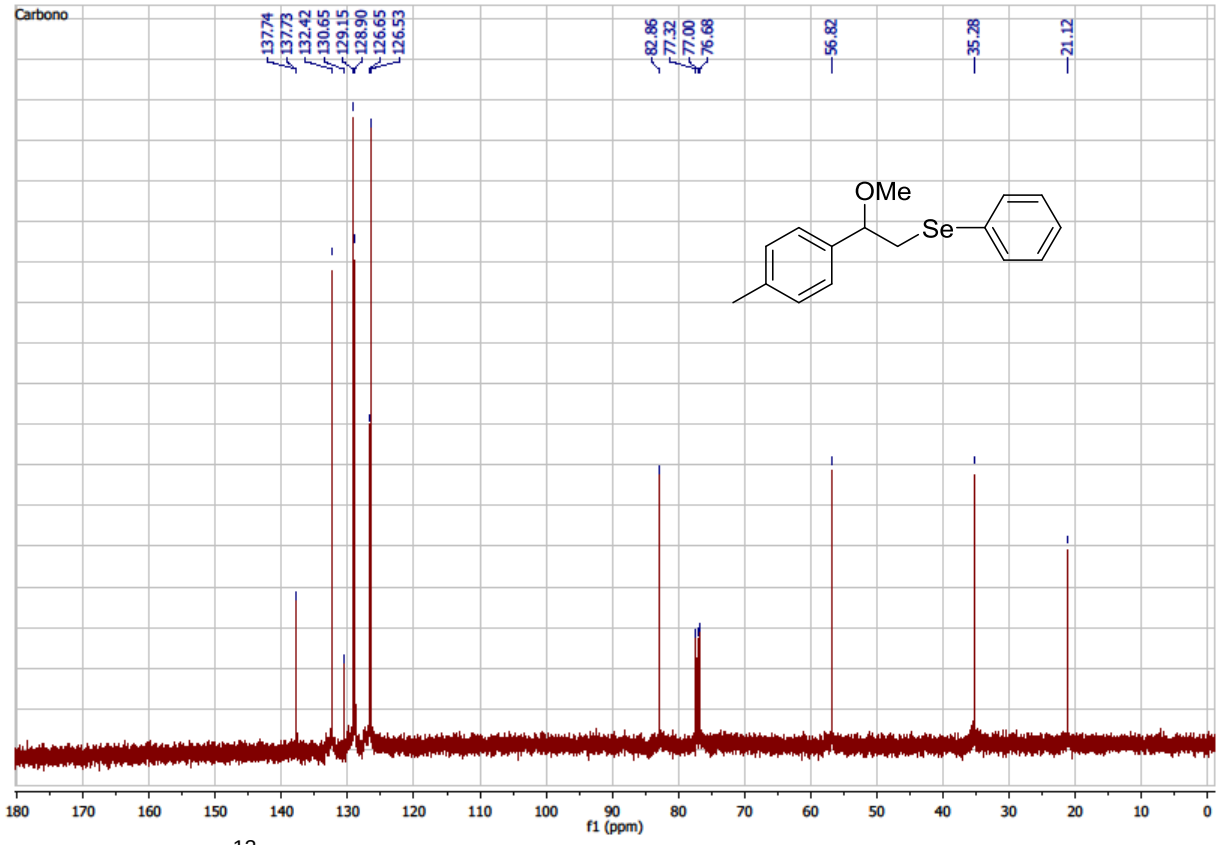
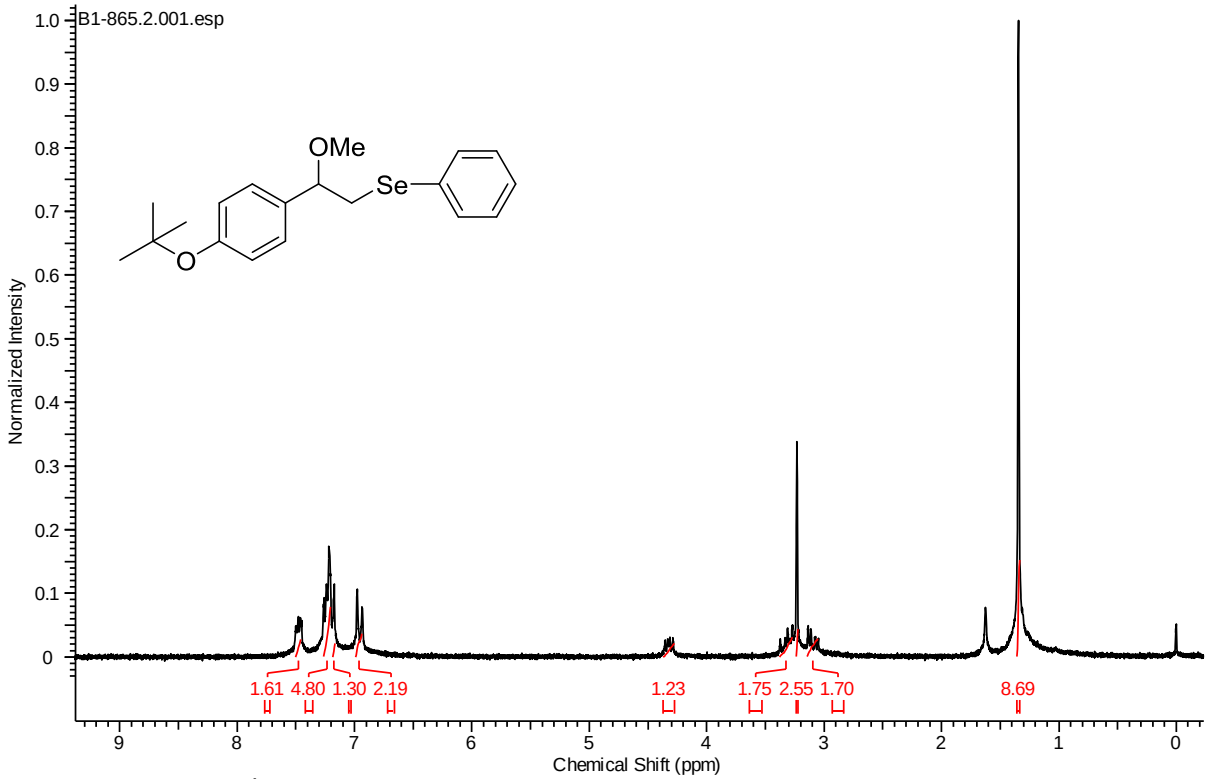


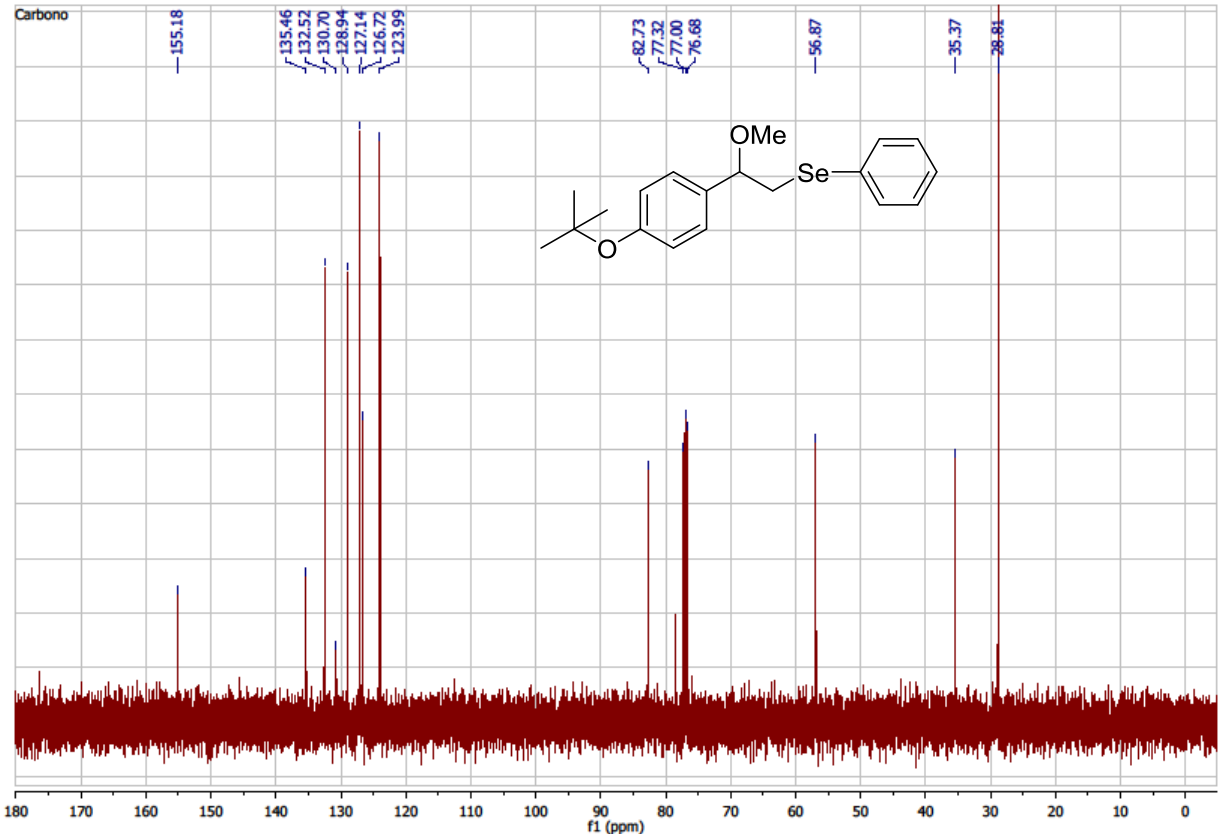
S15. ^{1}H NMR spectrum of compound **3i** in $CDCl_3$ (200 MHz).



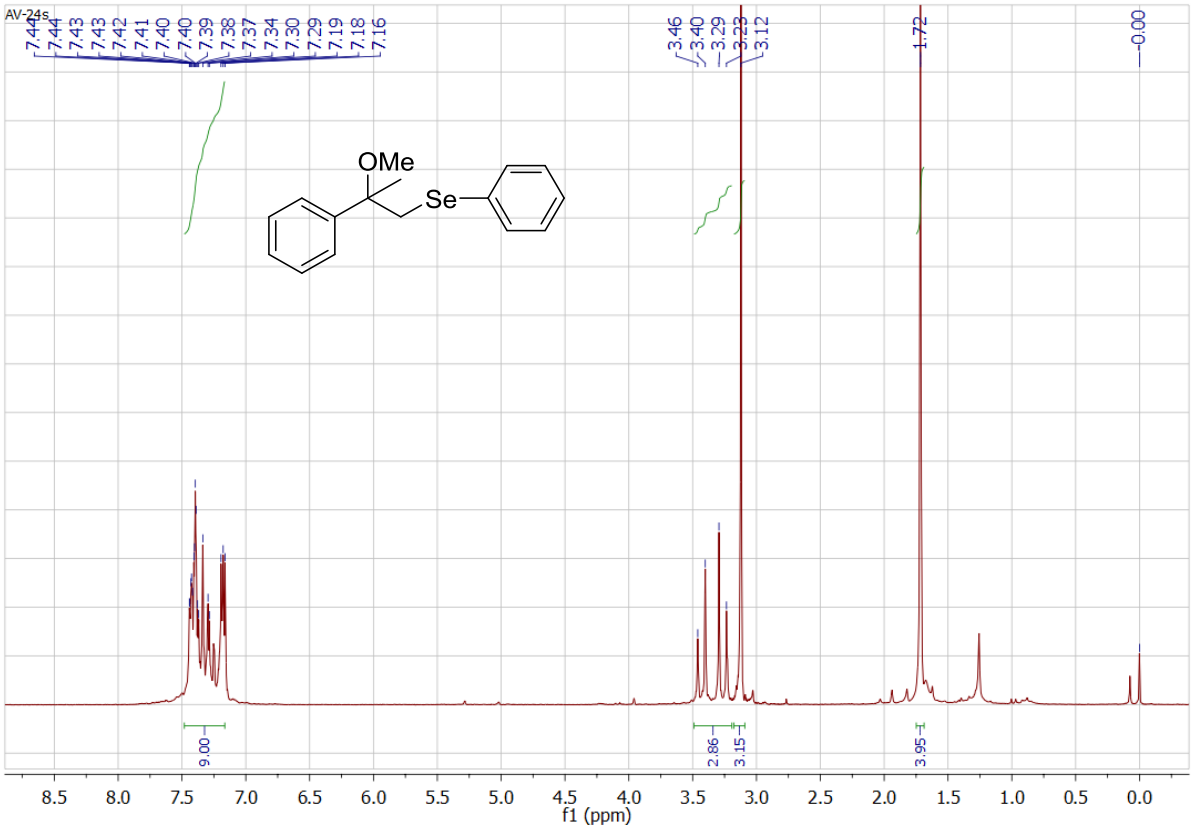
S16. ^{13}C NMR spectrum of compound **3i** in $CDCl_3$ (50 MHz).



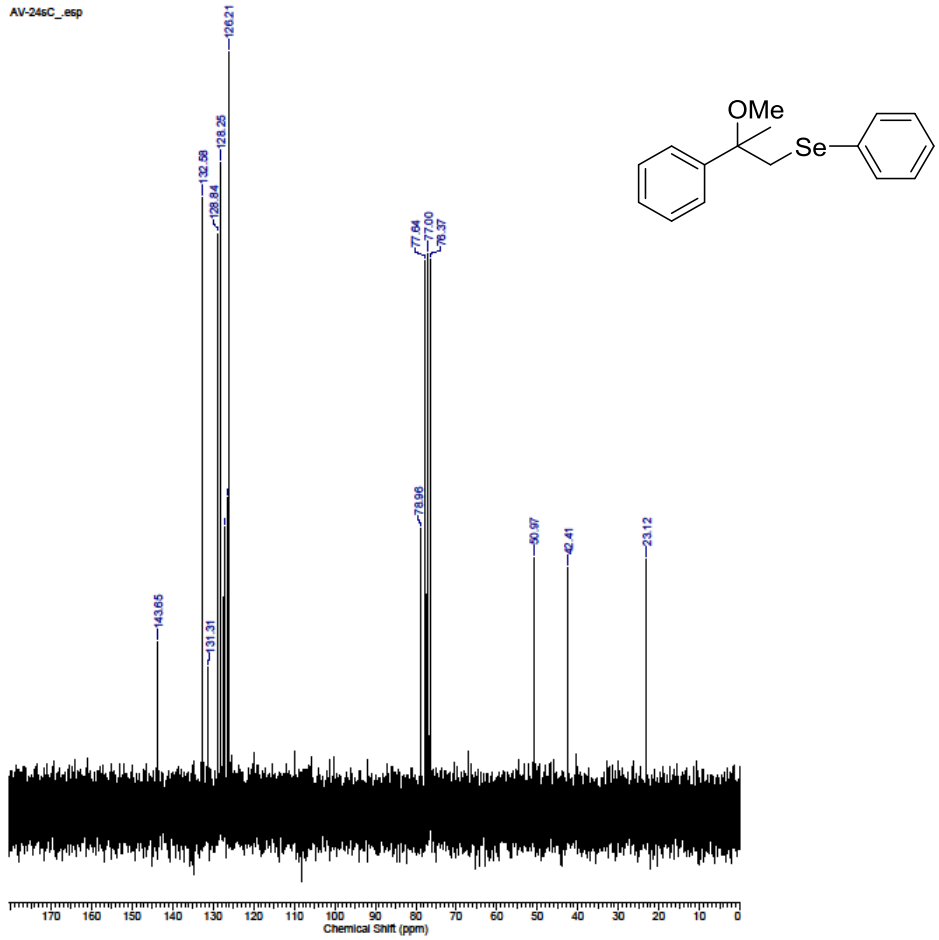
S17. ^{1}H NMR spectrum of compound **3j** in $CDCl_3$ (200 MHz).



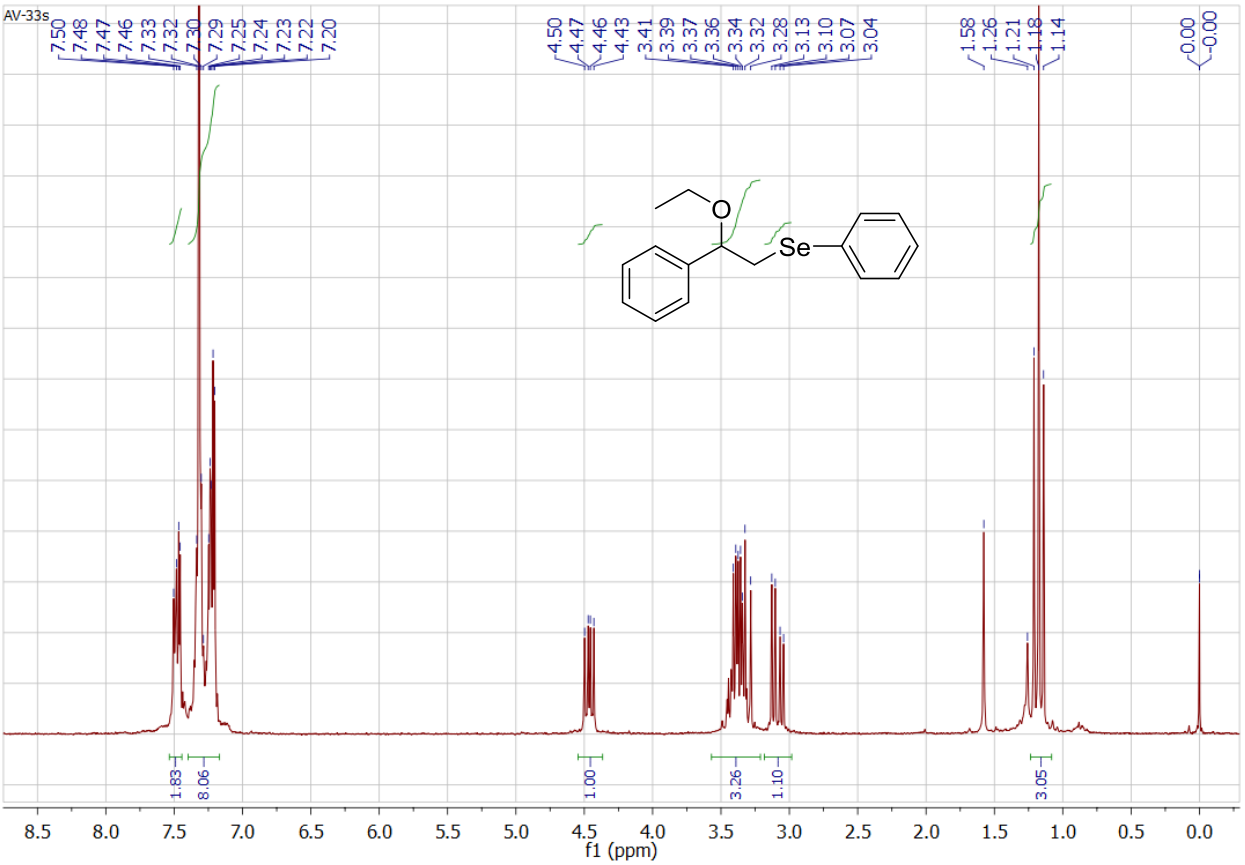
S18. ^{13}C NMR spectrum of compound **3j** in $CDCl_3$ (50 MHz).



S19. ^{1}H NMR spectrum of compound **3k** in $CDCl_3$ (200 MHz).



S20. ^{13}C NMR spectrum of compound **3k** in $CDCl_3$ (50 MHz).



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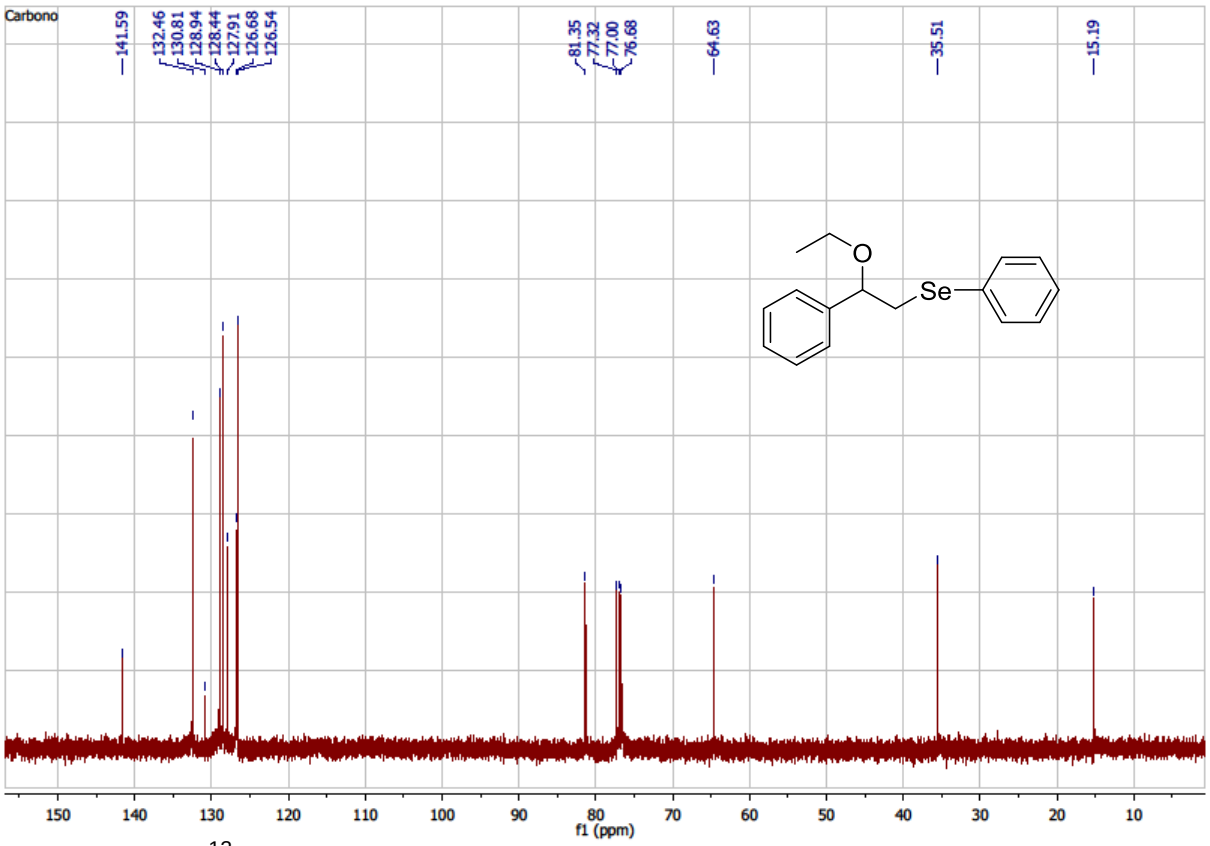
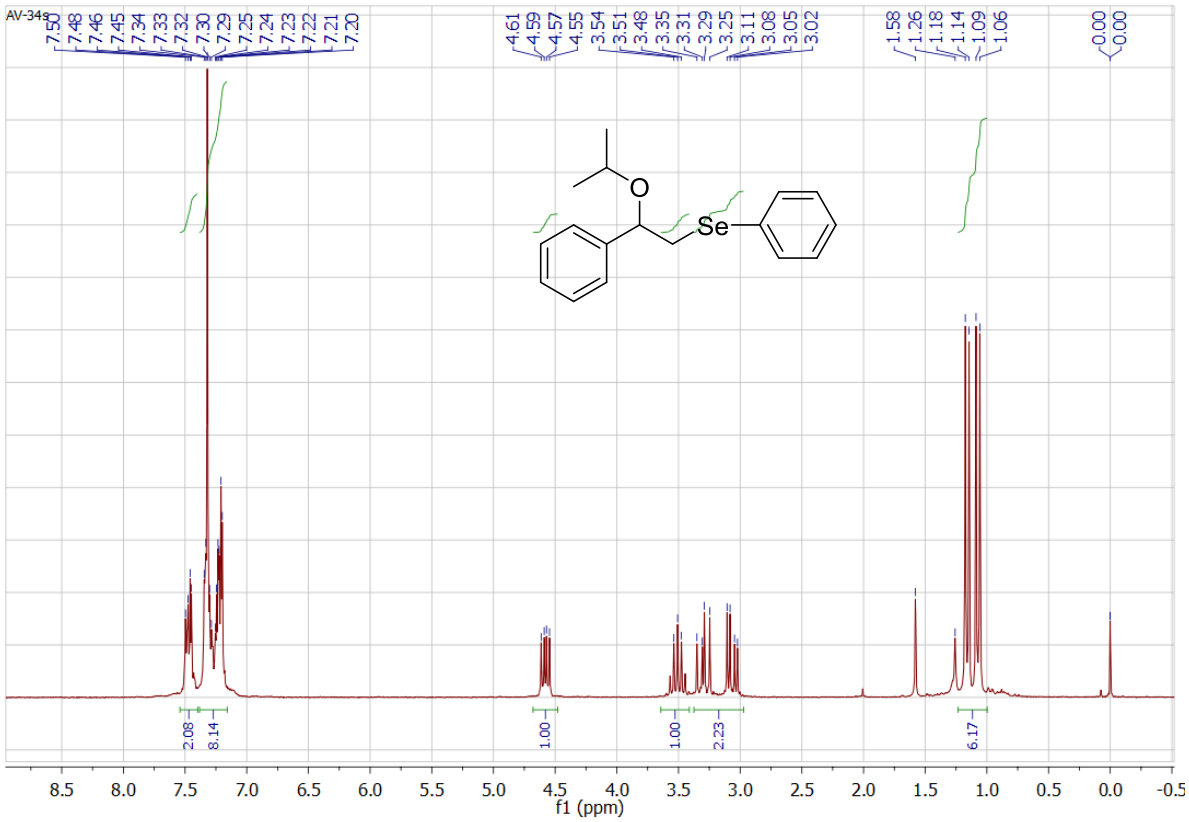
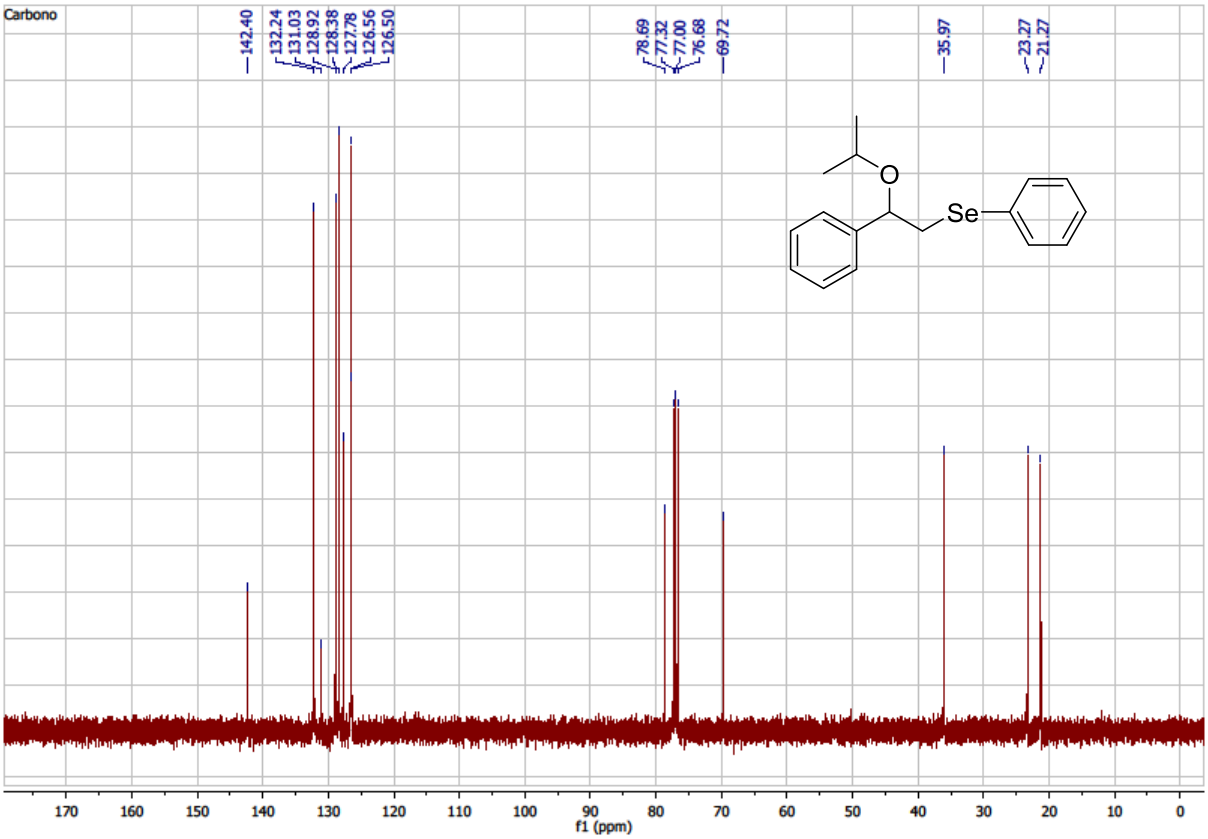


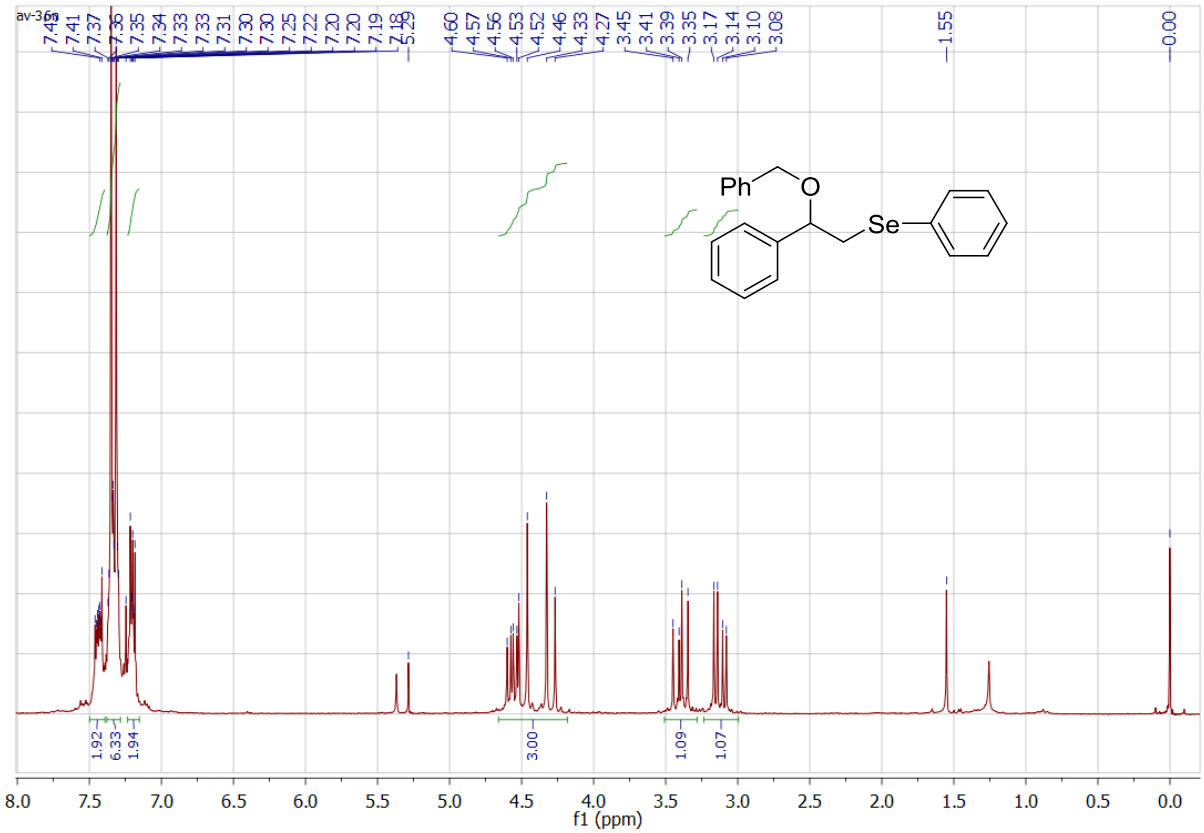
S22. ^{13}C NMR spectrum of compound **3m** in $CDCl_3$ (50 MHz).



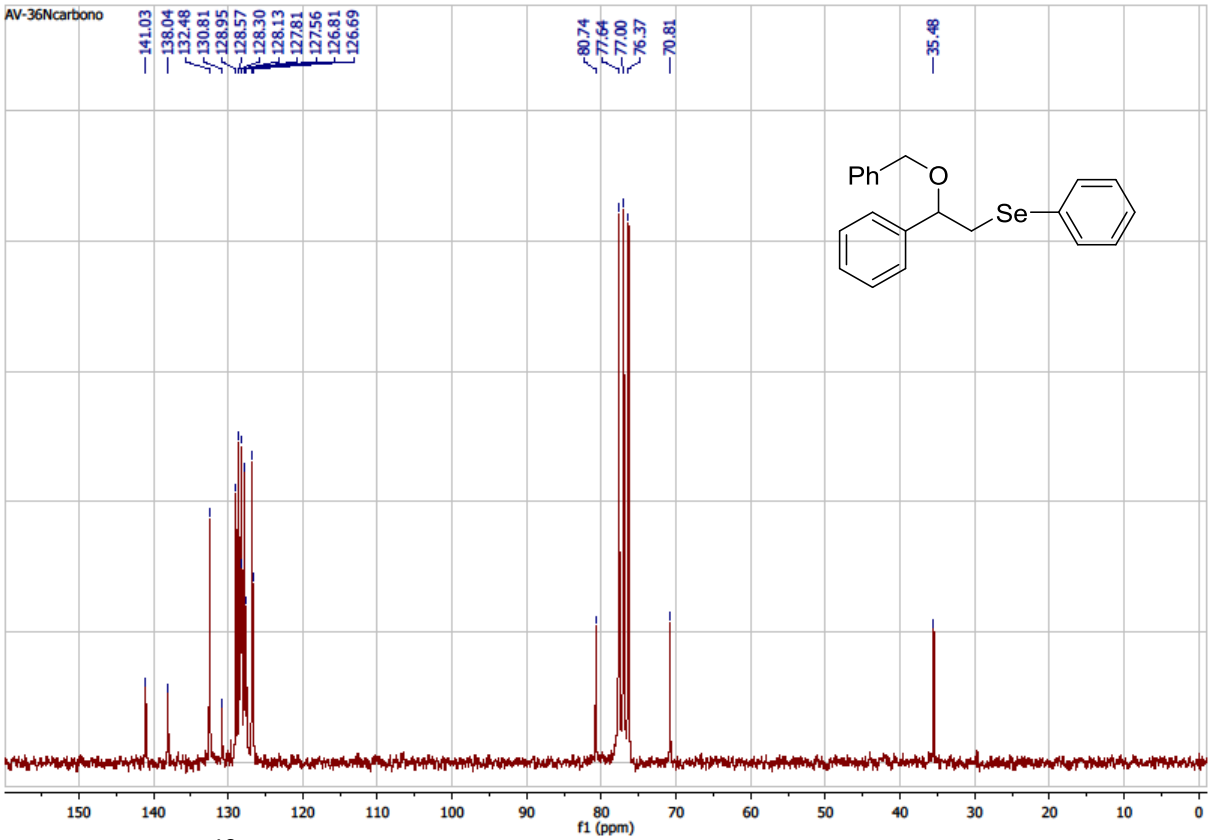
S23. ^{1}H NMR spectrum of compound **3n** in $CDCl_3$ (200 MHz).



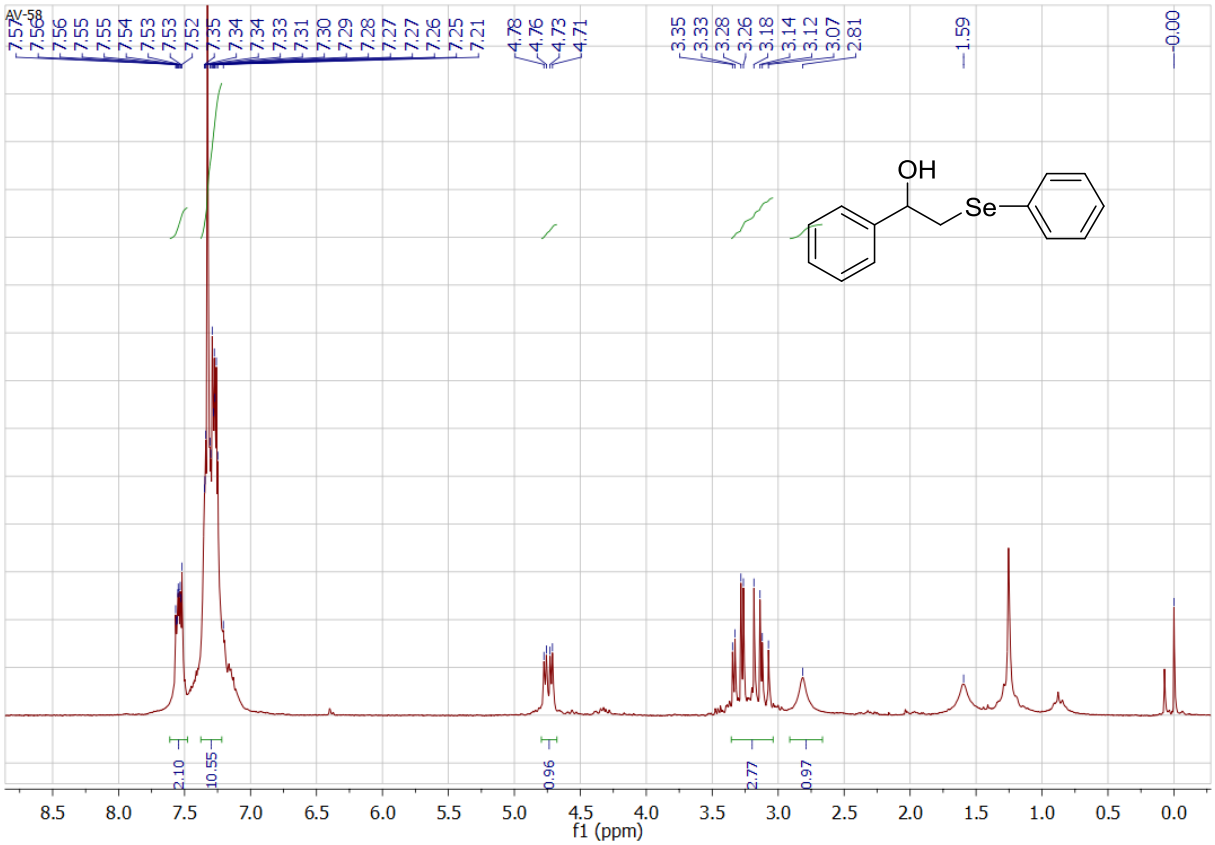
S24. ^{13}C NMR spectrum of compound **3n** in $CDCl_3$ (50 MHz).



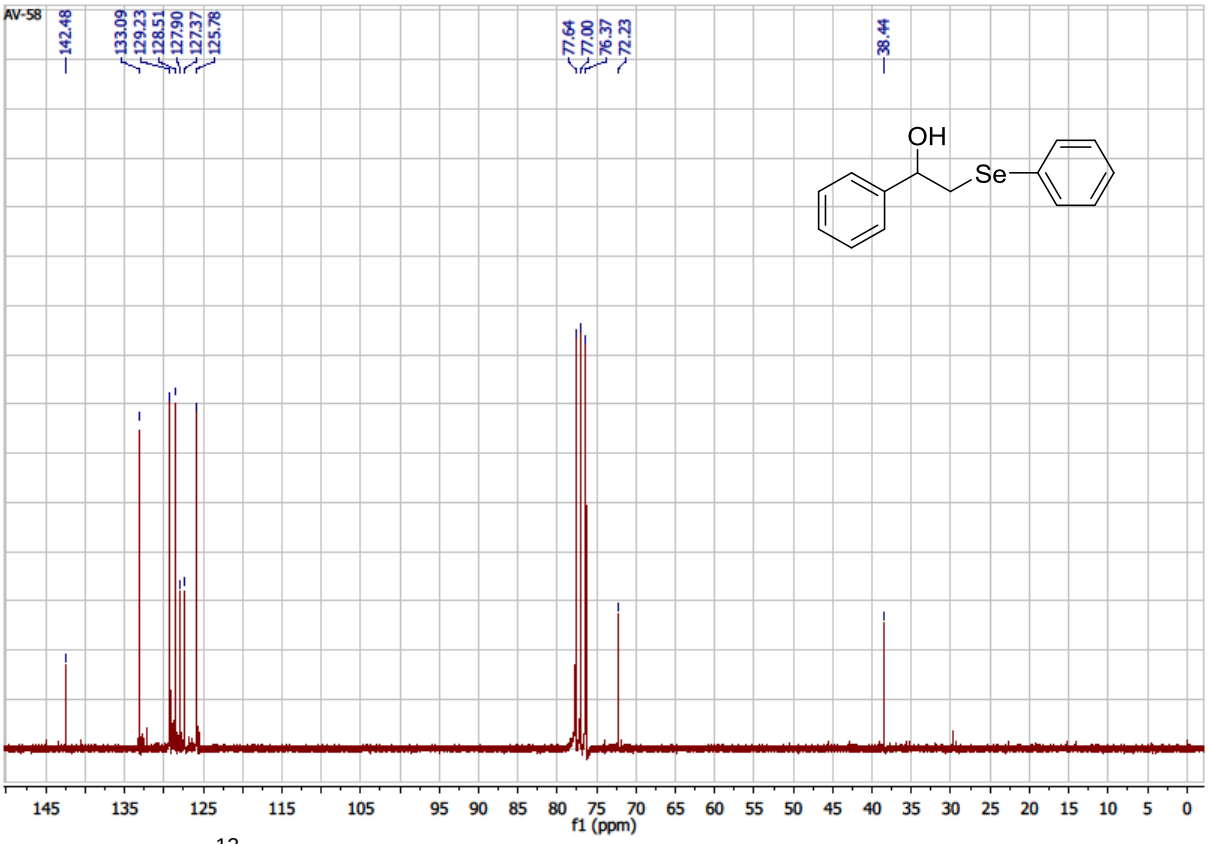
S25. ^{1}H NMR spectrum of compound **3o** in $CDCl_3$ (200 MHz).



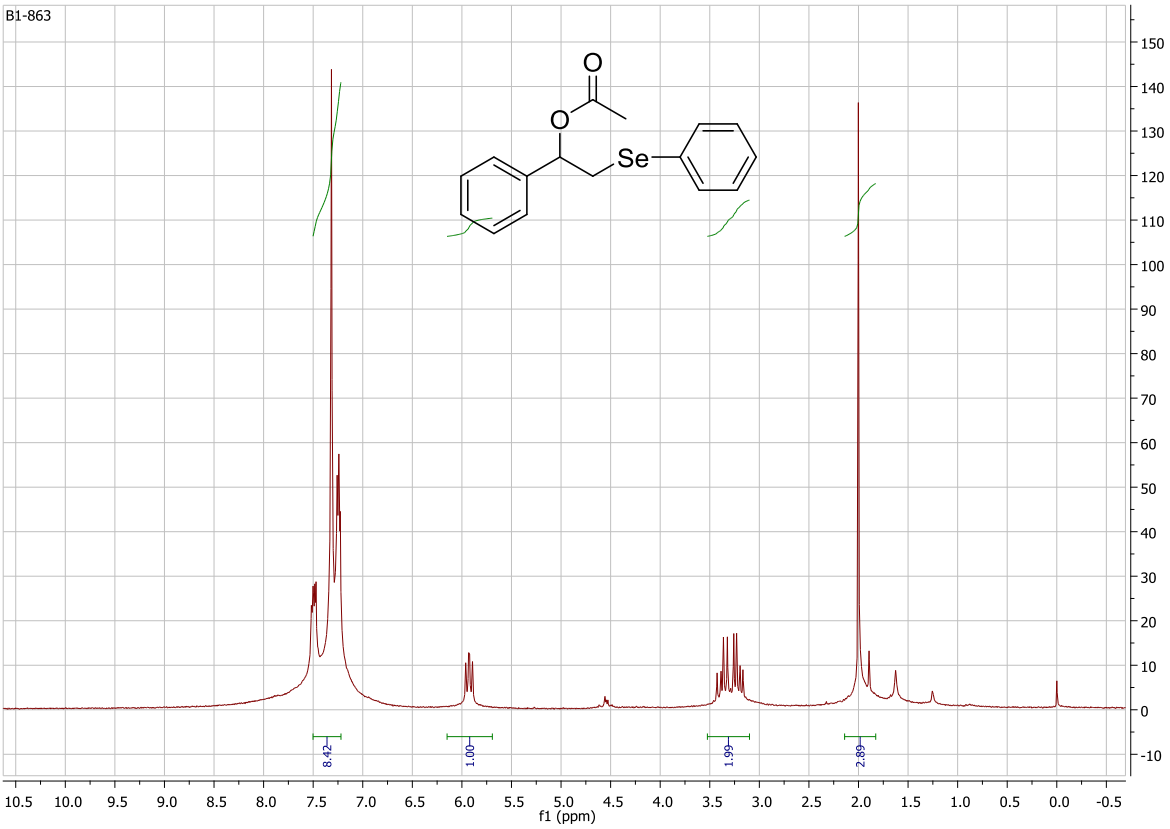
S26. ^{13}C NMR spectrum of compound **3o** in $CDCl_3$ (50 MHz).



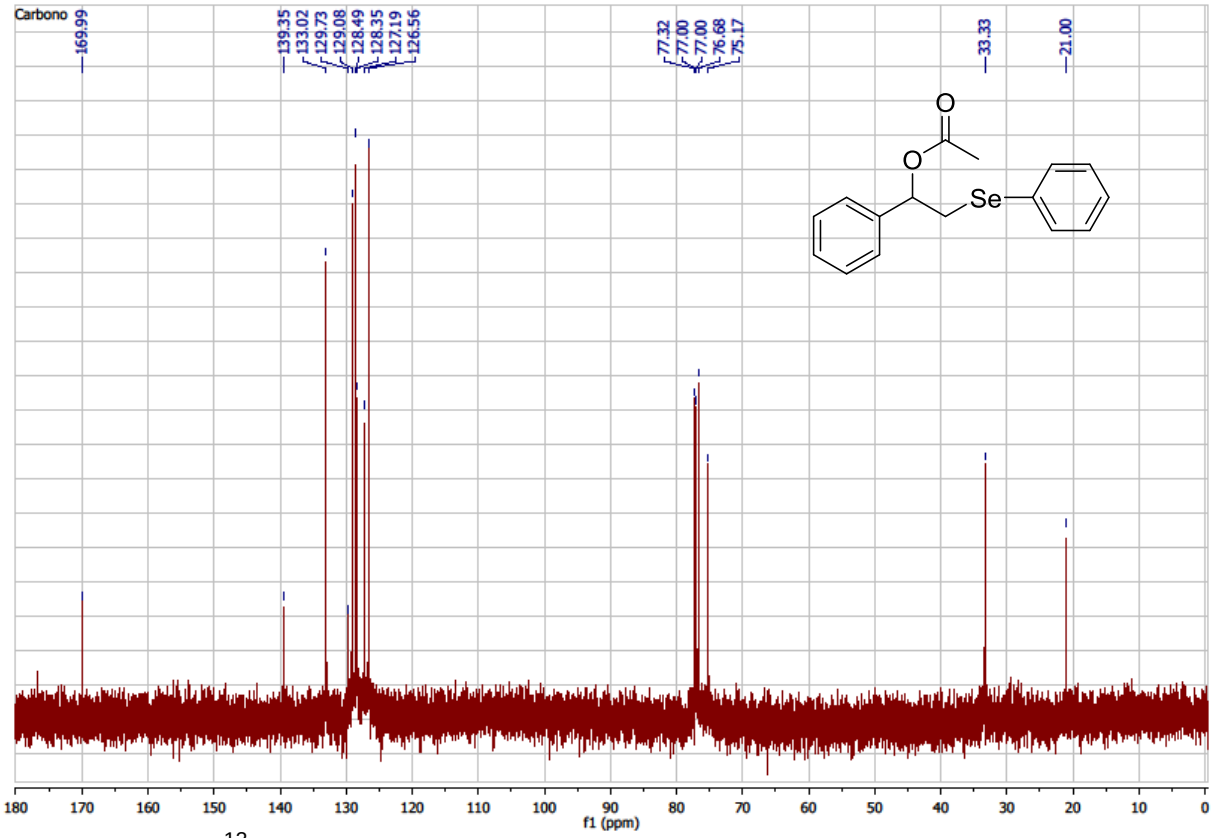
S27. ^{1}H NMR spectrum of compound **3r** in $CDCl_3$ (200 MHz)



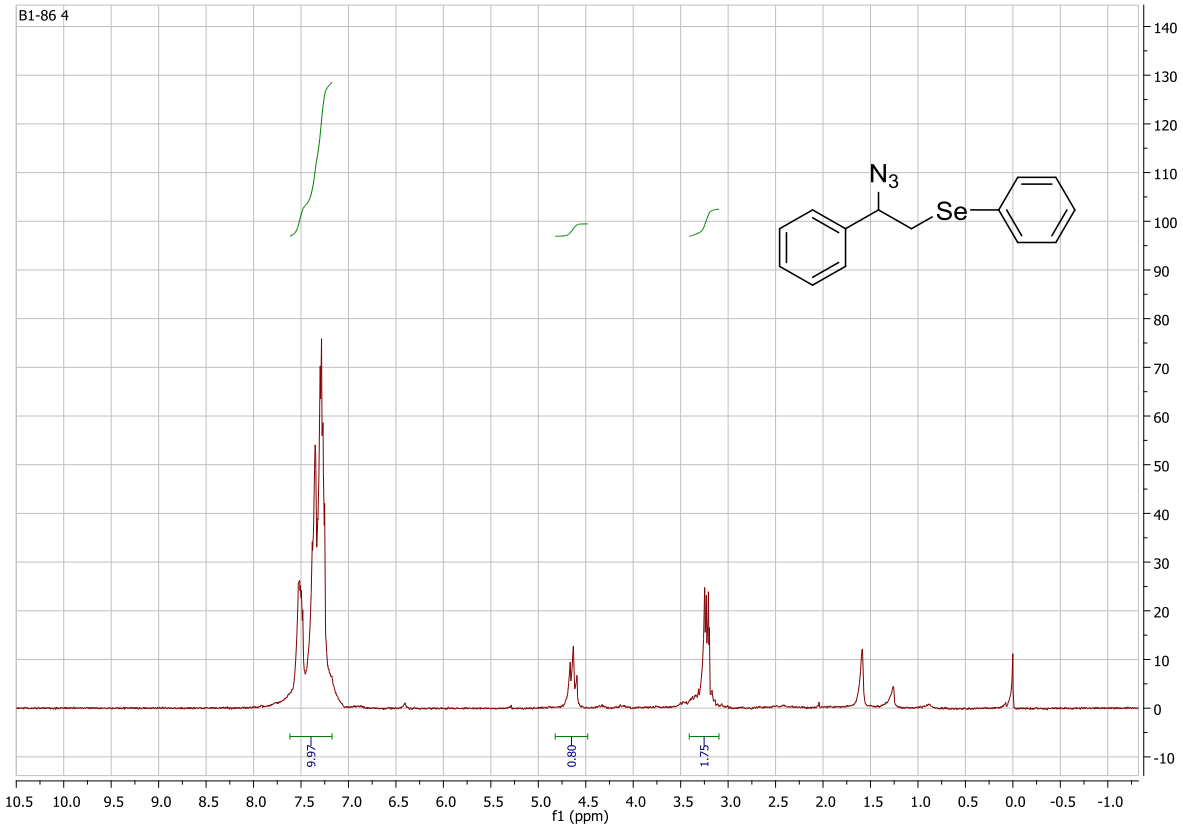
S28. ^{13}C NMR spectrum of compound **3r** in $CDCl_3$ (50 MHz).



S29. ^{1}H NMR spectrum of compound **3s** in $CDCl_3$ (200 MHz).



S30. ^{13}C NMR spectrum of compound **3s** in $CDCl_3$ (50 MHz).



S31. ^{1}H NMR spectrum of compound **3t** in $CDCl_3$ (200 MHz)

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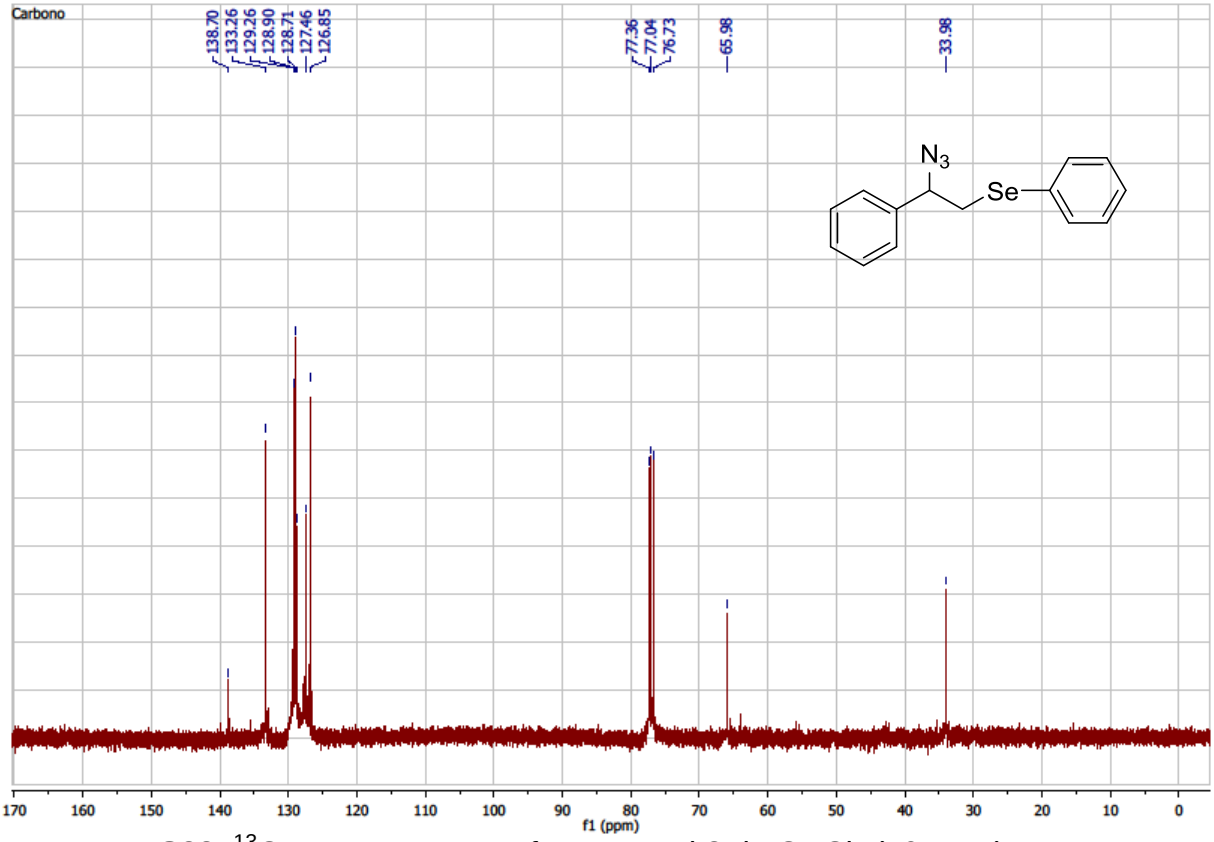
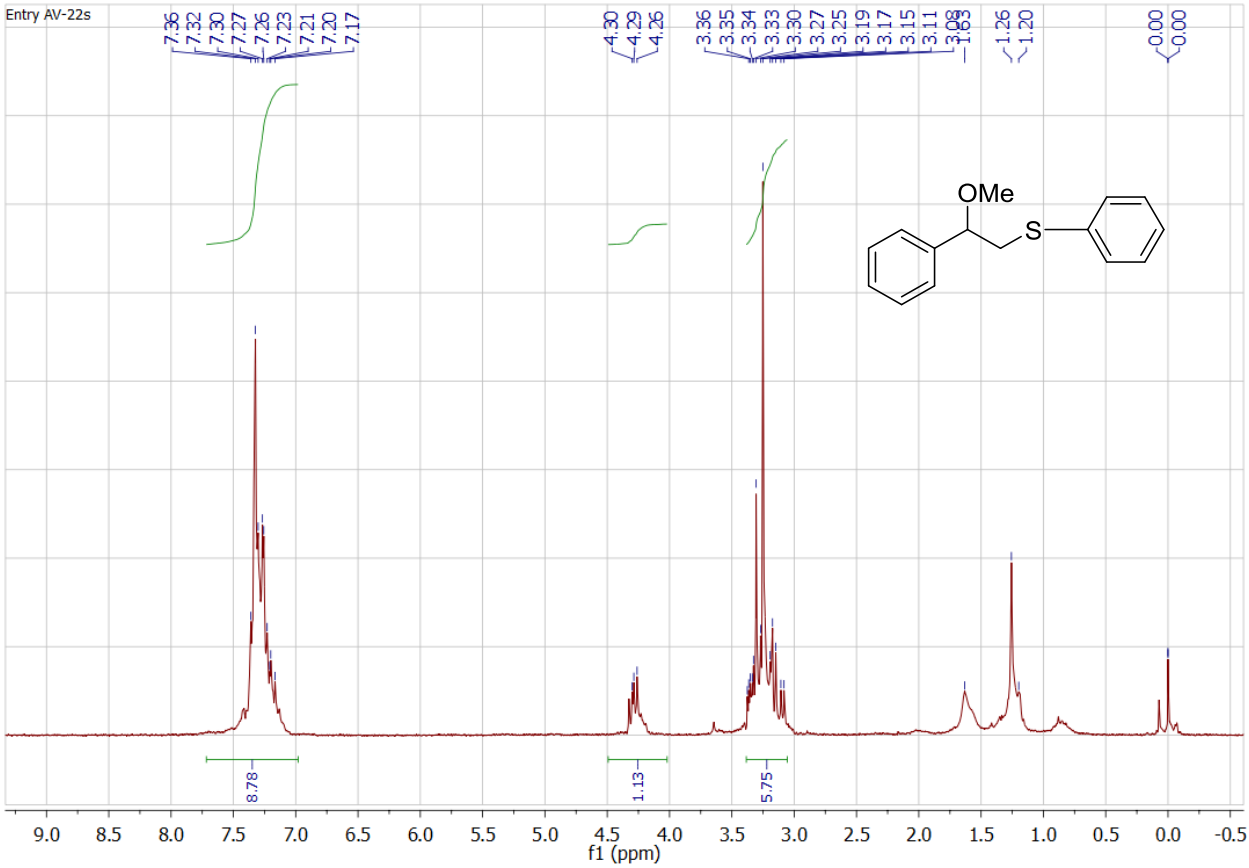
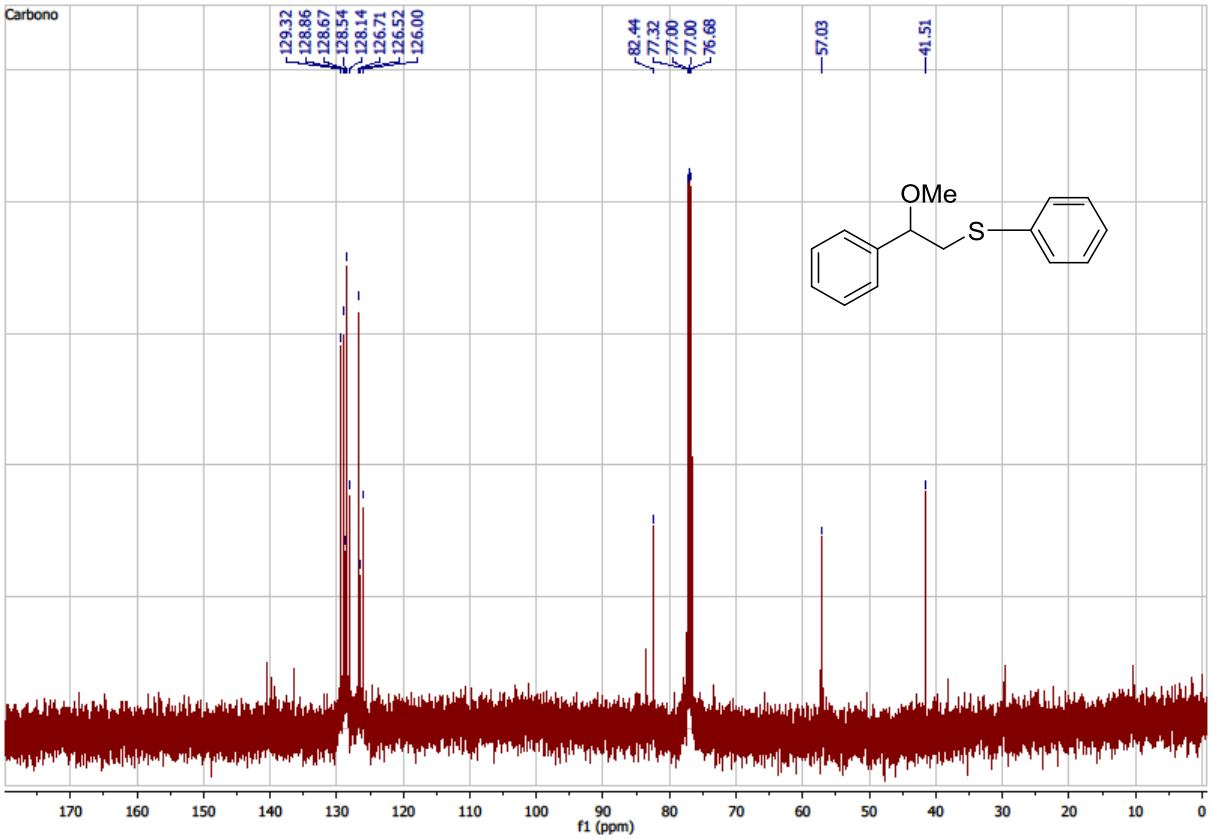


S32. ^{13}C NMR spectrum of compound **3t** in $CDCl_3$ (50 MHz).



S33. ^{1}H NMR spectrum of compound **5a** in $CDCl_3$ (200 MHz).



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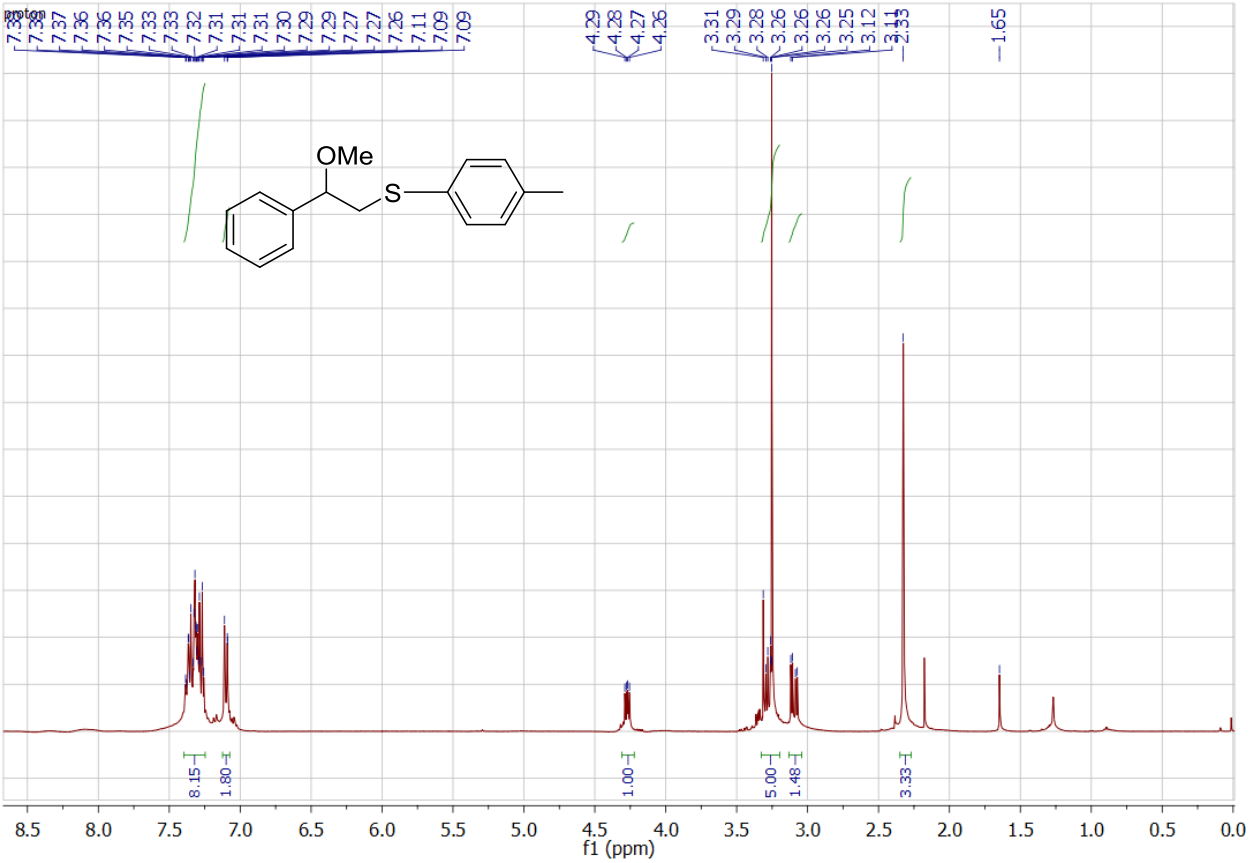
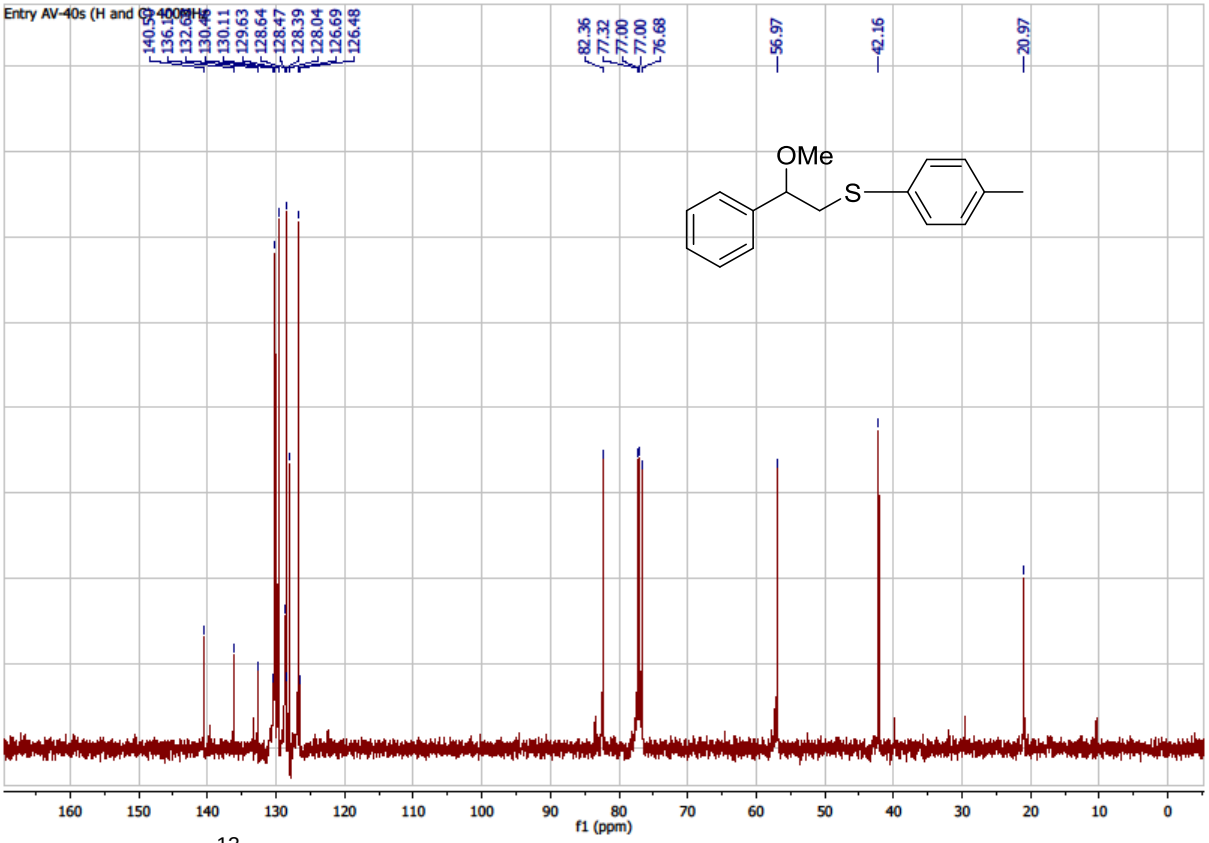
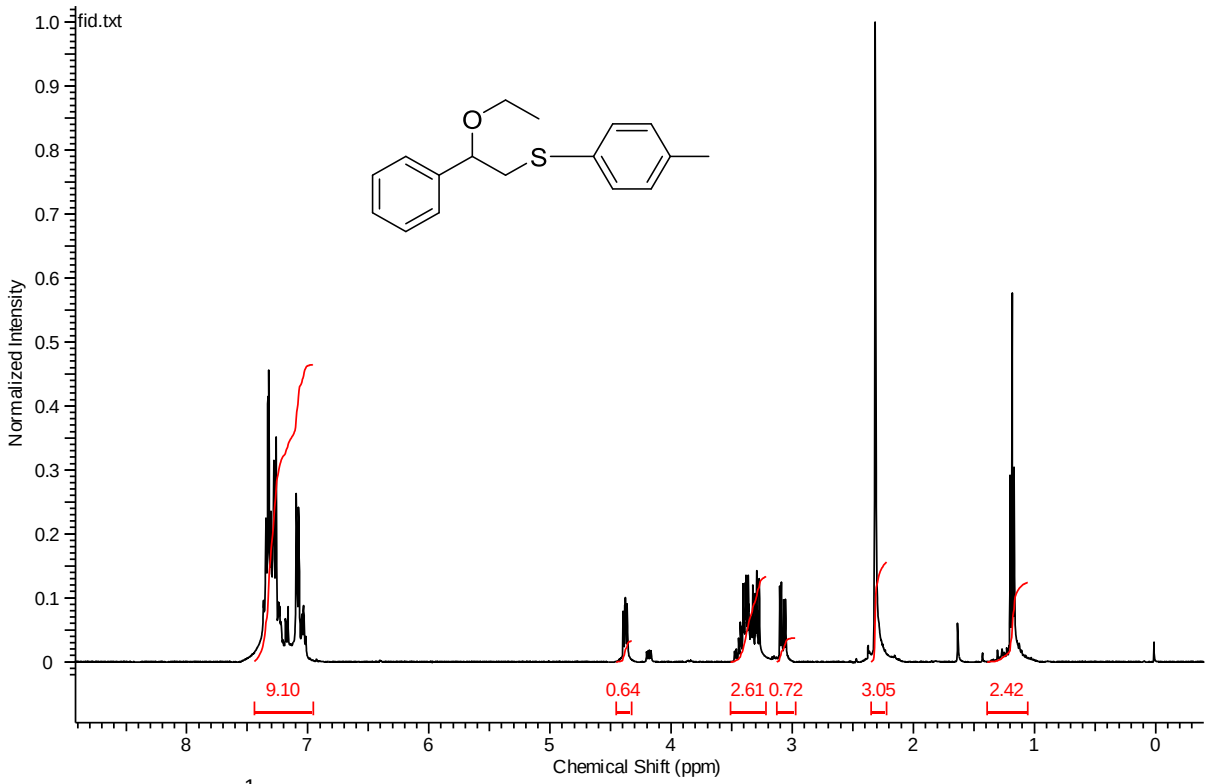


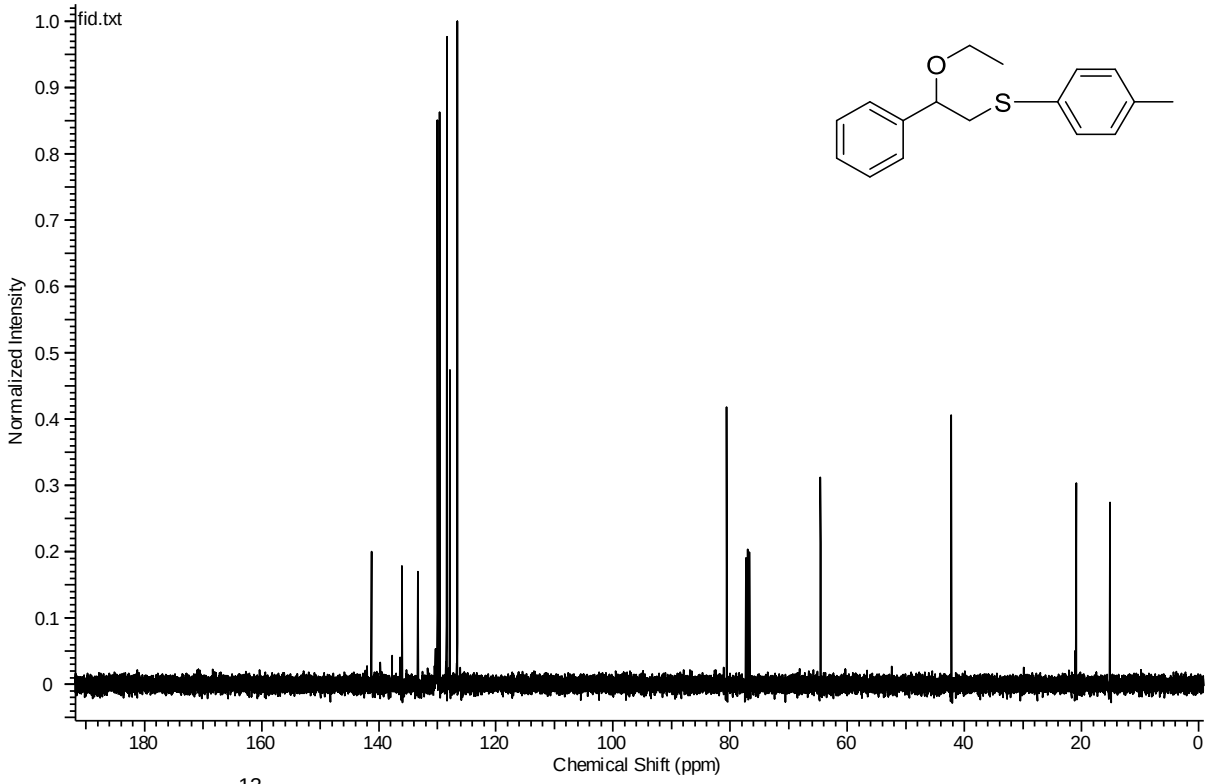
S35. ^{1}H NMR spectrum of compound **5b** in $CDCl_3$ (200 MHz).



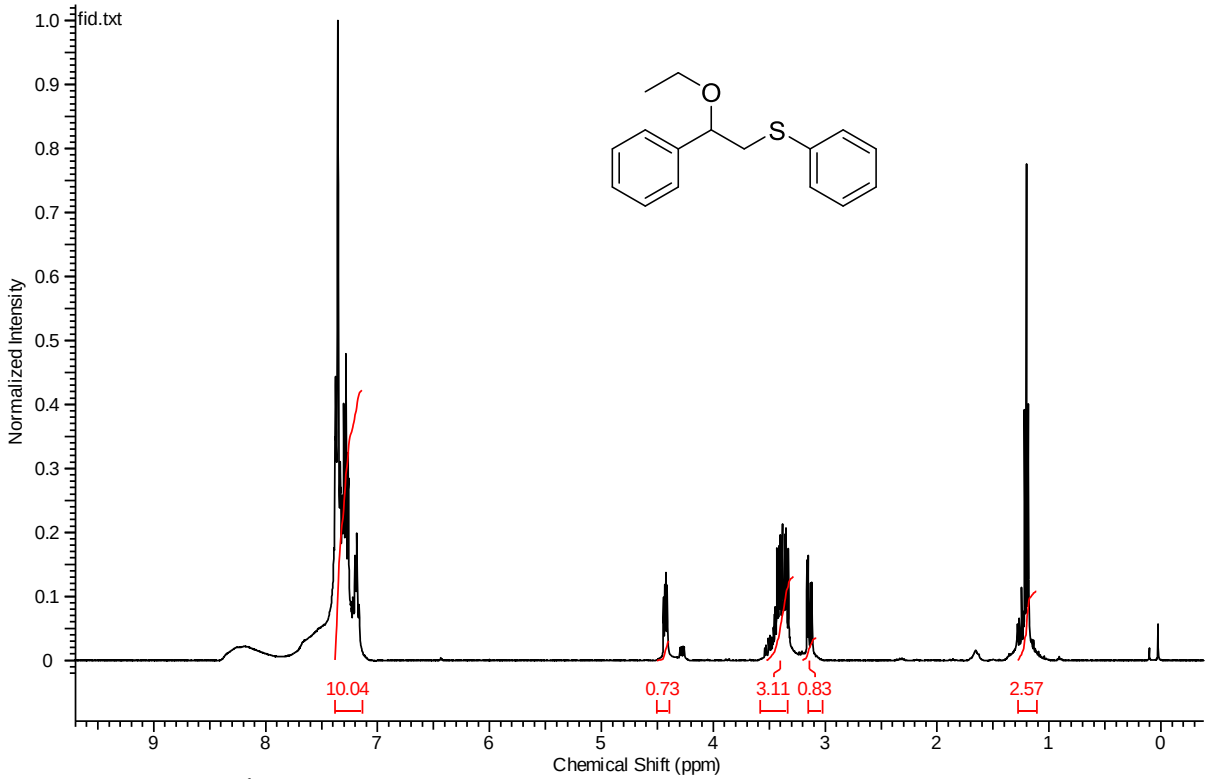
S36. ^{13}C NMR spectrum of compound **5b** in $CDCl_3$ (50 MHz).



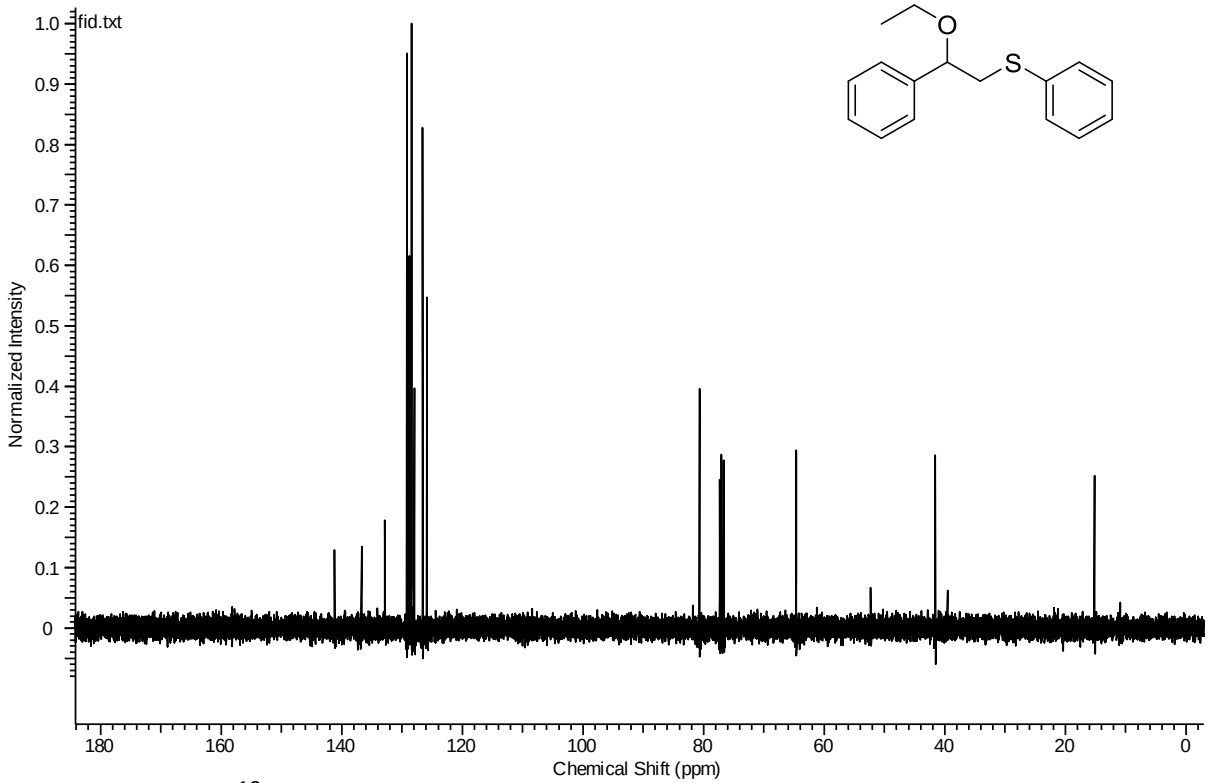
S37. ^{1}H NMR spectrum of compound **5c** in $CDCl_3$ (400 MHz).



S38. ^{13}C NMR spectrum of compound **5c** in $CDCl_3$ (100 MHz).



S39. ^{1}H NMR spectrum of compound **5d** in $CDCl_3$ (400 MHz).



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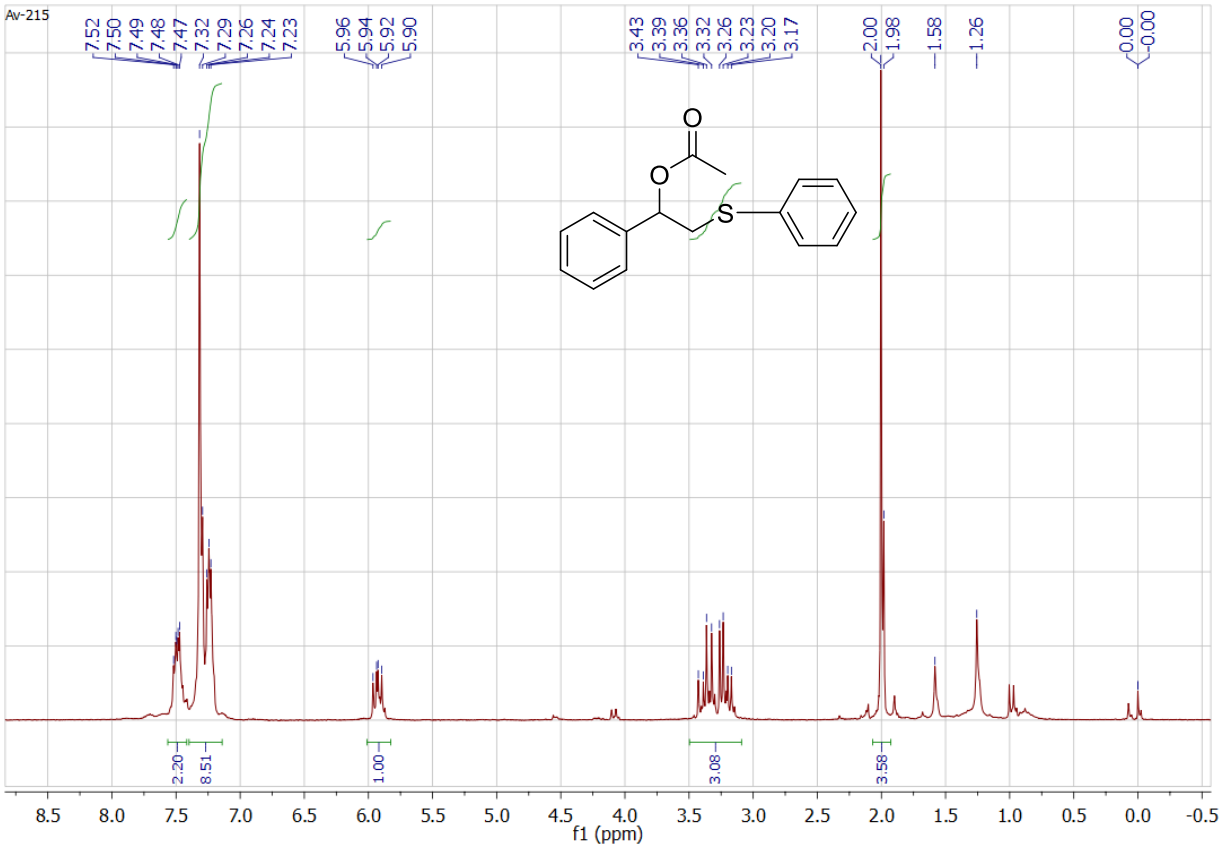
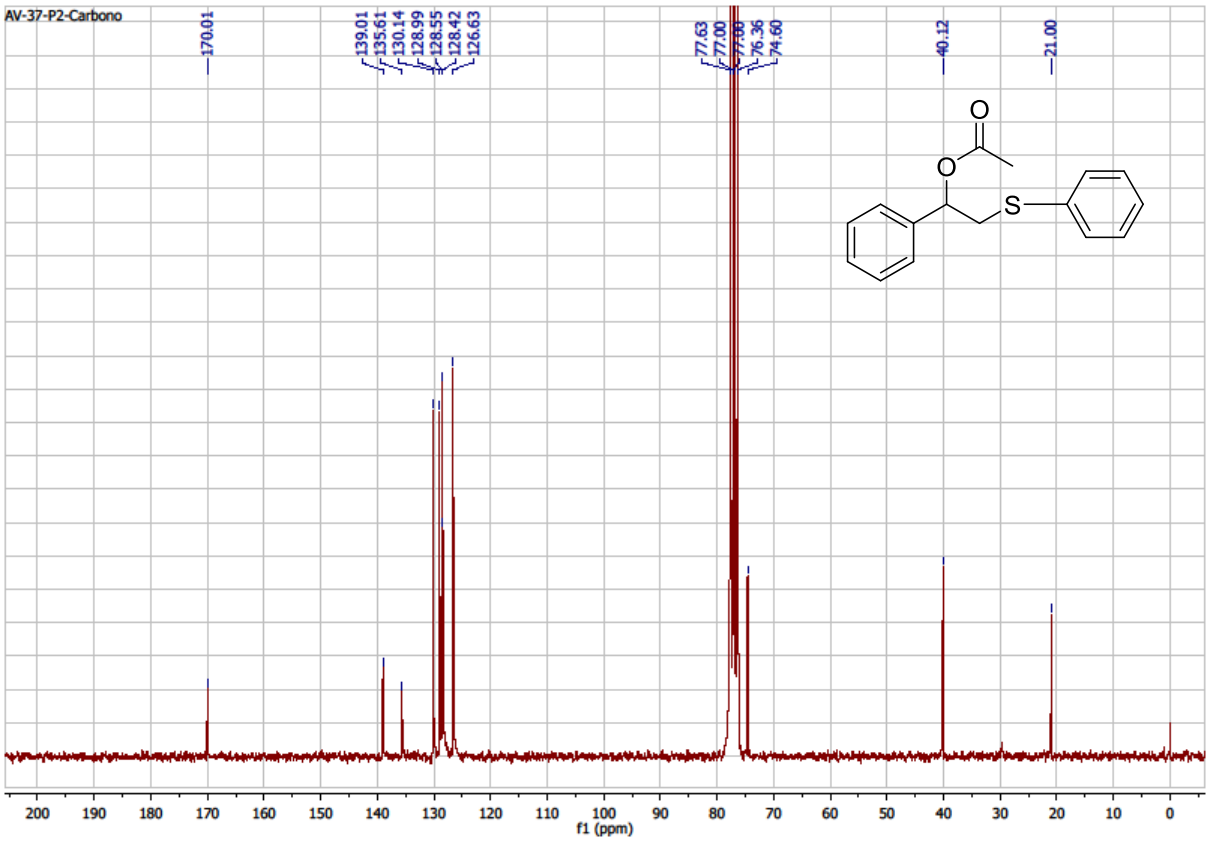
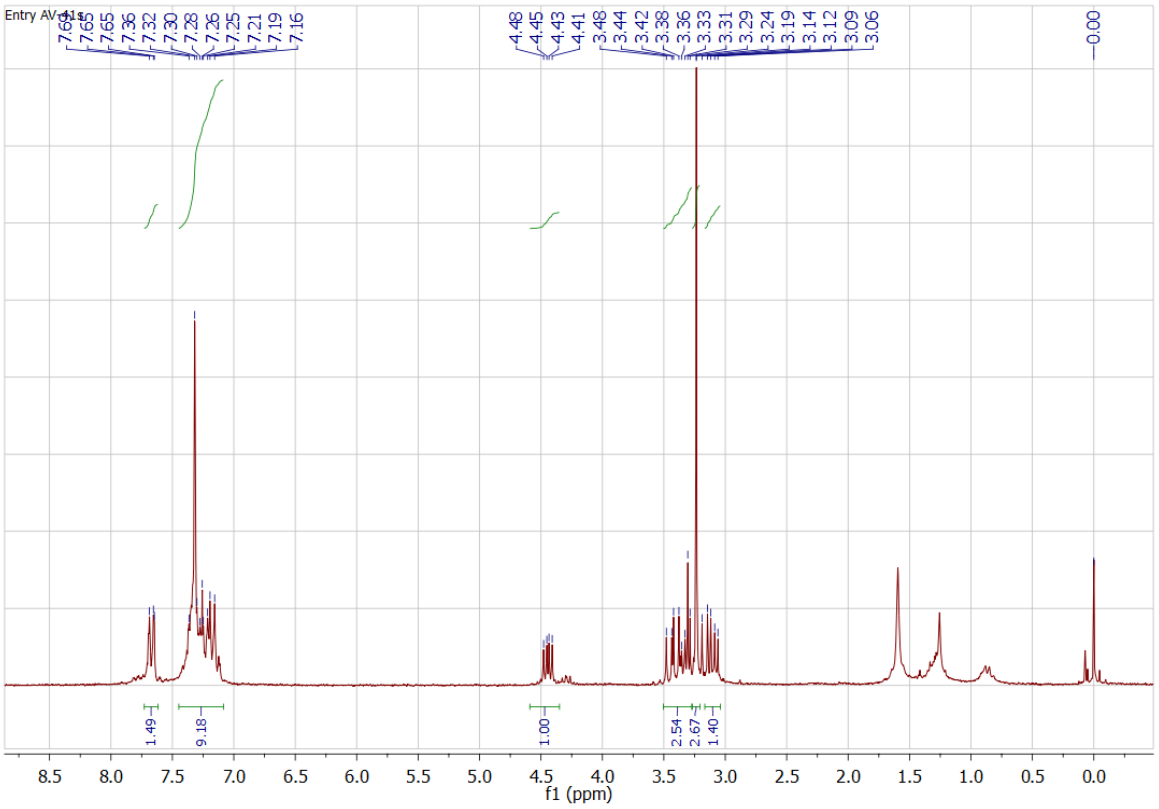


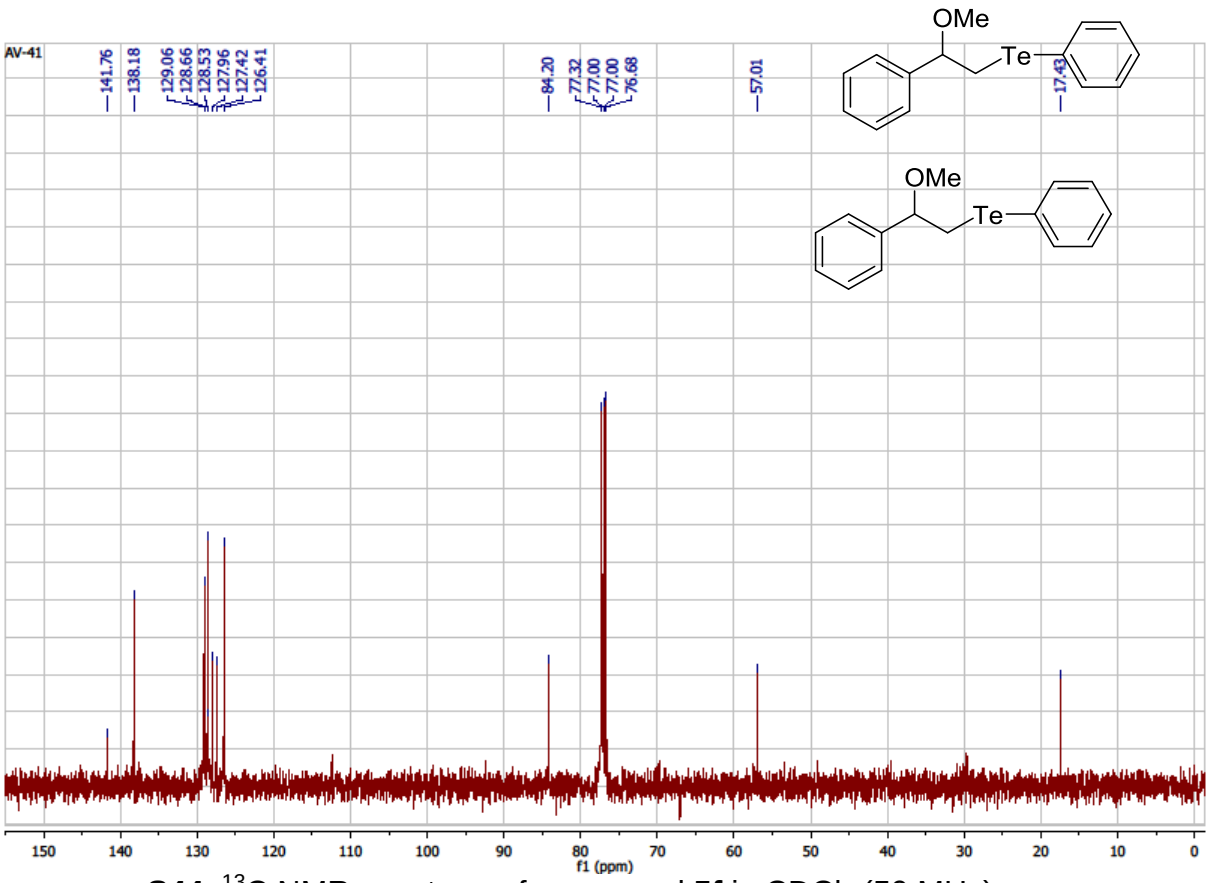
S41. ^{1}H NMR spectrum of compound **5e** in $CDCl_3$ (200 MHz).



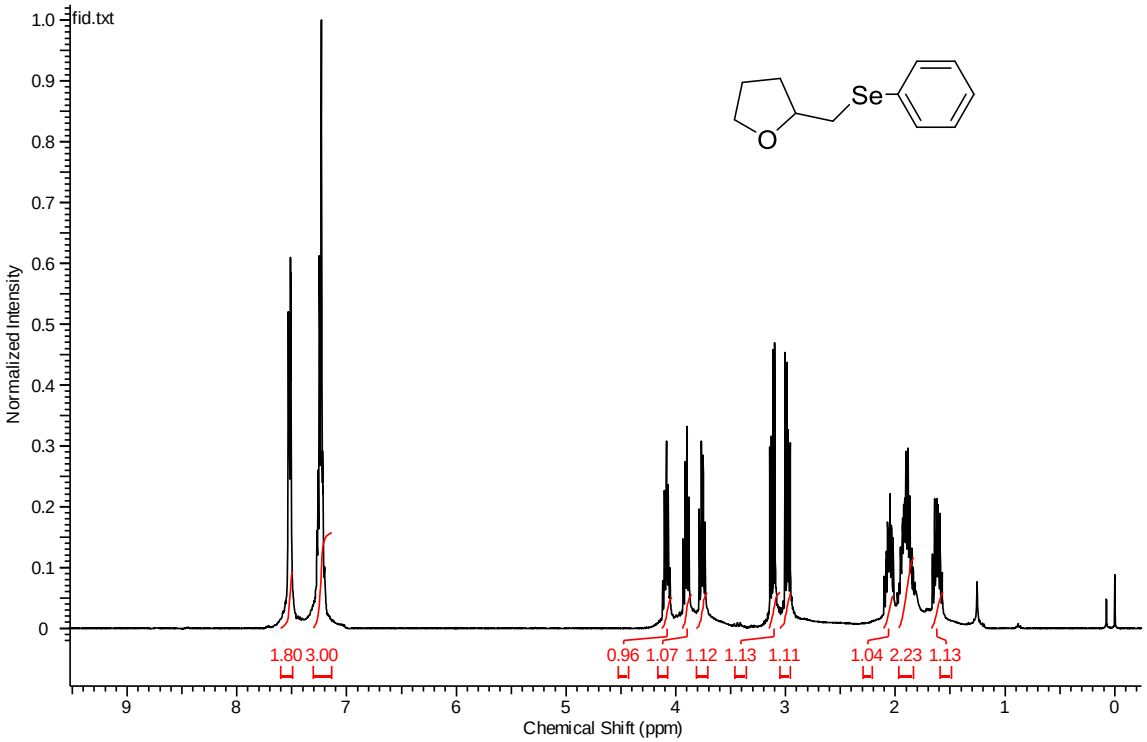
S42. ^{13}C NMR spectrum of compound **5e** in $CDCl_3$ (50 MHz).



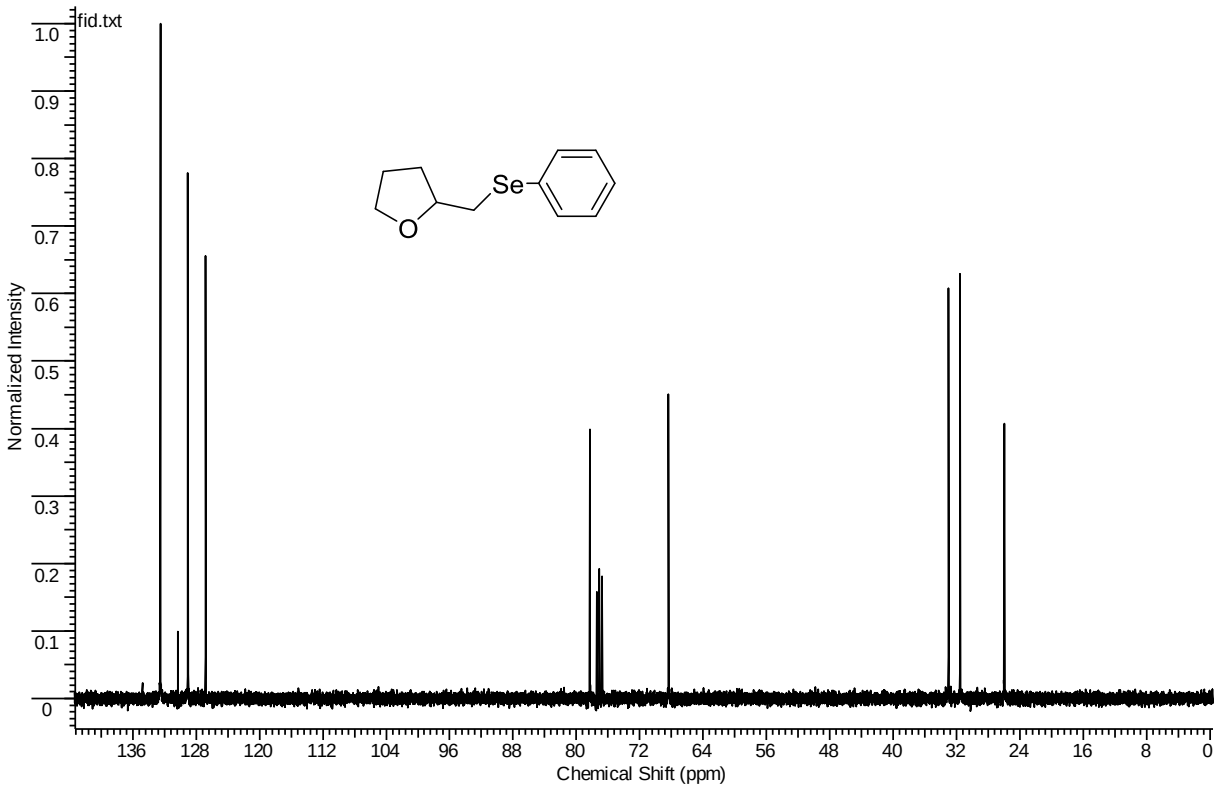
S43. ^{1}H NMR spectrum of compound **5f** in $CDCl_3$ (200 MHz).



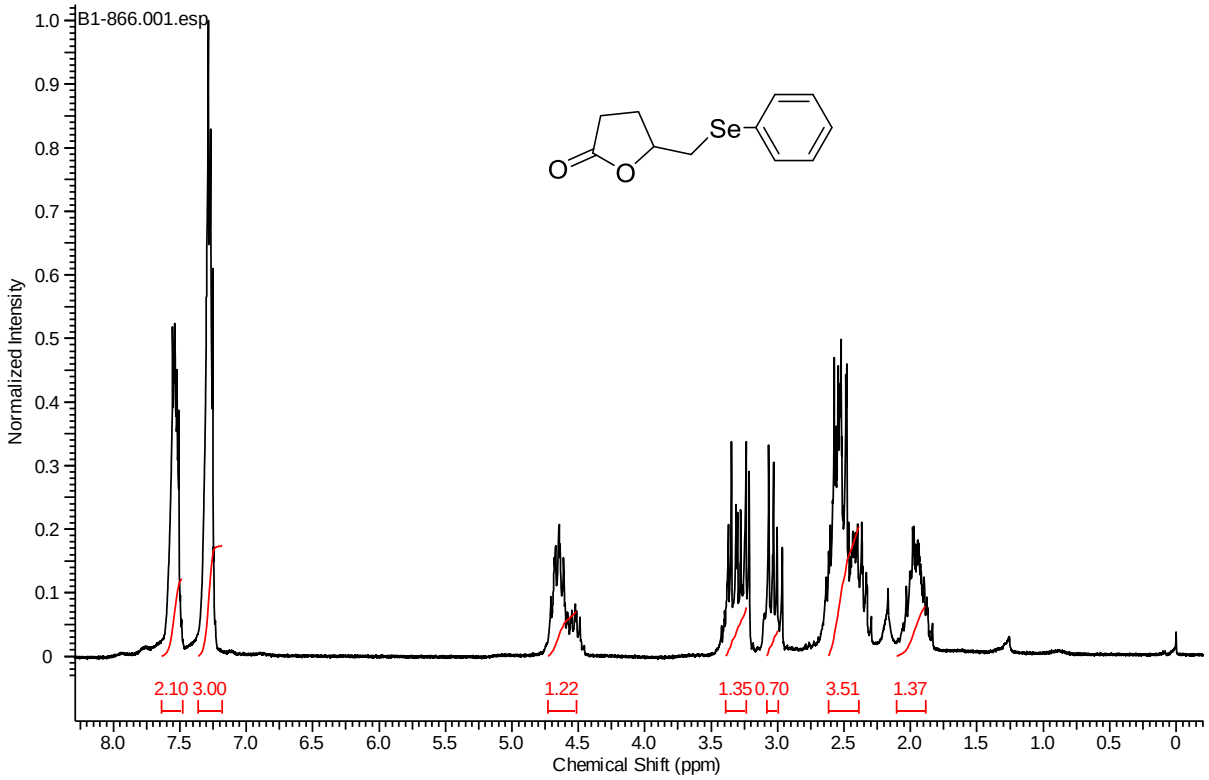
S44. ^{13}C NMR spectrum of compound **5f** in $CDCl_3$ (50 MHz).



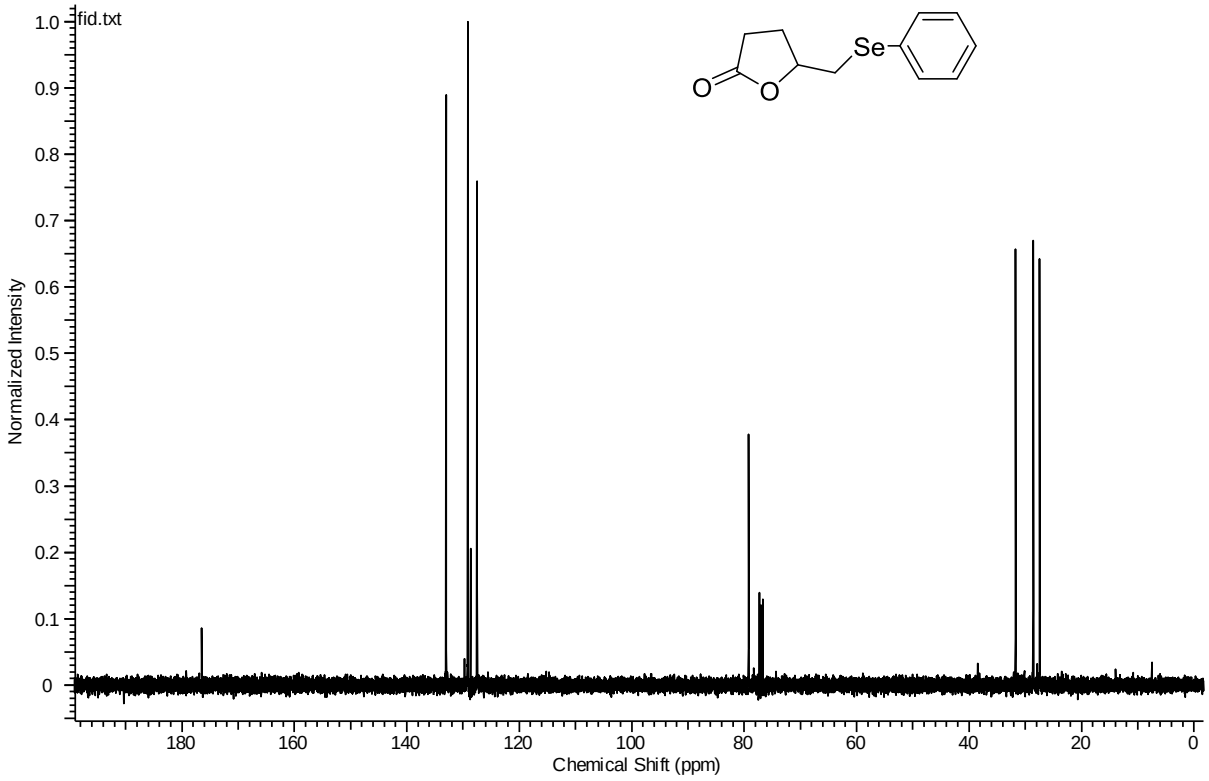
S45. ^{1}H NMR spectrum of compound **6a** in $CDCl_3$ (400 MHz).



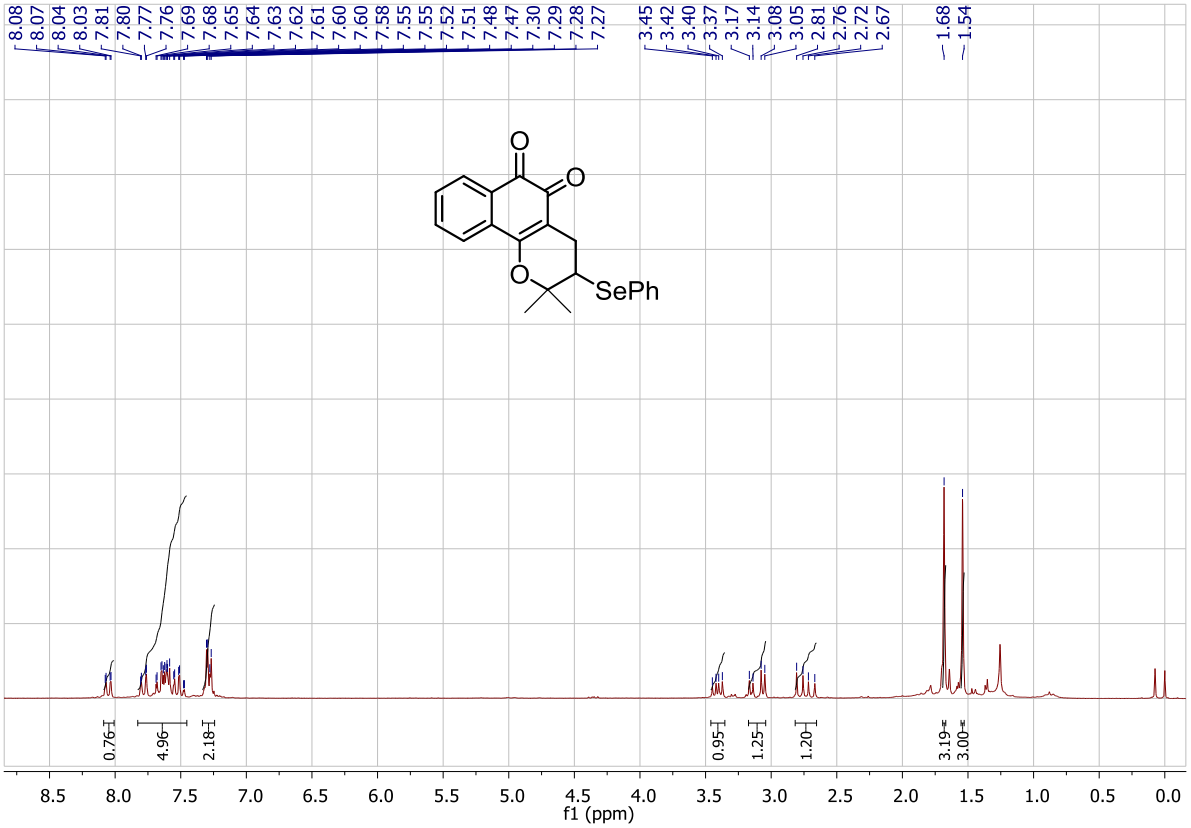
S46. ^{13}C NMR spectrum of compound **6a** in $CDCl_3$ (100 MHz).



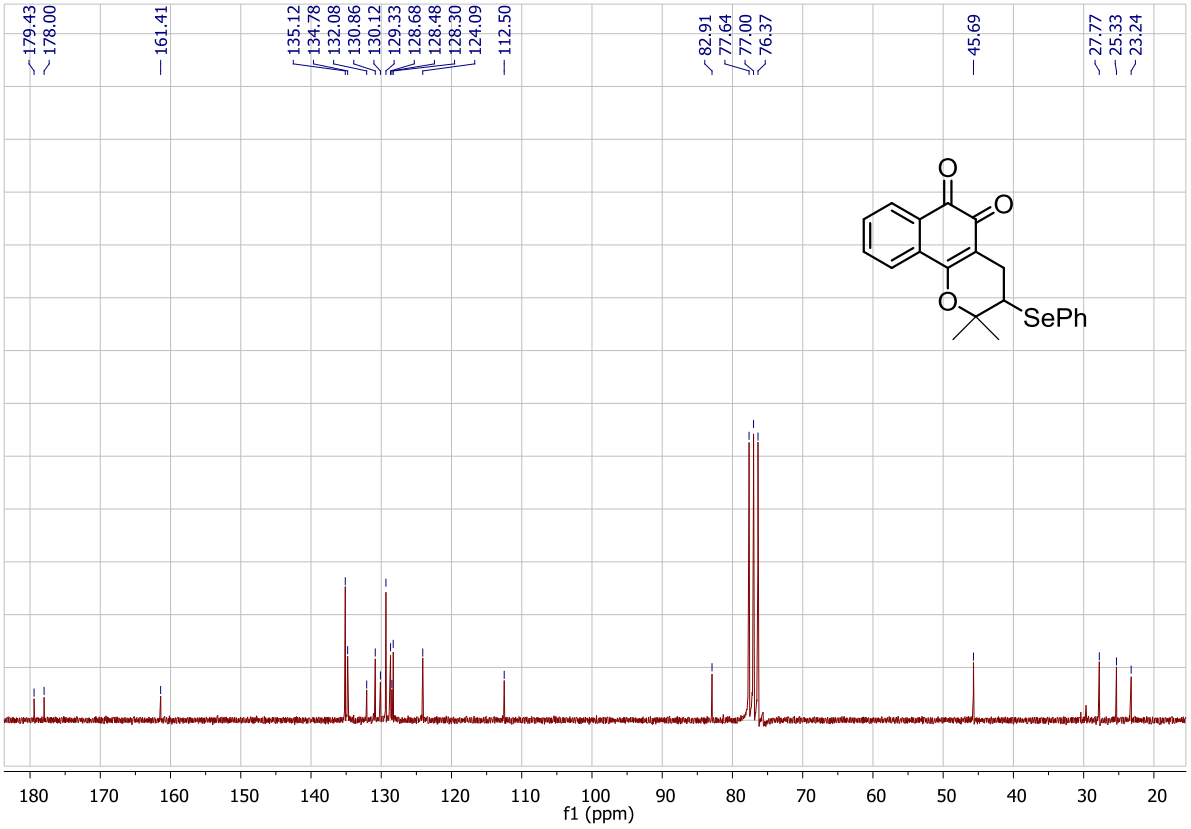
S47. ^{1}H NMR spectrum of compound **7a** in $CDCl_3$ (400 MHz)



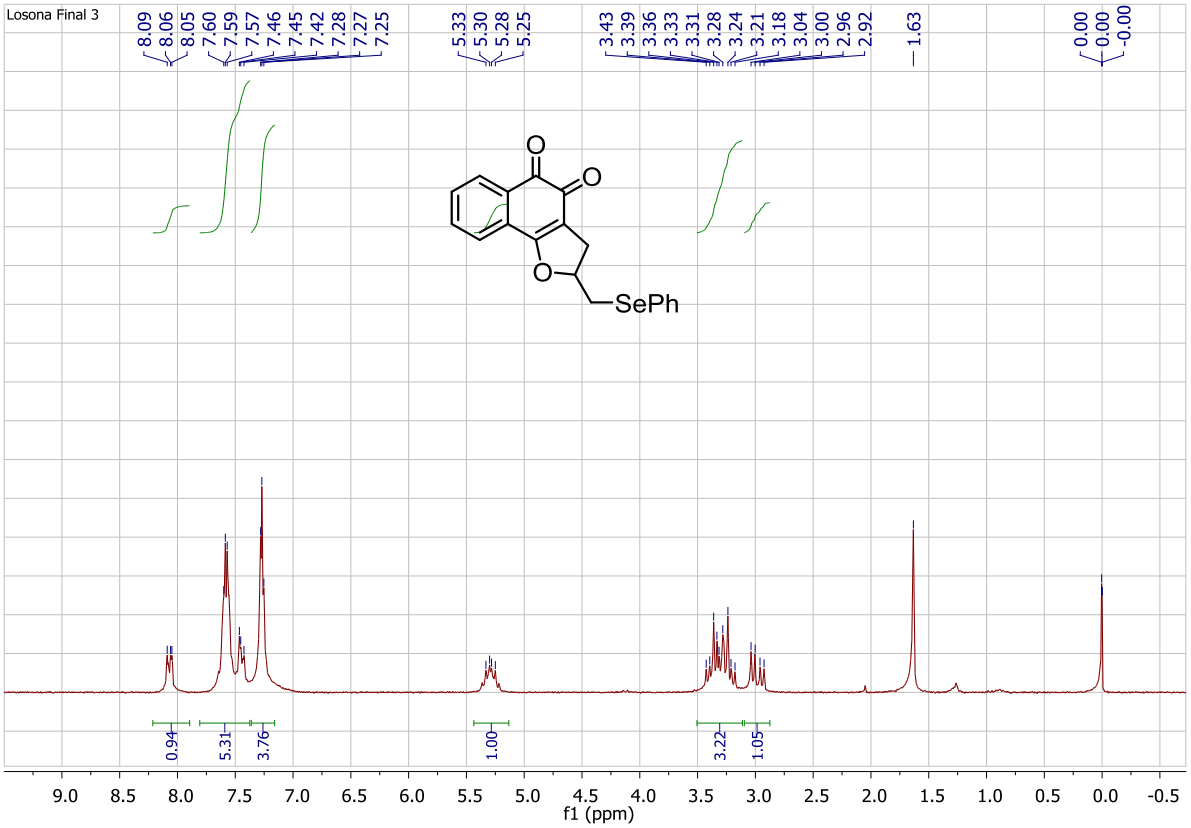
S48. ^{13}C NMR spectrum of compound **7a** in $CDCl_3$ (100 MHz).



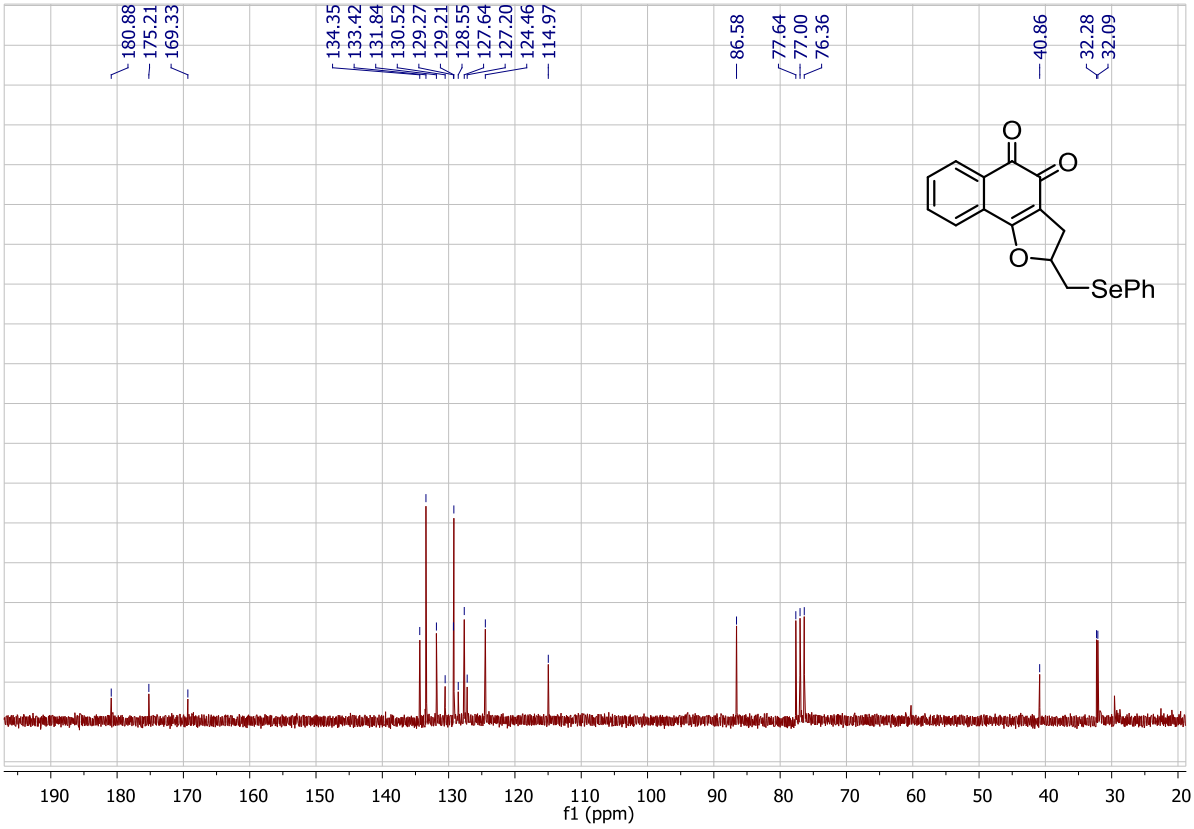
S49. ^{1}H NMR spectrum of compound **8a** in $CDCl_3$ (200 MHz).



S50. ^{13}C NMR spectrum of compound **8a** in $CDCl_3$ (100 MHz).

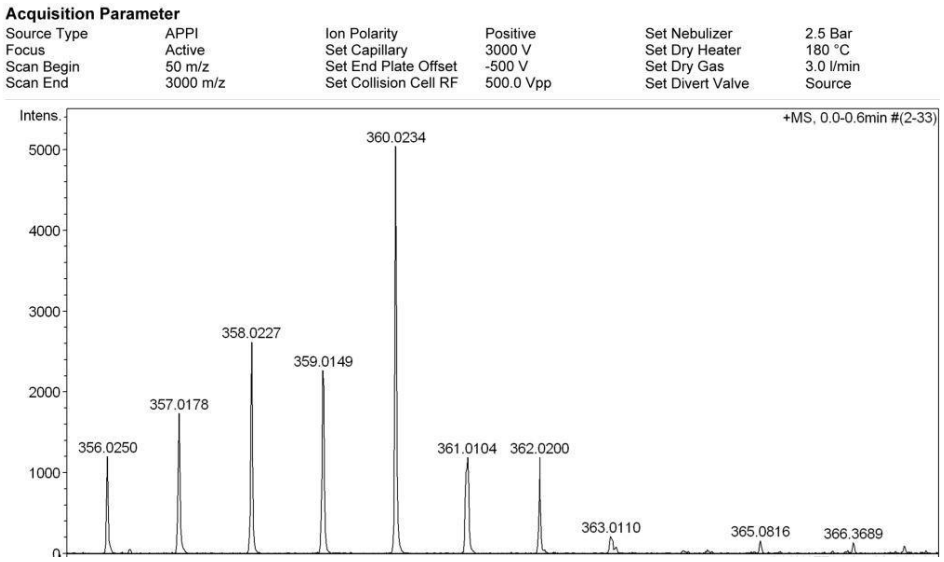


S51. ^{1}H NMR spectrum of compound **9a** in $CDCl_3$ (200 MHz).

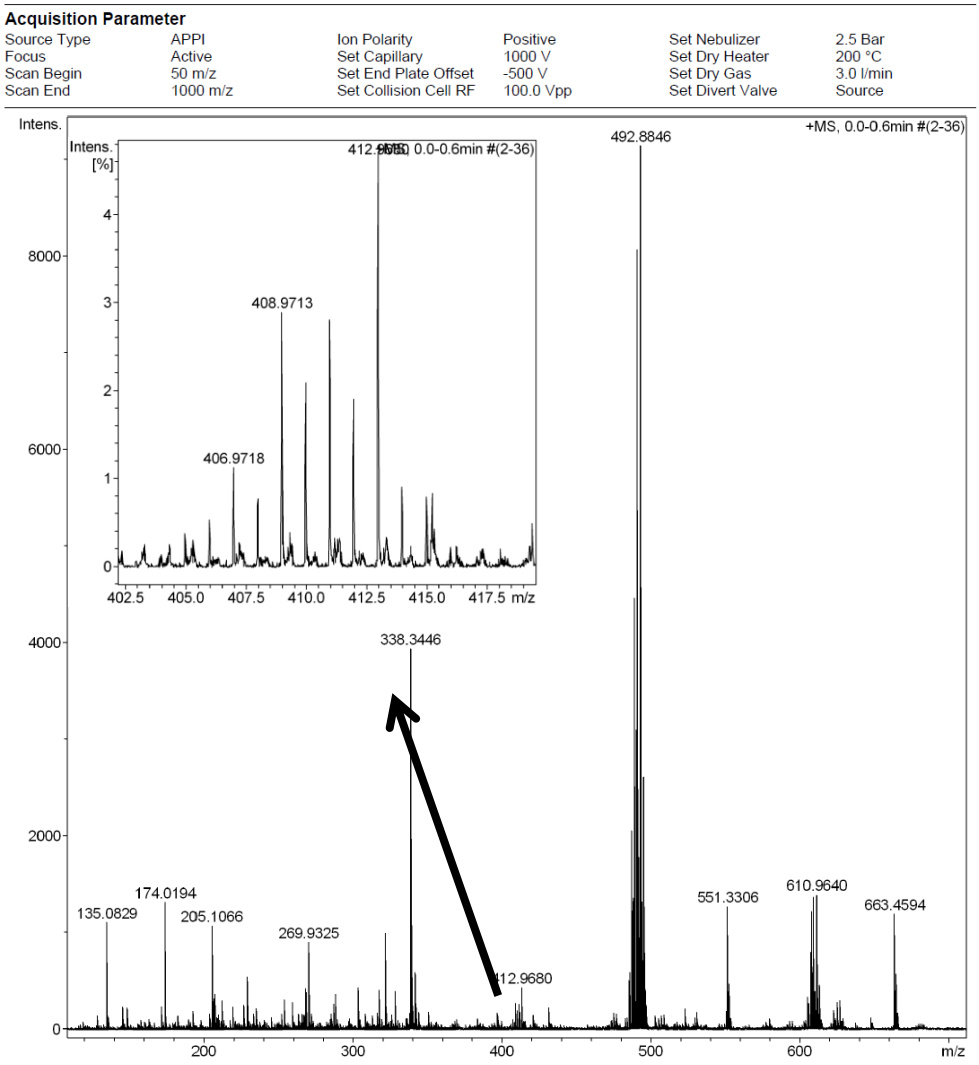


S52. ^{13}C NMR spectrum of compound **9a** in $CDCl_3$ (50 MHz).

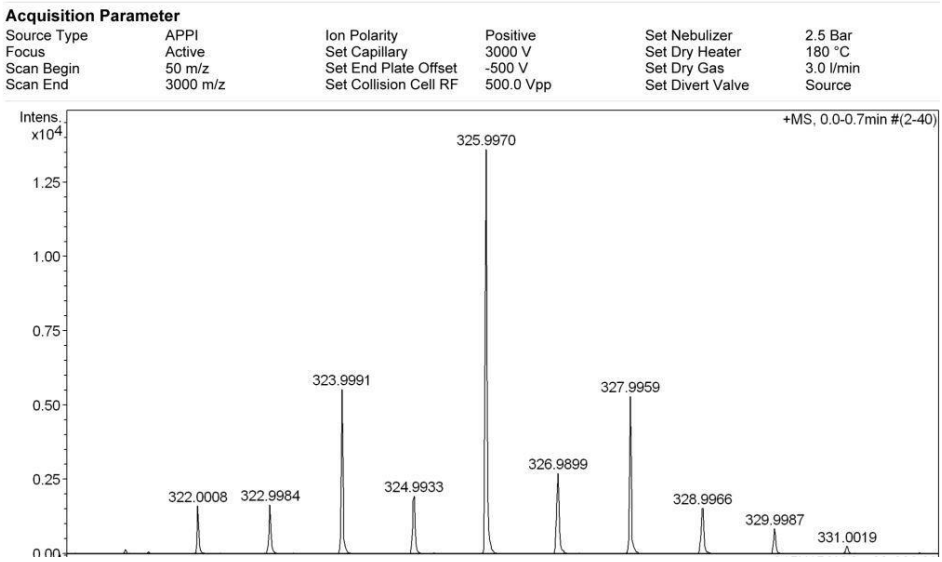
1.2. Mass Spectra



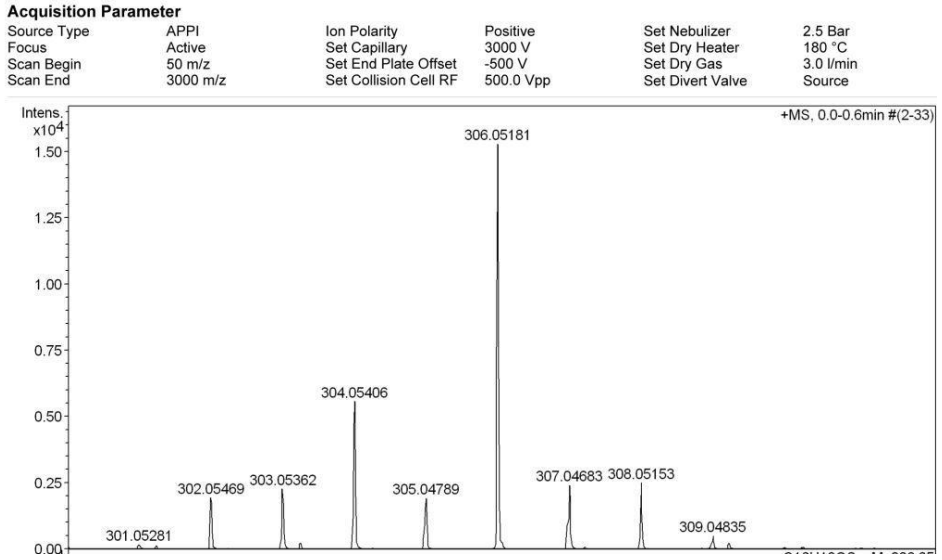
S53. High Resolution Chemical Ionization Mass Spectra for Compound **3b**.



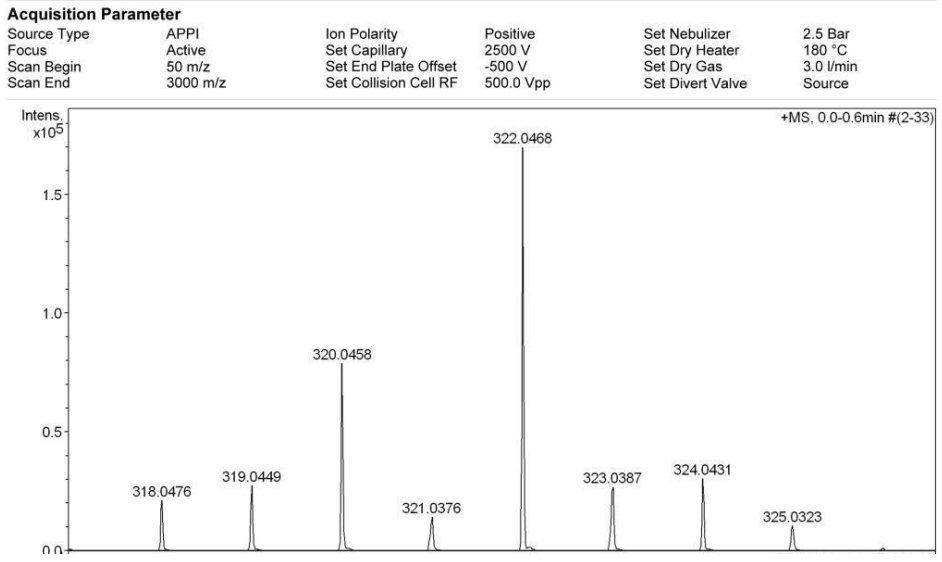
S54. High Resolution Chemical Ionization Mass Spectra for traces of Compound **3c**.



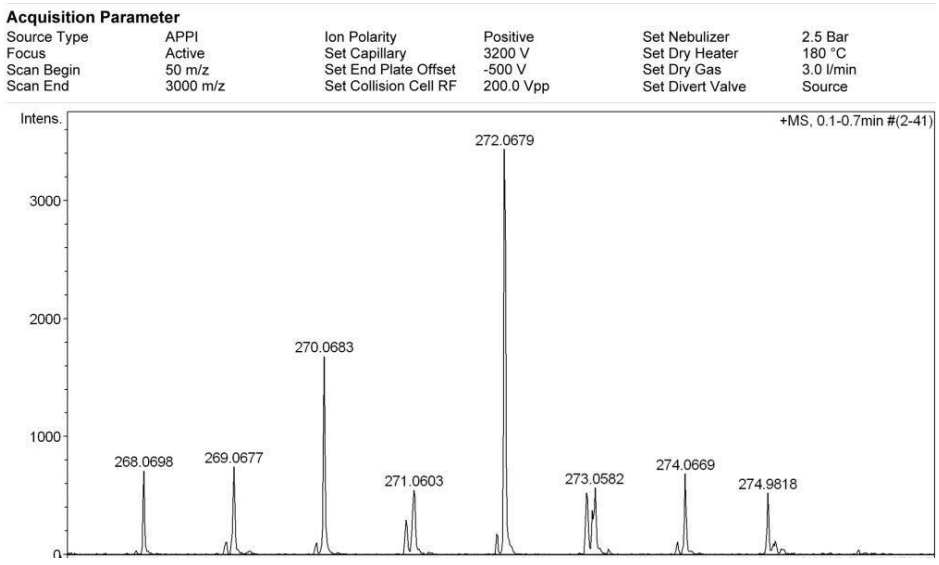
S55. High Resolution Chemical Ionization Mass Spectra for Compound **3d**.



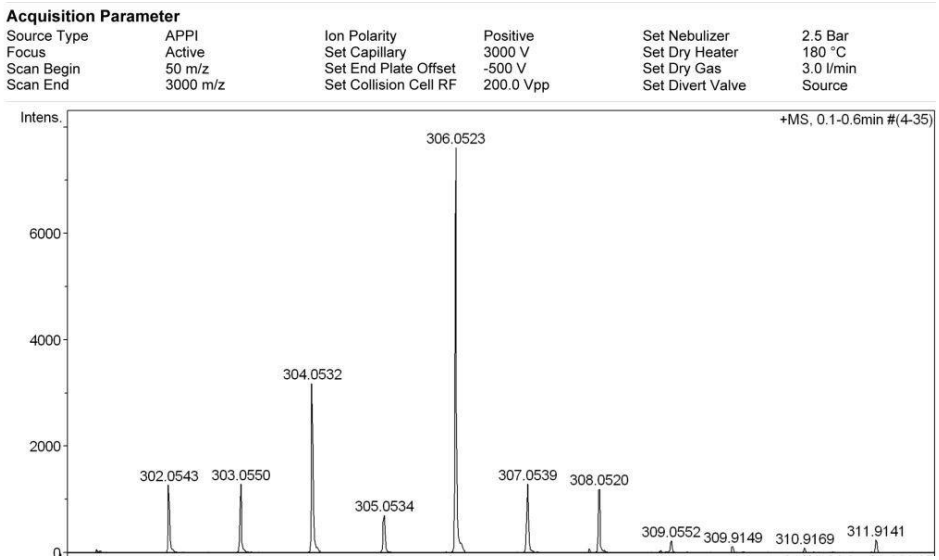
S56. High Resolution Chemical Ionization Mass Spectra for Compound **3e**.



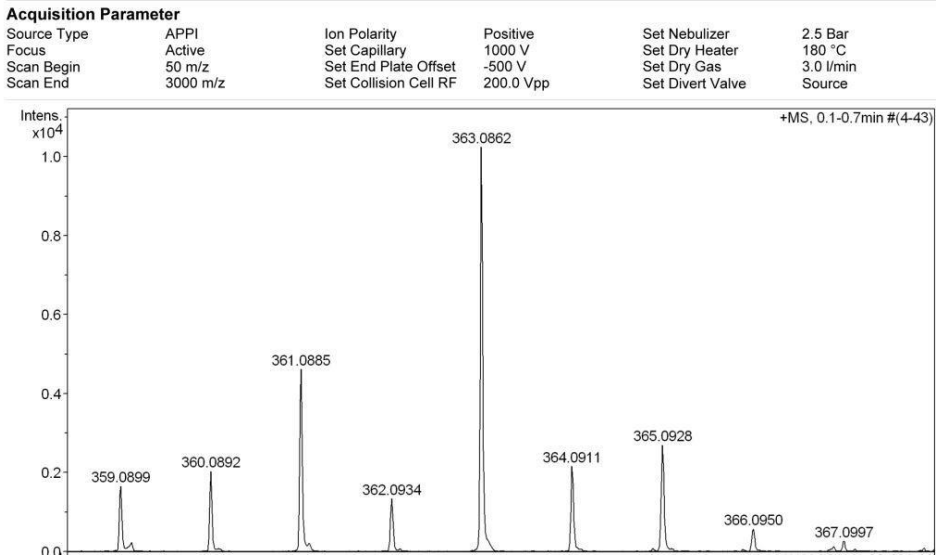
S57. High Resolution Chemical Ionization Mass Spectra for Compound **3f**.



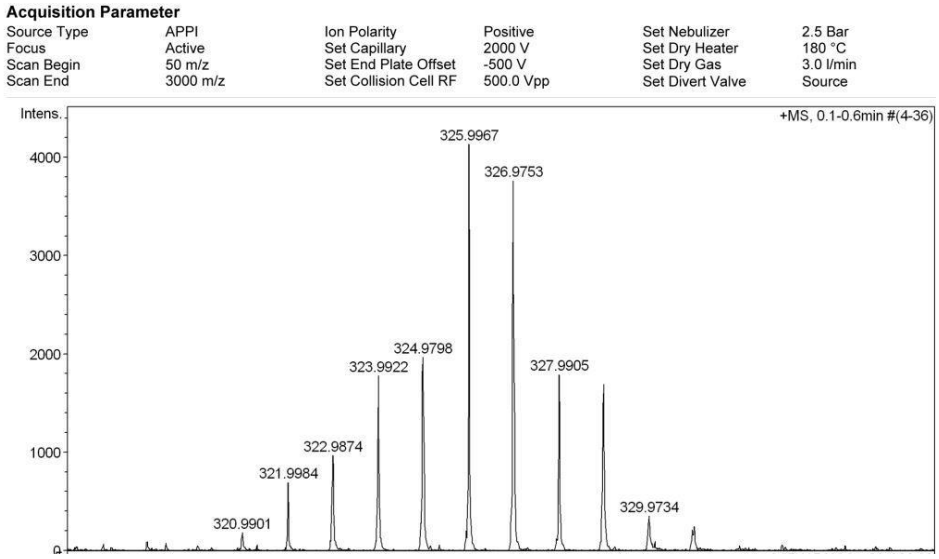
S58. High Resolution Chemical Ionization Mass Spectra for Compound **3g**.



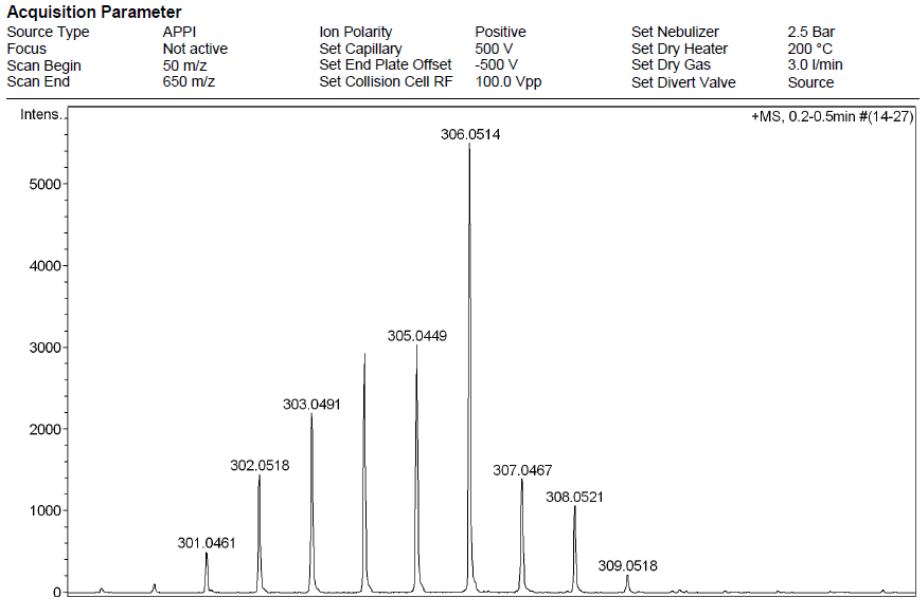
S59. High Resolution Chemical Ionization Mass Spectra for Compound **3i**.



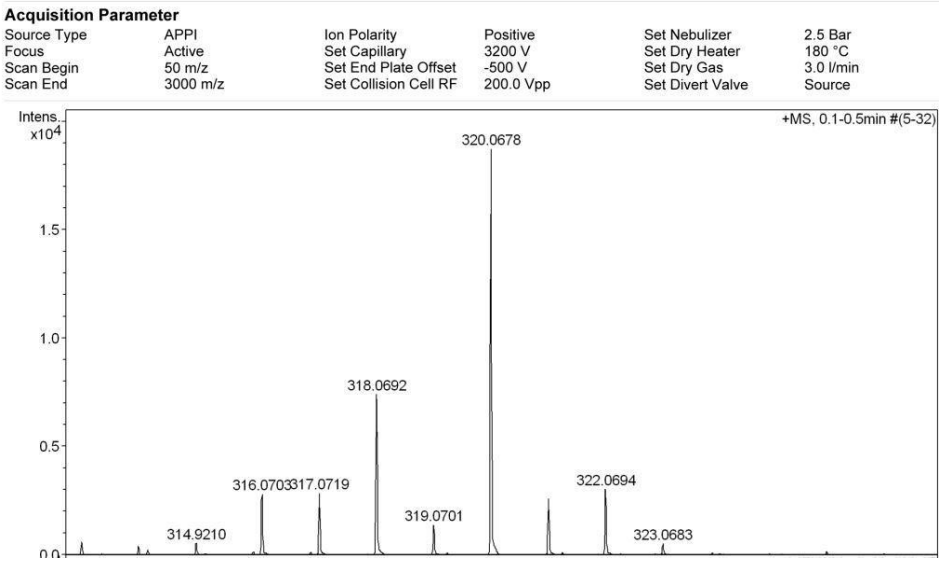
S60. High Resolution Chemical Ionization Mass Spectra for Compound **3j**.



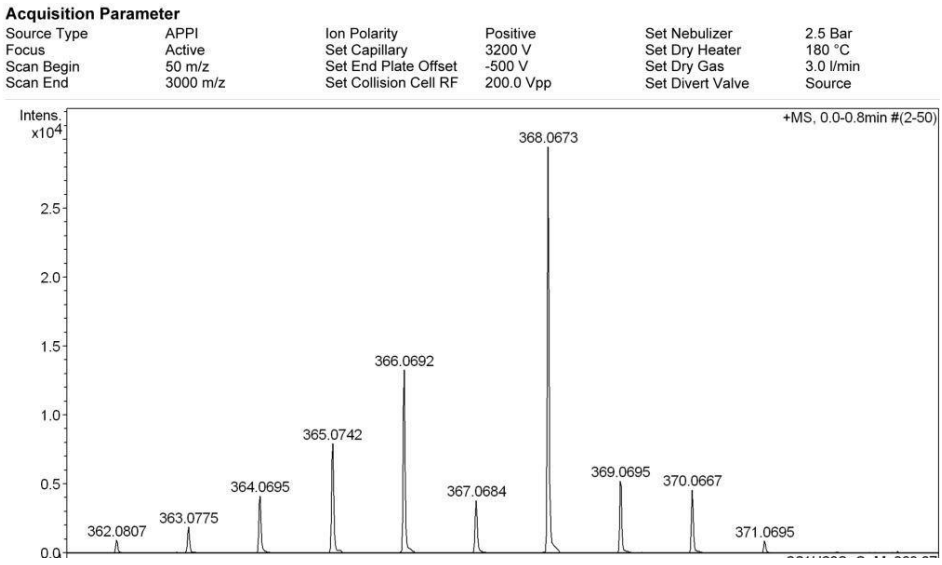
S61. High Resolution Chemical Ionization Mass Spectra for Compound **3h**.



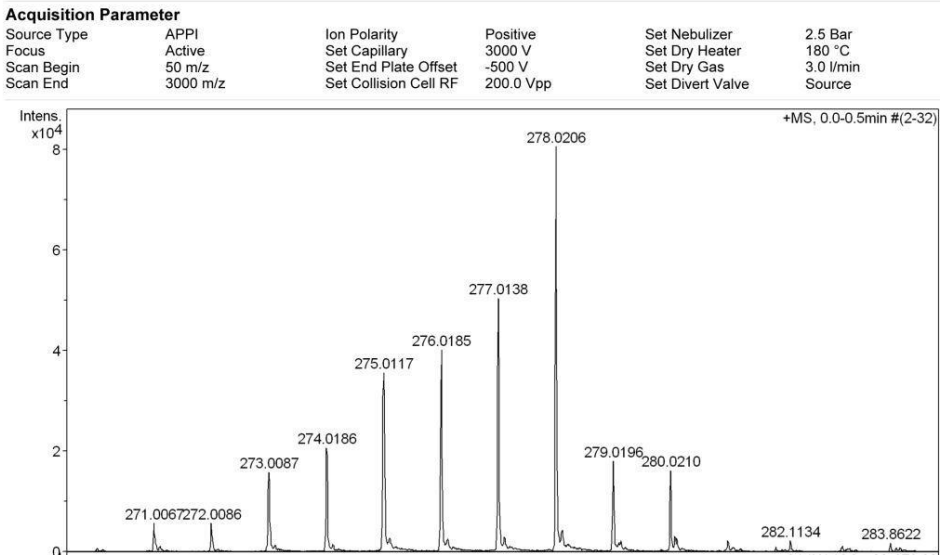
S62. High Resolution Chemical Ionization Mass Spectra for Compound **3k**.



S63. High Resolution Chemical Ionization Mass Spectra for Compound **3m**.



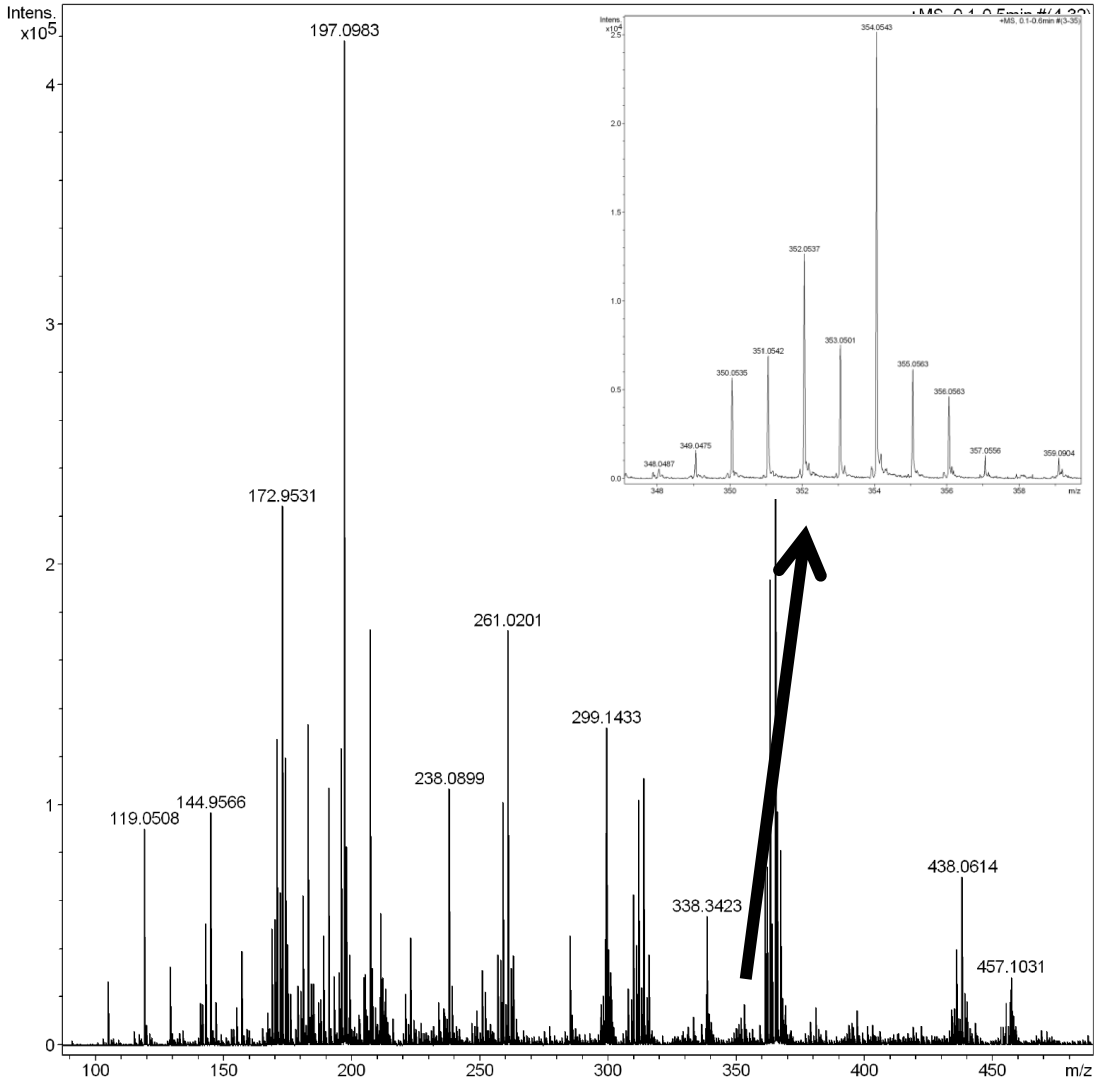
S64. High Resolution Chemical Ionization Mass Spectra for Compound **3o**.



S65. High Resolution Chemical Ionization Mass Spectra for Compound **3r**.

Acquisition Parameter

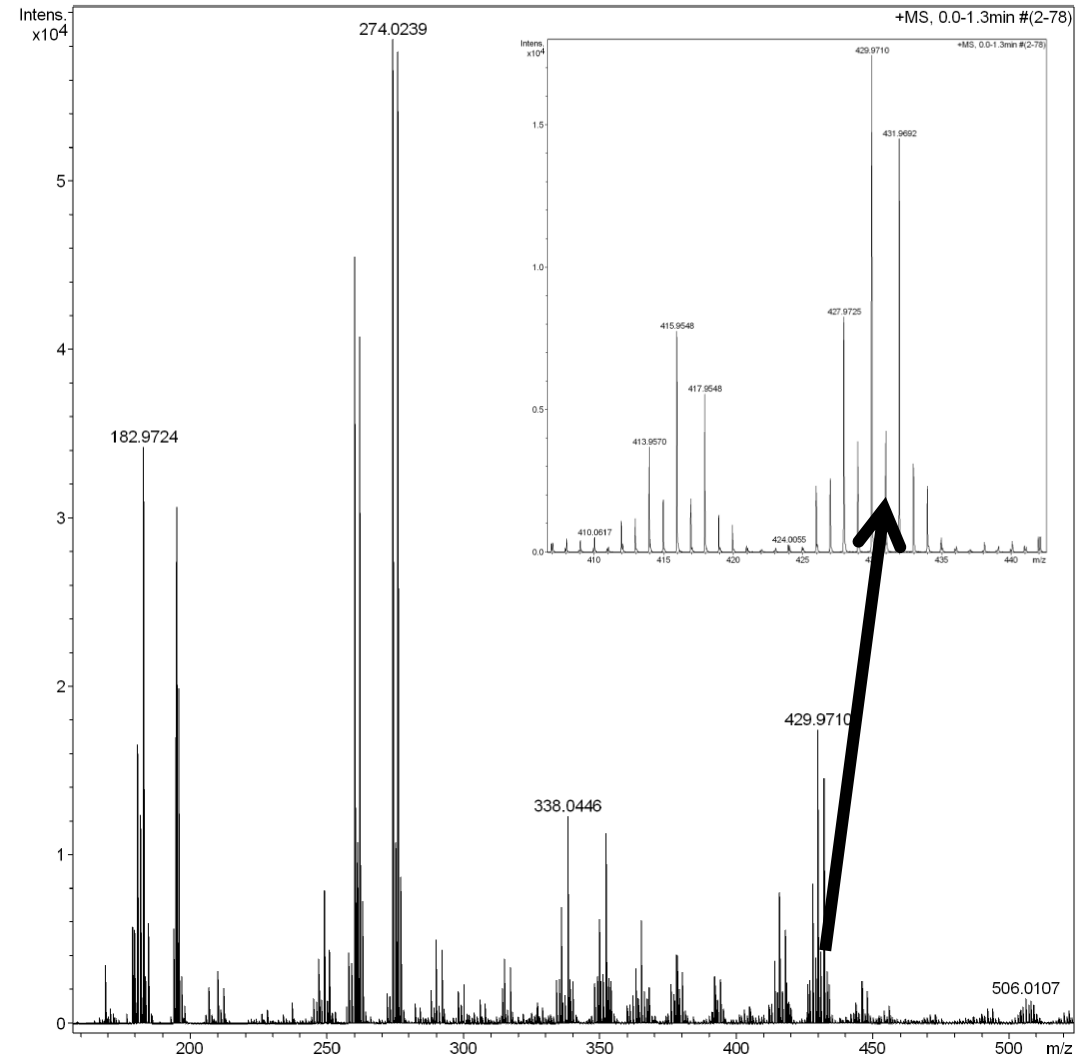
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	1200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



S66. High Resolution Chemical Ionization Mass Spectra for traces of Compound **3p**.

Acquisition Parameter

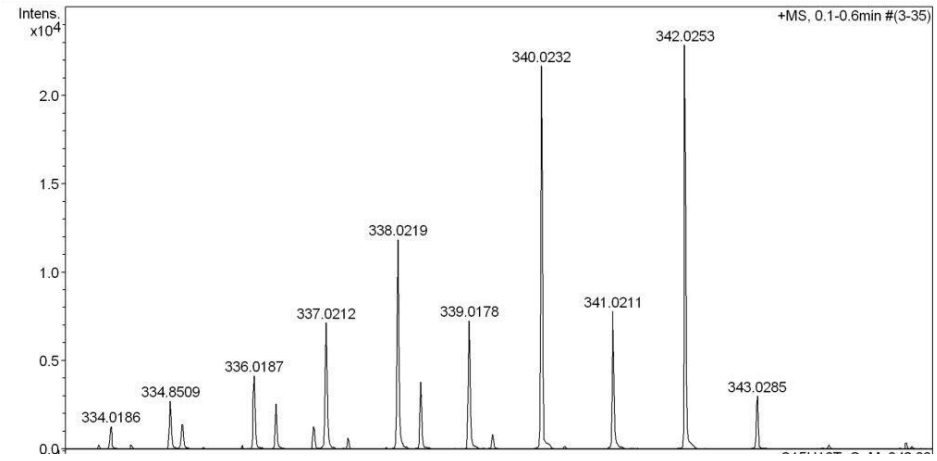
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	2.5 Bar
Focus	Active	Set Capillary	1000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



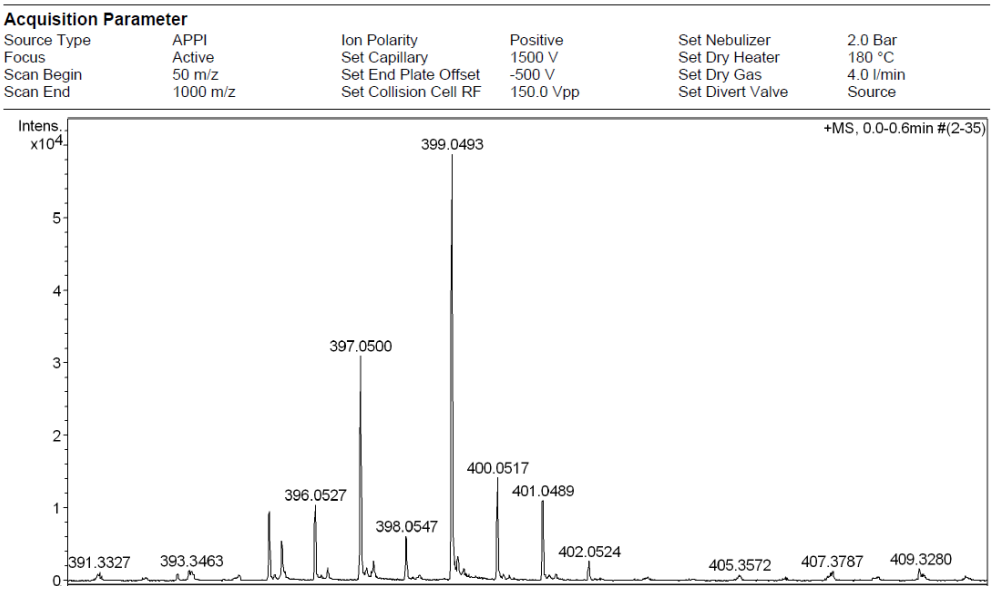
S67. High Resolution Chemical Ionization Mass Spectra for traces of Compound **3q**.

Acquisition Parameter

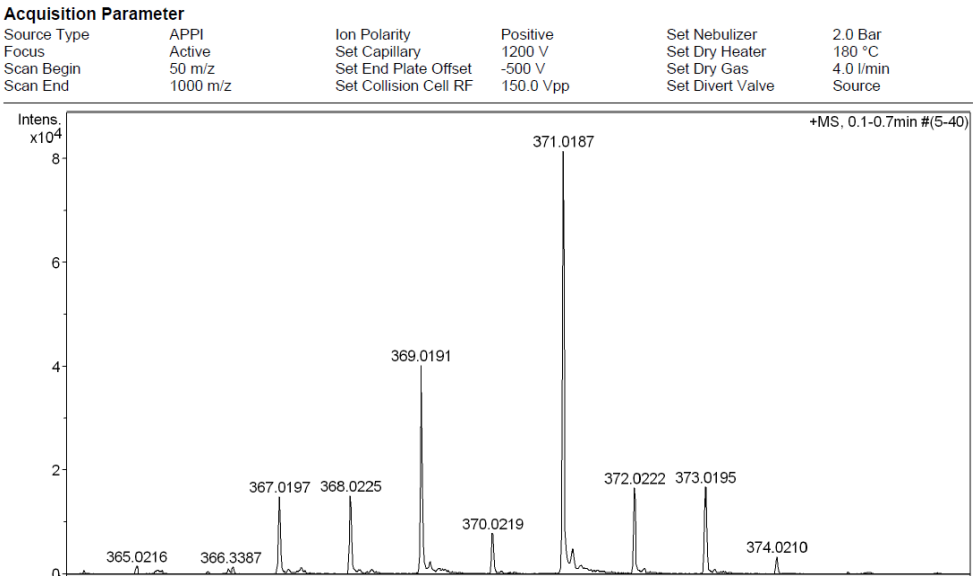
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	2.5 Bar
Focus	Active	Set Capillary	700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



S68. High Resolution Chemical Ionization Mass Spectra for Compound **5f**.

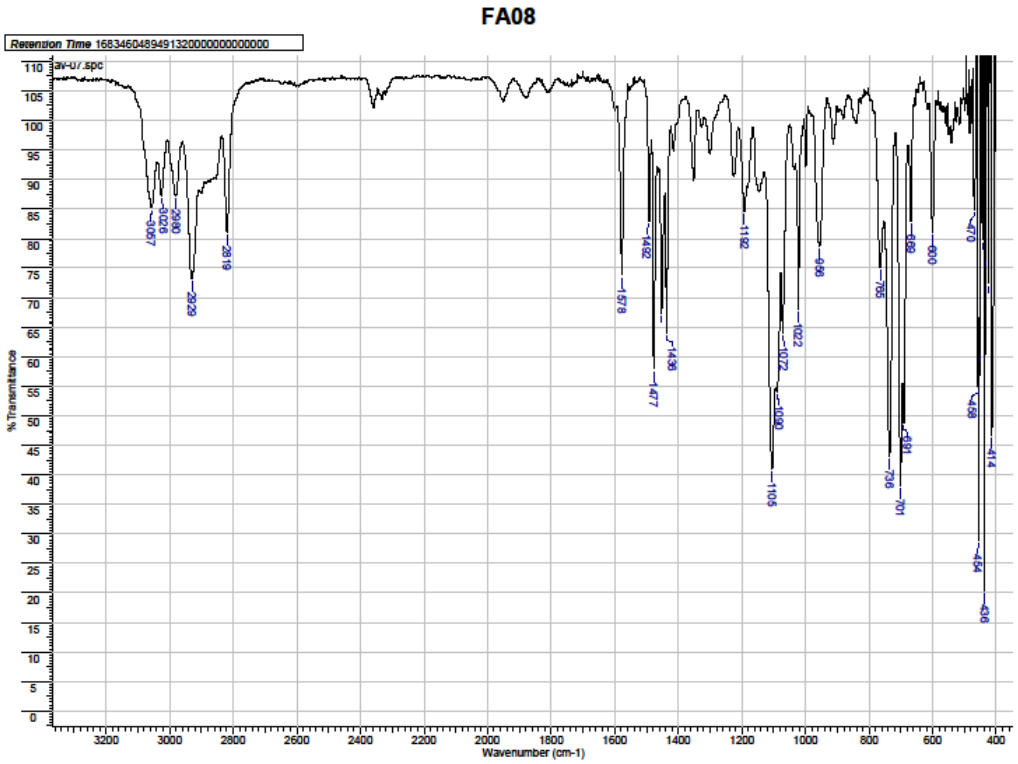


S69. High Resolution Chemical Ionization Mass Spectra for Compound **8a**.

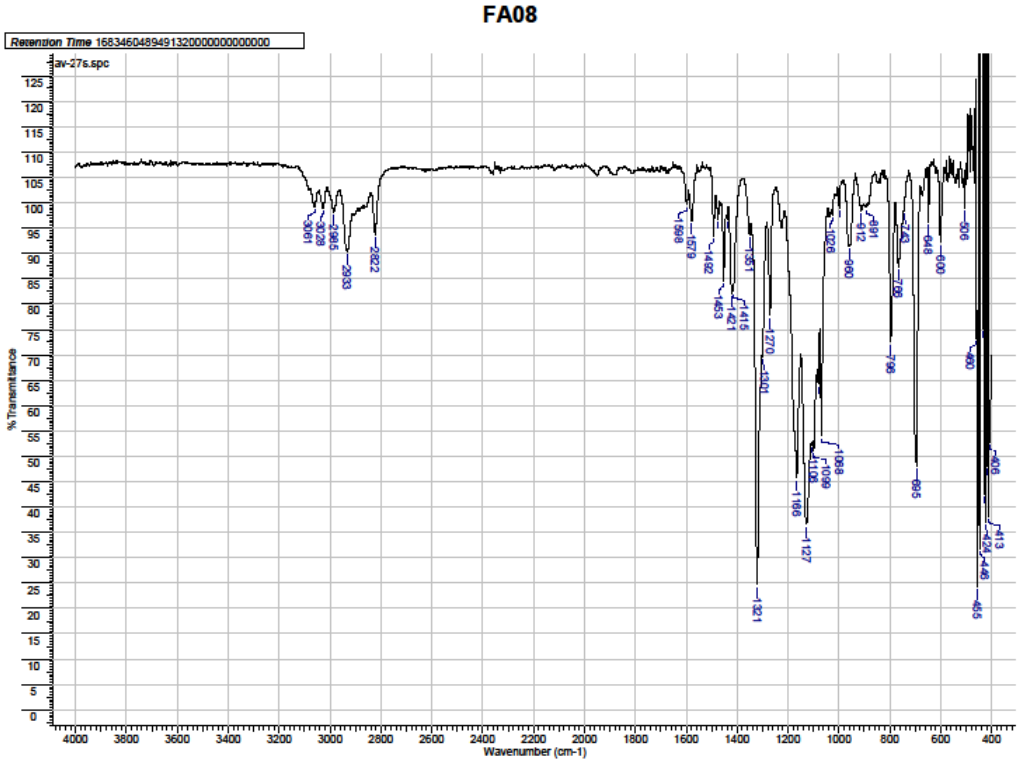


S70. High Resolution Chemical Ionization Mass Spectra for Compound **9a**.

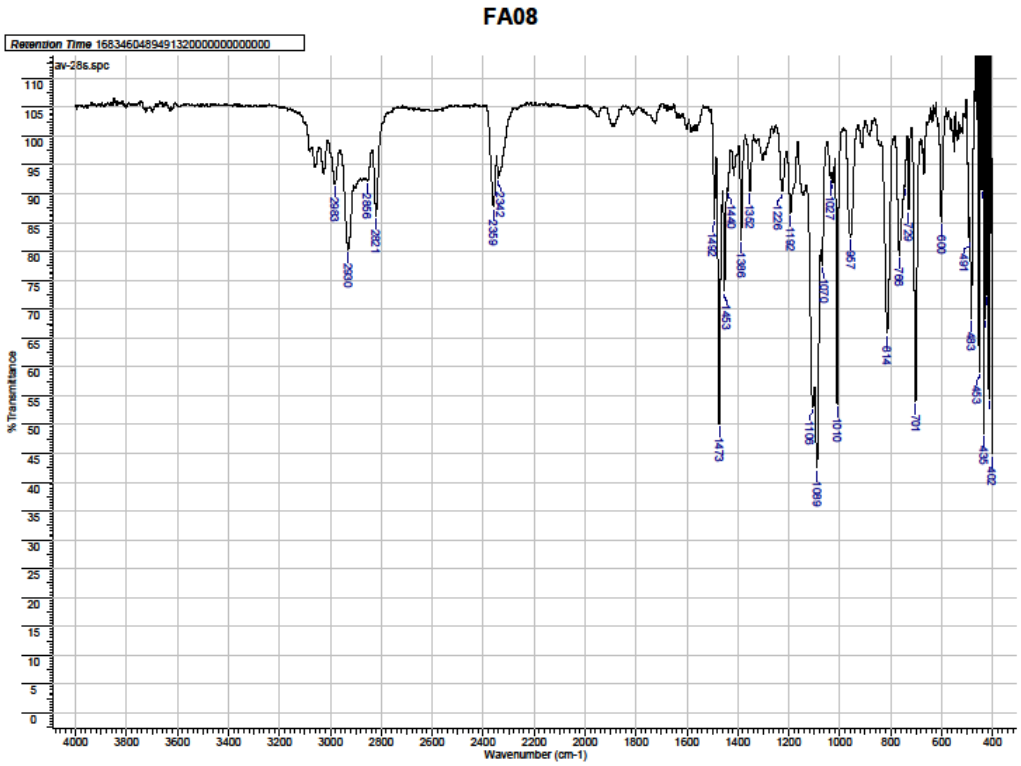
1.3. IR spectra



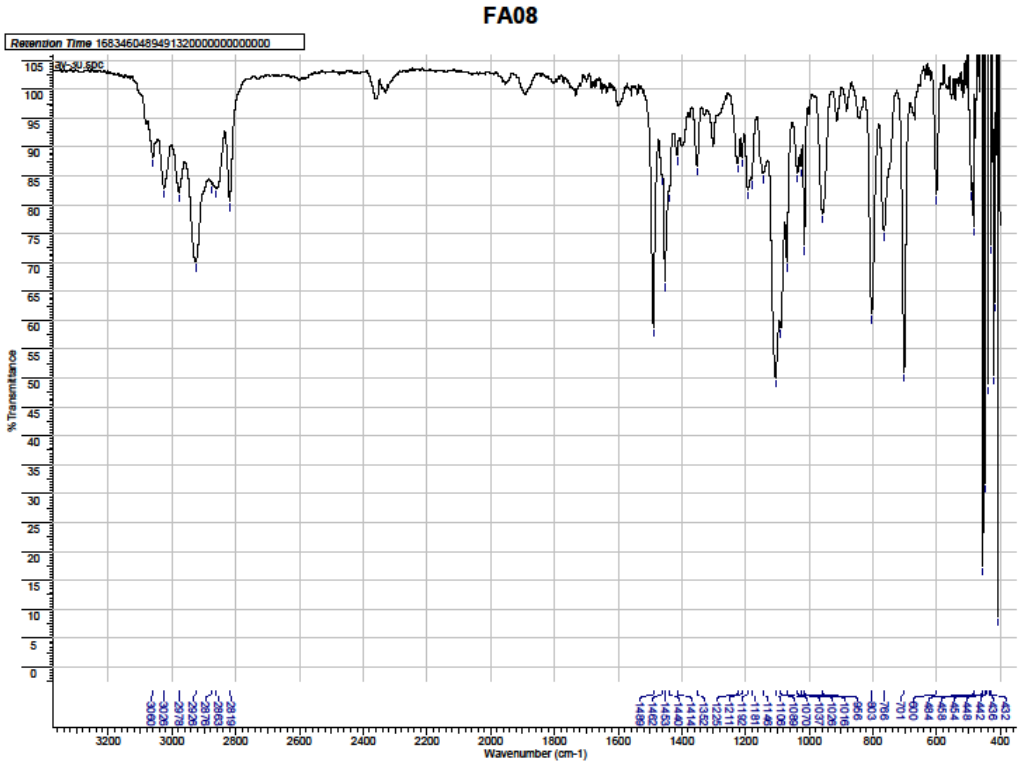
S71. IR spectrum of compound **3a** (KBr pellet).



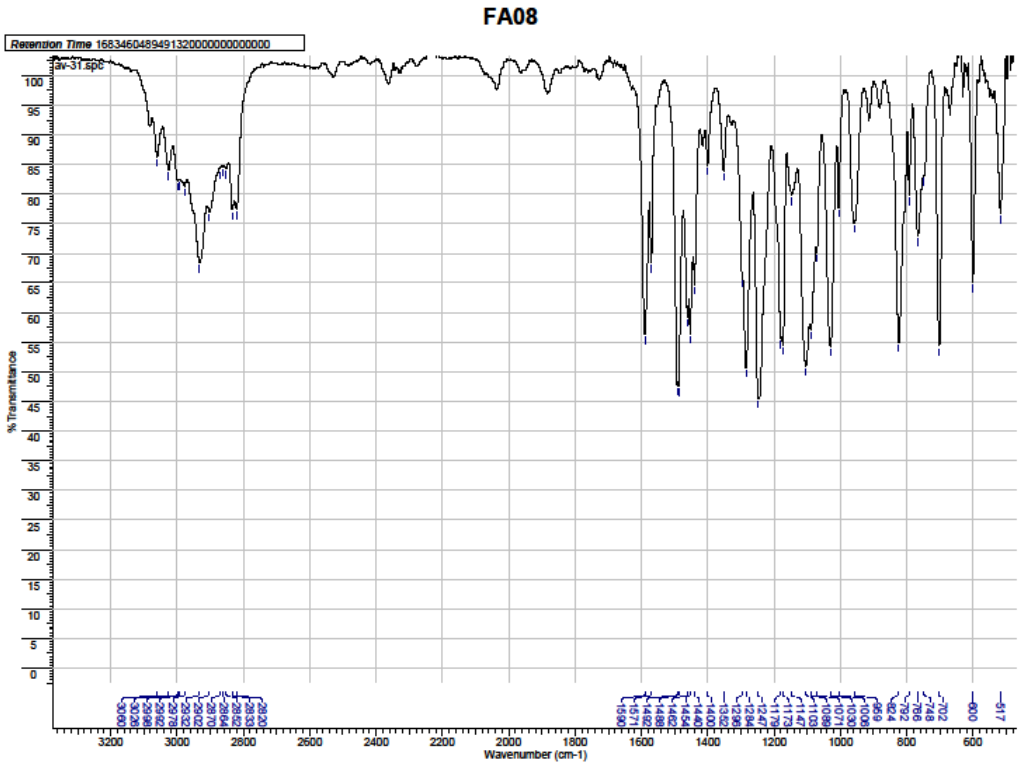
S72. IR spectrum of compound **3b** (KBr pellet).



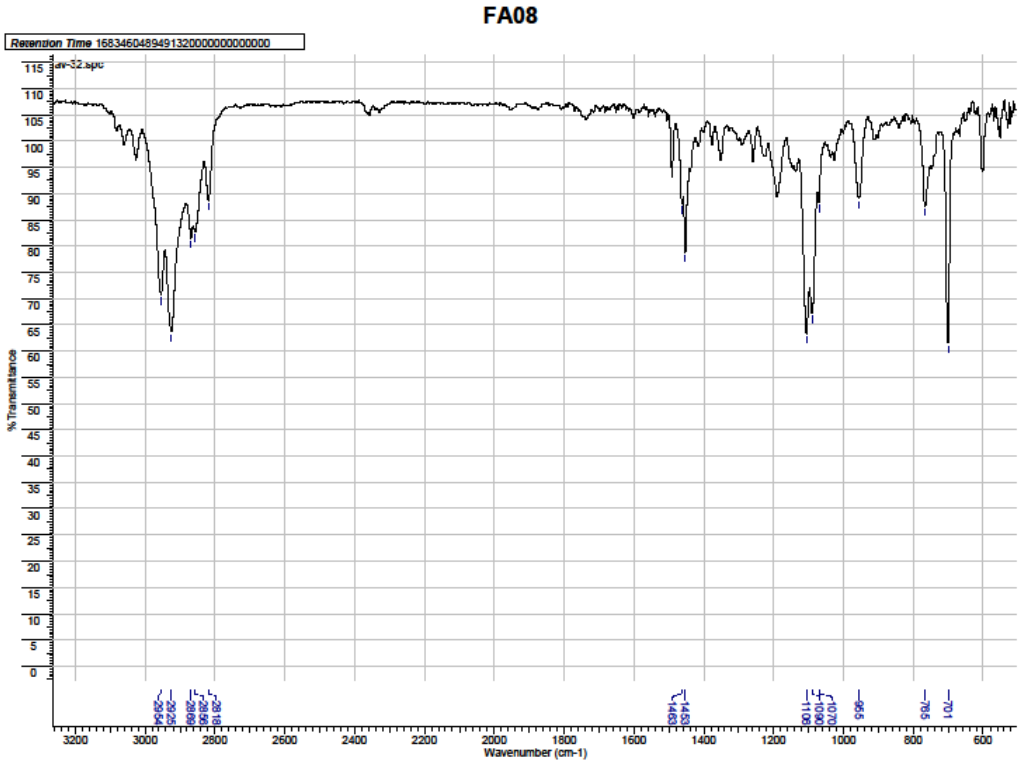
S73. IR spectrum of compound **3d** (KBr pellet).



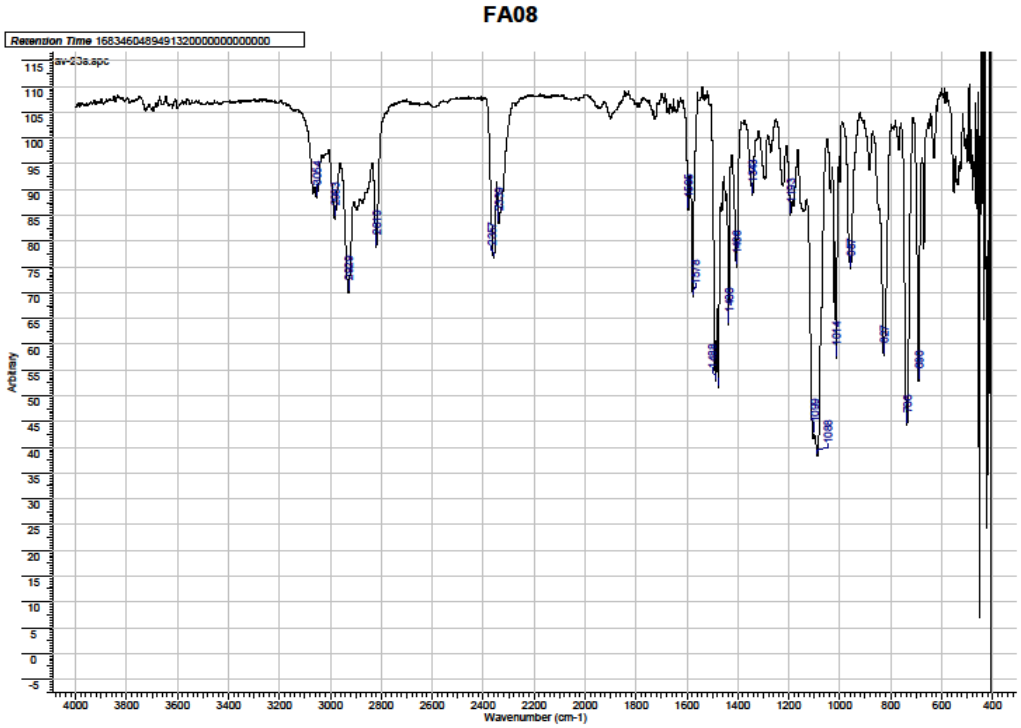
S74. IR spectrum of compound **3e** (KBr pellet).



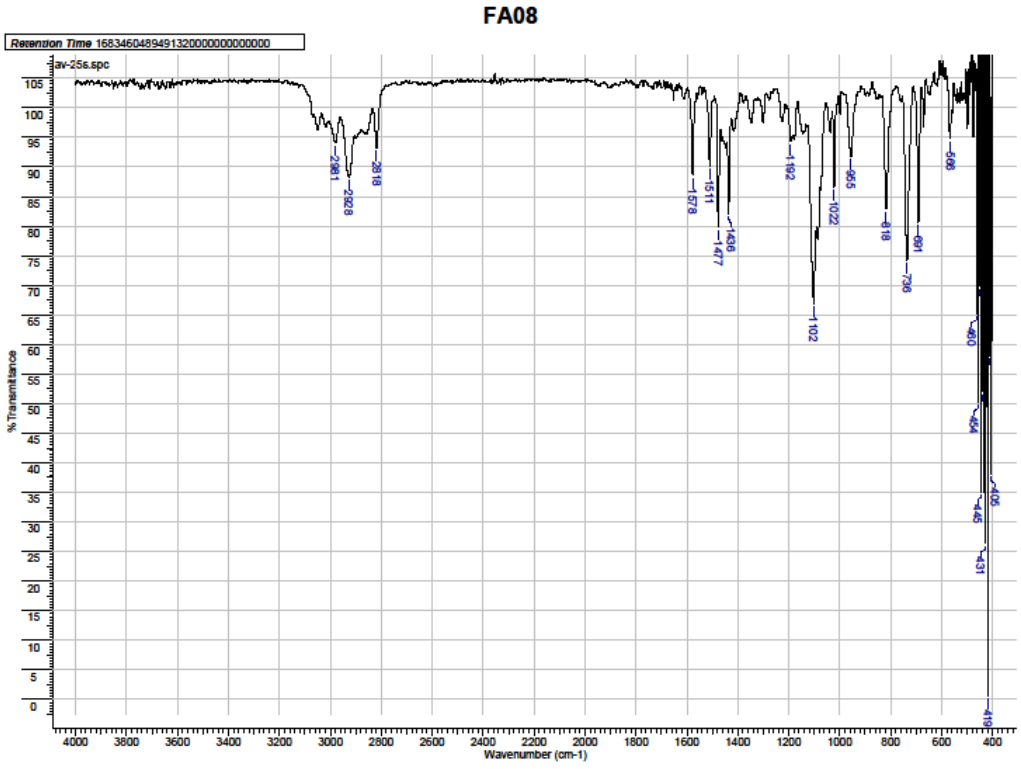
S75. IR spectrum of compound **3f** (KBr pellet).



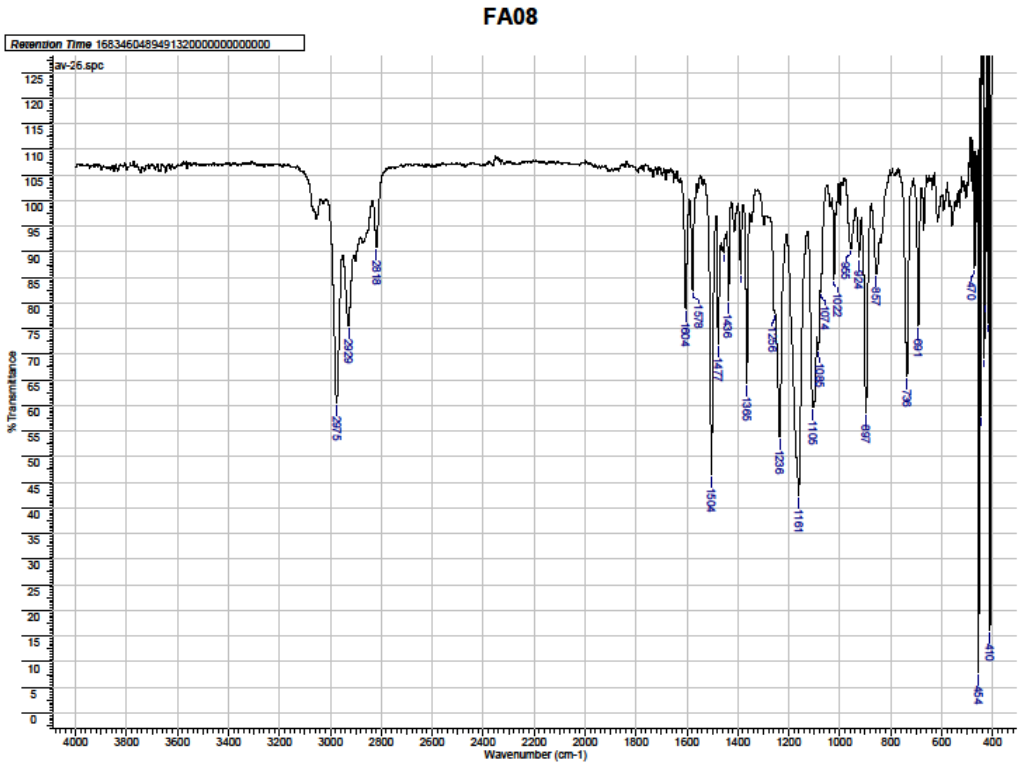
S76. IR spectrum of compound **3g** (KBr pellet).



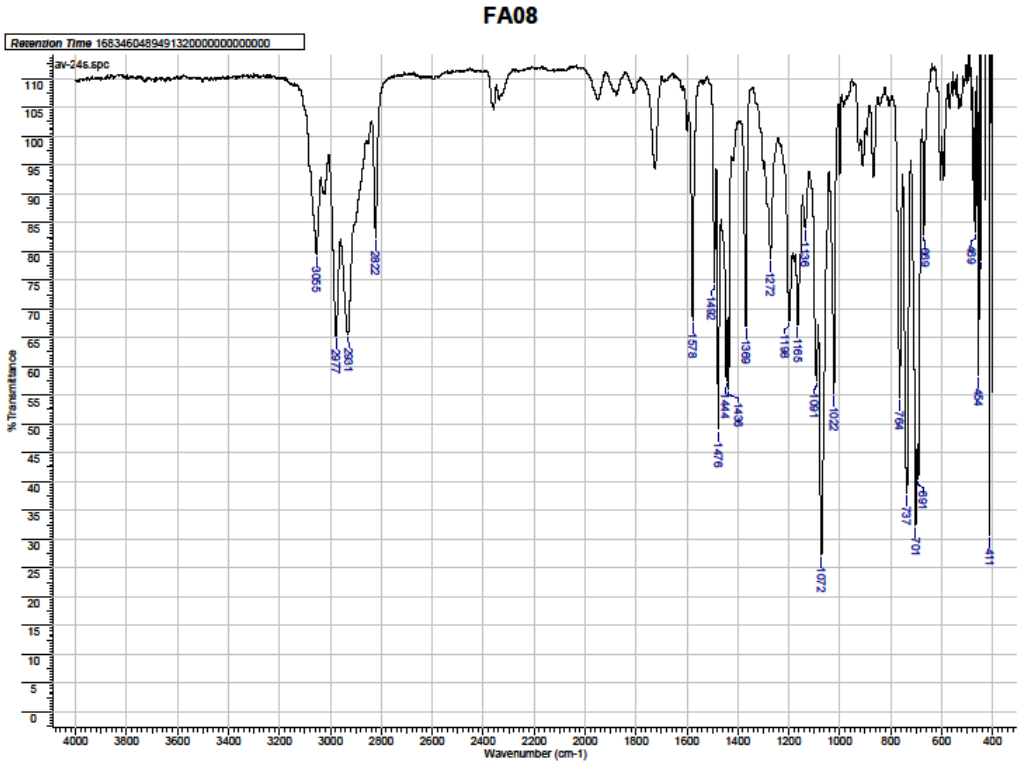
S77. IR spectrum of compound **3h** (KBr pellet).



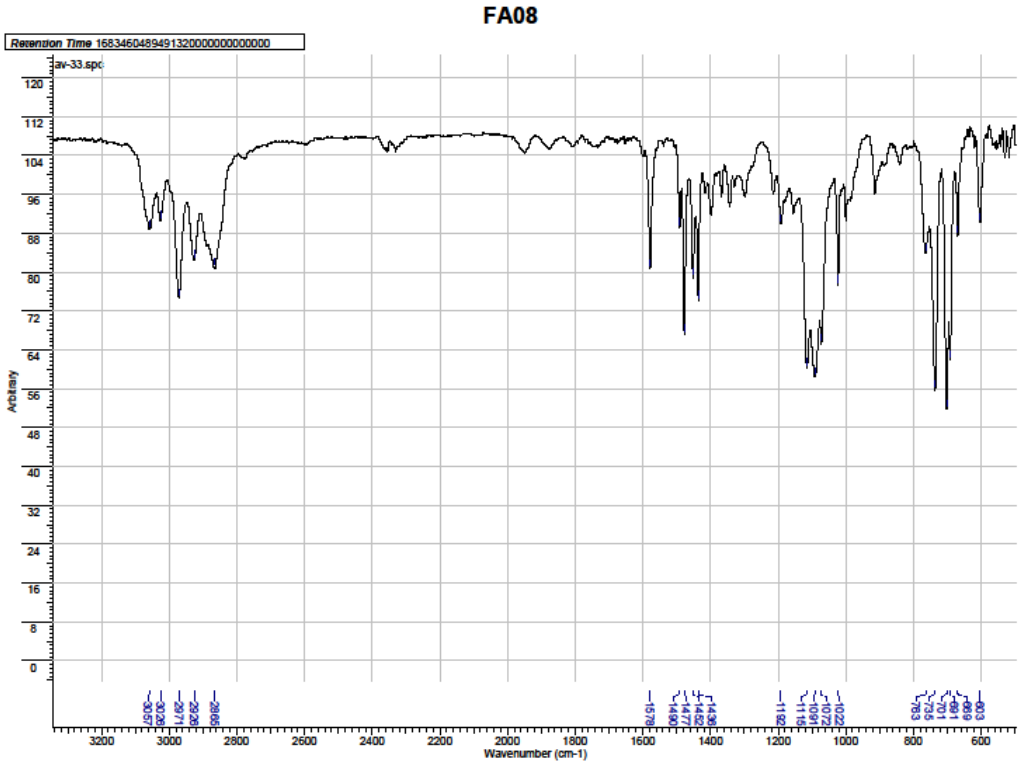
S78. IR spectrum of compound **3i** (KBr pellet).



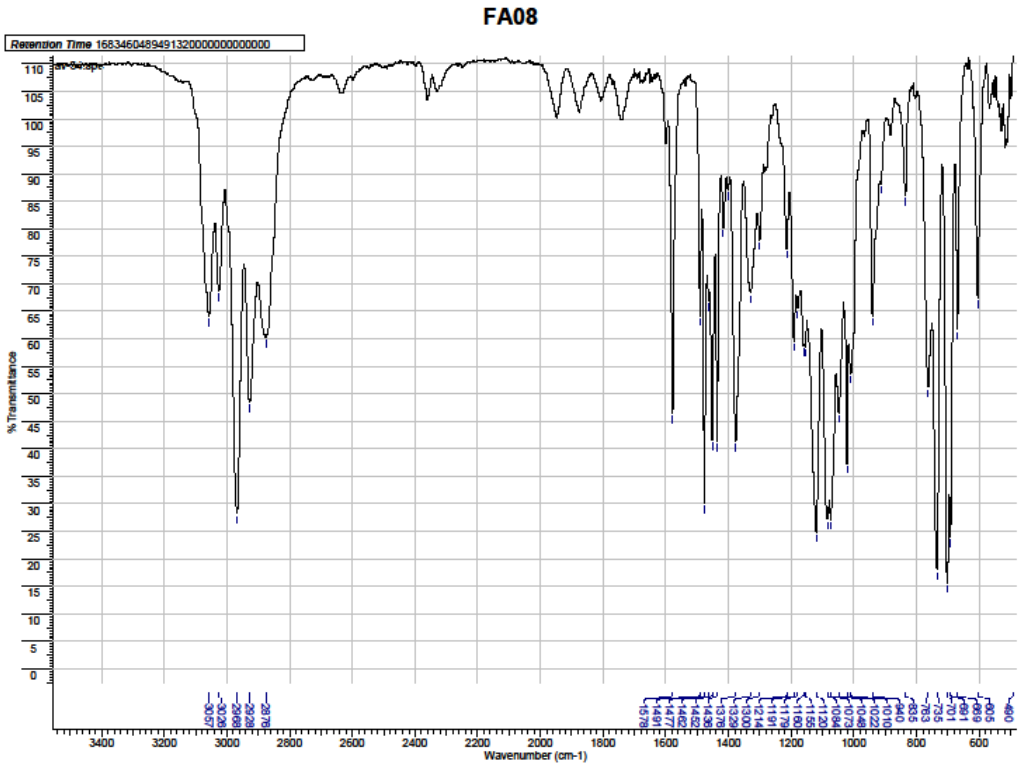
S79. IR spectrum of compound **3j** (KBr pellet).



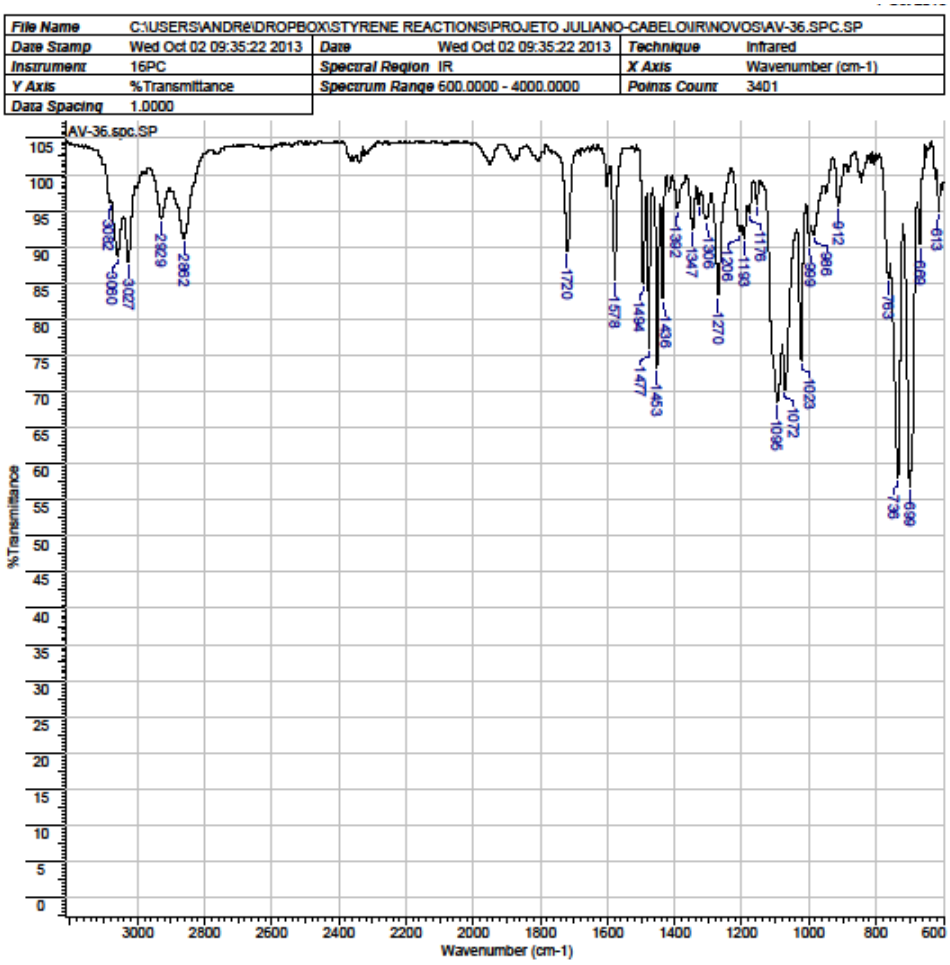
S80. IR spectrum of compound **3k** (KBr pellet).



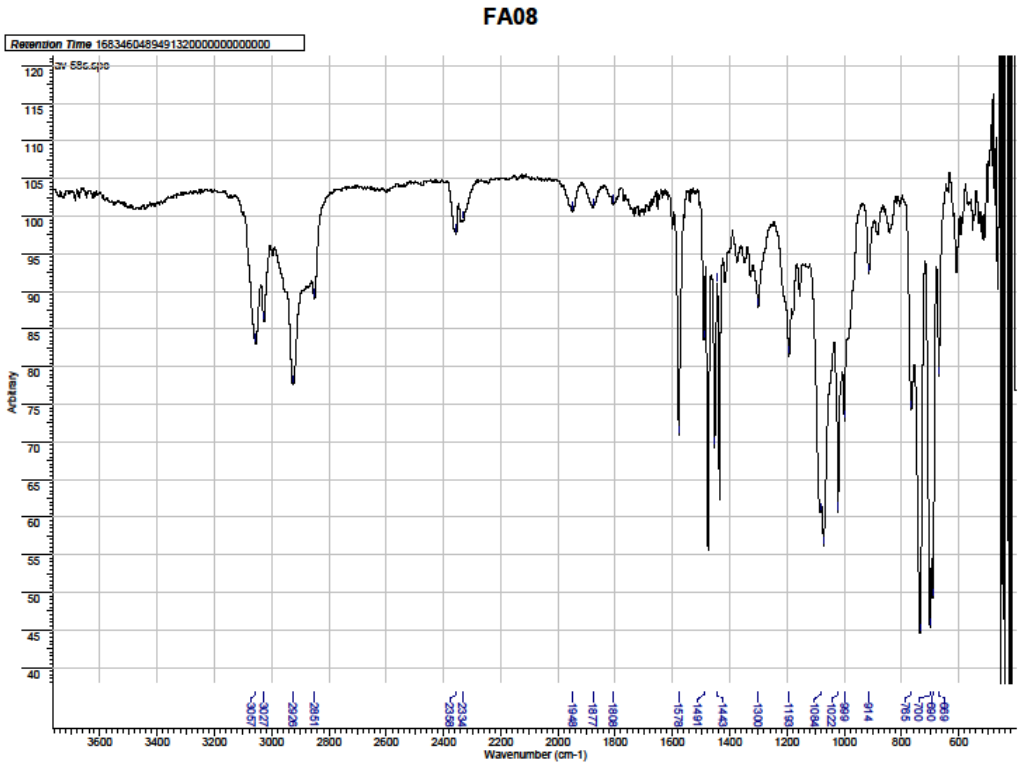
S81. IR spectrum of compound **3m** (KBr pellet).



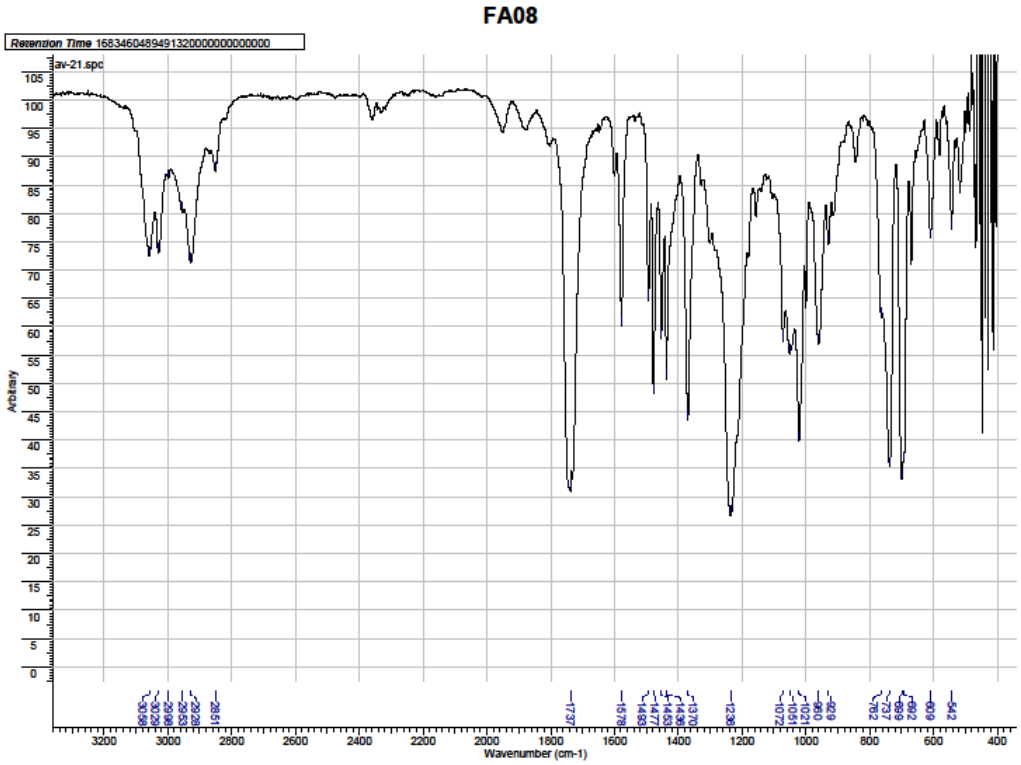
S82. IR spectrum of compound **3n**(KBr pellet).



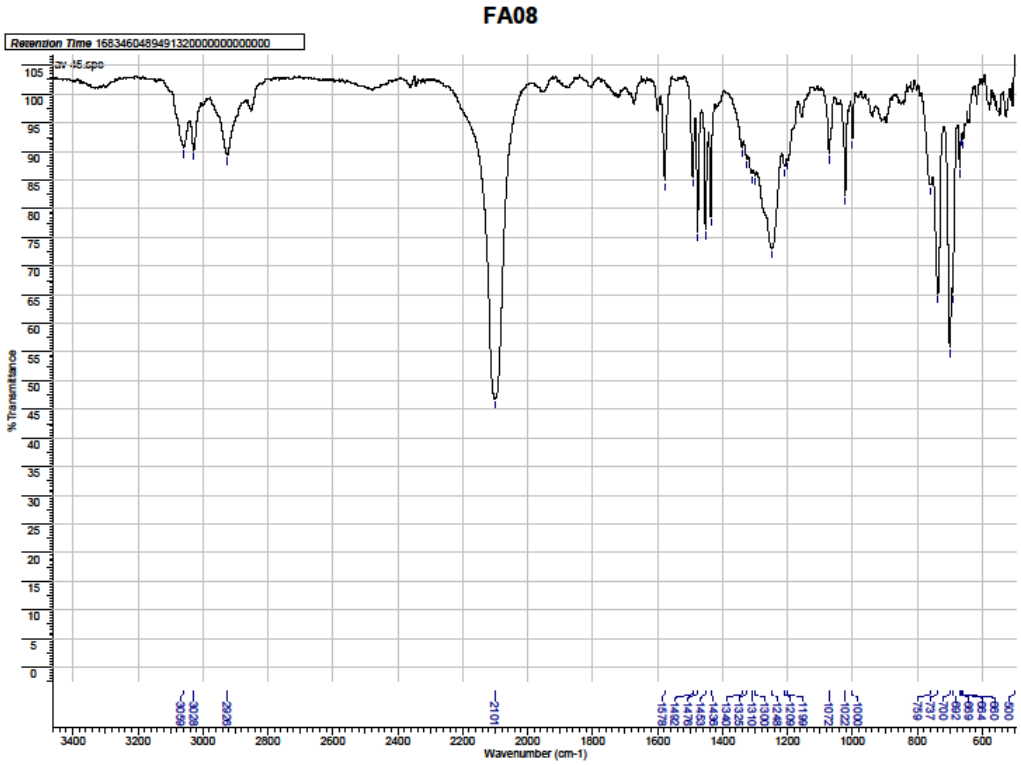
S83. IR spectrum of compound **3o** (KBr pellet).



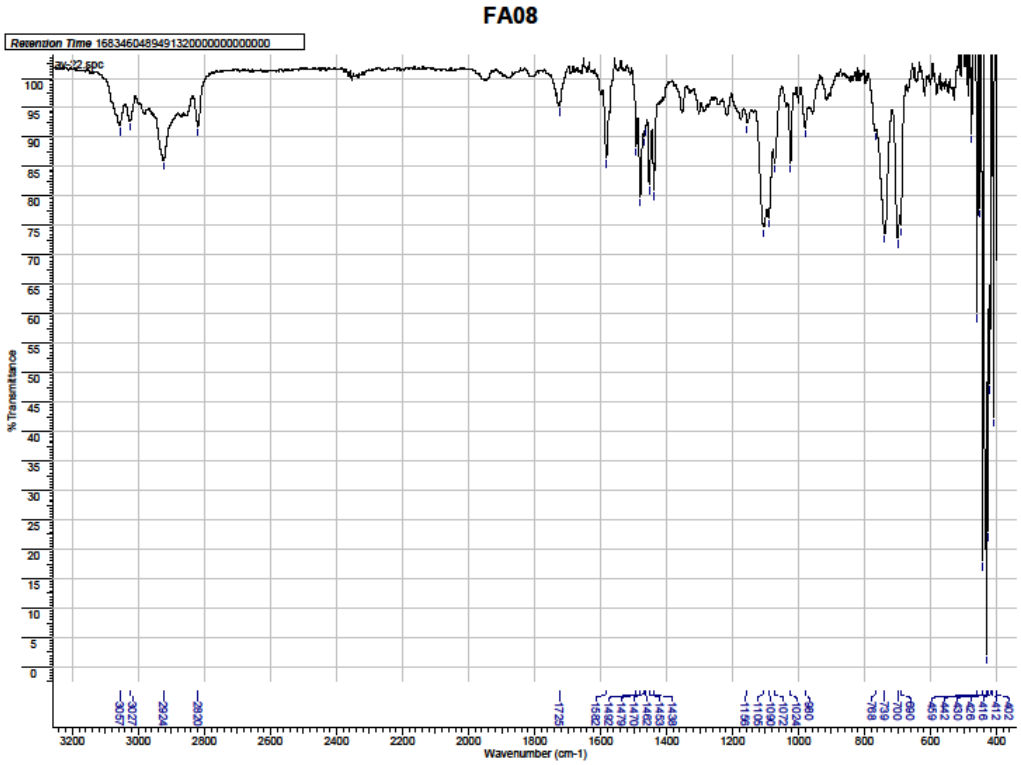
S84. IR spectrum of compound **3r**(KBr pellet).



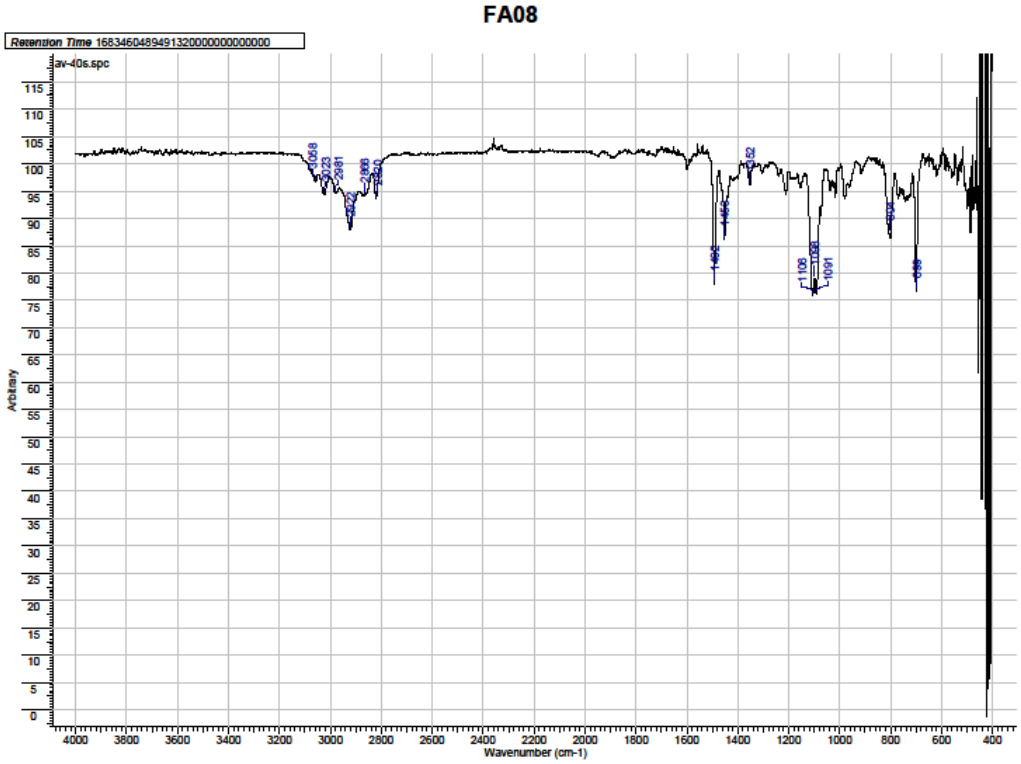
S85. IR spectrum of compound **3s** (KBr pellet).



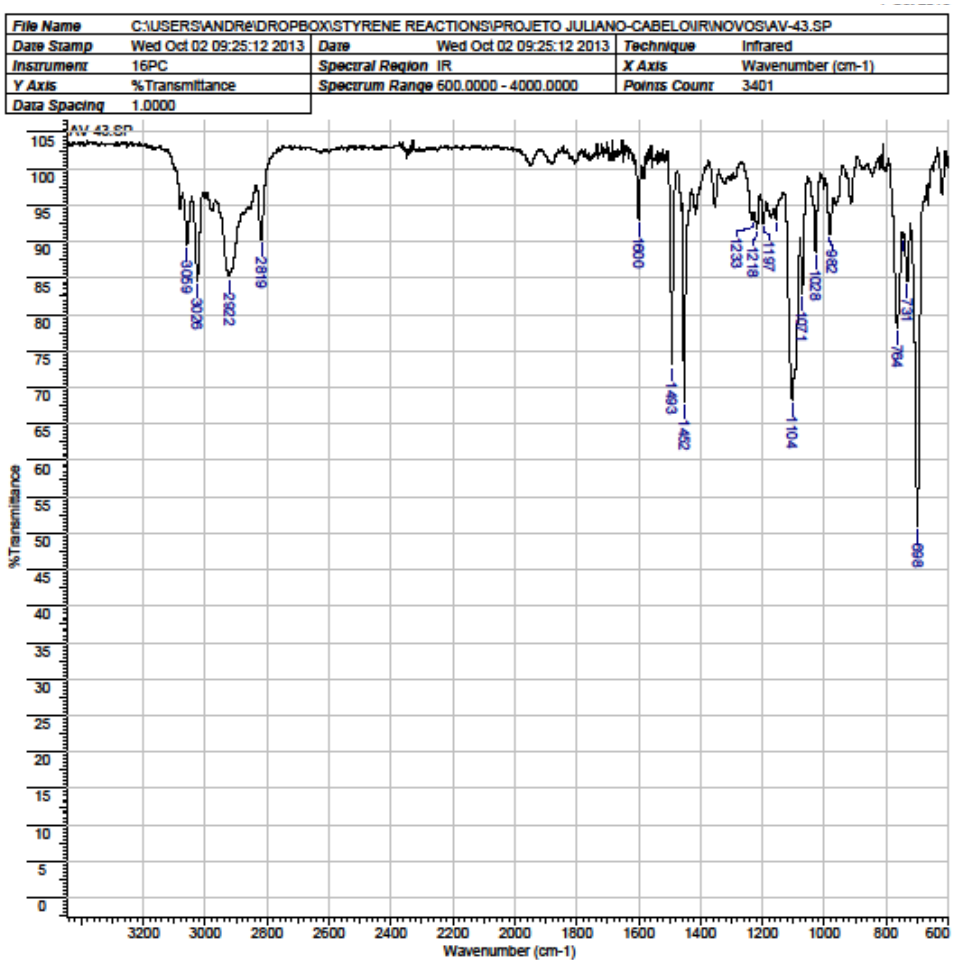
S86. IR spectrum of compound **3t** (KBr pellet).



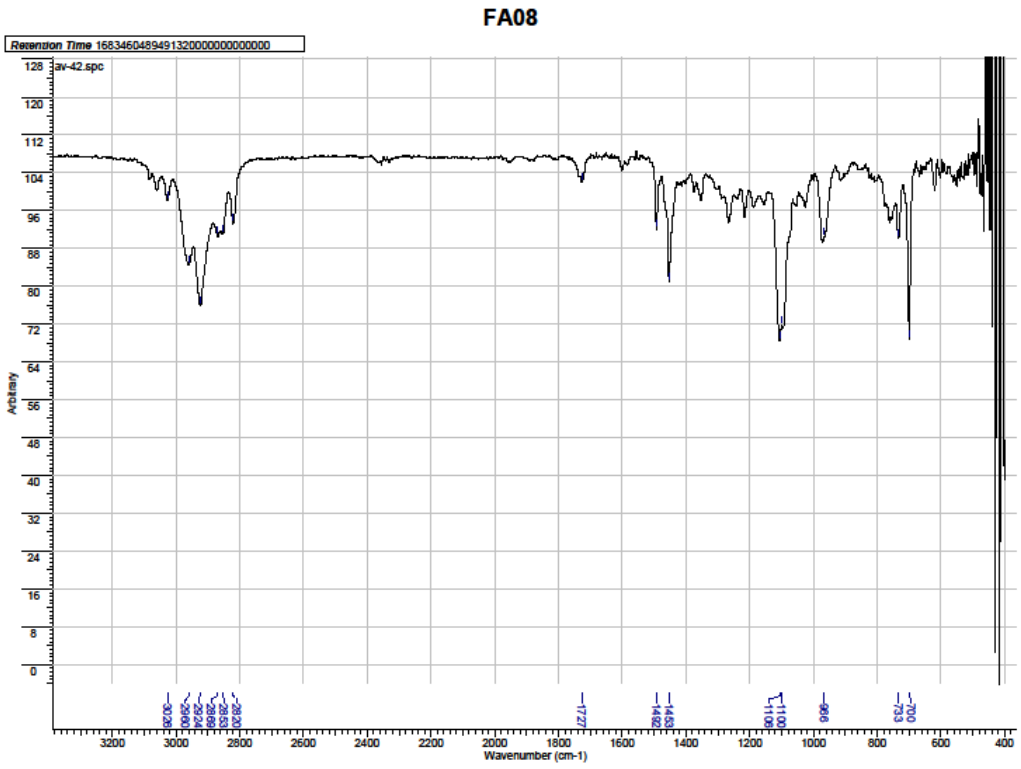
S87. IR spectrum of compound **5a** (KBr pellet).



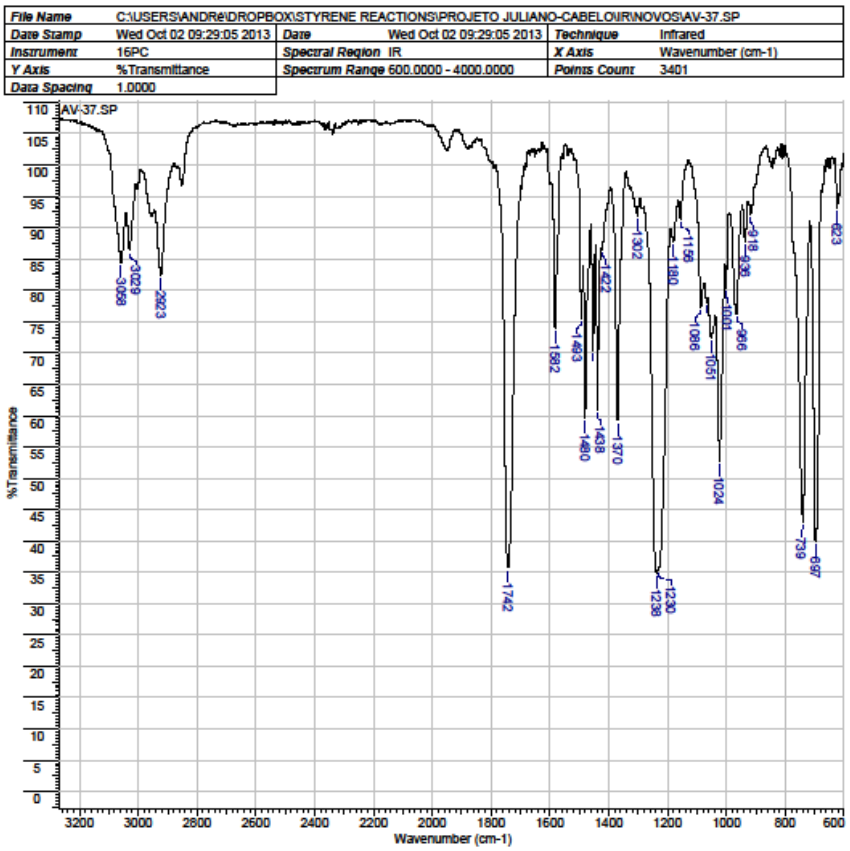
S88. IR spectrum of compound **5b** (KBr pellet).



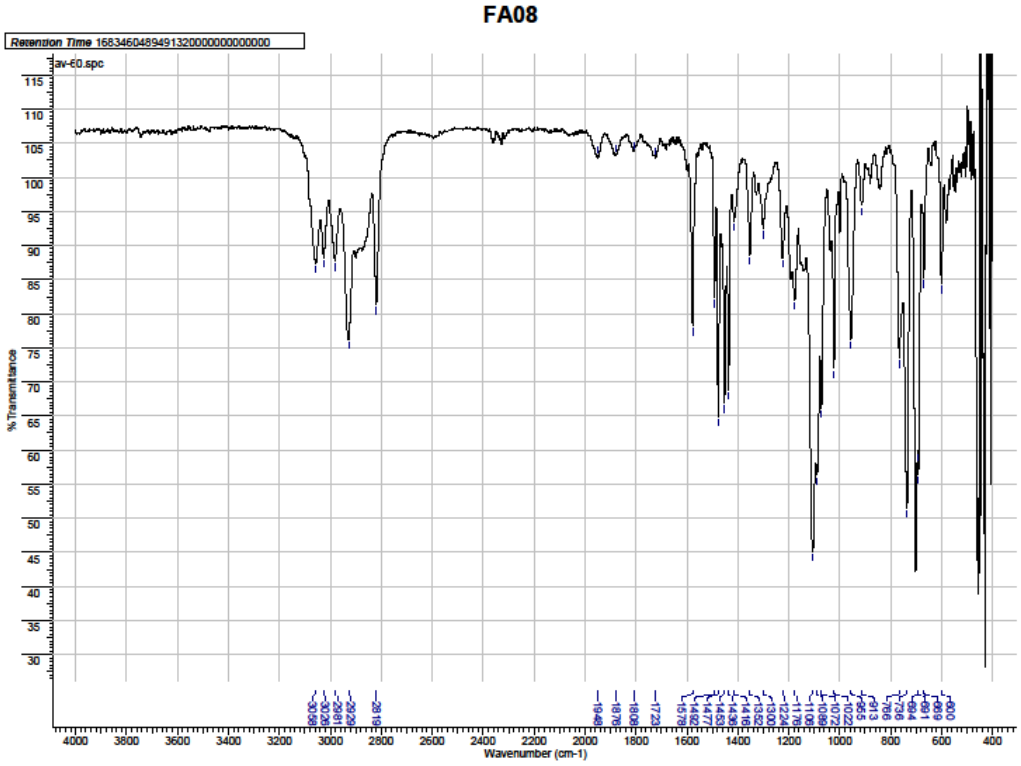
S89. IR spectrum of compound **5c** (KBr pellet).



S90. IR spectrum of compound **5d** (KBr pellet).



S91. IR spectrum of compound **5e** (KBr pellet).



S92. IR spectrum of compound **5f** (KBr pellet).