

Supporting Information For

Synthesis of Unsaturated Precursors for Parahydrogen Induced Polarization and Molecular Imaging of 1-¹³C-acetates and 1-¹³C-pyruvates via Side Arm Hydrogenation

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1. Additional Figures (S1-S29): ^1H NMR and ^{13}C NMR spectra of acetates and pyruvates in CDCl_3 .

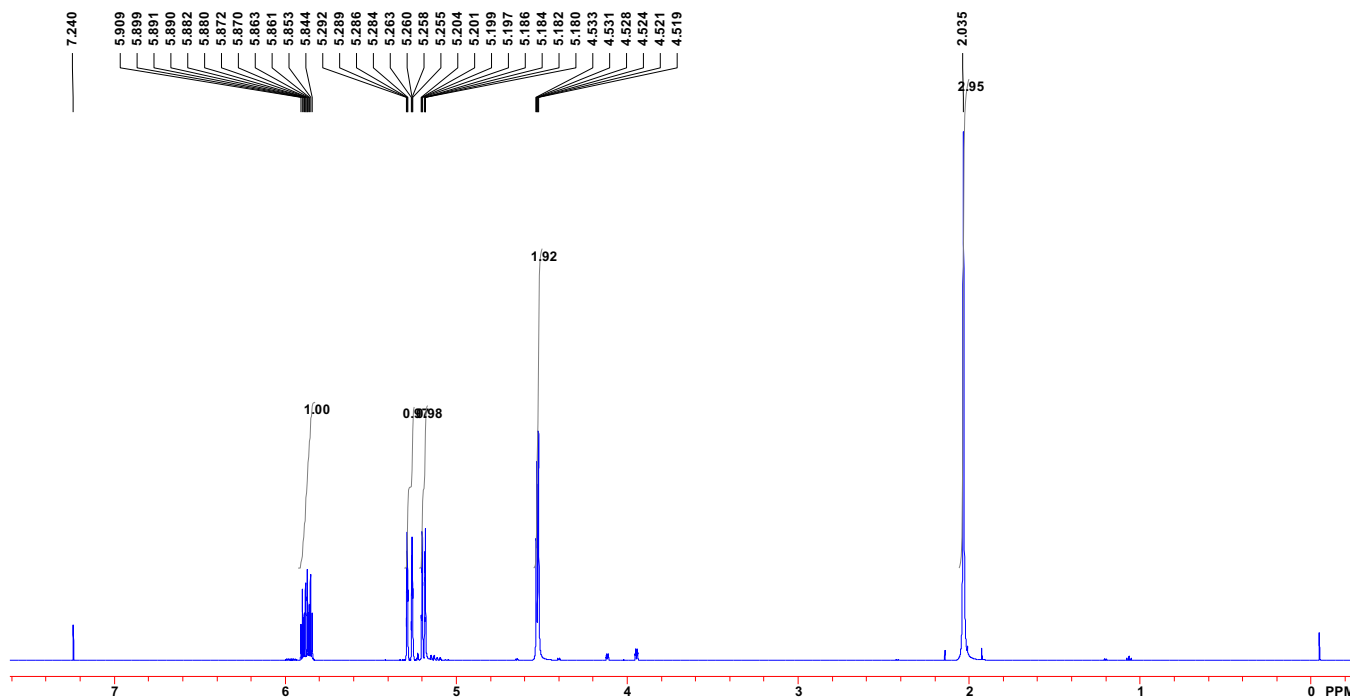


Figure S1. ^1H NMR spectroscopy of allyl acetate 5a

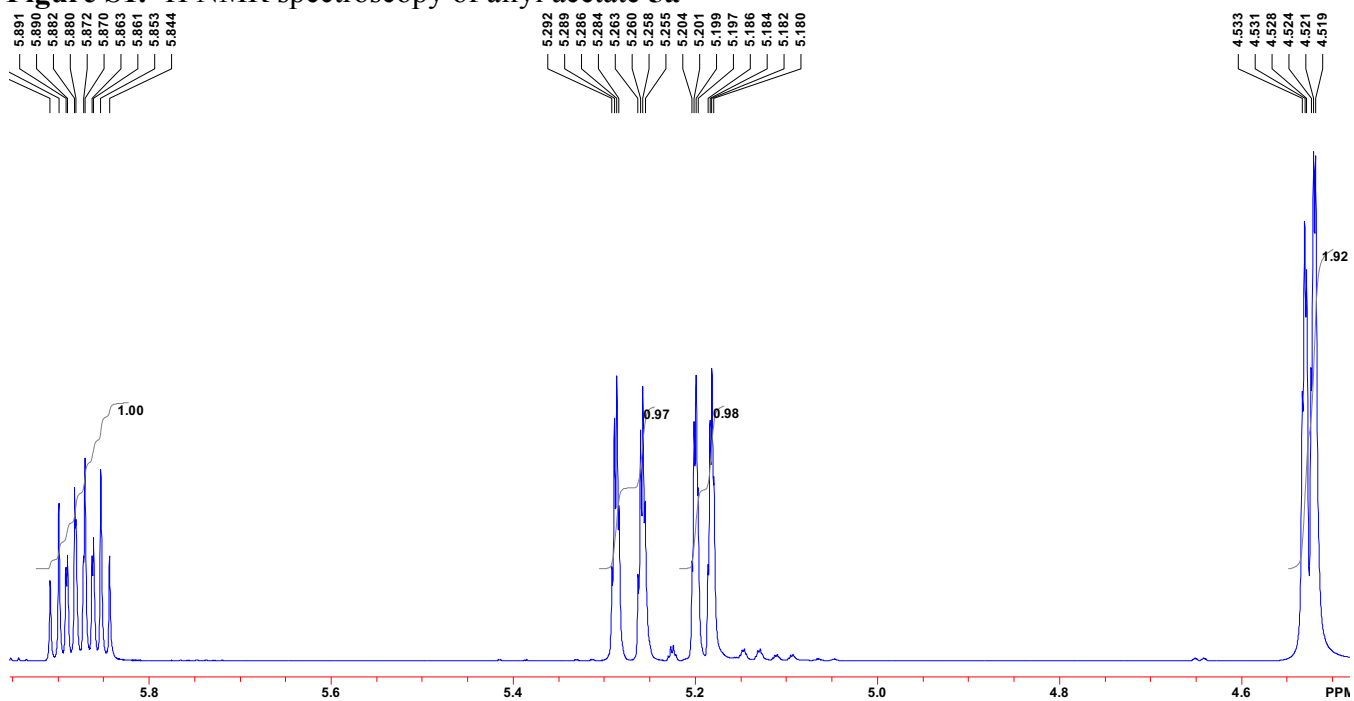


Figure S2. ^1H NMR spectroscopy of allyl acetate 5a

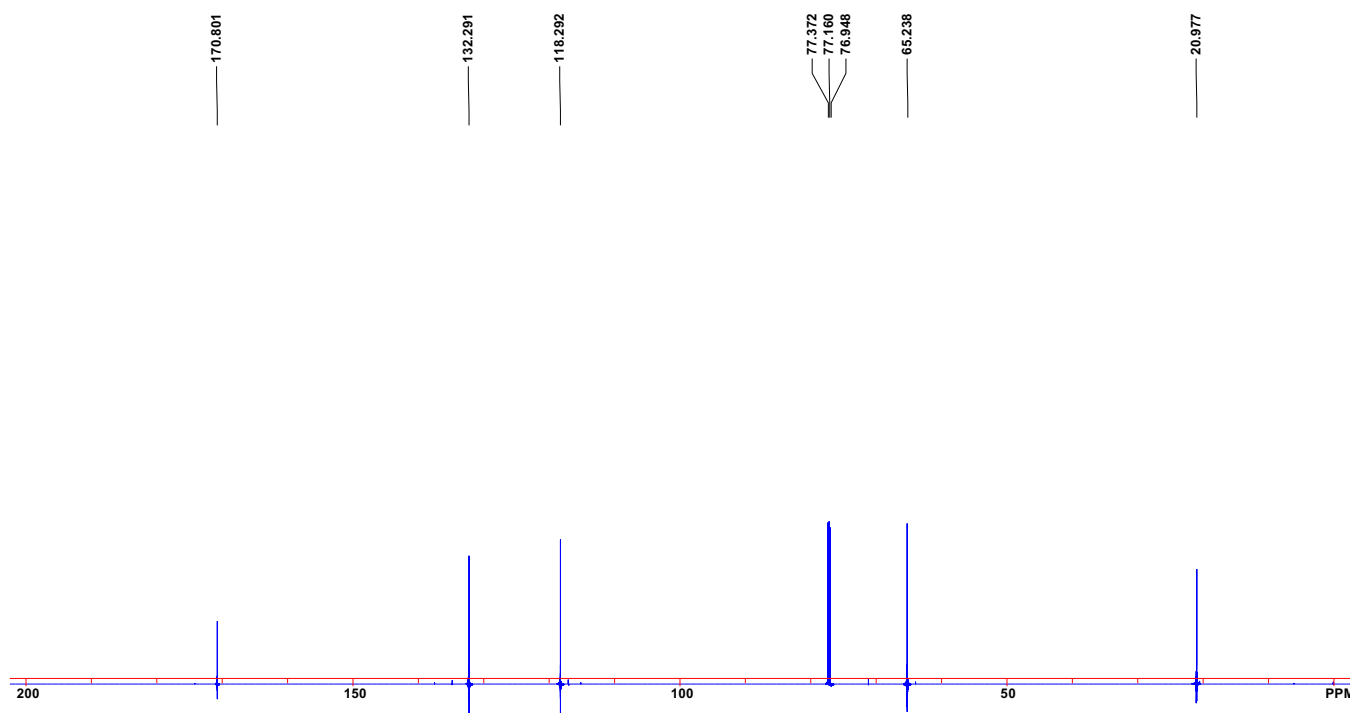


Figure S3. ^{13}C NMR spectroscopy of allyl acetate **5a**

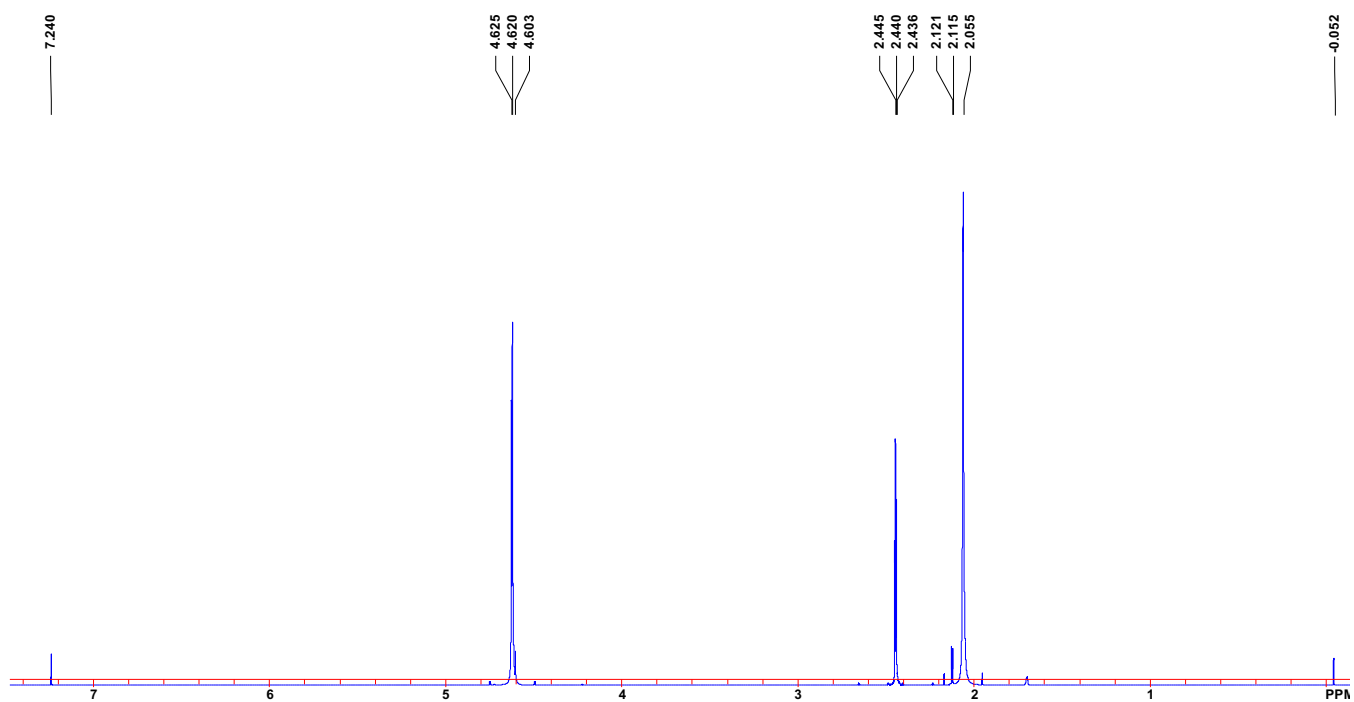


Figure S4. ^1H NMR spectroscopy of propargyl acetate **6a**

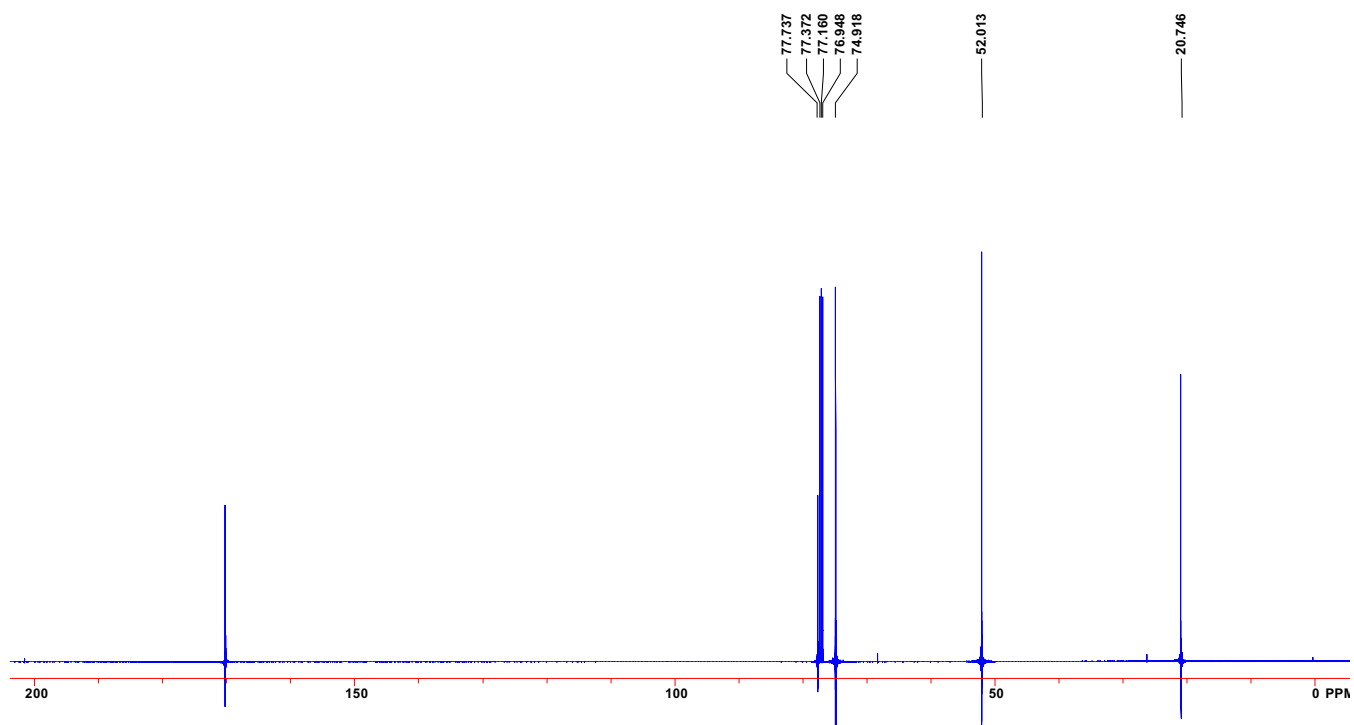


Figure S5. ^{13}C NMR spectroscopy of propargyl acetate **6a**

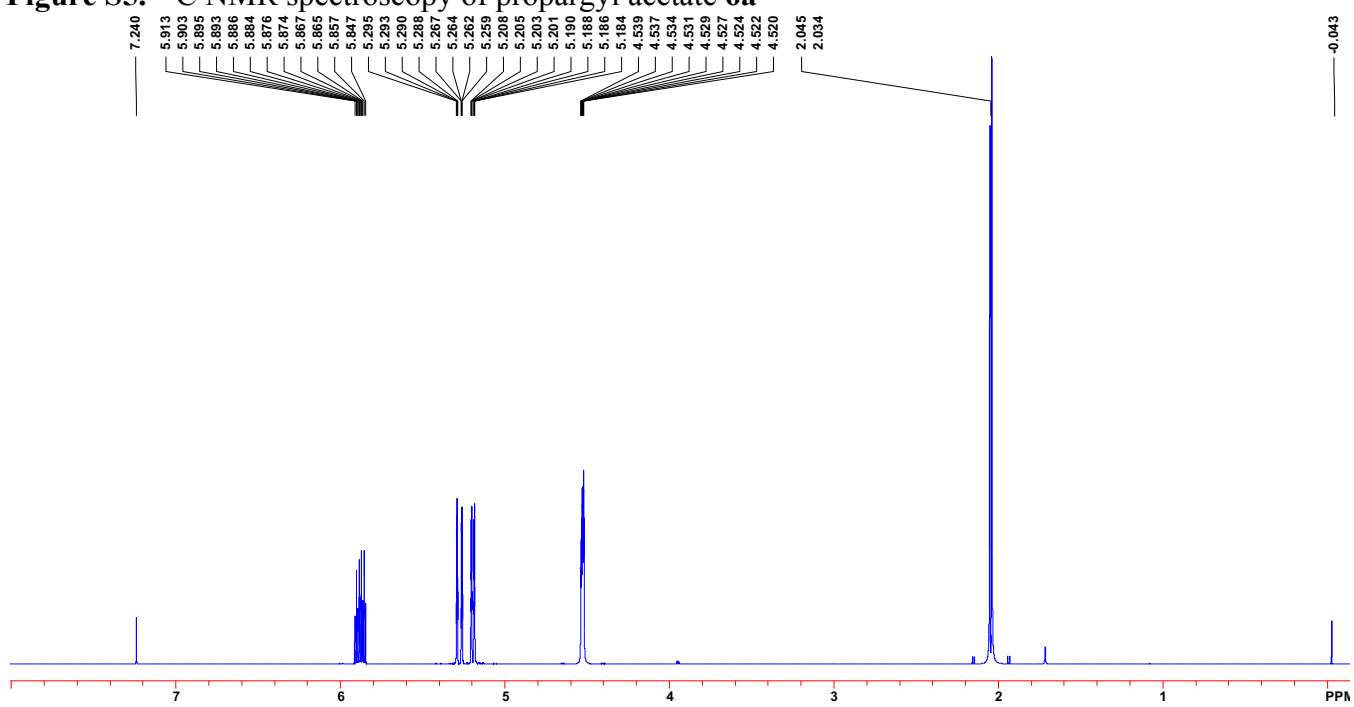


Figure S6. ^1H NMR spectroscopy of allyl acetate- $1\text{-}^{13}\text{C}$ **5b**

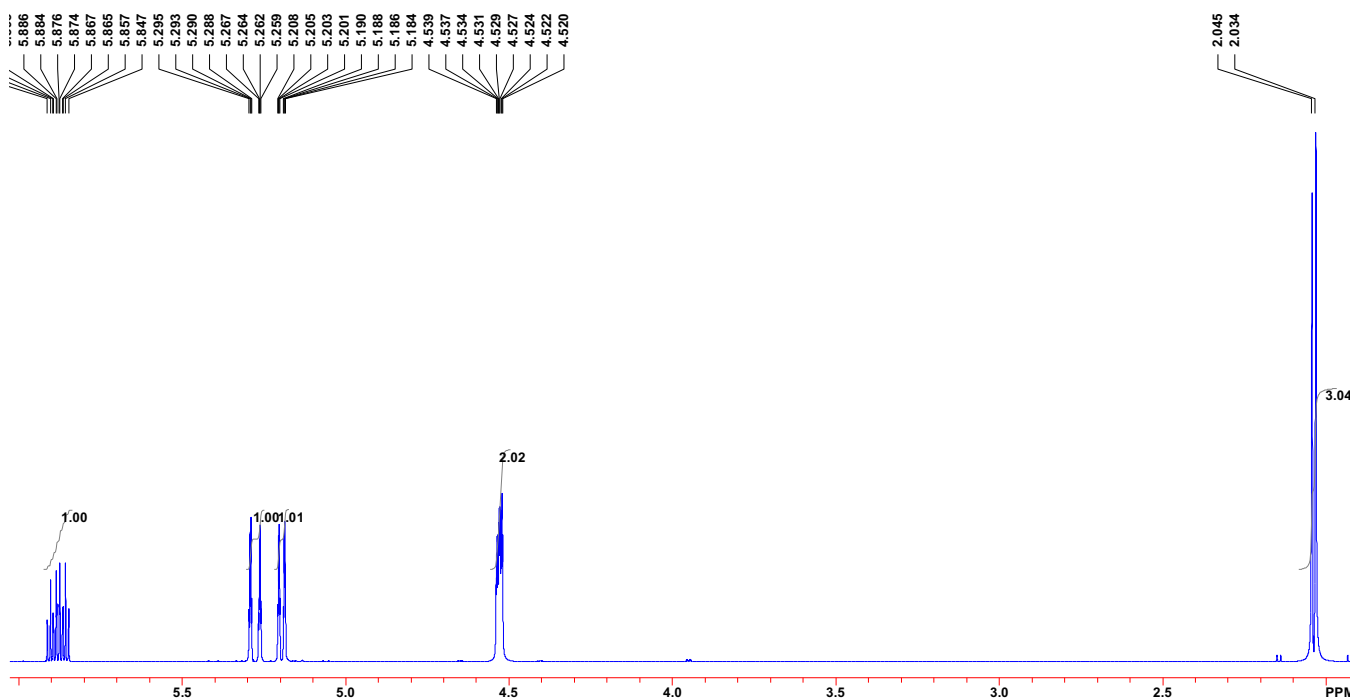


Figure S7. ^1H NMR spectroscopy of allyl acetate- $1\text{-}^{13}\text{C}$ **5b**

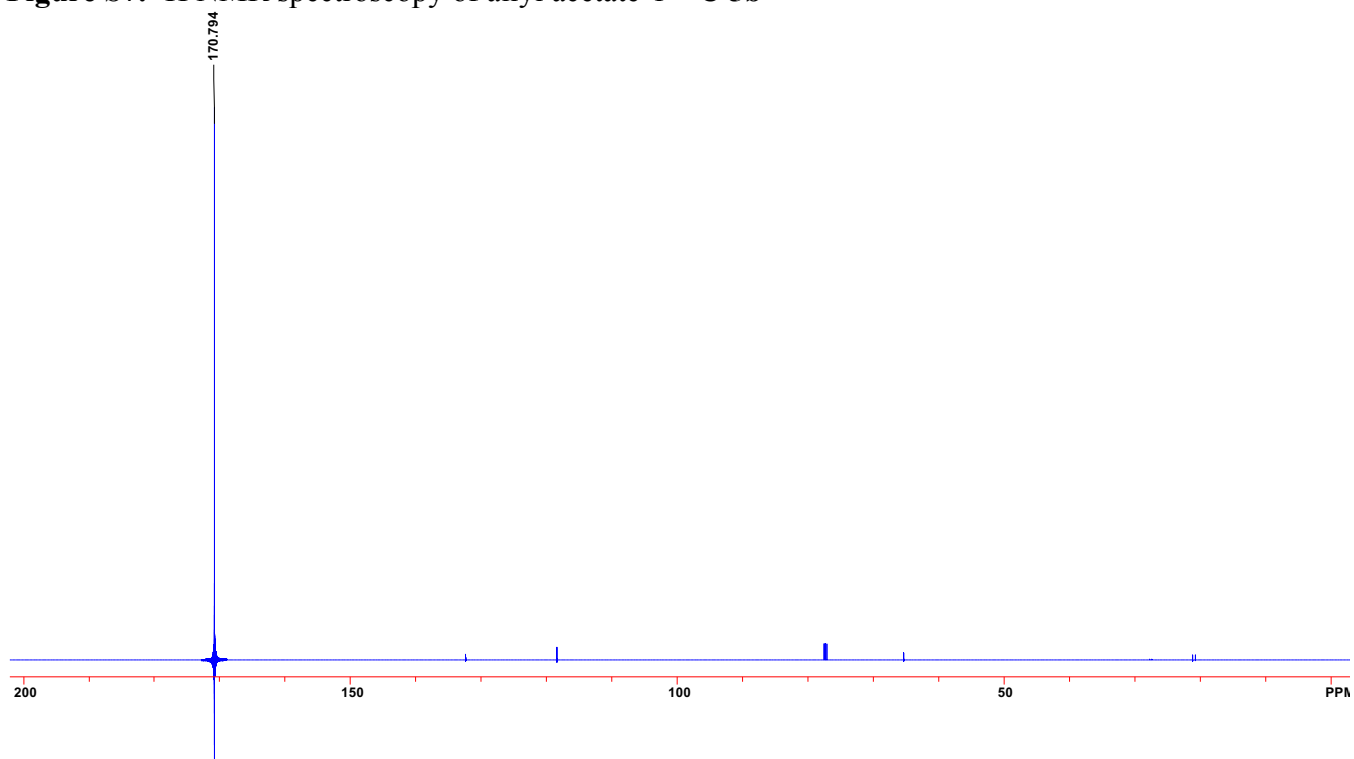


Figure S8. ^{13}C NMR spectroscopy of allyl acetate- $1\text{-}^{13}\text{C}$ **5b**

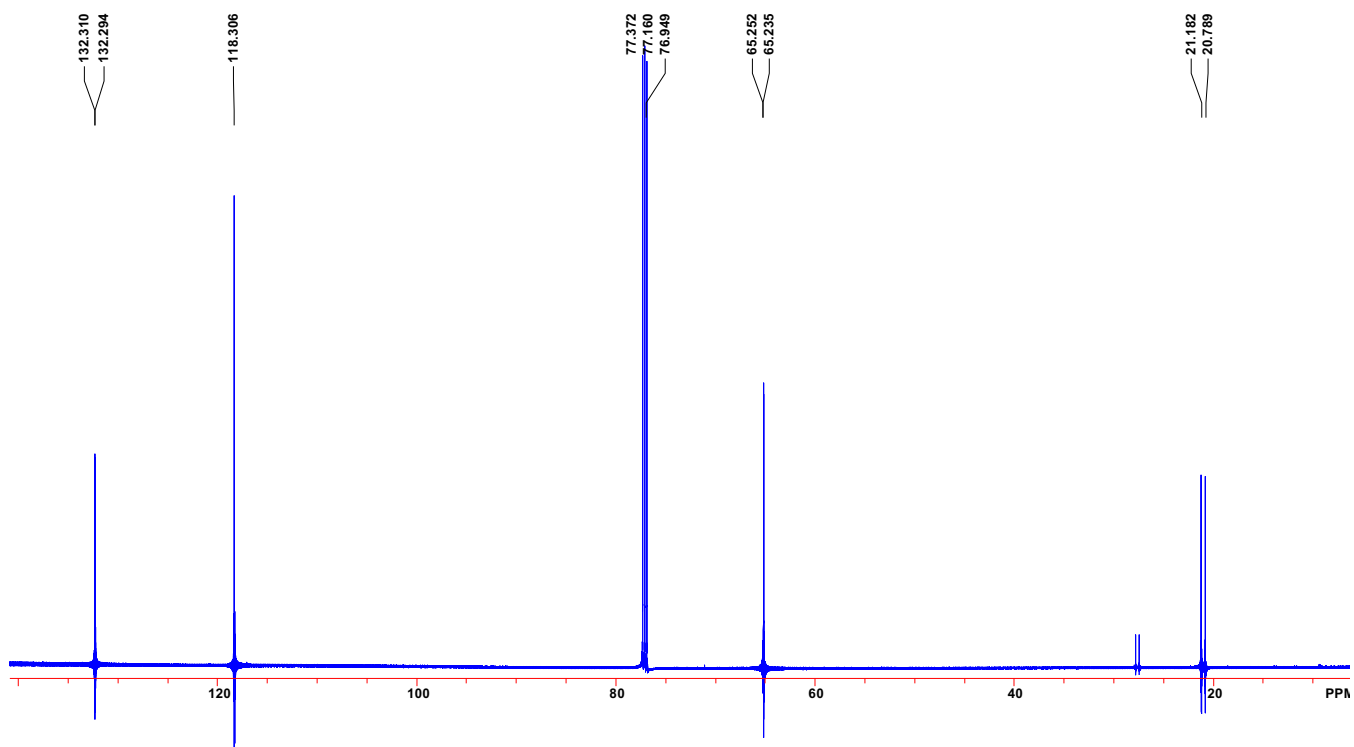


Figure S9. ^{13}C NMR spectroscopy of allyl acetate-1- ^{13}C **5b**

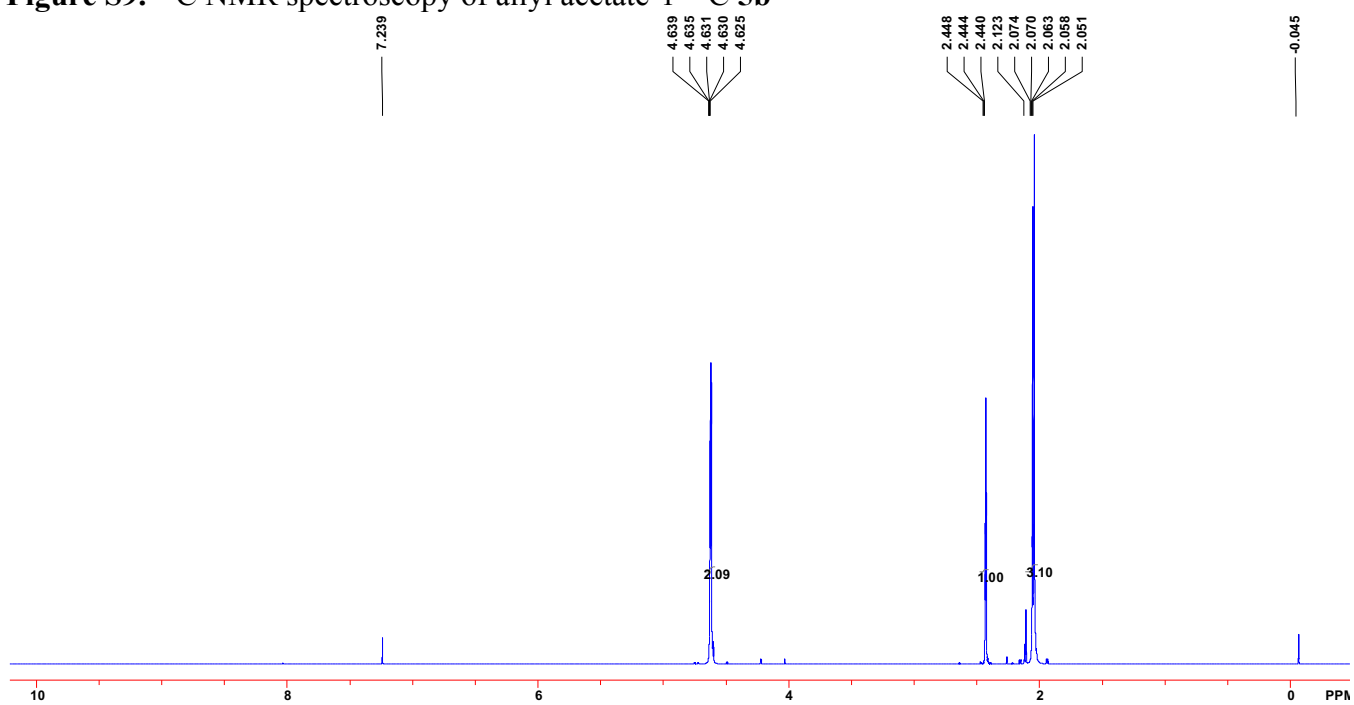


Figure S10. ^1H NMR spectroscopy of propargyl acetate-1- ^{13}C **6b**



Figure S11. ^1H NMR spectroscopy of propargyl acetate-1- ^{13}C **6b**

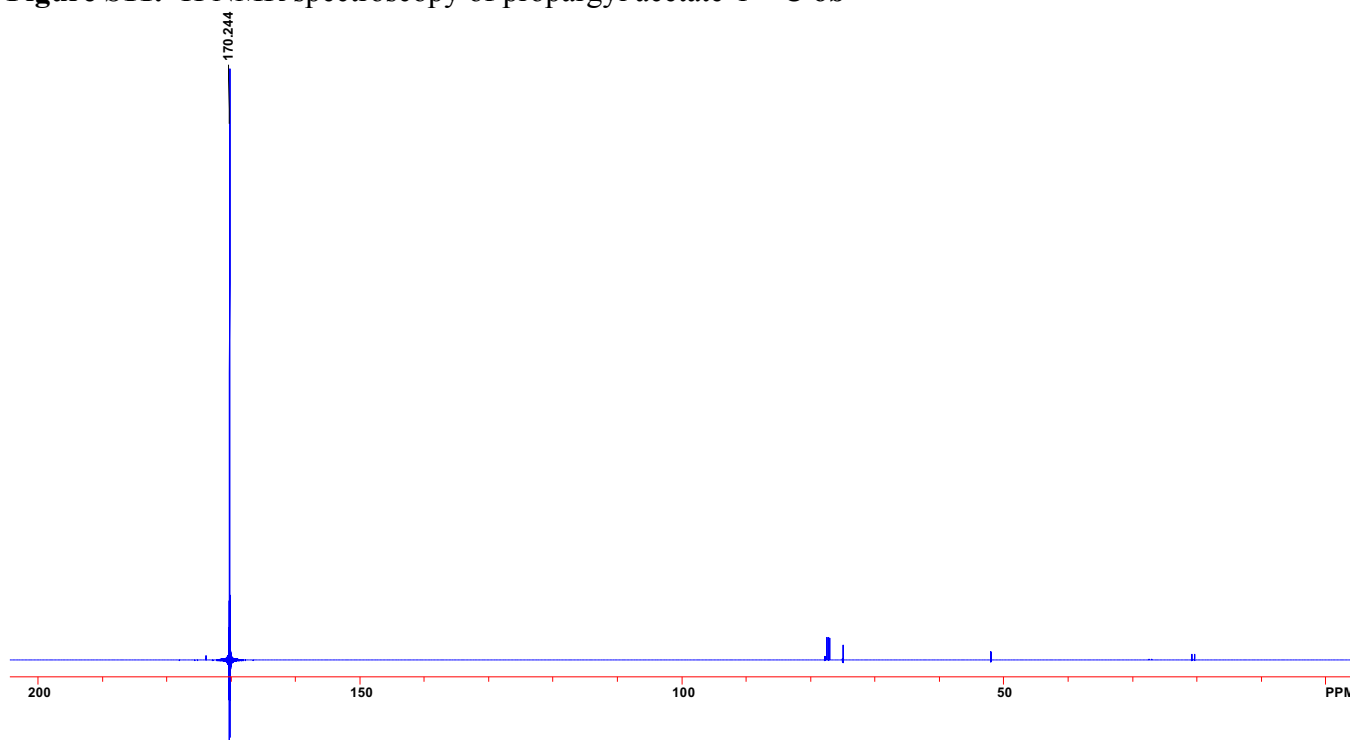


Figure S12. ^{13}C NMR spectroscopy of propargyl acetate-1- ^{13}C **6b**

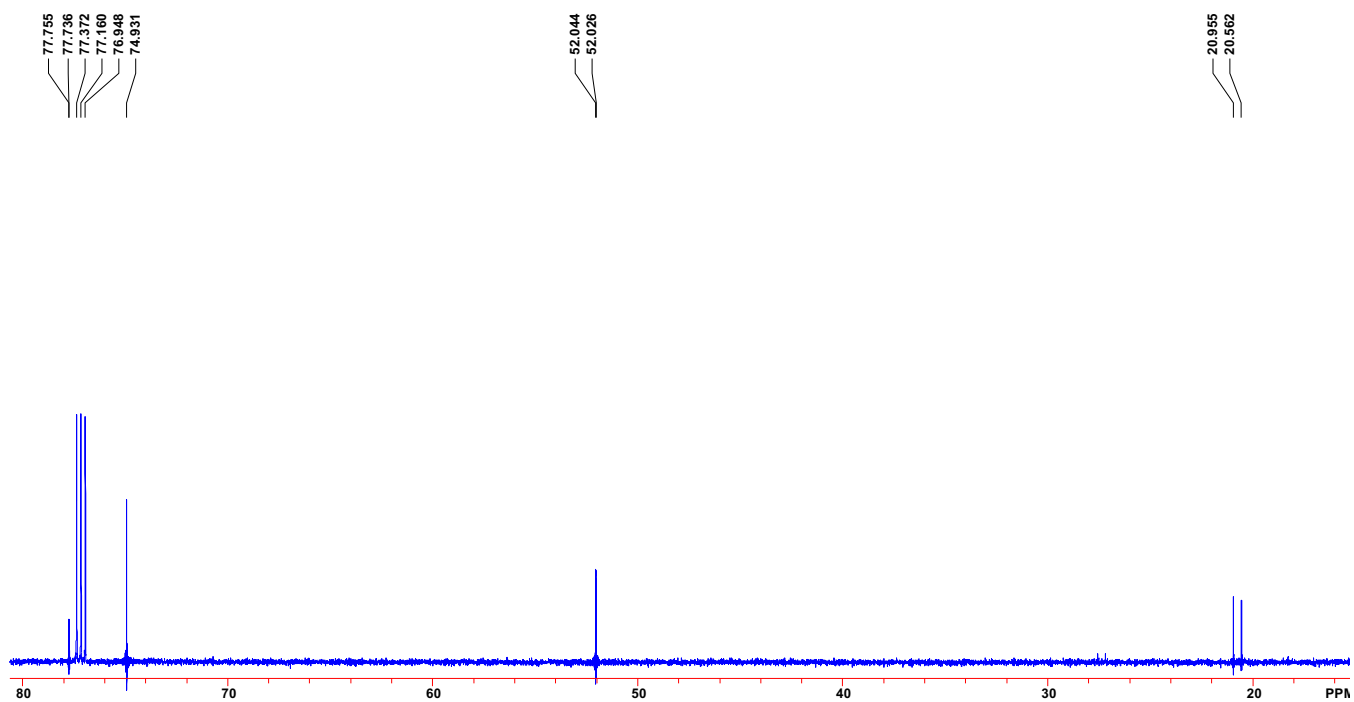


Figure S13. ^{13}C NMR spectroscopy of propargyl acetate- $1\text{-}^{13}\text{C}$ **6b**

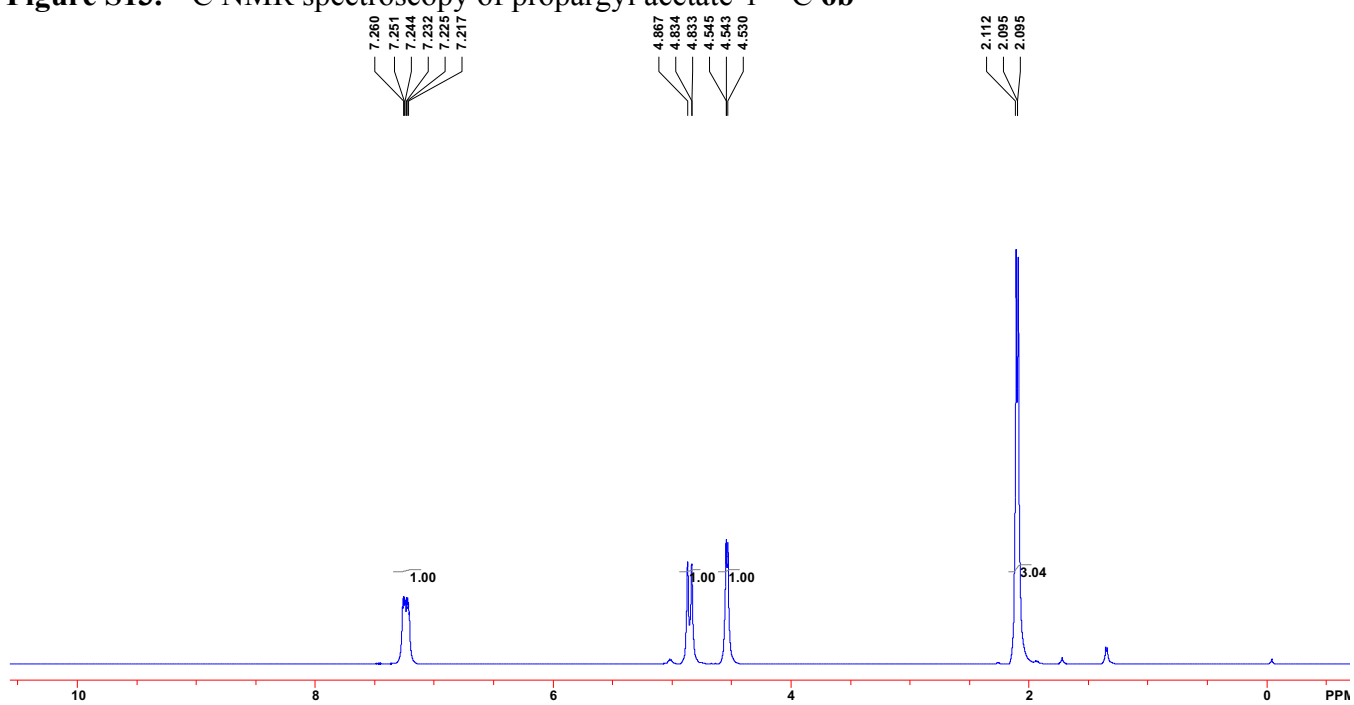


Figure S14. ^1H NMR spectroscopy of vinyl acetate- $1\text{-}^{13}\text{C}$ **7b**

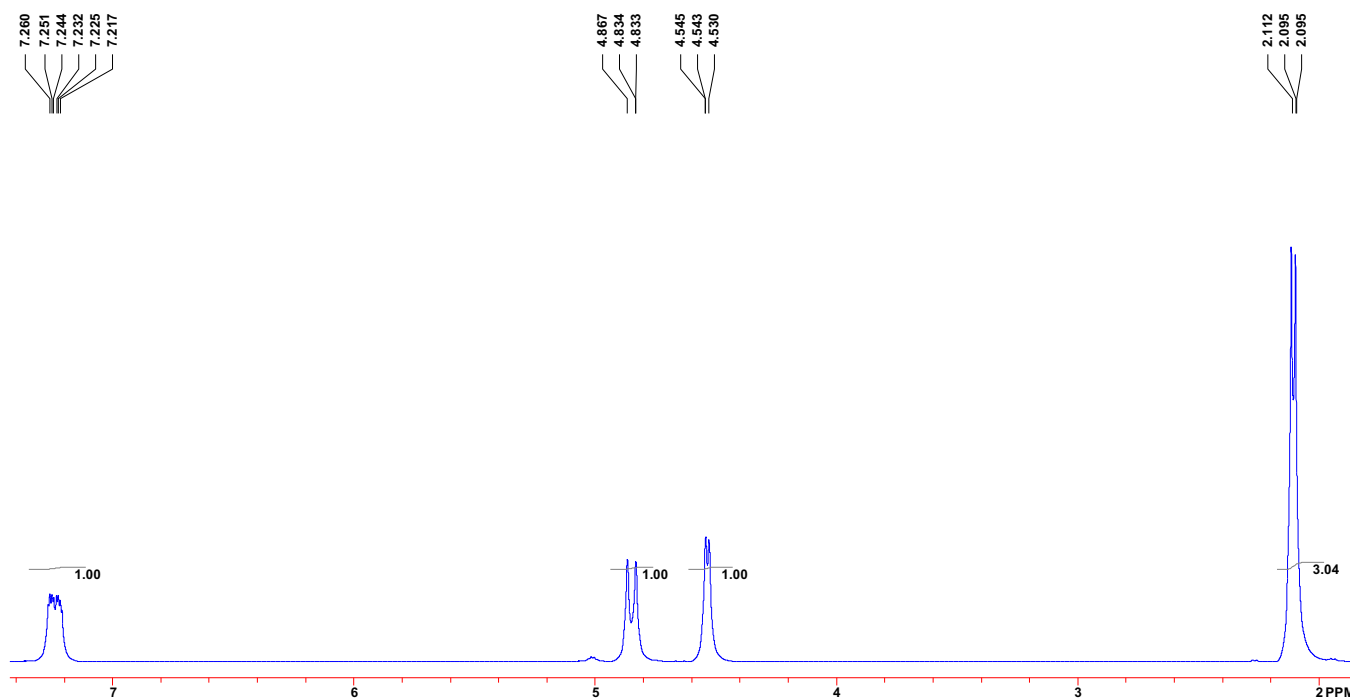


Figure S15. ^1H NMR spectroscopy of vinyl acetate-1- ^{13}C **7b**

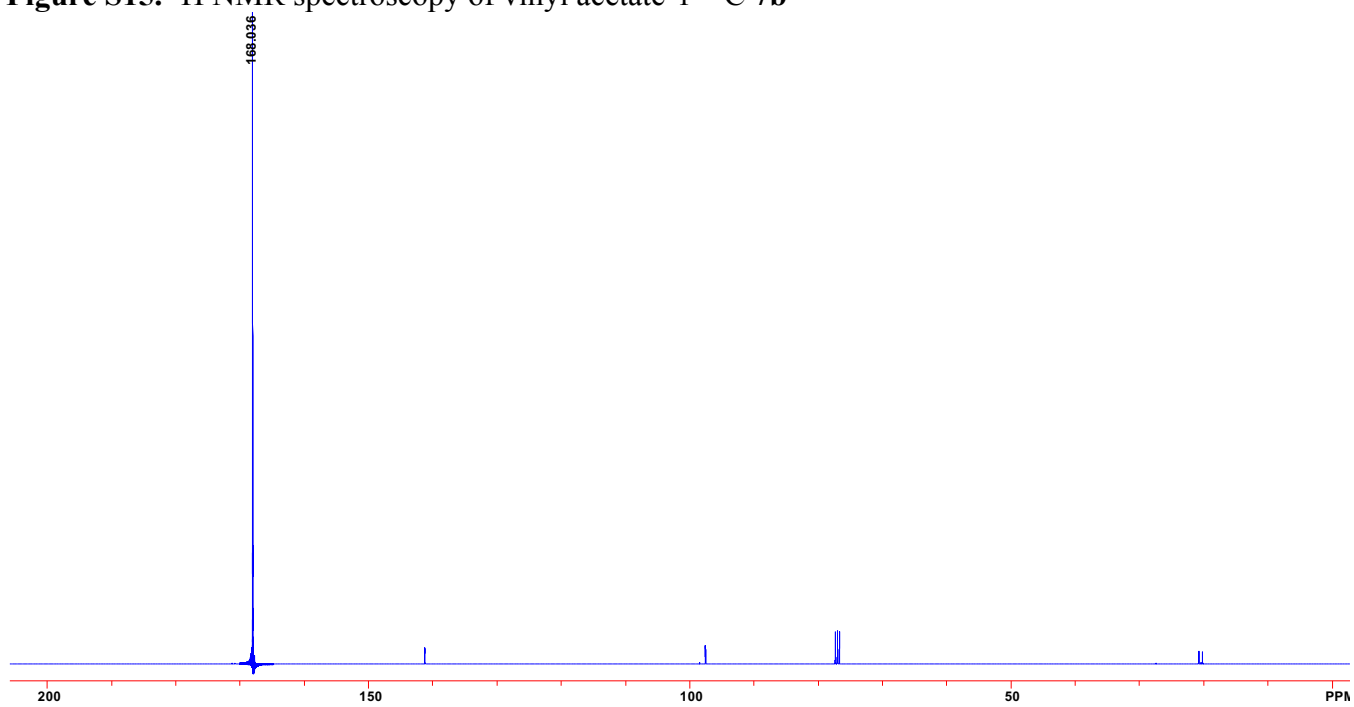


Figure S16. ^{13}C NMR spectroscopy of vinyl acetate-1- ^{13}C **7b**

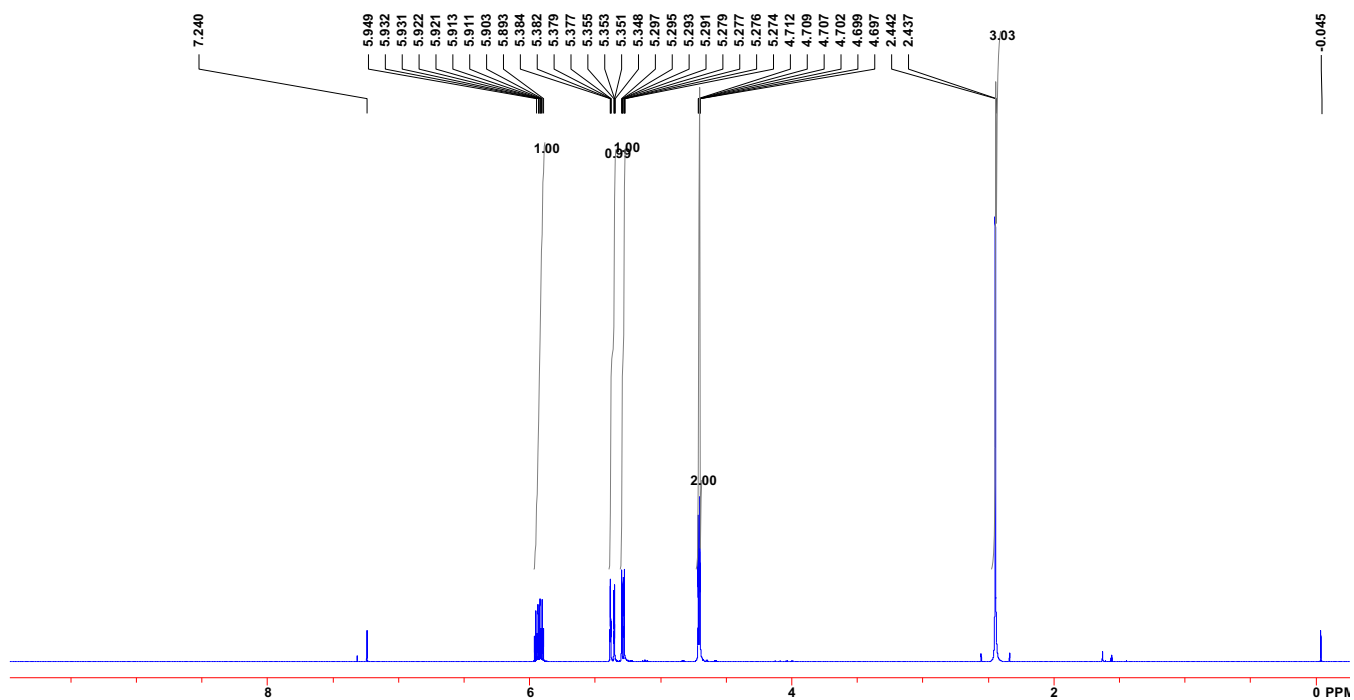


Figure S17. ^1H NMR spectroscopy of allyl pyruvate **8a**

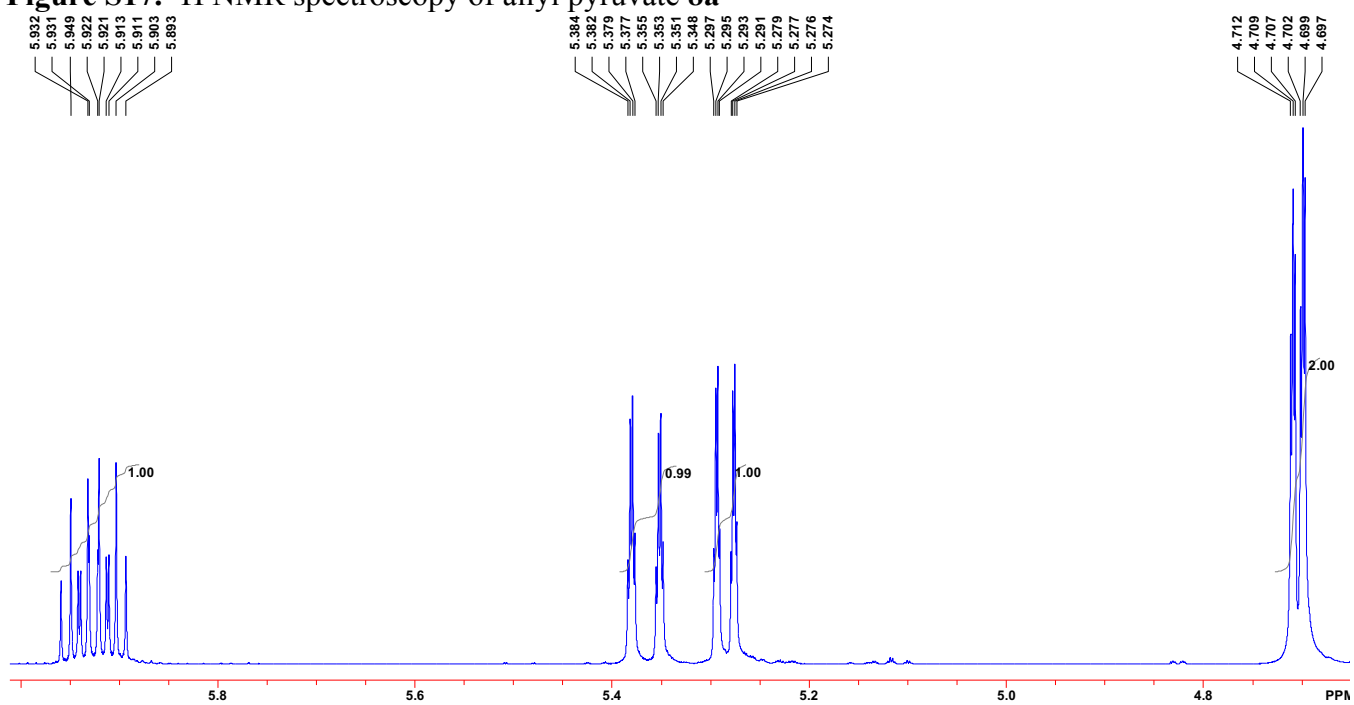


Figure S18. ^1H NMR spectroscopy of allyl pyruvate **8a**

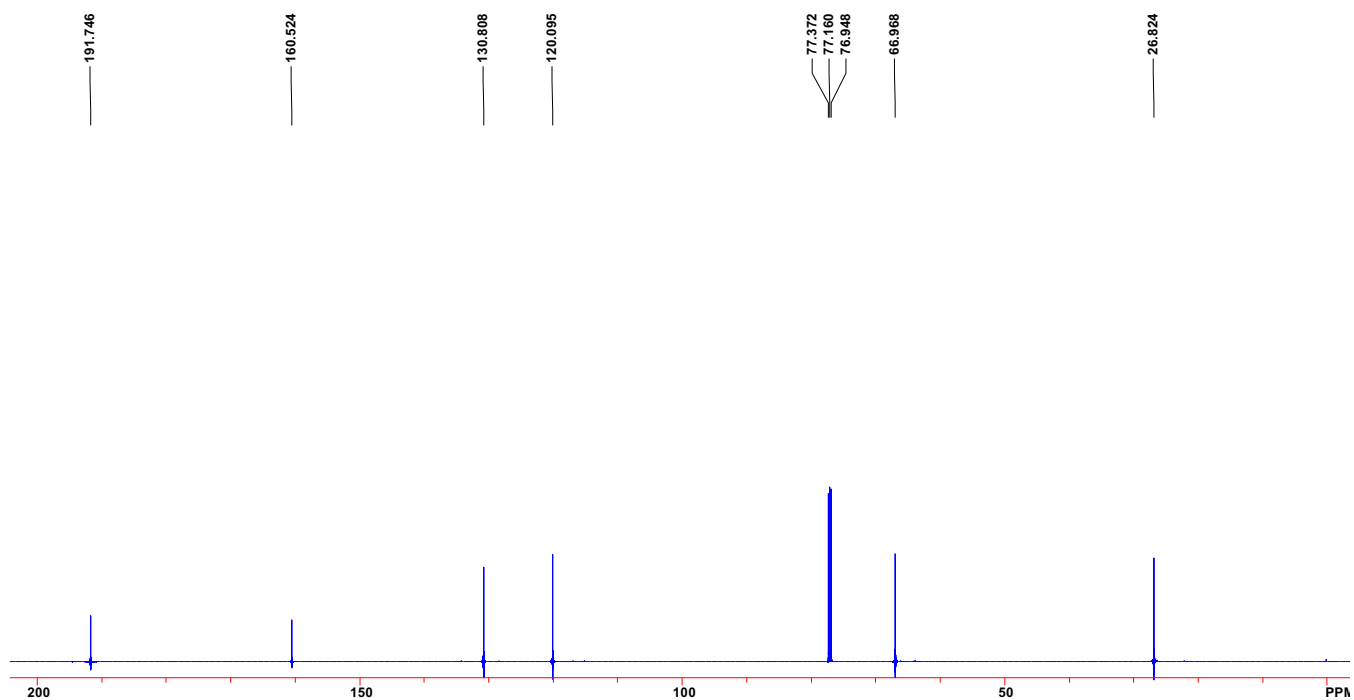


Figure S19. ^{13}C NMR spectroscopy of allyl pyruvate **8a**

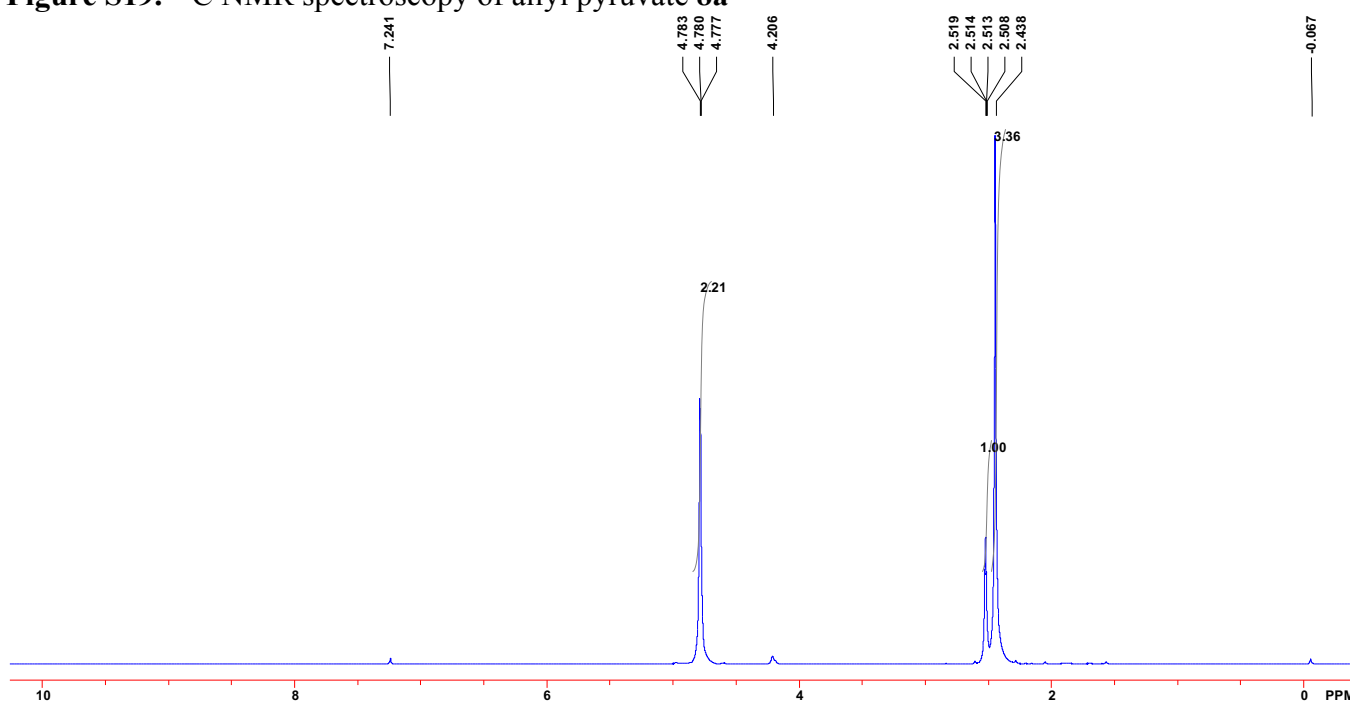


Figure S20. ^1H NMR spectroscopy of propargyl pyruvate **9a**

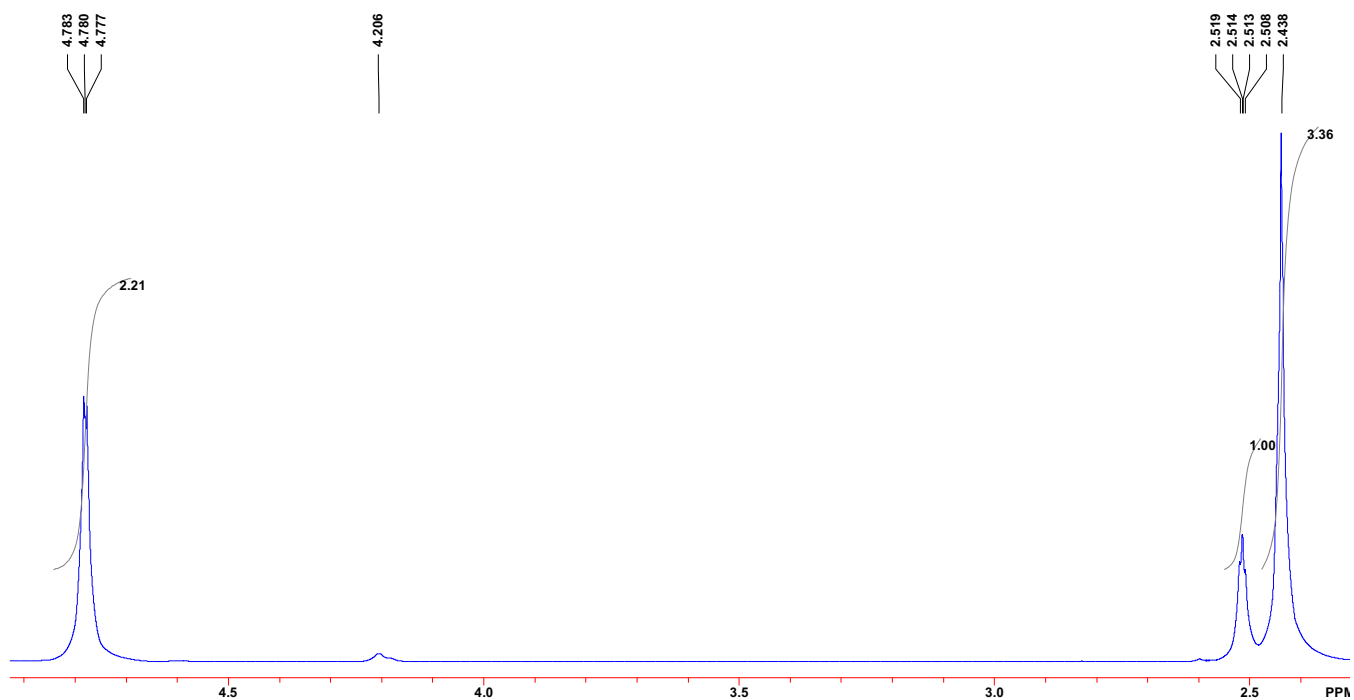


Figure S21. ^1H NMR spectroscopy of propargyl pyruvate **9a**

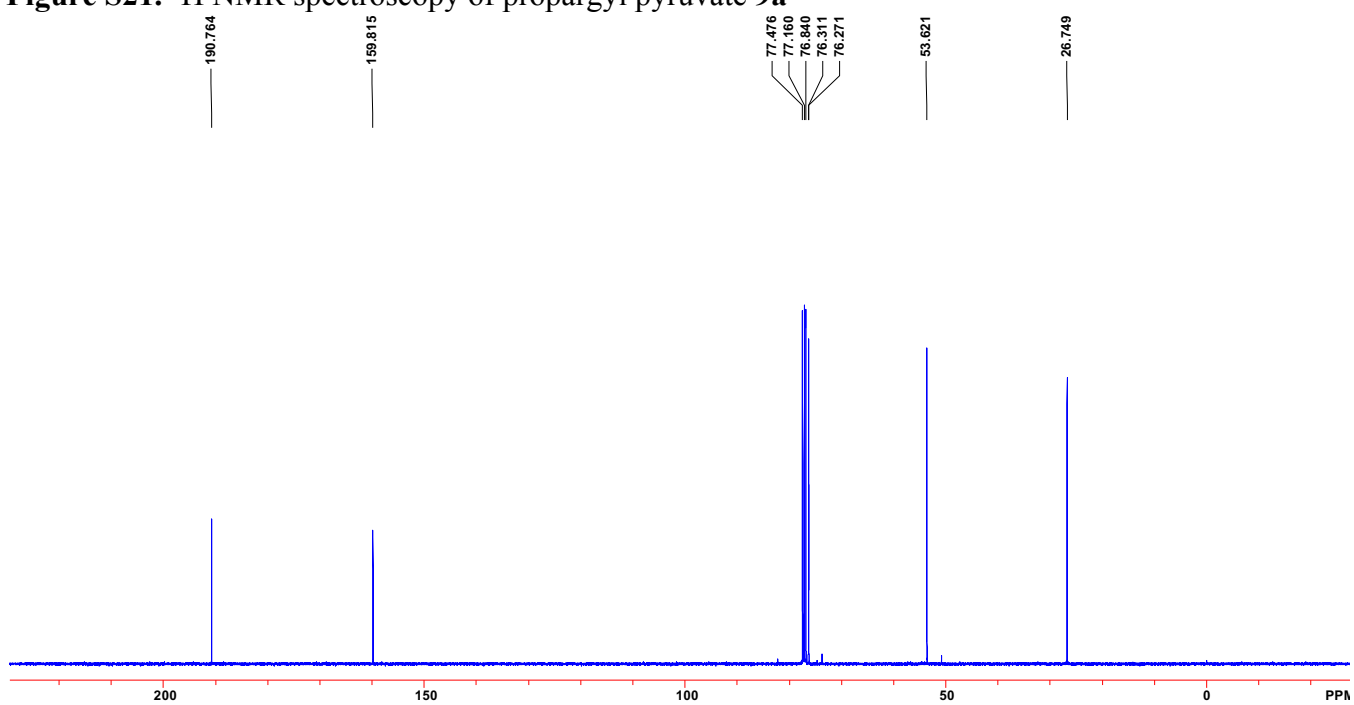


Figure S22. ^{13}C NMR spectroscopy of propargyl pyruvate **9a**

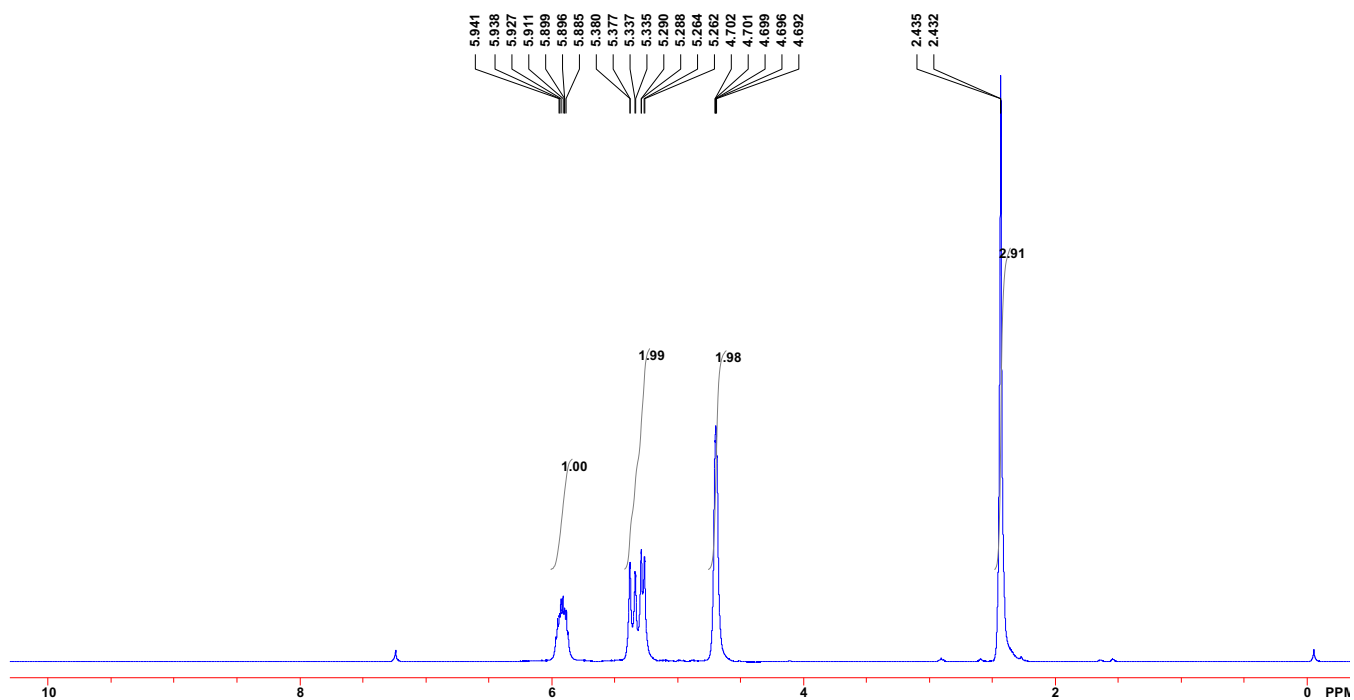


Figure S23. ^1H NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

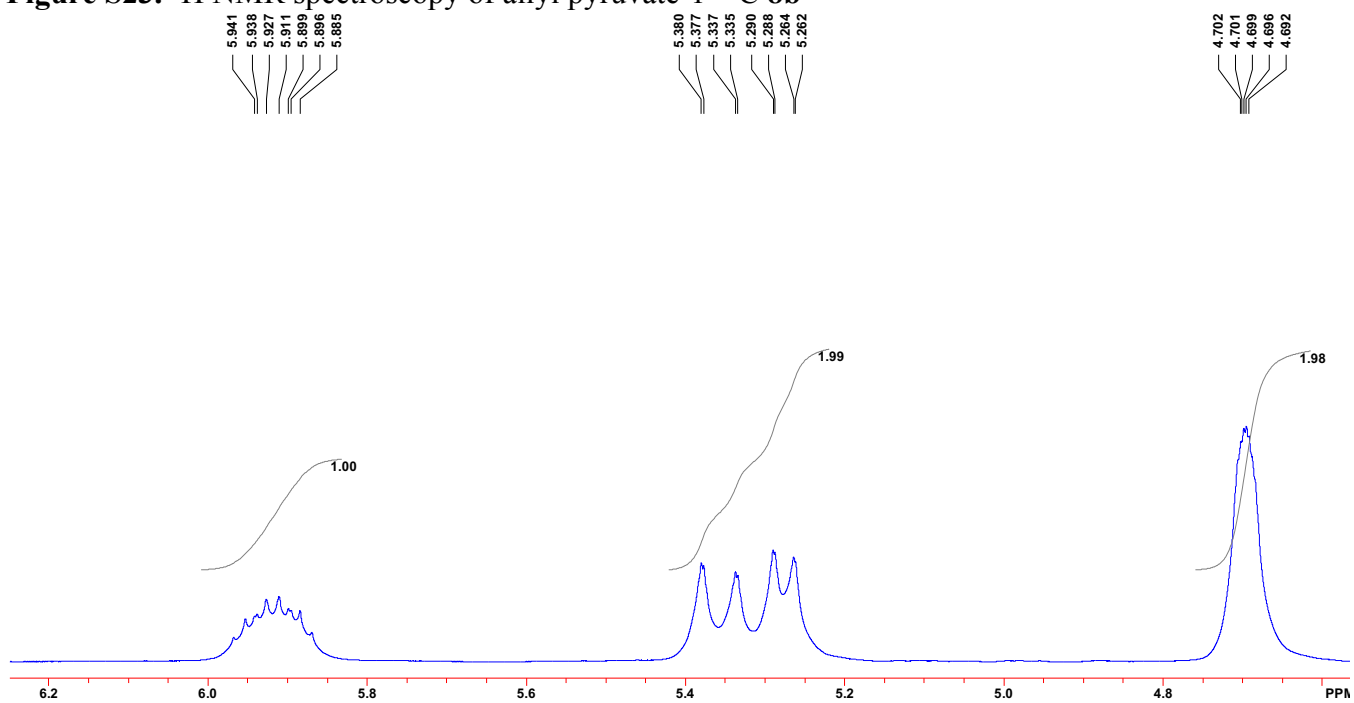


Figure S24. ^1H NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

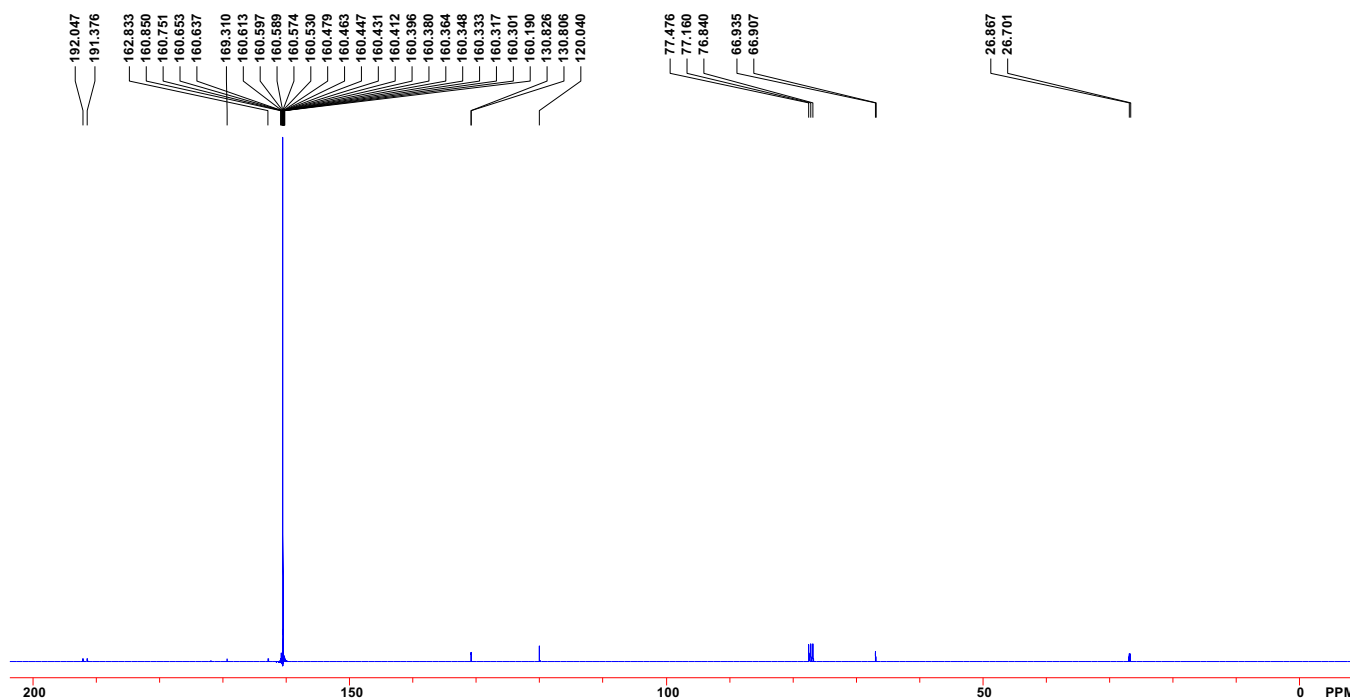


Figure S25. ^{13}C NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

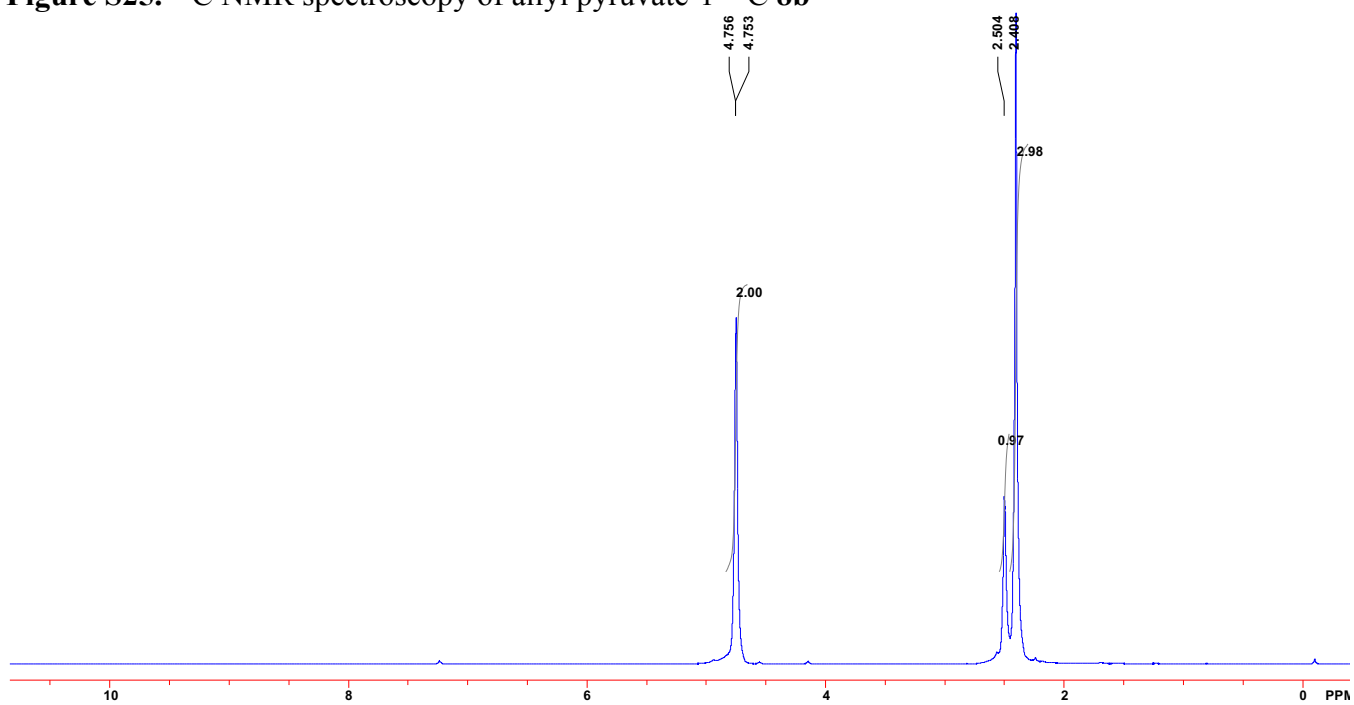


Figure S26. ^1H NMR spectroscopy of propargyl pyruvate-1- ^{13}C

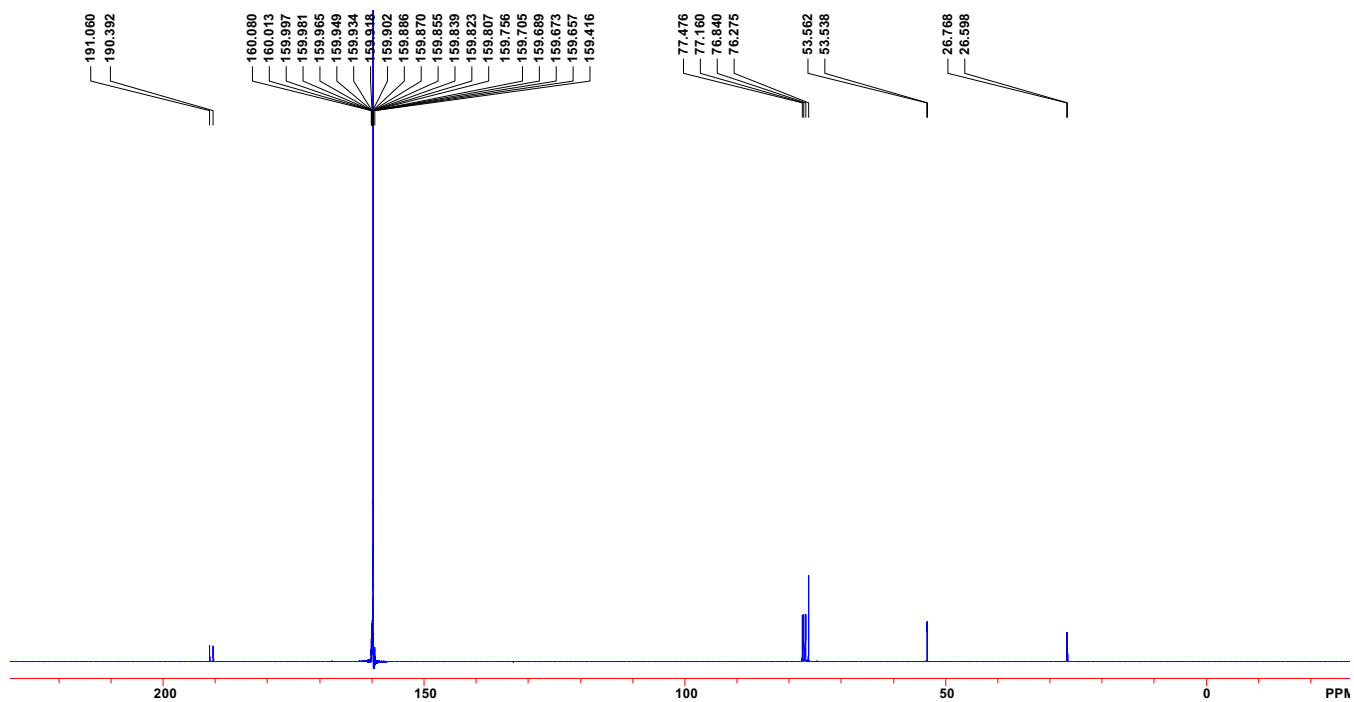


Figure S27. ^{13}C NMR spectroscopy of propargyl pyruvate-1- ^{13}C **9b**

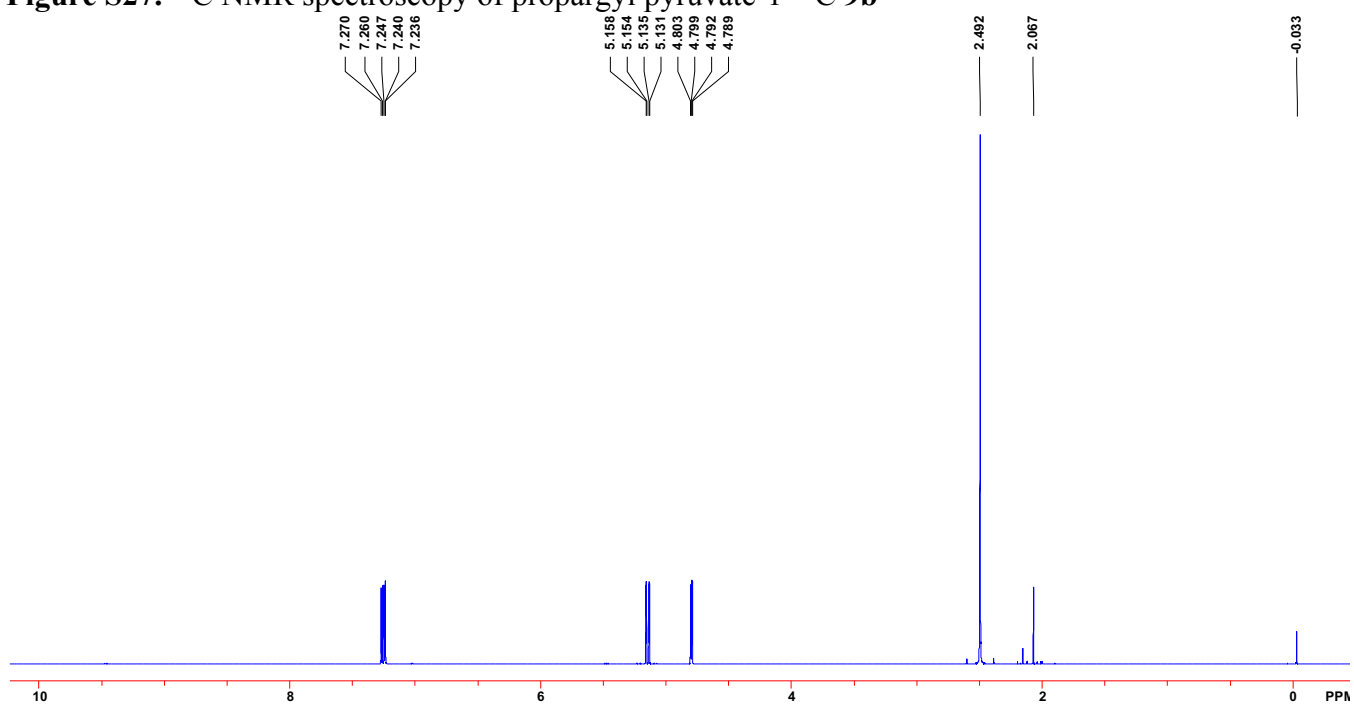


Figure S28. ^1H NMR spectroscopy of vinyl pyruvate **10a**

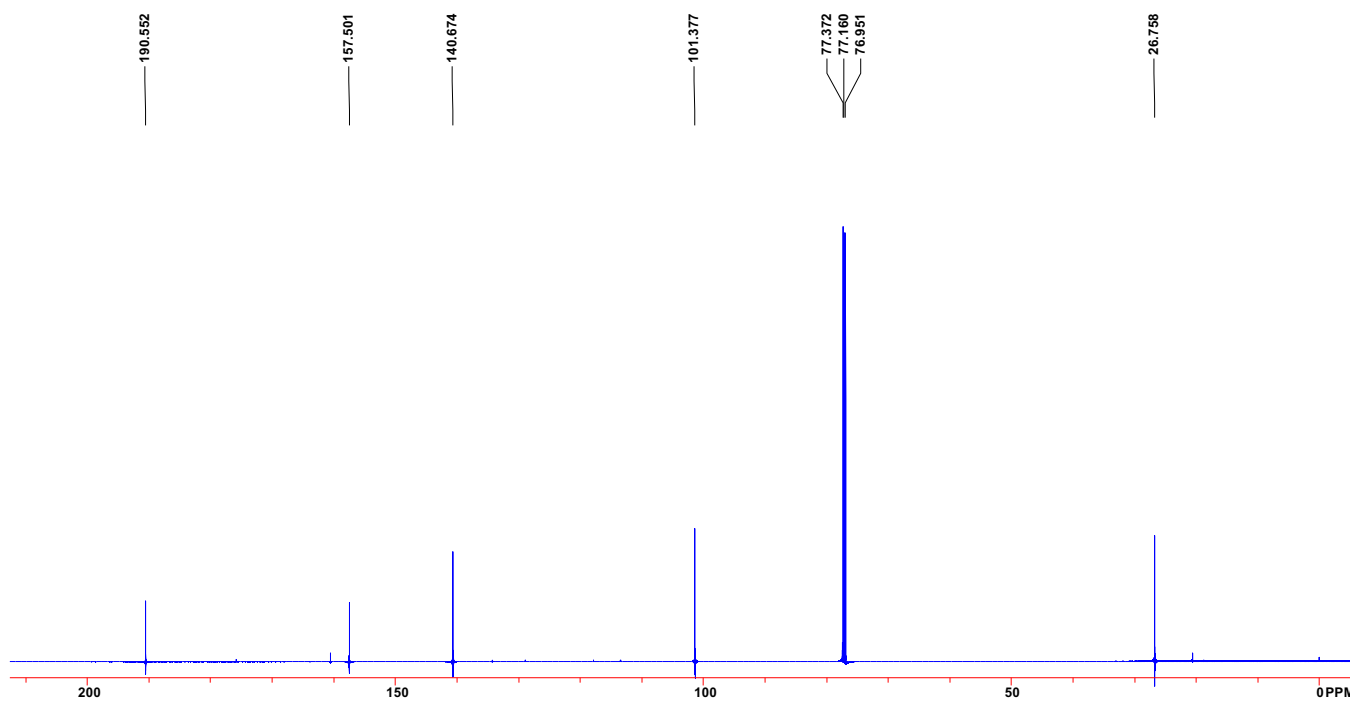


Figure S29. ¹³C NMR spectroscopy of vinyl pyruvate **10a**

2. Additional Figures (S30-S39): ^1H NMR and ^{13}C NMR spectra of pyruvates in CD_3OD .

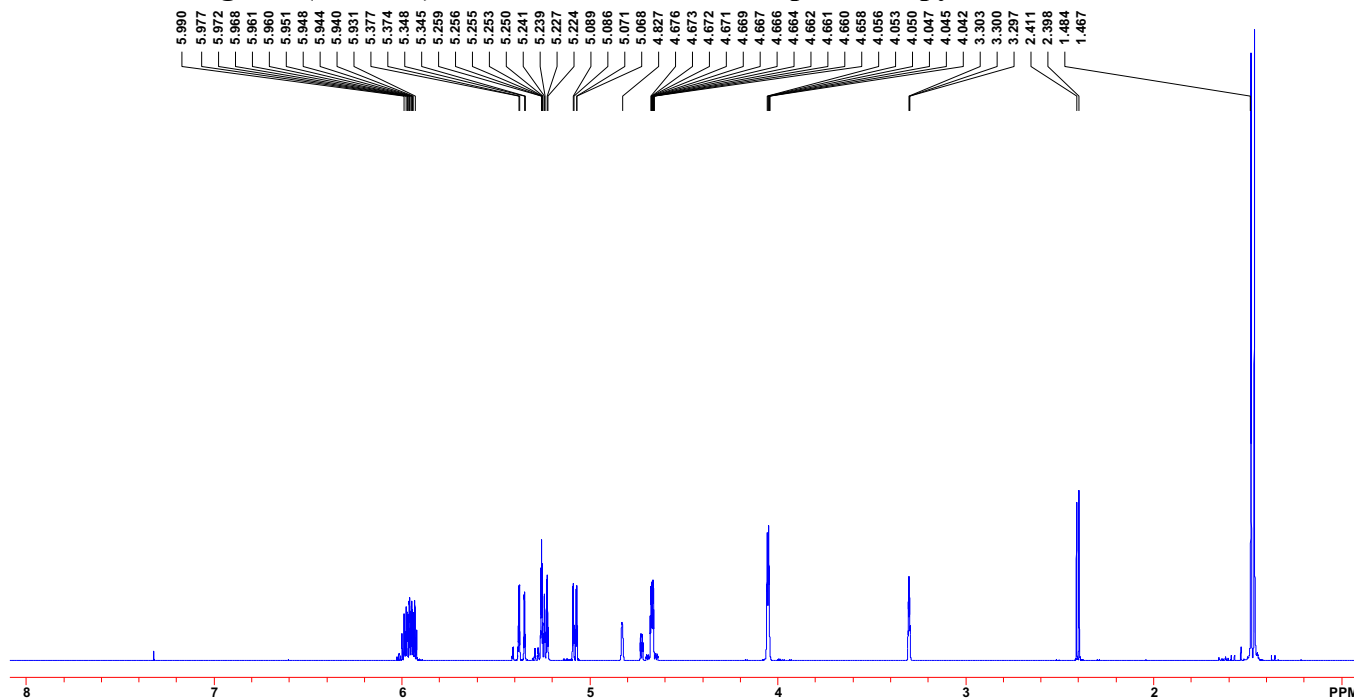


Figure S30. ^1H NMR spectroscopy of allyl pyruvate **8a**

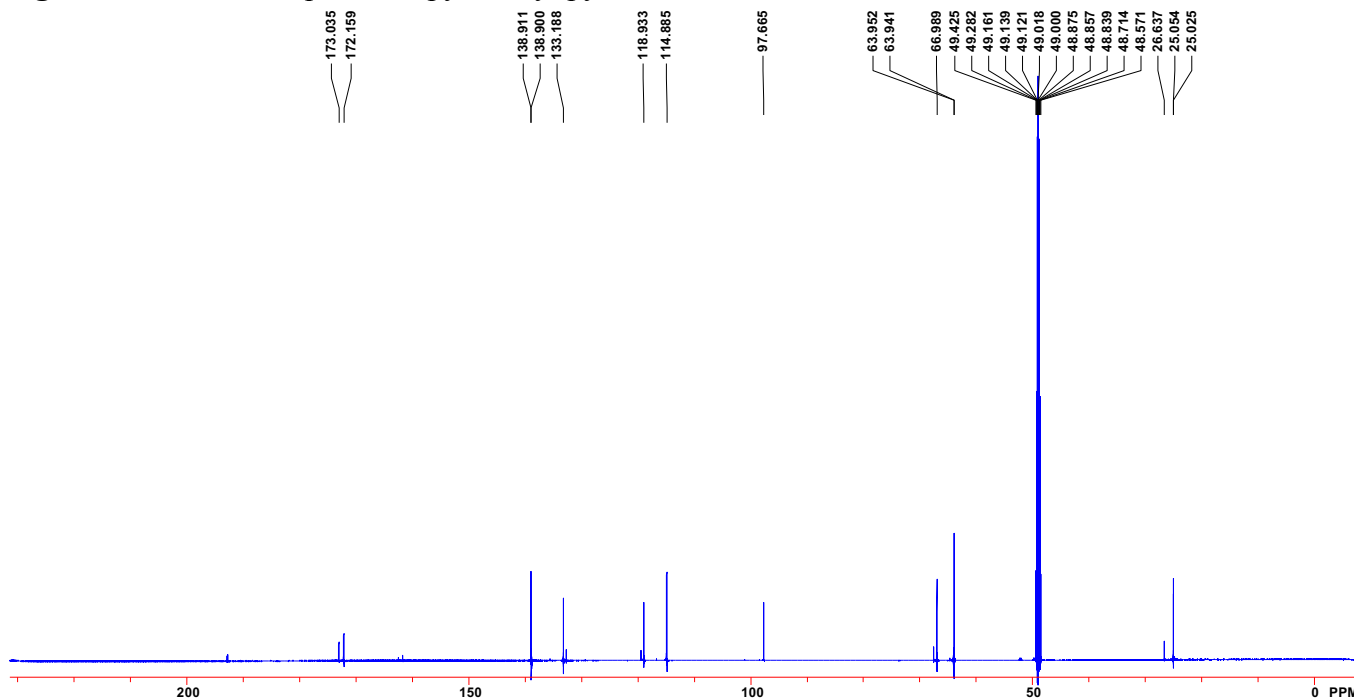


Figure S31. ^{13}C NMR spectroscopy of allyl pyruvate **8a**

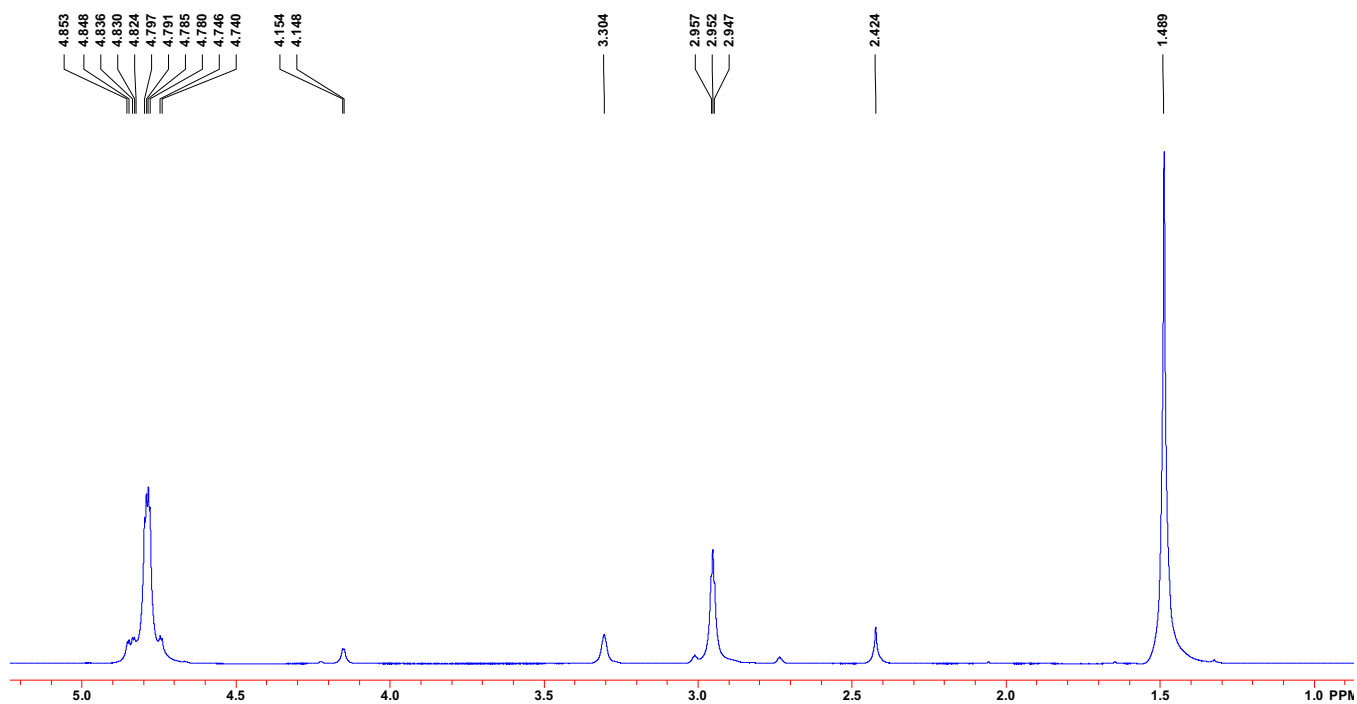


Figure S32. ^1H NMR spectroscopy of propargyl pyruvate **9a**

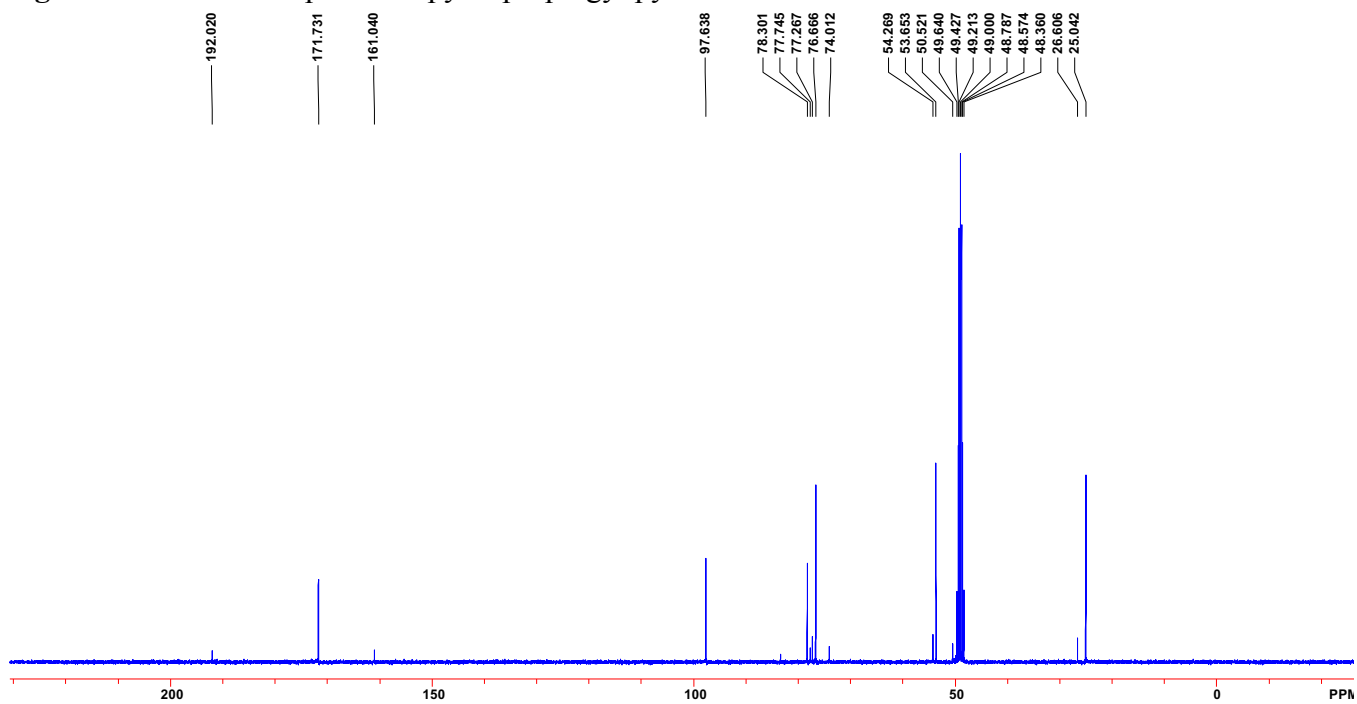


Figure S33. ^{13}C NMR spectroscopy of propargyl pyruvate **9a**

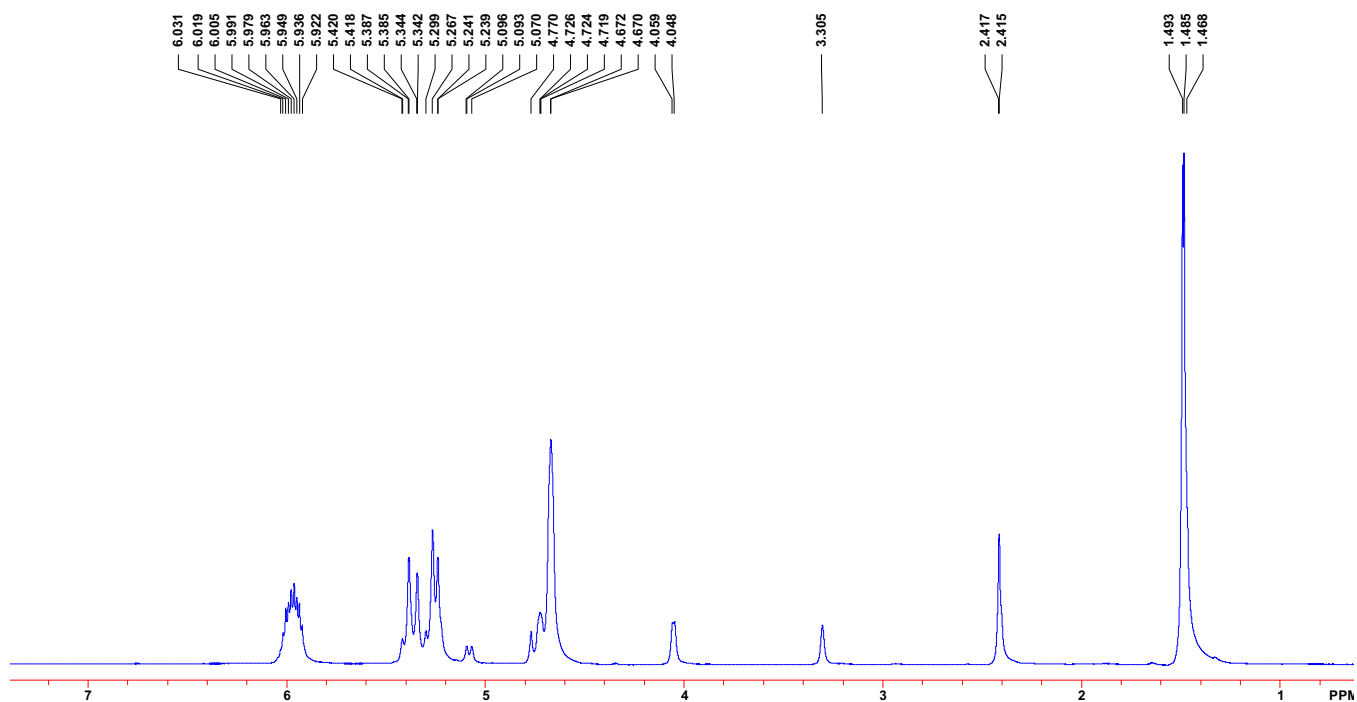


Figure S34. ^1H NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

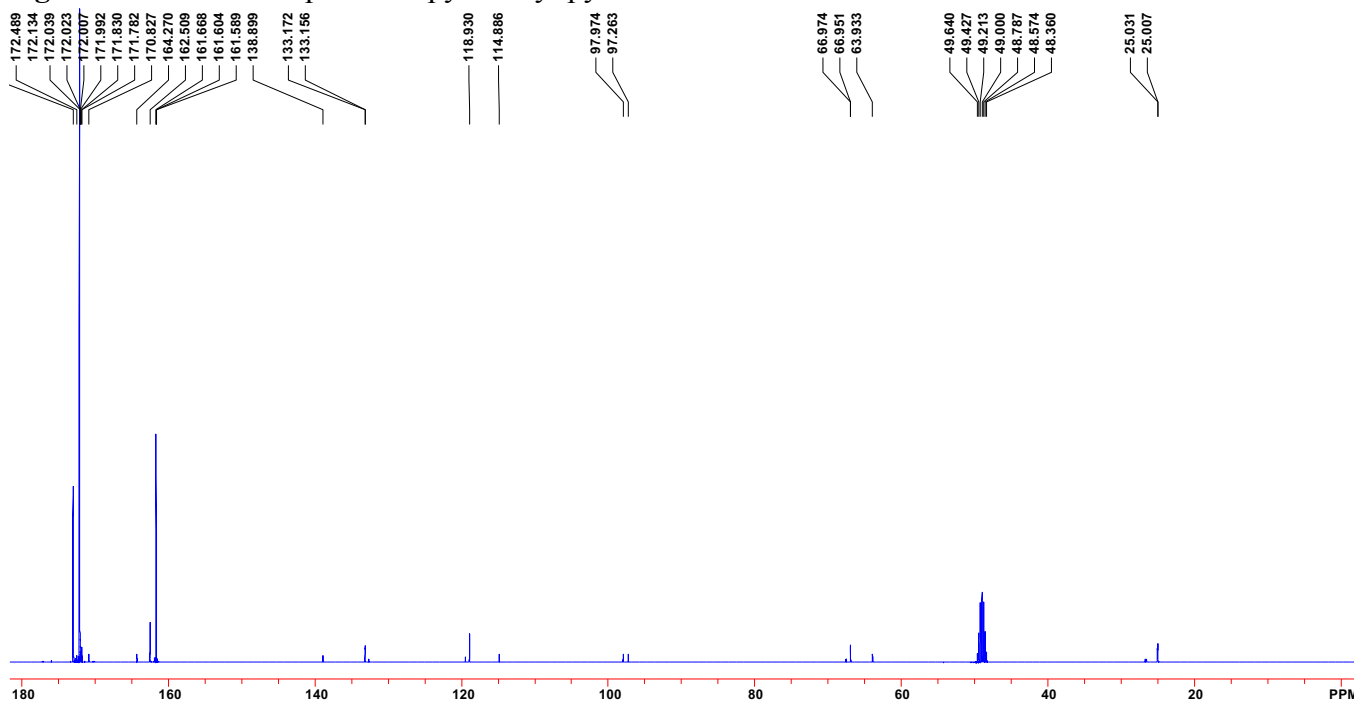


Figure S35. ^{13}C NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

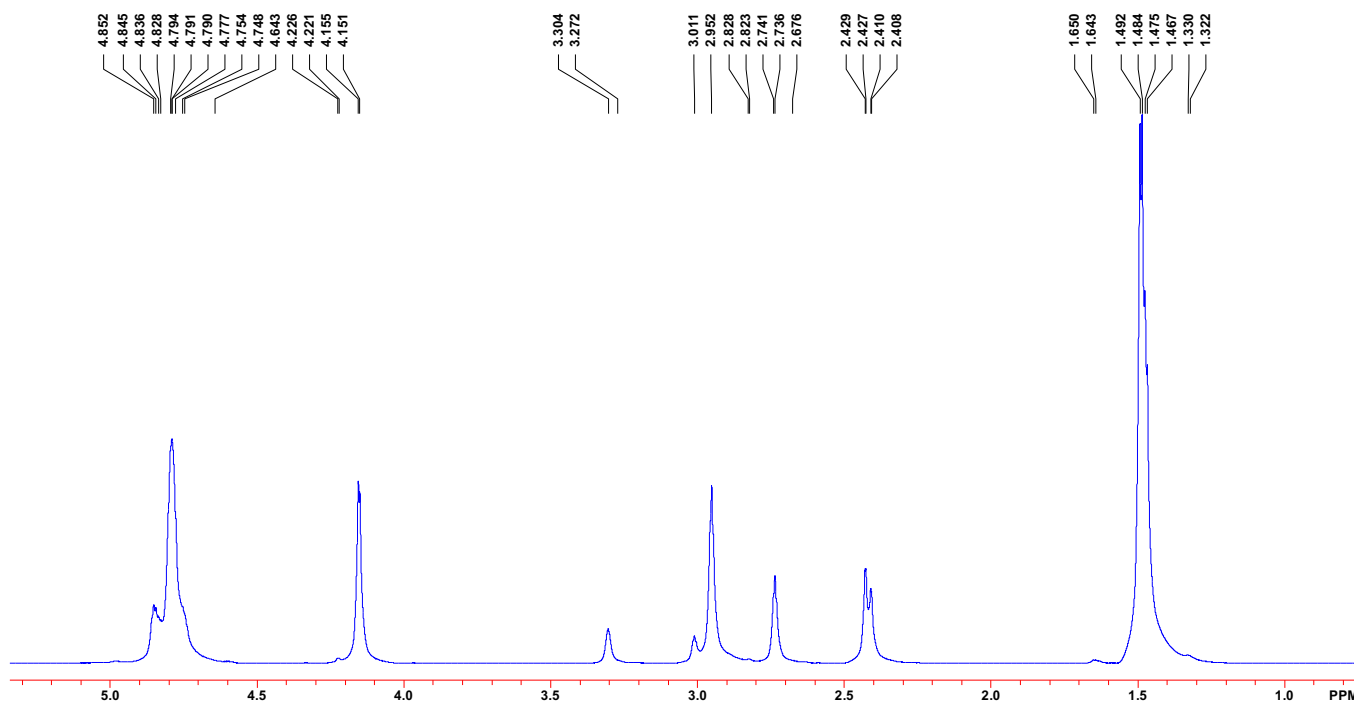


Figure S36. ^1H NMR spectroscopy of propargyl pyruvate-1- ^{13}C **9b**

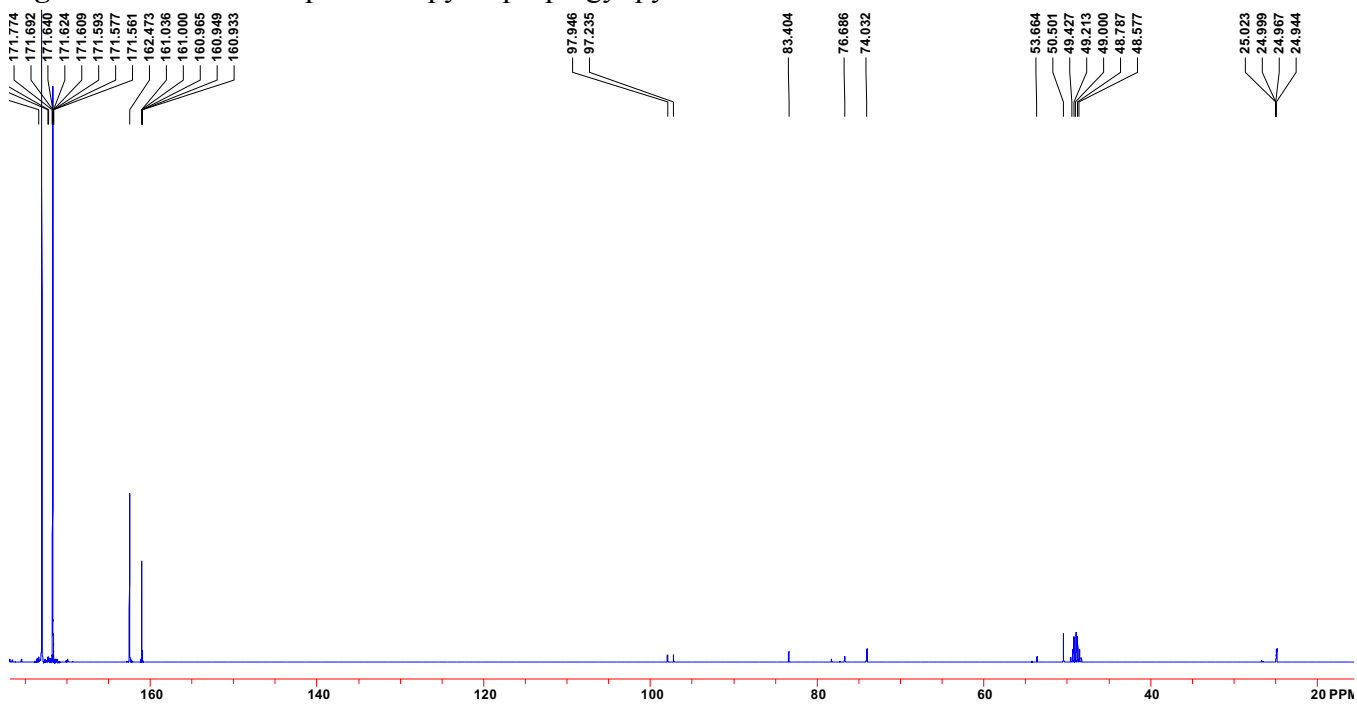


Figure S37. ^{13}C NMR spectroscopy of propargyl pyruvate-1- ^{13}C **9b**

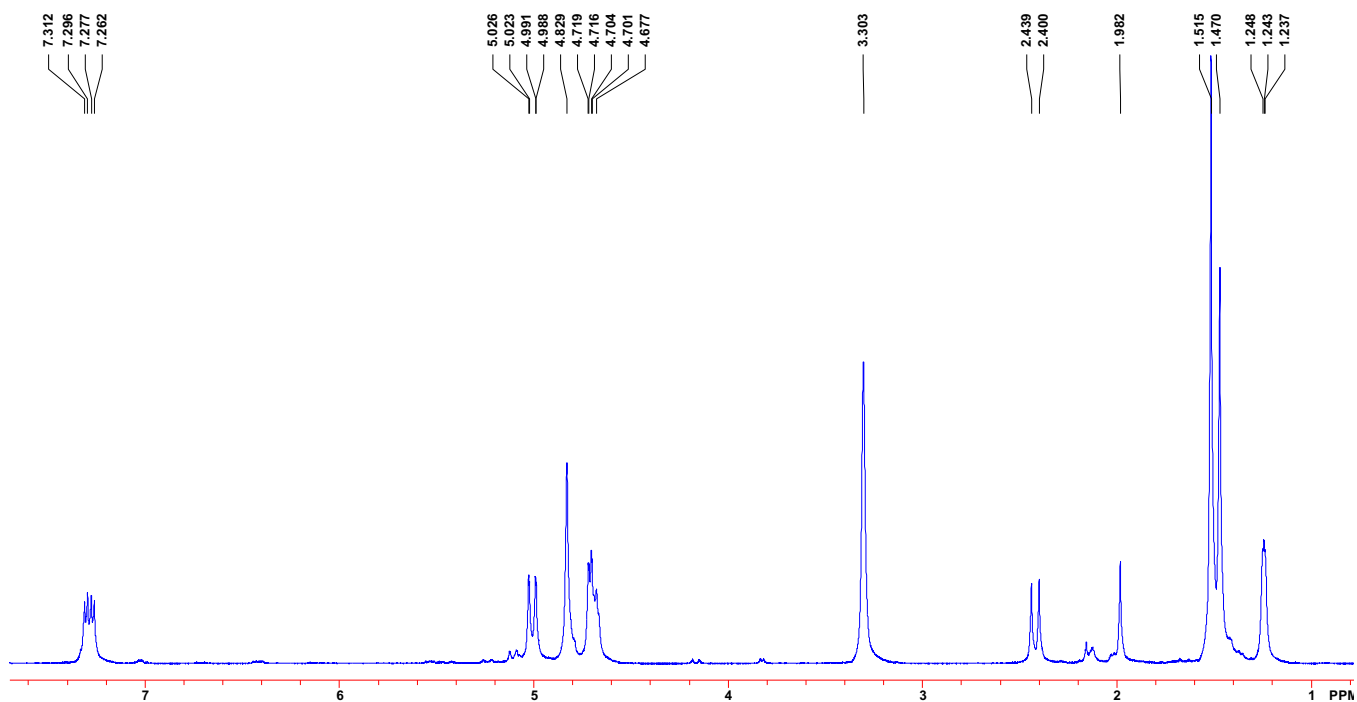


Figure S38. ^1H NMR spectroscopy of vinyl pyruvate **10a**

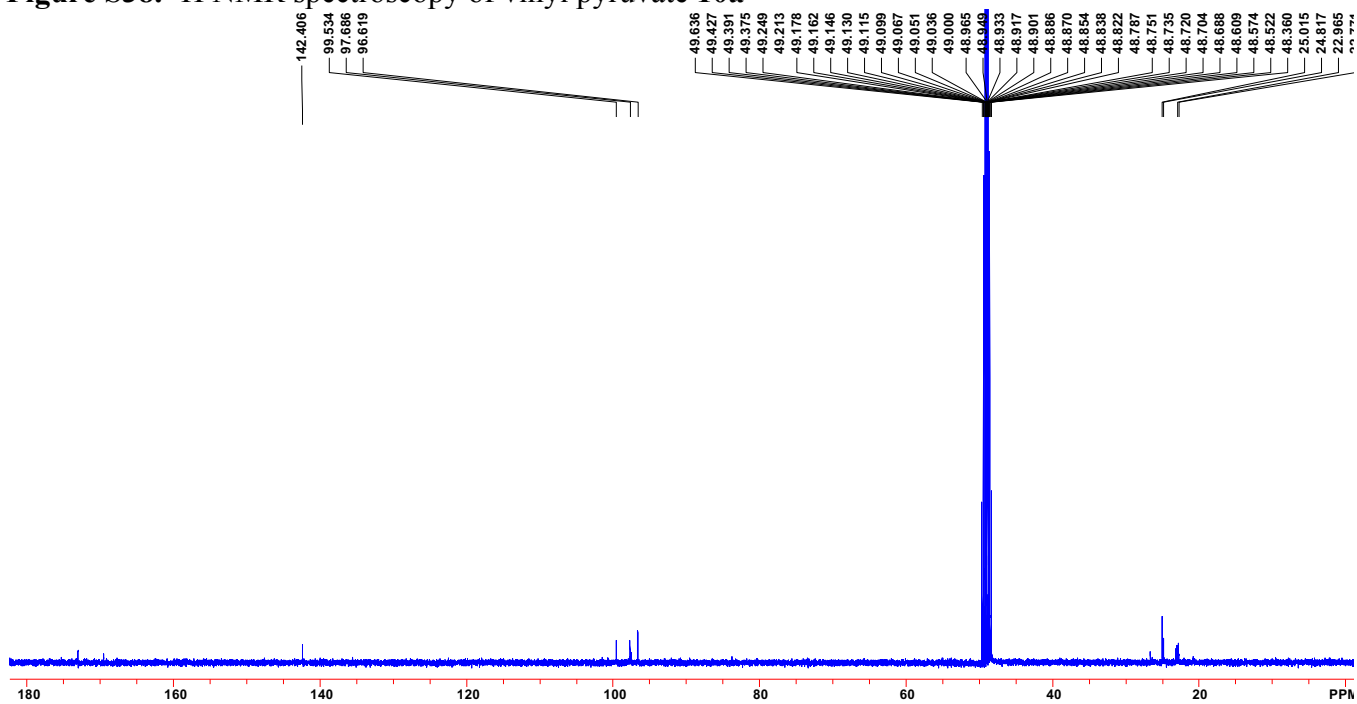


Figure S39. ^{13}C NMR spectroscopy of vinyl pyruvate **10a**

3. Additional Figures (S40-S57): ^1H NMR and ^{13}C NMR spectra of neat acetates and pyruvates.

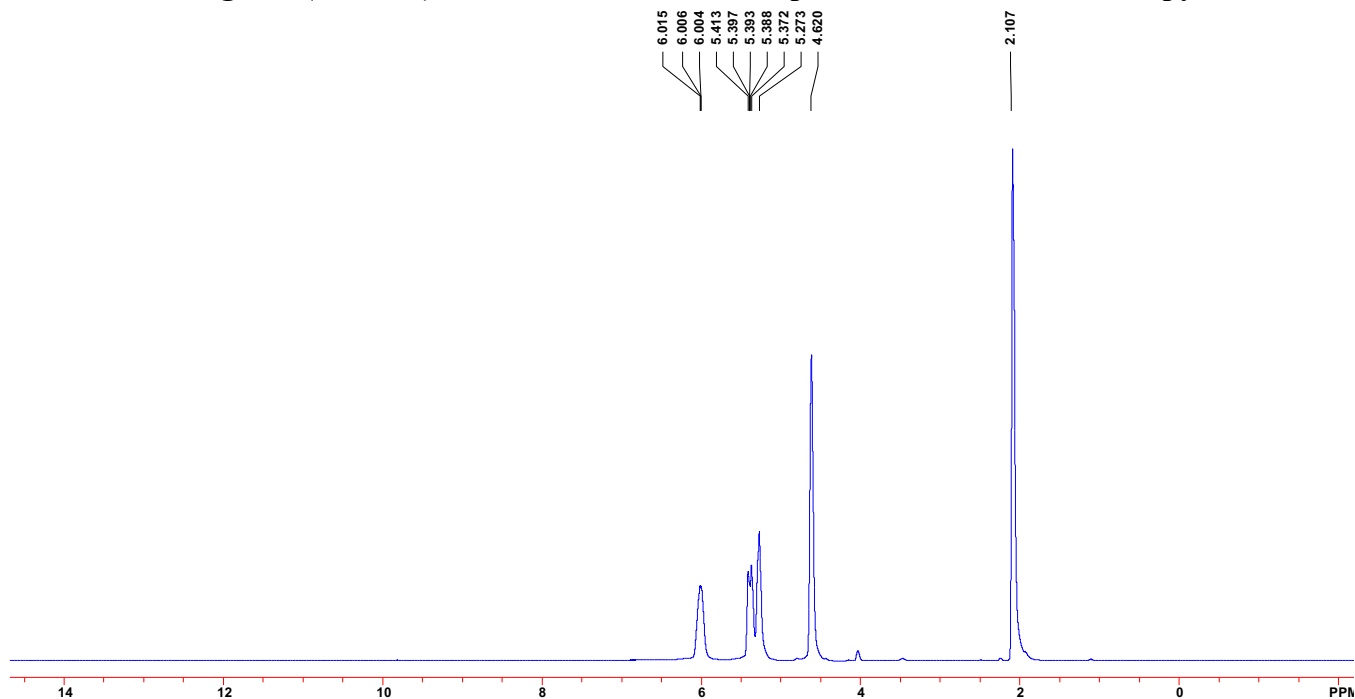


Figure S40. ^1H NMR spectroscopy of allyl acetate **5a**

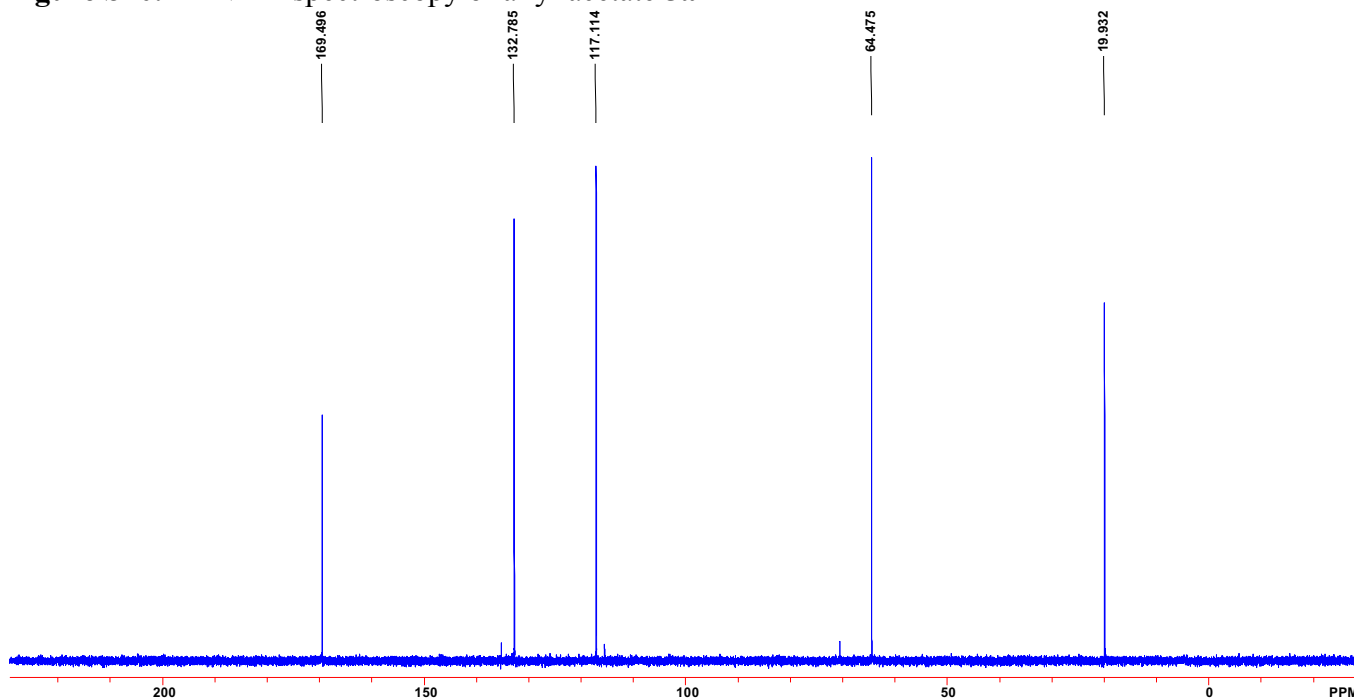


Figure S41. ^{13}C NMR spectroscopy of allyl acetate **5a**

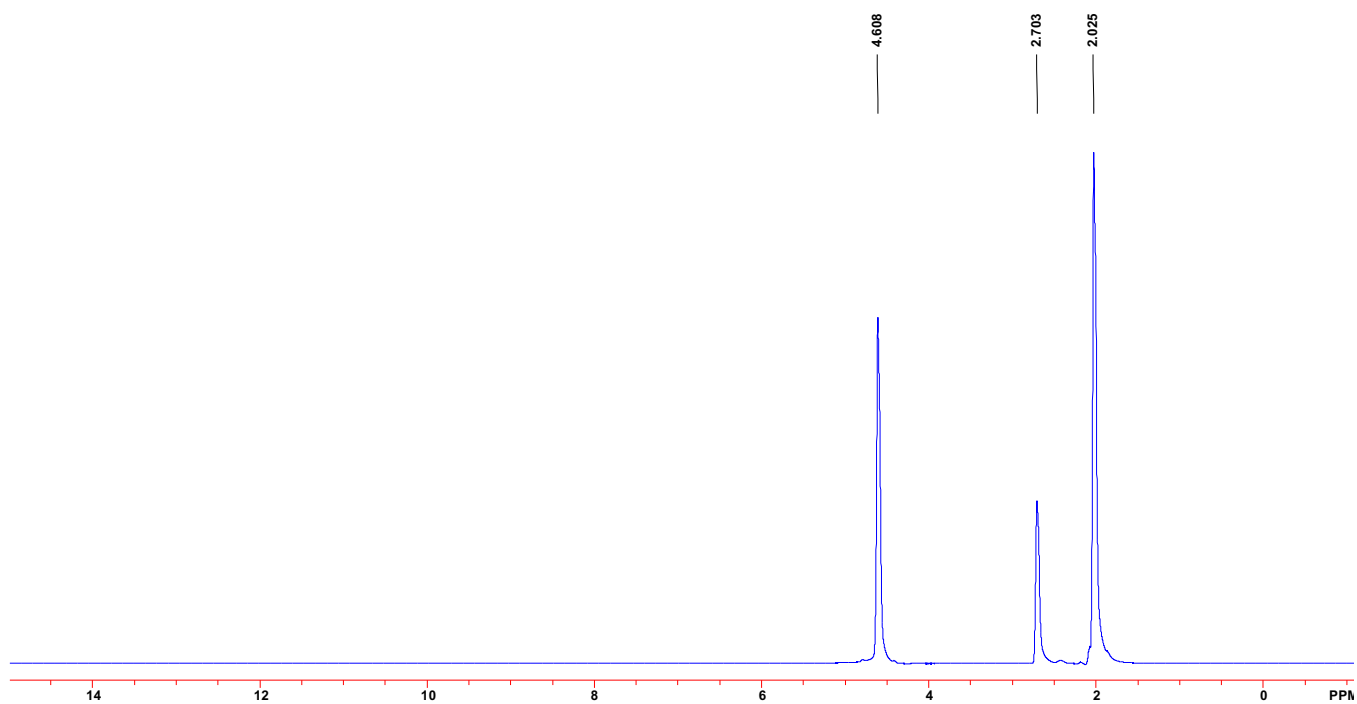


Figure S42. ¹H NMR spectroscopy of propargyl acetate **6a**

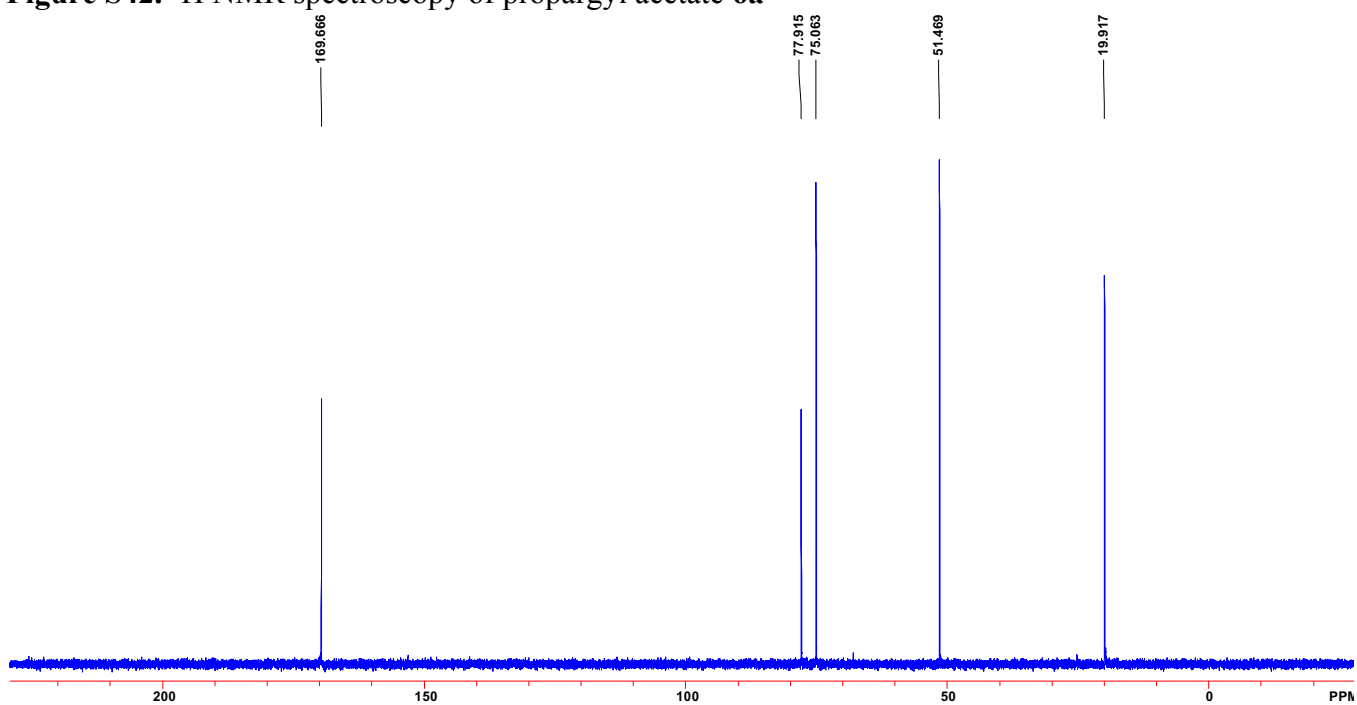


Figure S43. ¹³C NMR spectroscopy of propargyl acetate **6a**

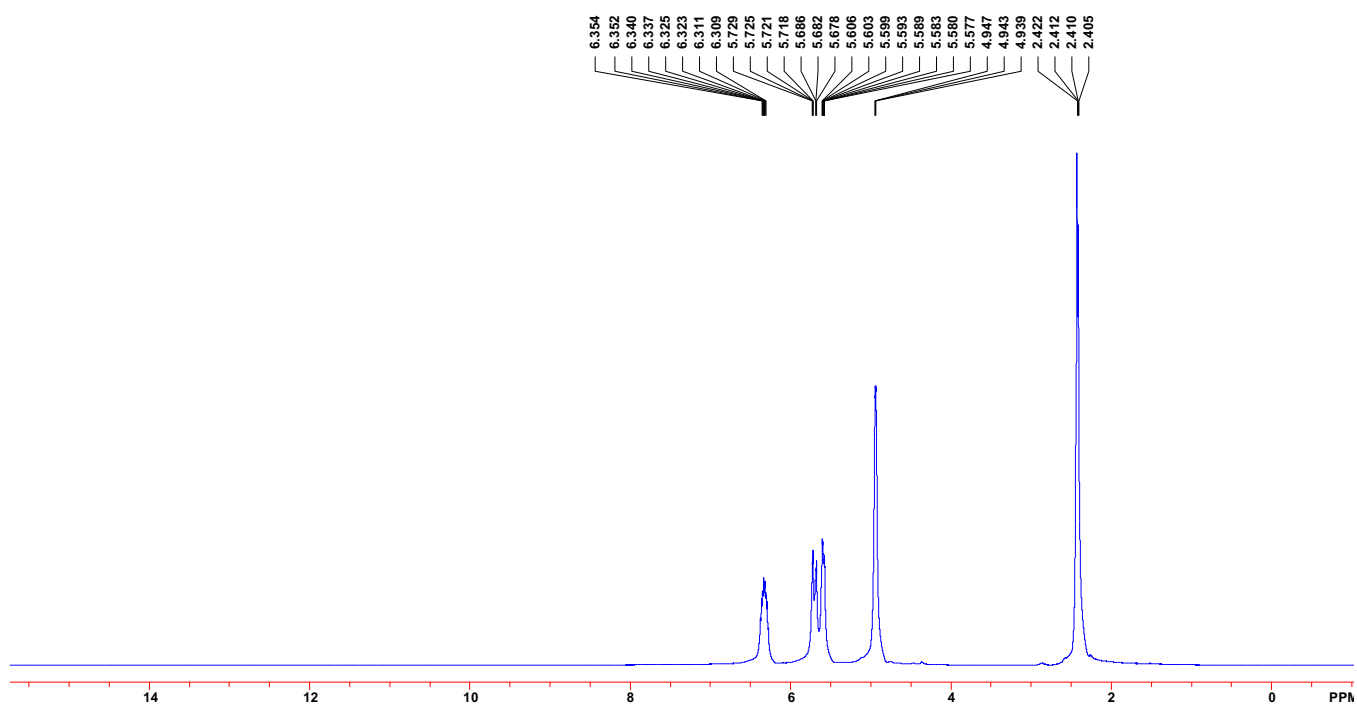


Figure S44. ^1H NMR spectroscopy of allyl acetate- $1\text{-}^{13}\text{C}$ **5b**

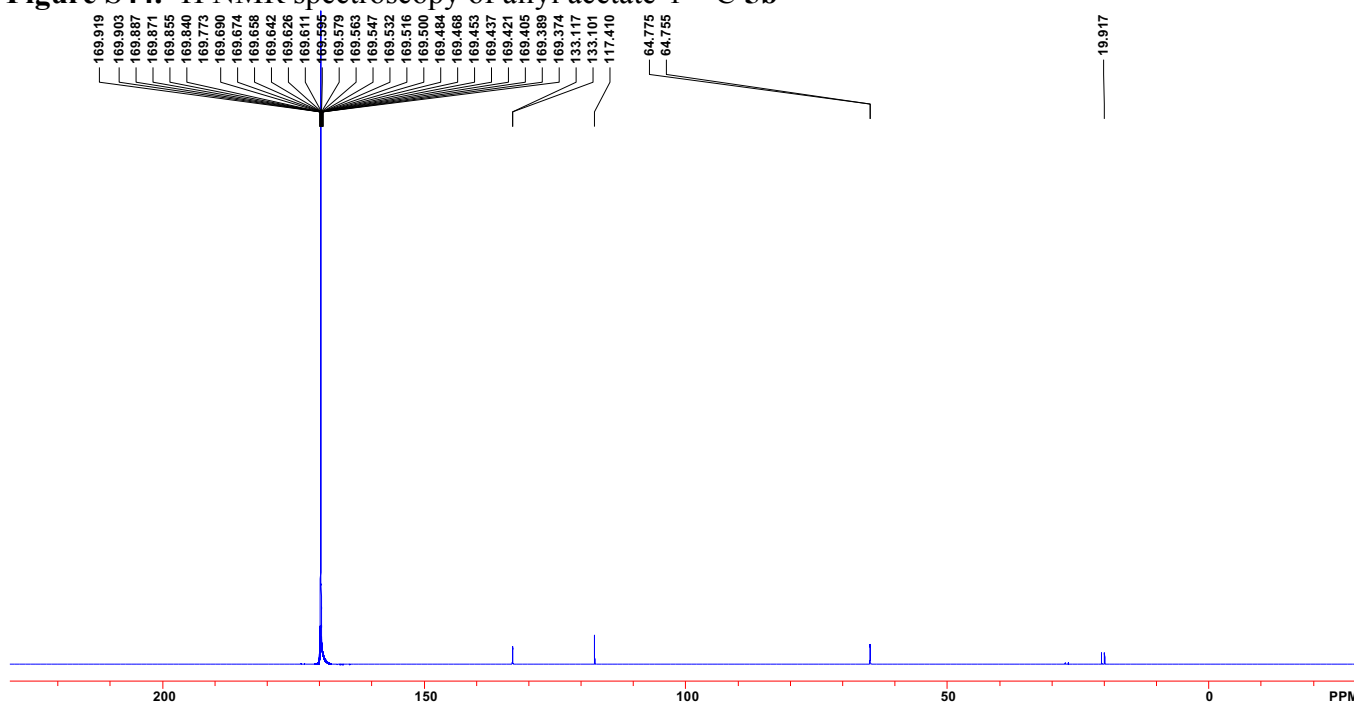


Figure S45. ^{13}C NMR spectroscopy of allyl acetate- $1\text{-}^{13}\text{C}$ **5b**

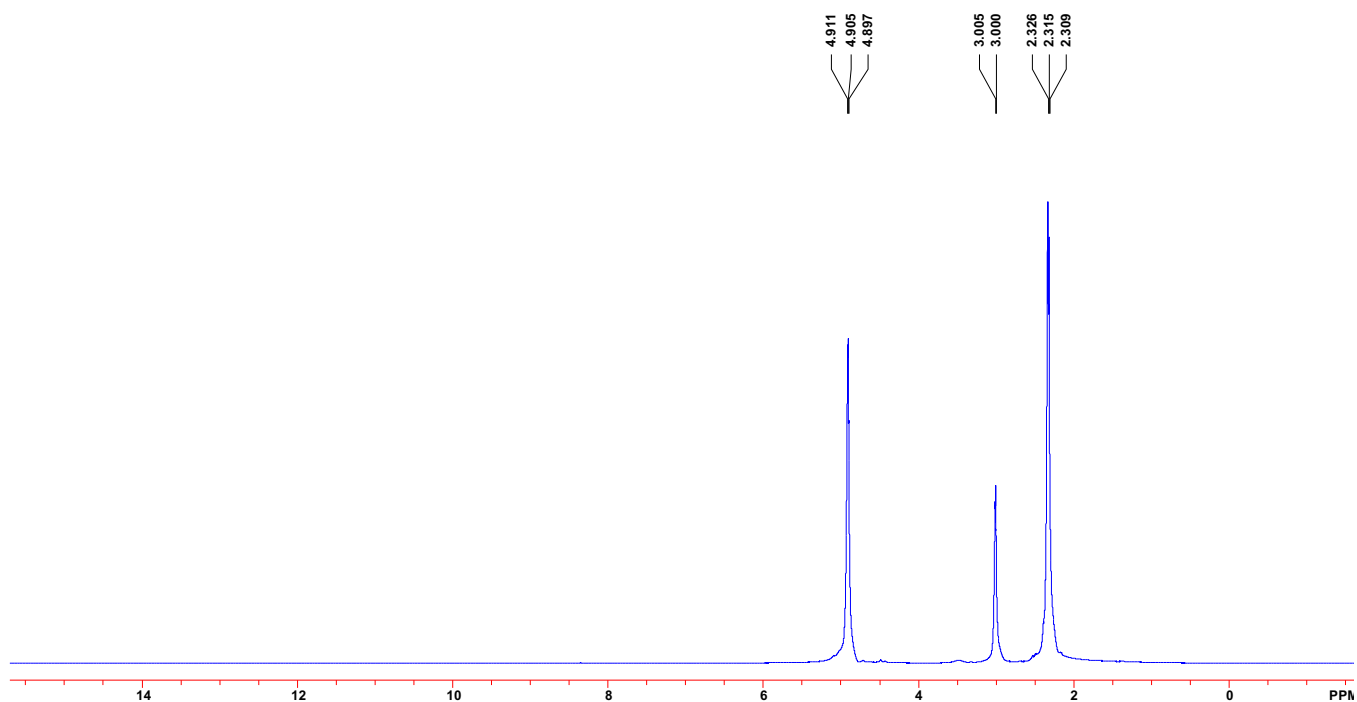


Figure S46. ¹H NMR spectroscopy of propargyl acetate-1-¹³C **6b**

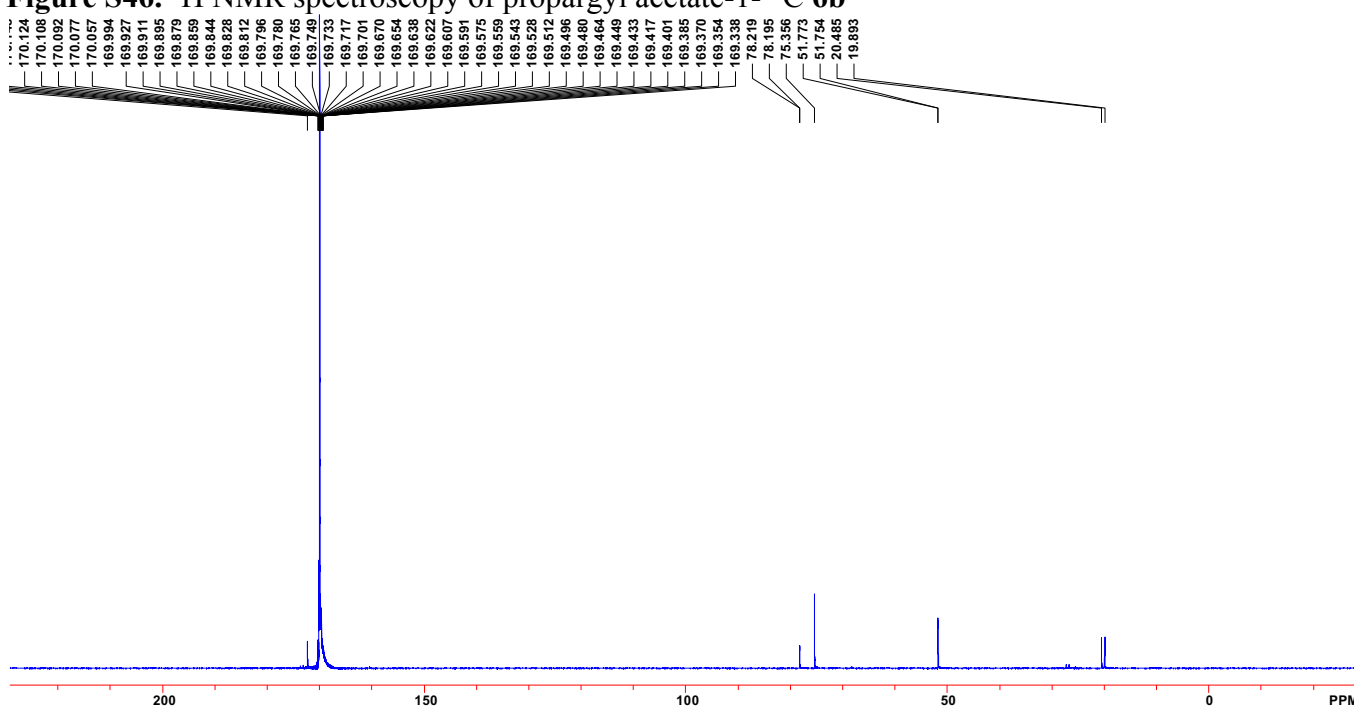


Figure S47. ¹³C NMR spectroscopy of propargyl acetate-1-¹³C **6b**

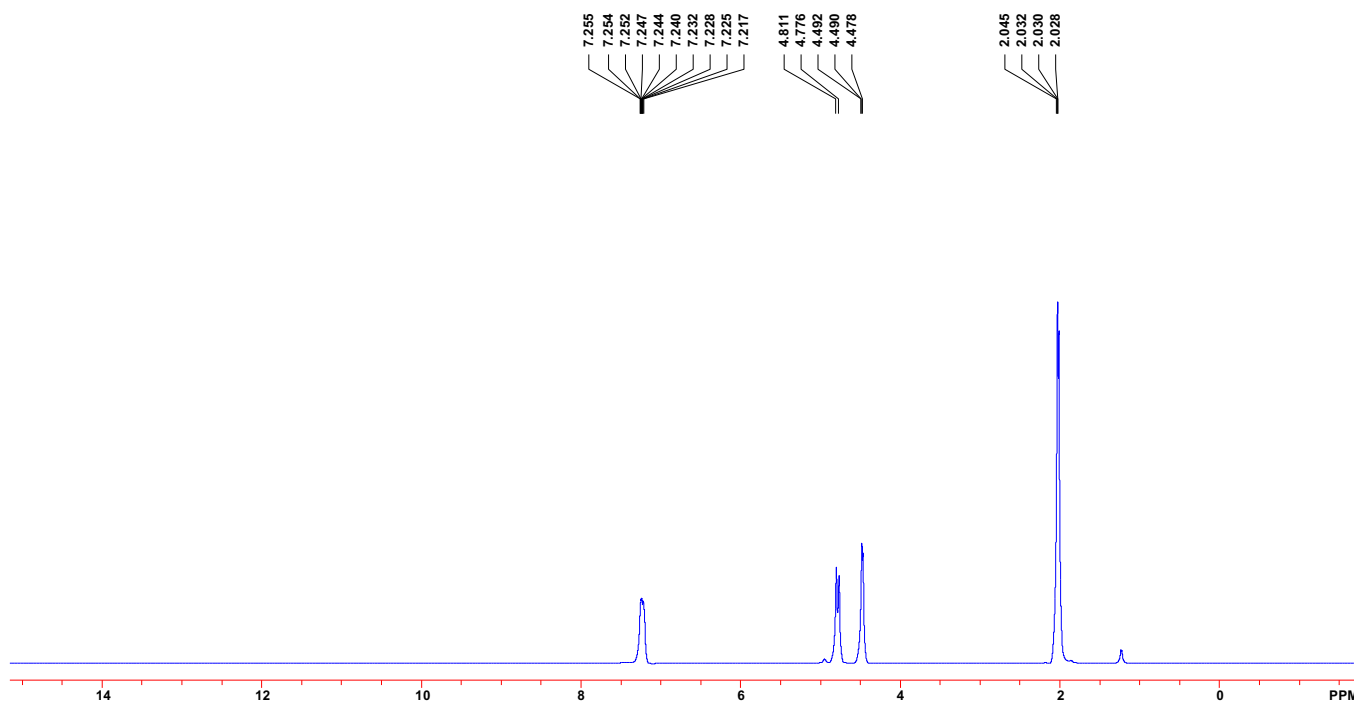


Figure S48. ^1H NMR spectroscopy of vinyl acetate-1- ^{13}C **7b**

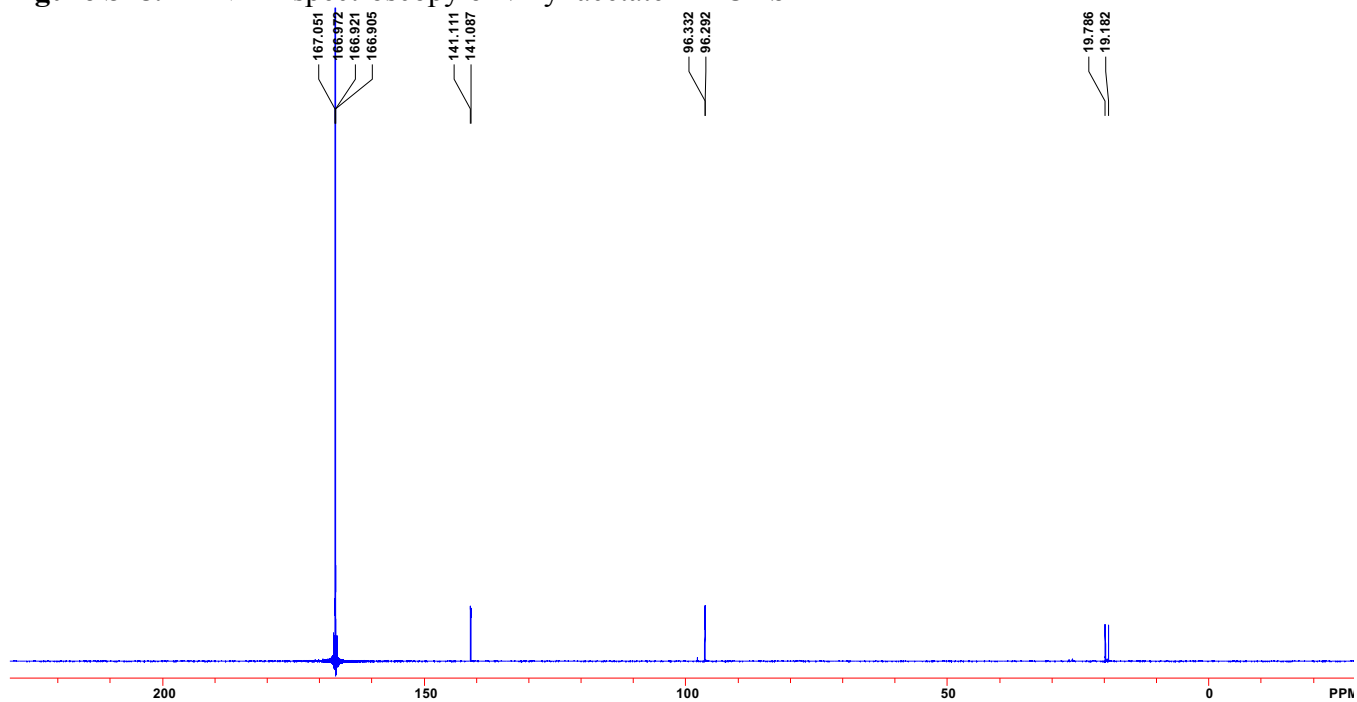


Figure S49. ^{13}C NMR spectroscopy of vinyl acetate-1- ^{13}C **7b**

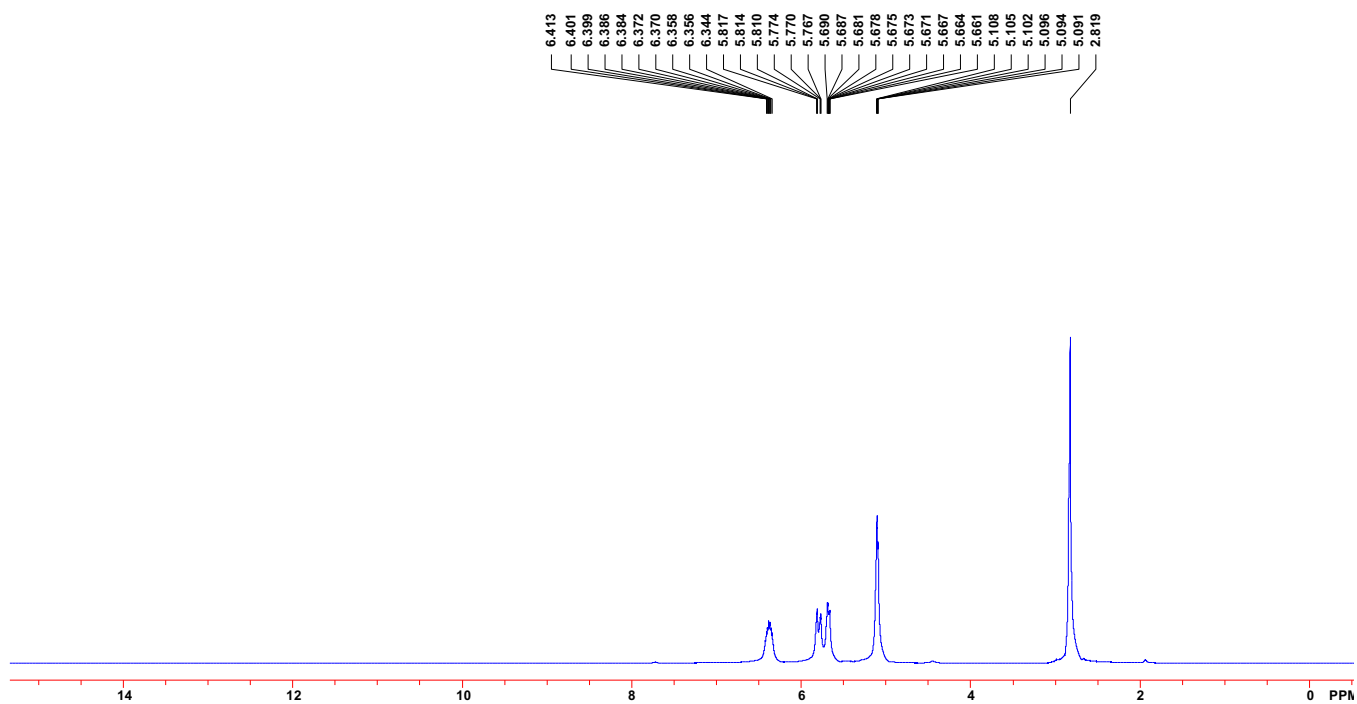


Figure S50. ^1H NMR spectroscopy of allyl pyruvate **8a**

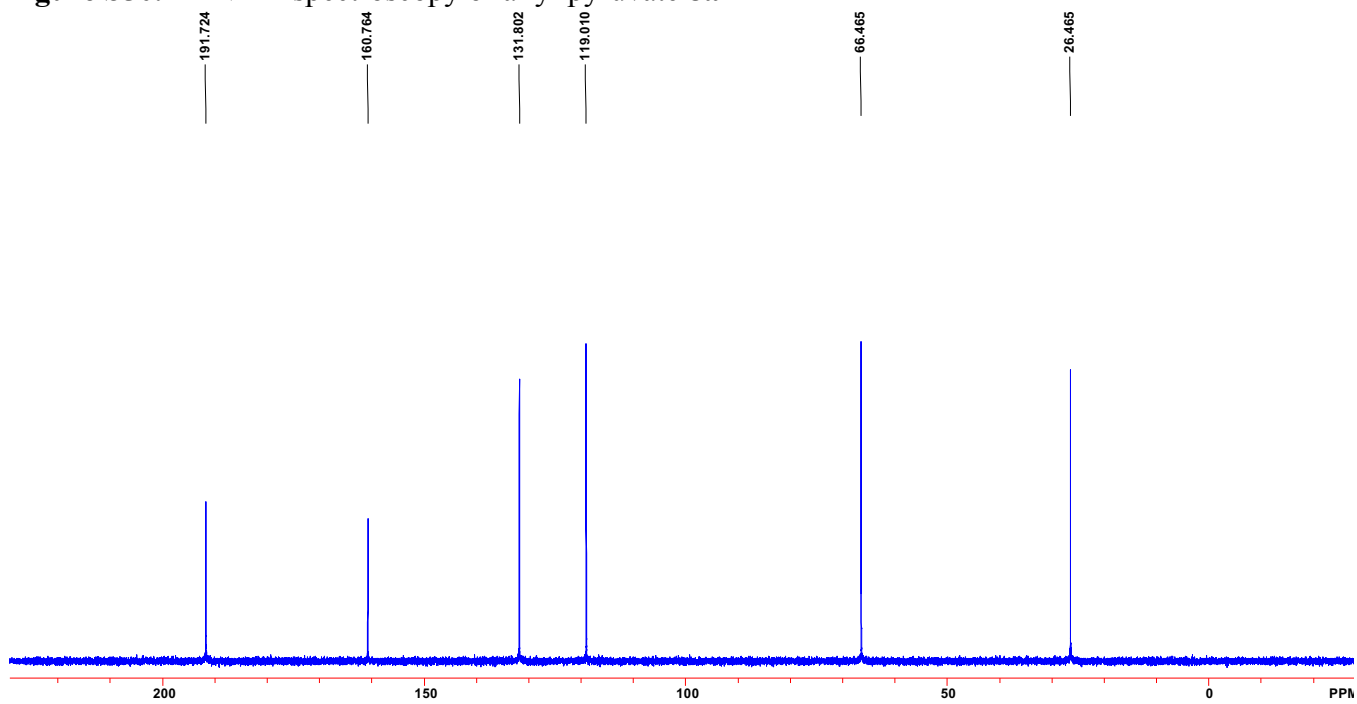


Figure S51. ^{13}C NMR spectroscopy of allyl pyruvate **8a**

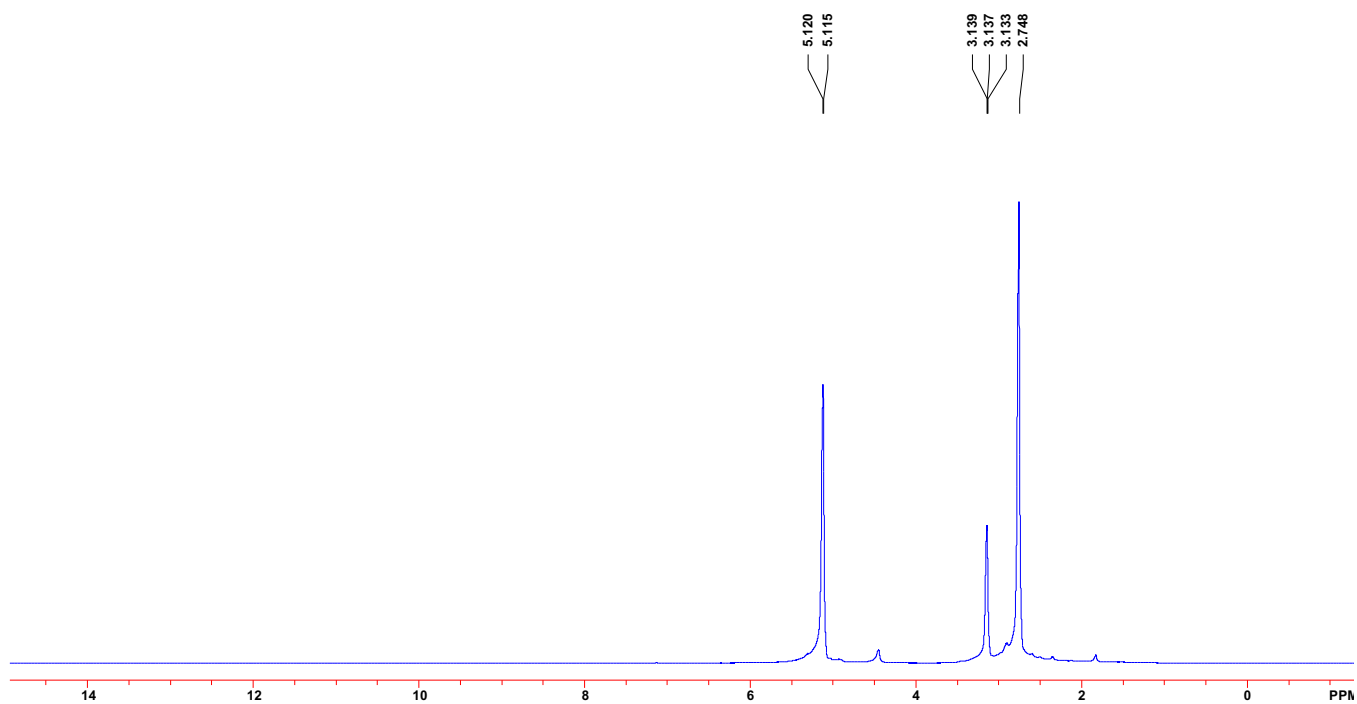


Figure S52. ¹H NMR spectroscopy of propargyl pyruvate **9a**

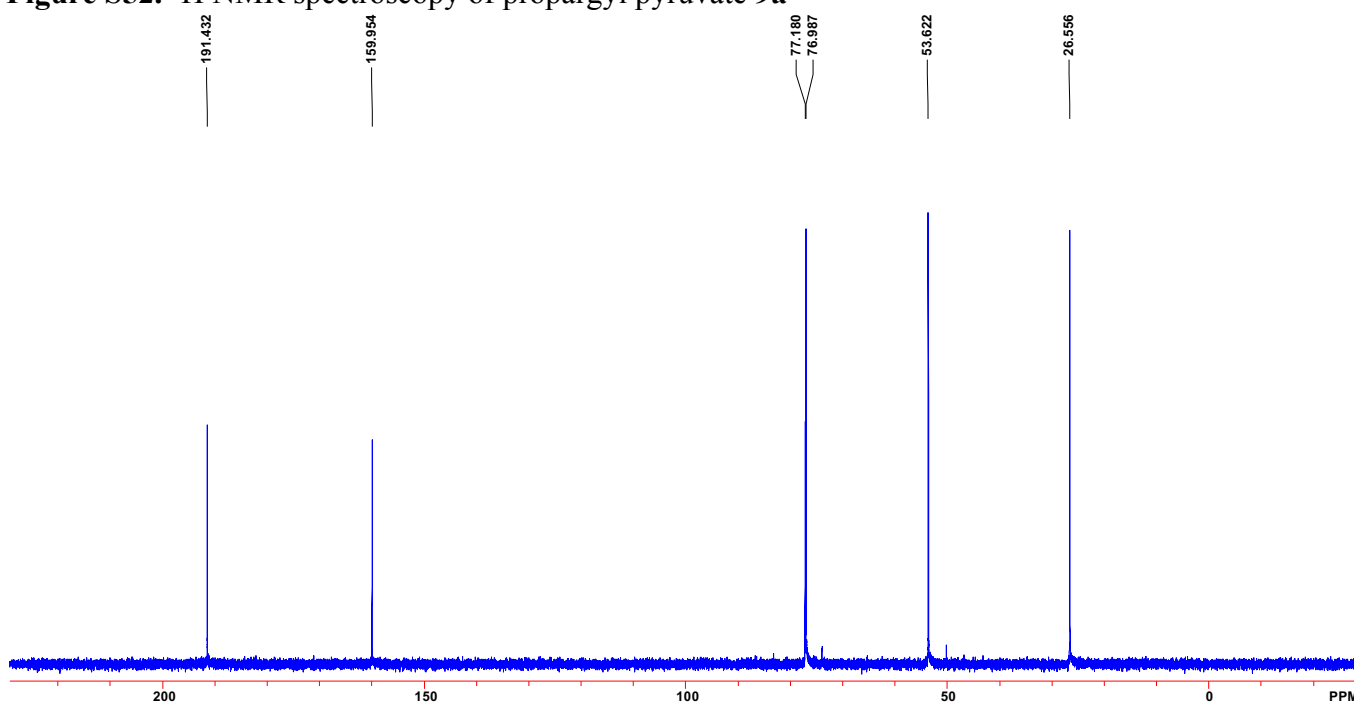


Figure S53. ¹³C NMR spectroscopy of propargyl pyruvate **9a**

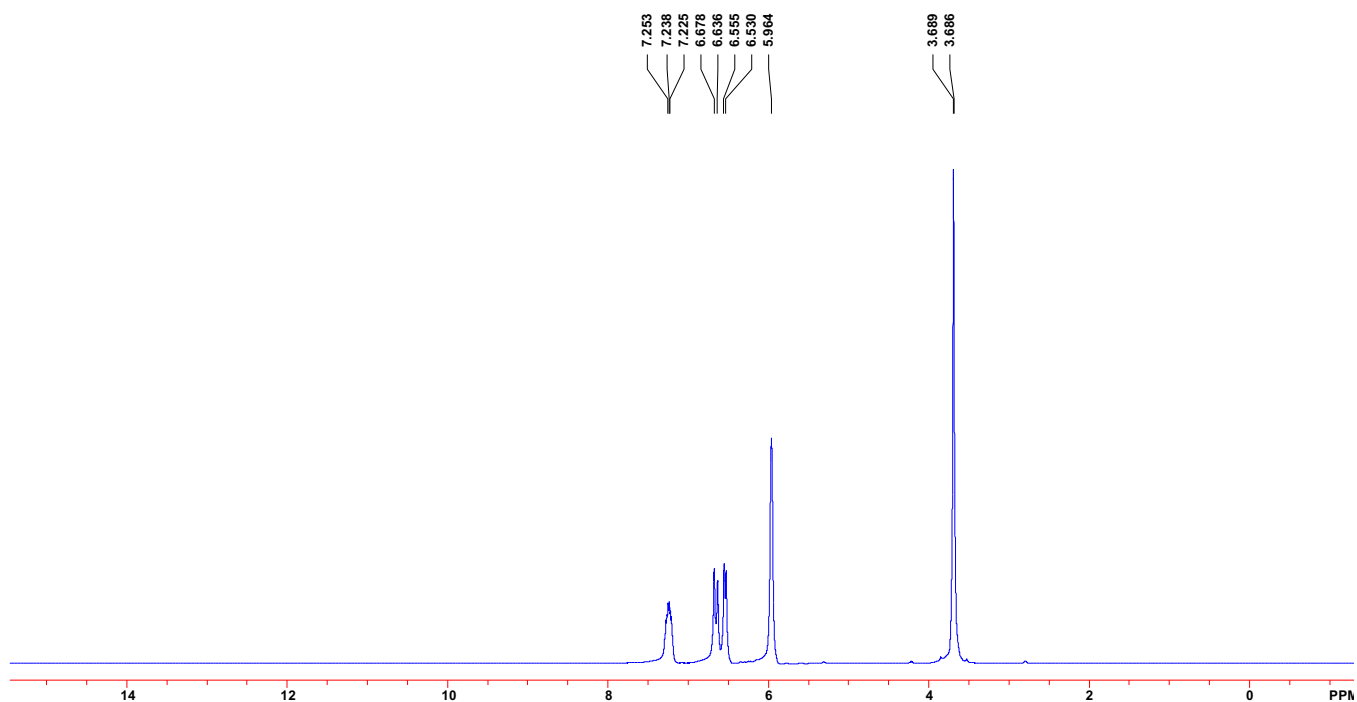


Figure S54. ^1H NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

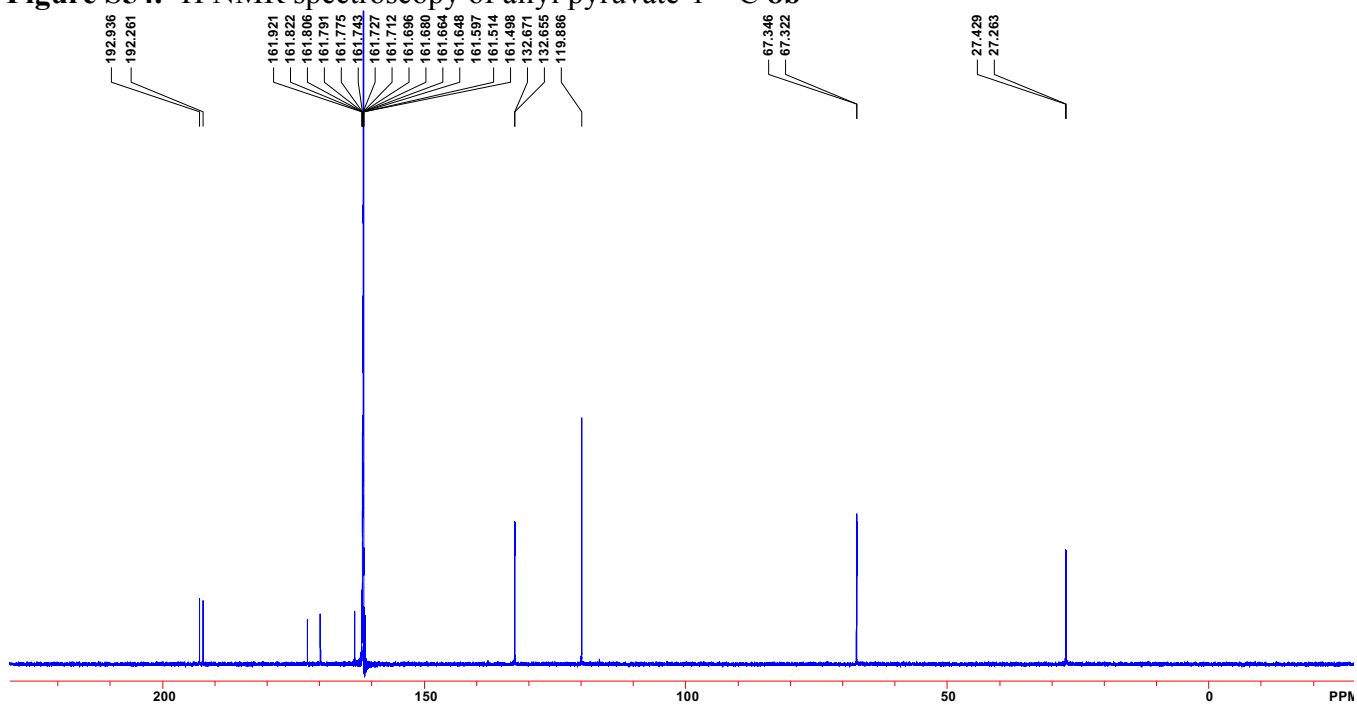


Figure S55. ^{13}C NMR spectroscopy of allyl pyruvate-1- ^{13}C **8b**

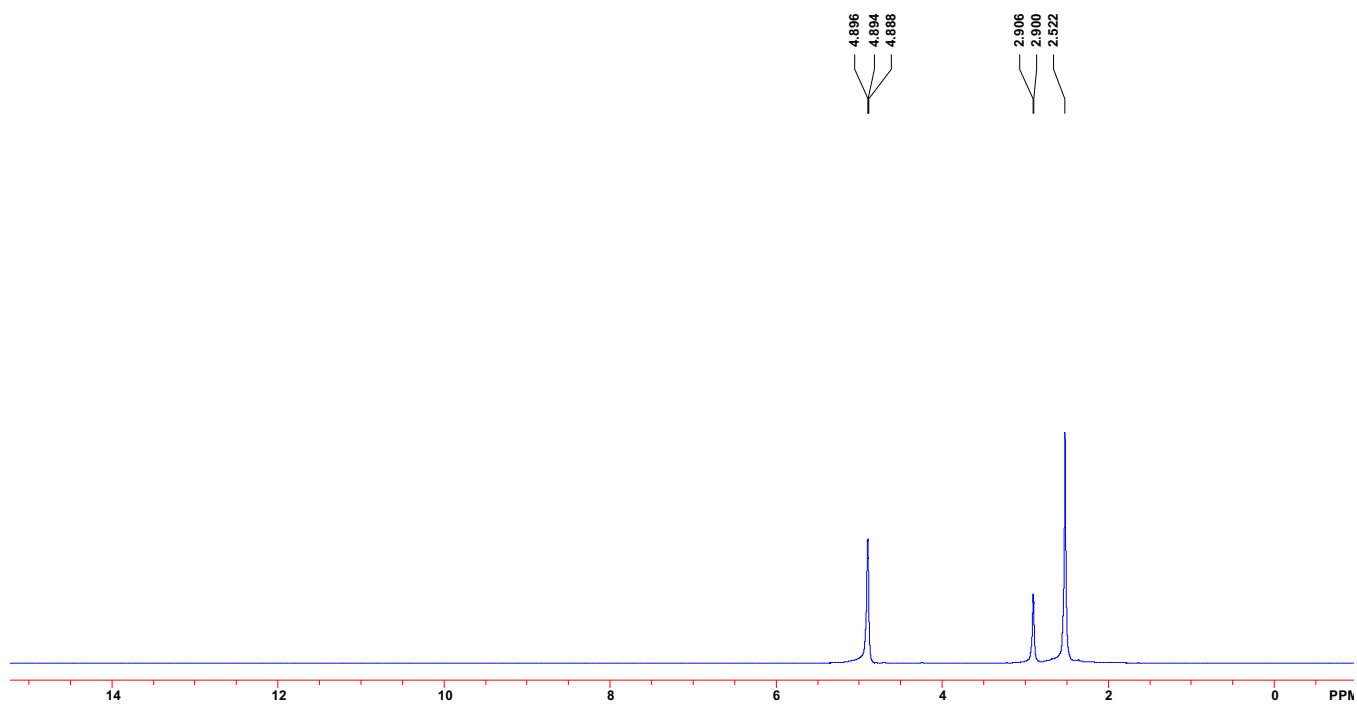


Figure S56. ¹H NMR spectroscopy of propargyl pyruvate-1-¹³C **9b**

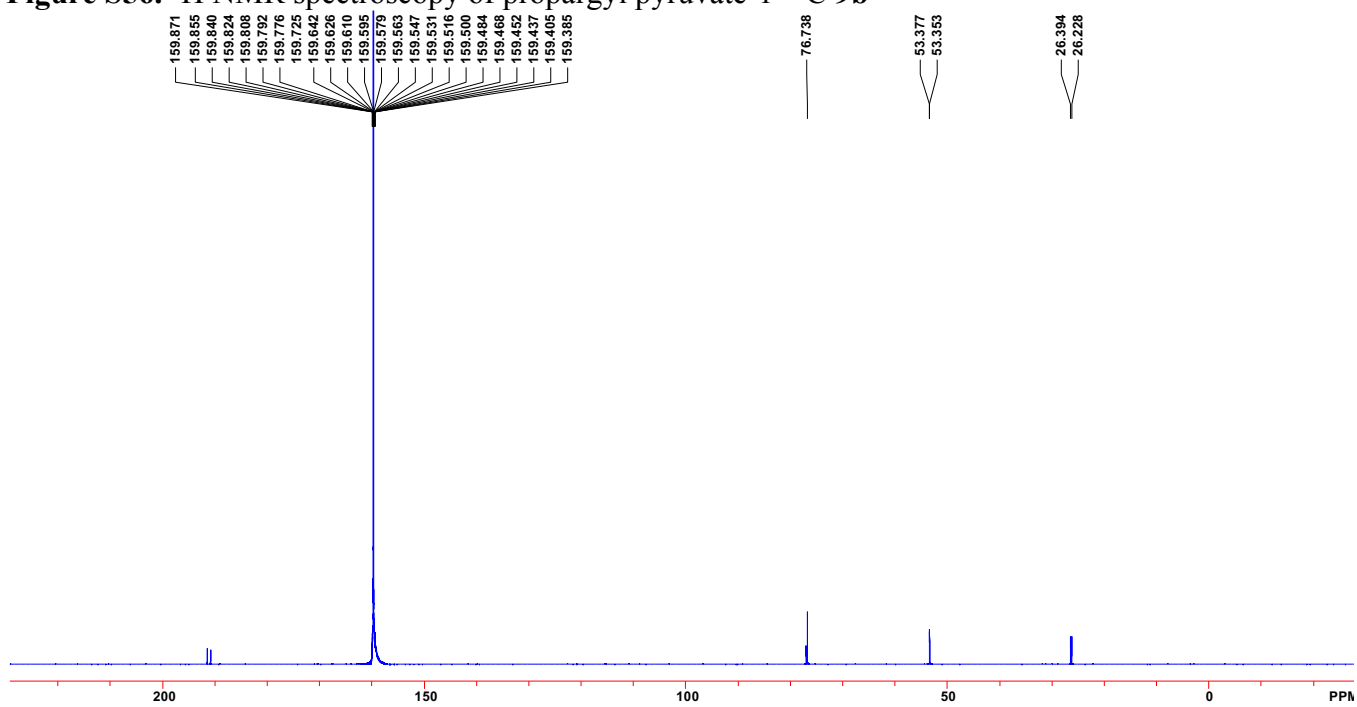


Figure S57. ¹³C NMR spectroscopy of propargyl pyruvate-1-¹³C **9b**