

Supplementary Information

Preparation, characterization and application of MgFe₂O₄/Cu nanocomposite as a new magnetic catalyst for one-pot regioselective synthesis of β -thiol-1,4-disubstituted-1,2,3-triazoles

Ronak Eisavi* and Kazhal Naseri

Department of Chemistry, Payame Noor University, PO BOX 19395-3697, Tehran, Iran

Email: roonak.isavi@gmail.com

FT-IR, ¹H NMR and ¹³C NMR spectra of β -Thiol-1,4-disubstituted-1,2,3-triazoles (**1-11b**) and FT-IR spectrum of 2-azido-2-phenylethanethiol intermediate are presented as following:

2-Phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethane-1-thiol (**1b**)

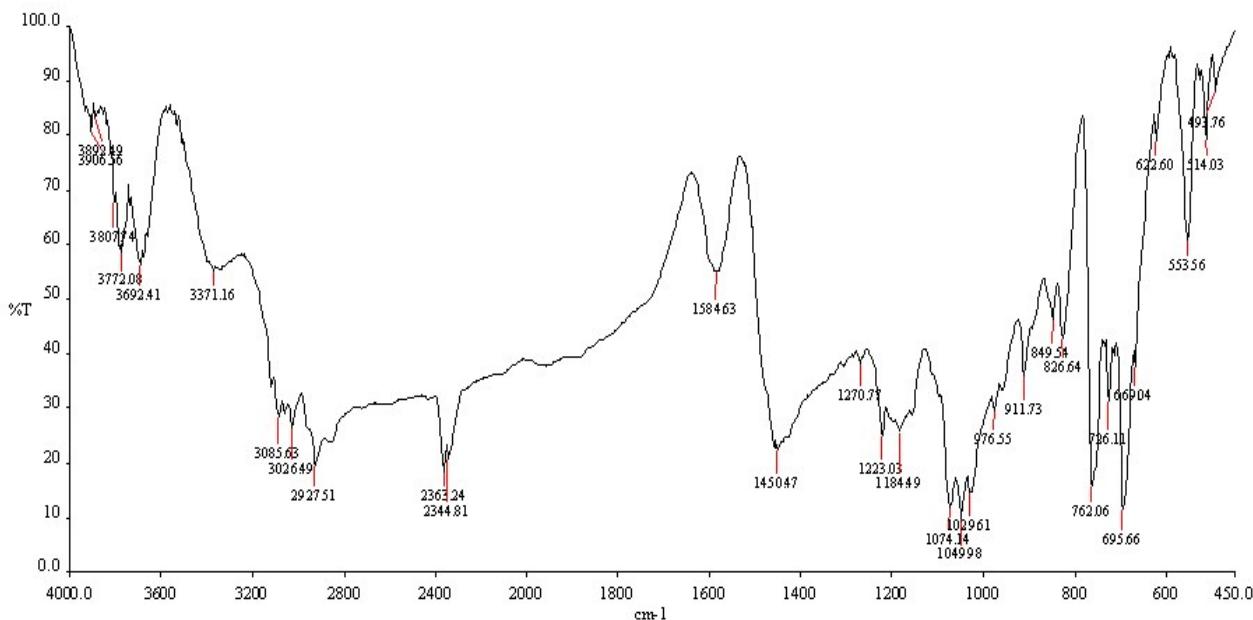
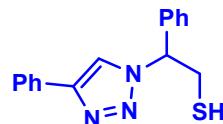


Figure S1. FT-IR Spectrum of 2-phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethane-1-thiol (**1b**)

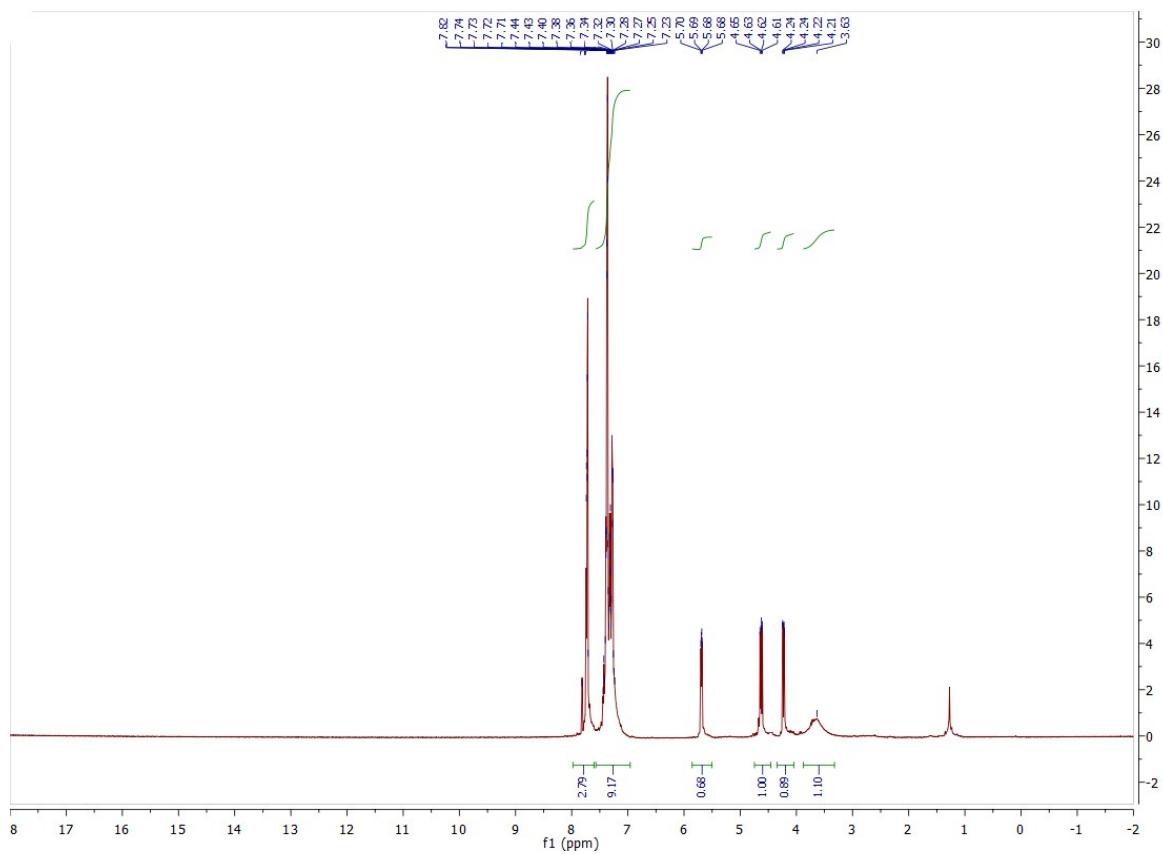


Figure S2. ¹H NMR Spectrum of 2-phenyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethane-1-thiol (1b)

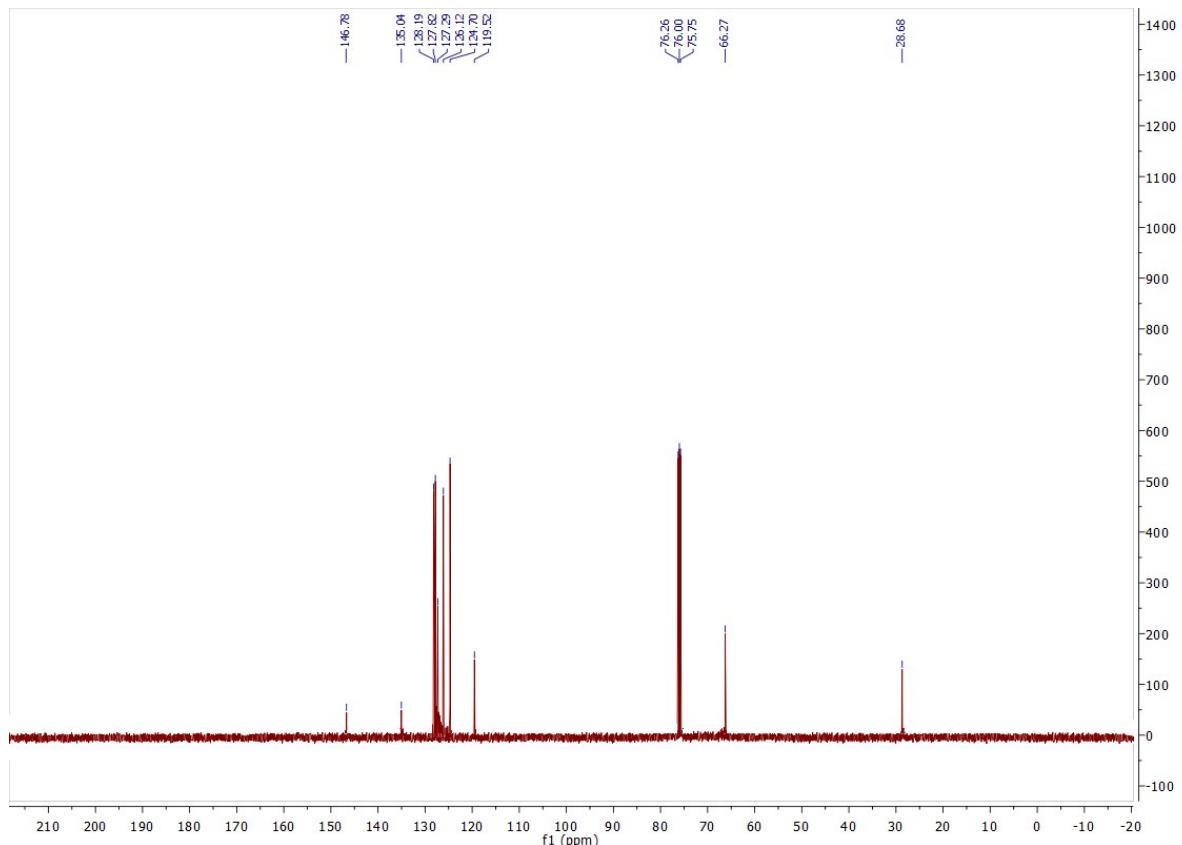


Figure S3. ¹³C NMR Spectrum of 2-phenyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethane-1-thiol (1b)
*1-Phenoxy-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (2b)*

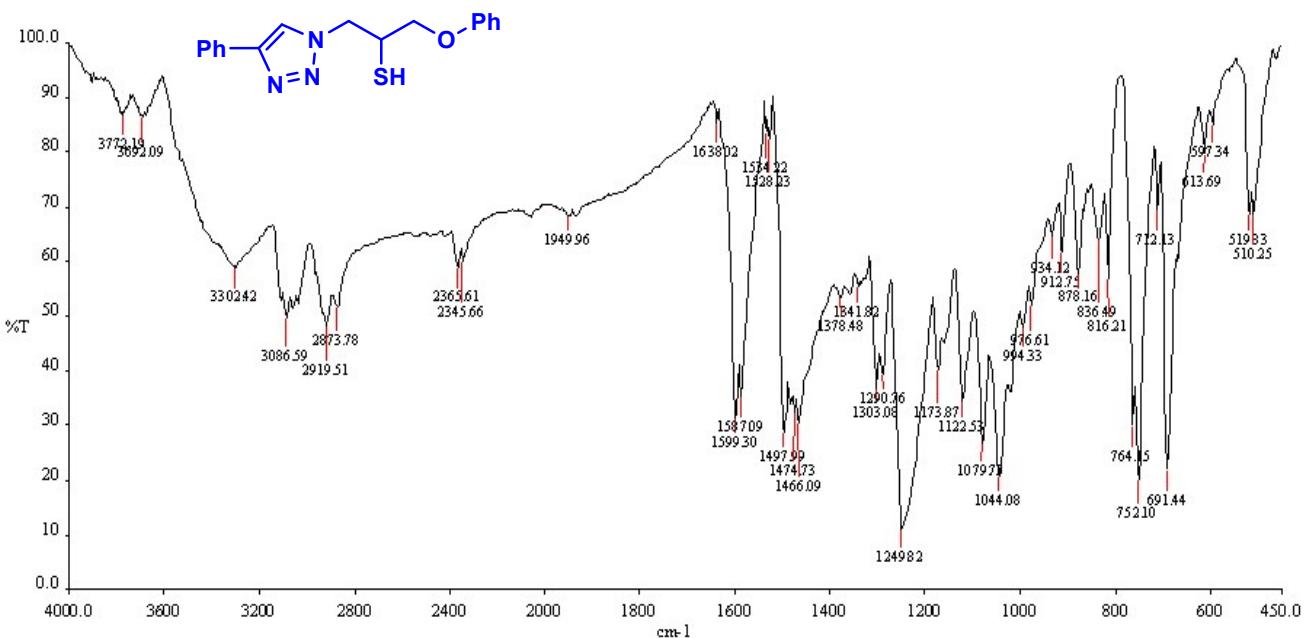


Figure S4. FT-IR Spectrum of 1-phenoxy-3-(4-phenyl-1H-1,2,3-triazol-1-yl)propane-2-thiol (2b)

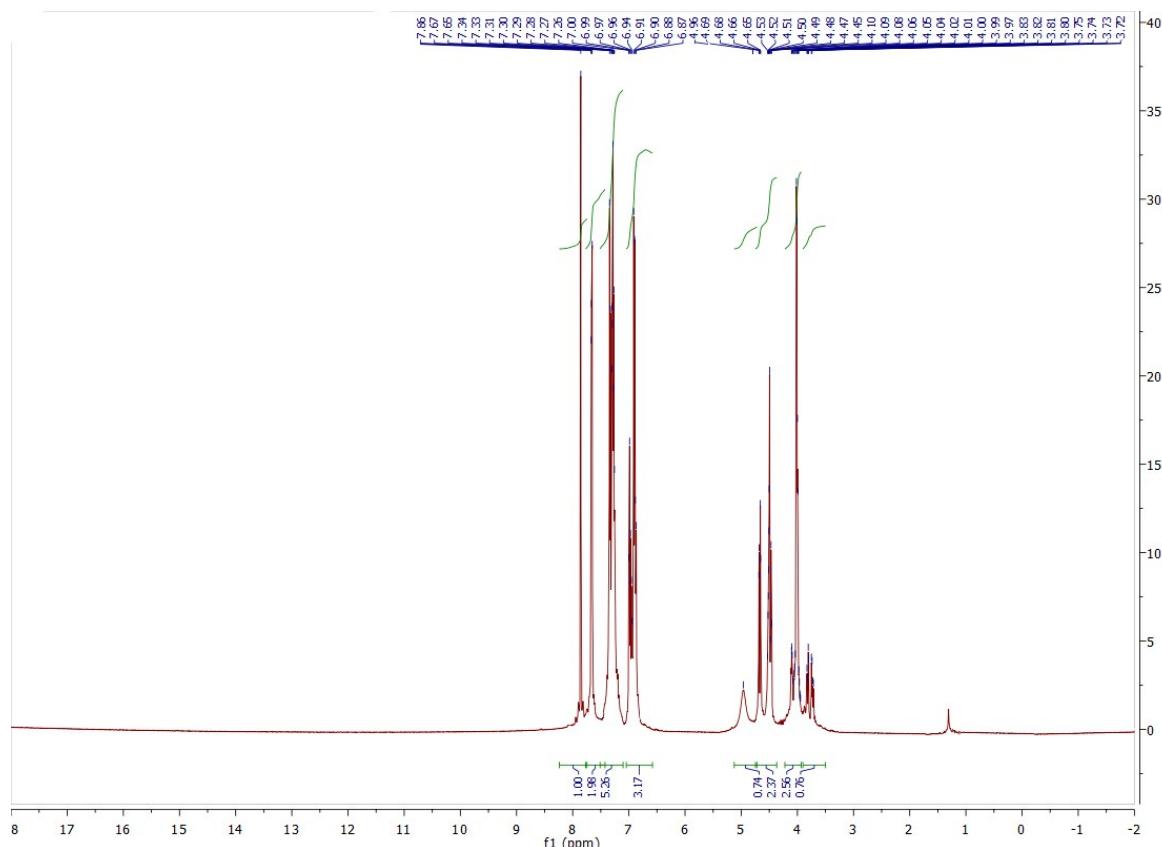


Figure S5. ¹H NMR Spectrum of 1-phenoxy-3-(4-phenyl-1H-1,2,3-triazol-1-yl)propane-2-thiol (2b)

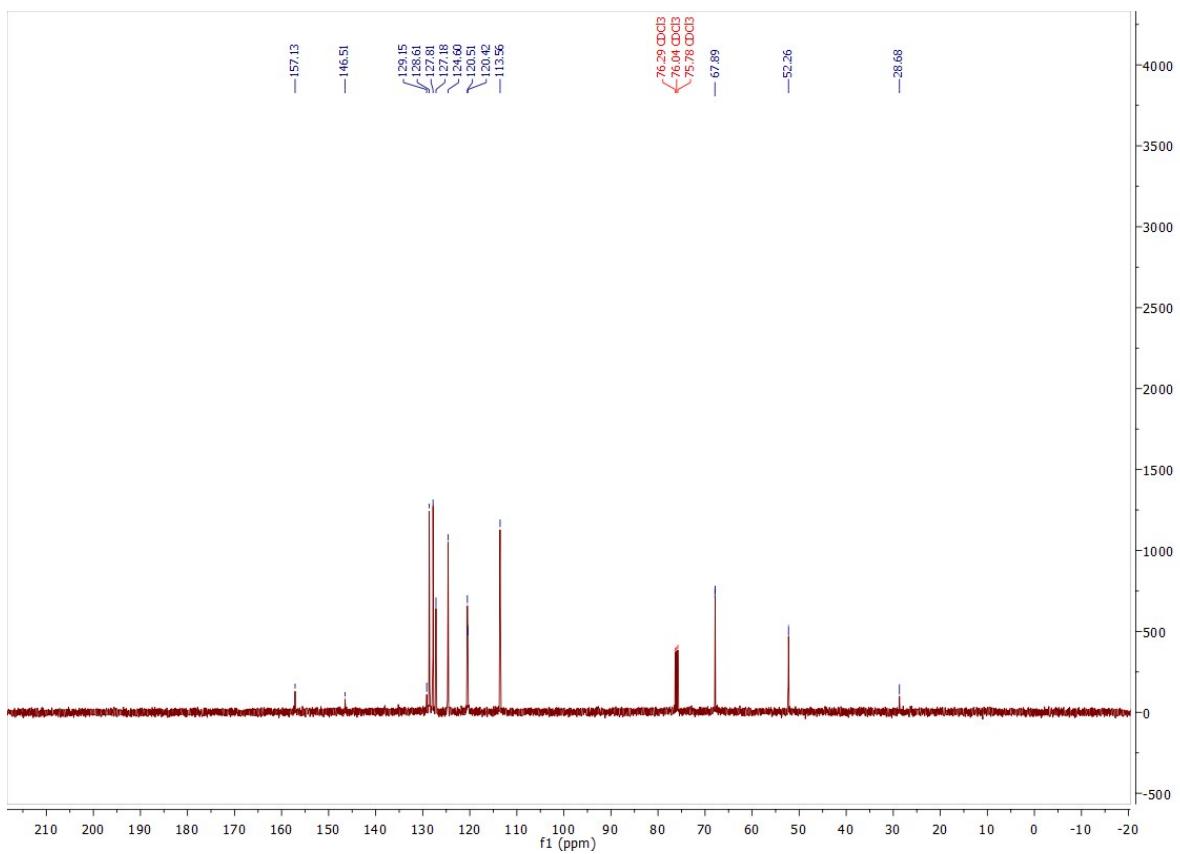
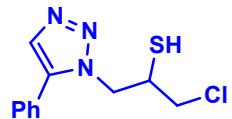


Figure S6. ^{13}C NMR Spectrum of 1-phenoxy-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (2b)

*1-Chloro-3-(5-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (3b)*



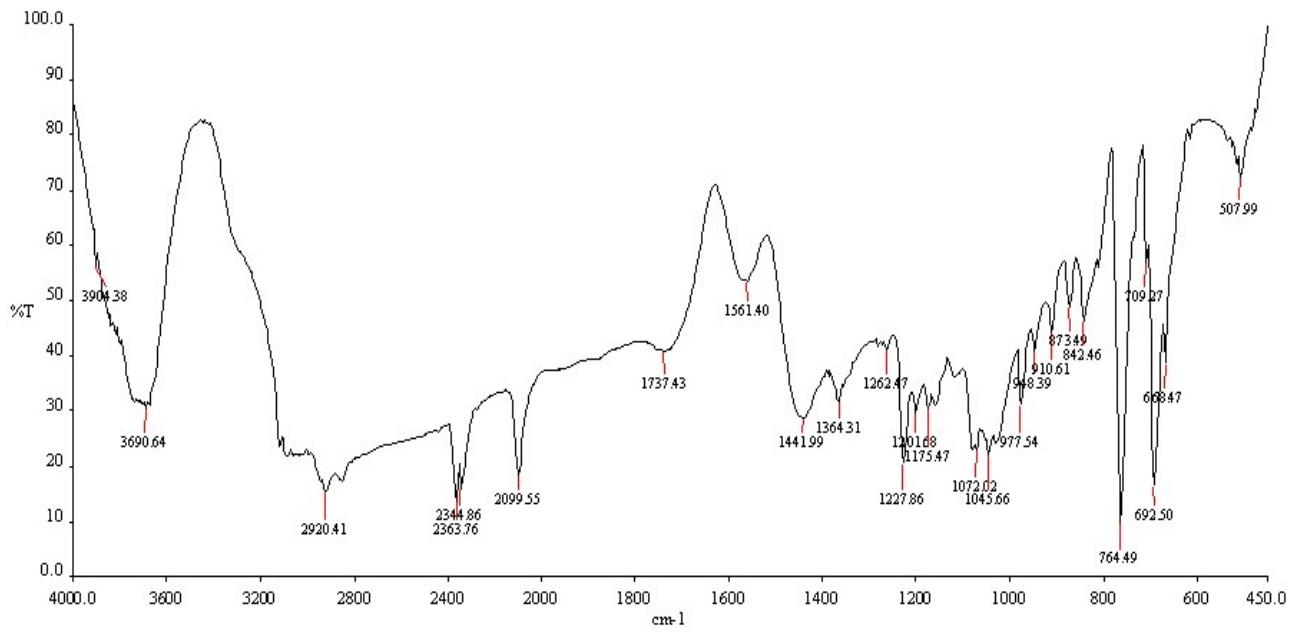


Figure S7. FT-IR Spectrum of 1-chloro-3-(5-phenyl-1H-1,2,3-triazol-1-yl)propane-2-thiol (**3b**)

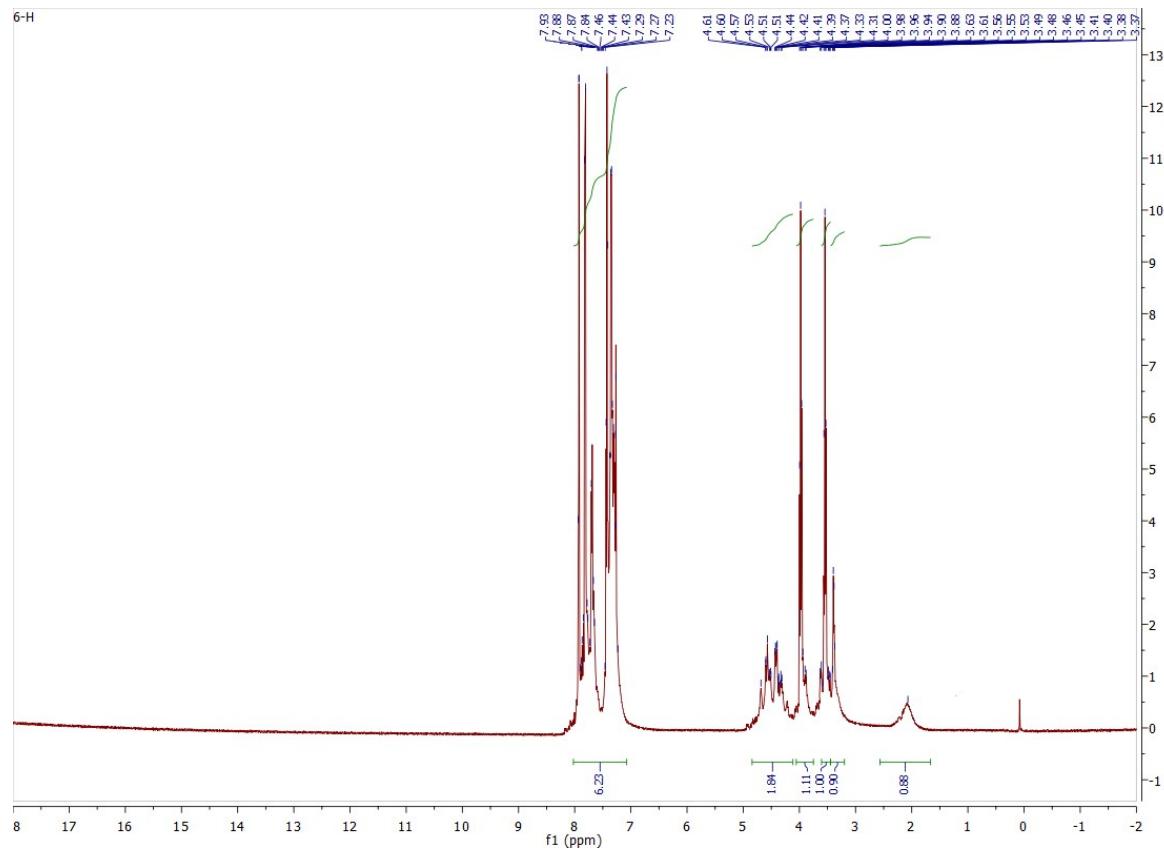


Figure S8. ^1H NMR Spectrum of 1-chloro-3-(5-phenyl-1H-1,2,3-triazol-1-yl)propane-2-thiol (**3b**)

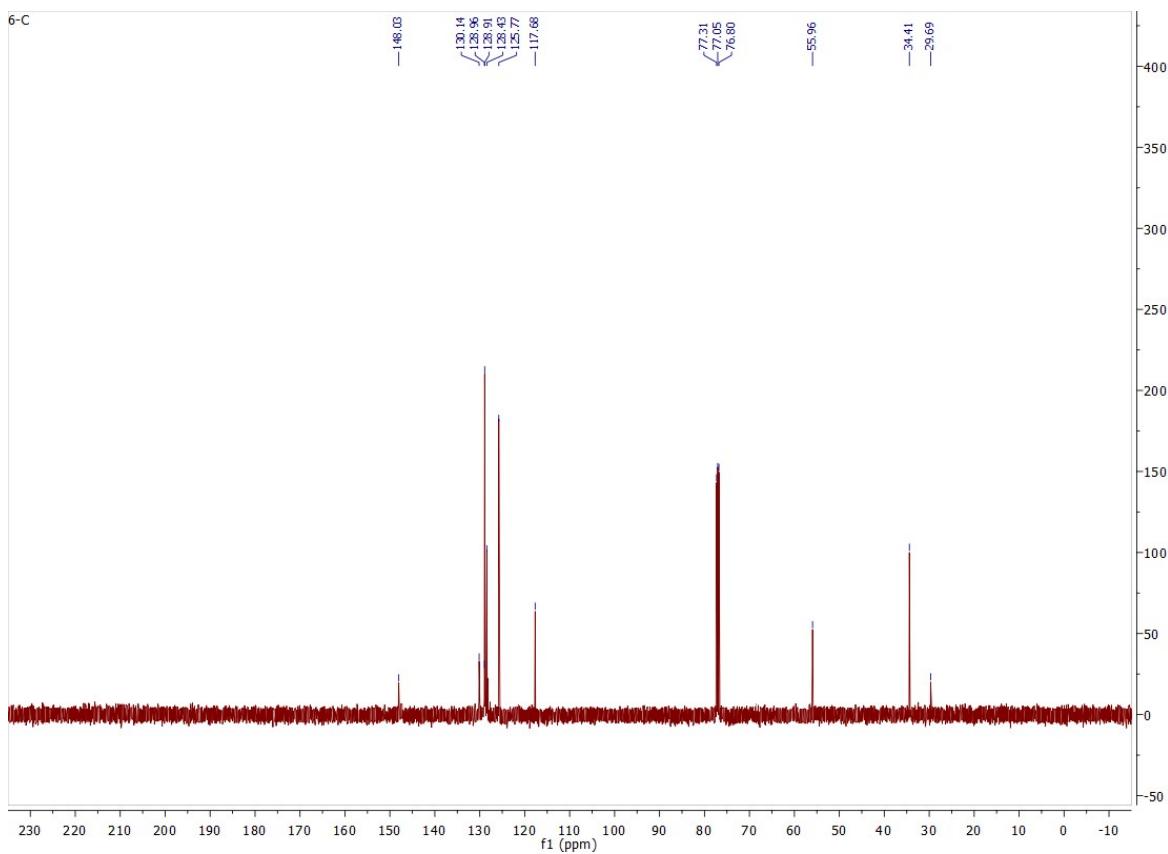


Figure S9. ¹³C NMR Spectrum of 1-chloro-3-(5-phenyl-1H-1,2,3-triazol-1-yl)propane-2-thiol (3b)

1-(4-Phenyl-1H-1,2,3-triazol-1-yl)butane-2-thiol (4b)



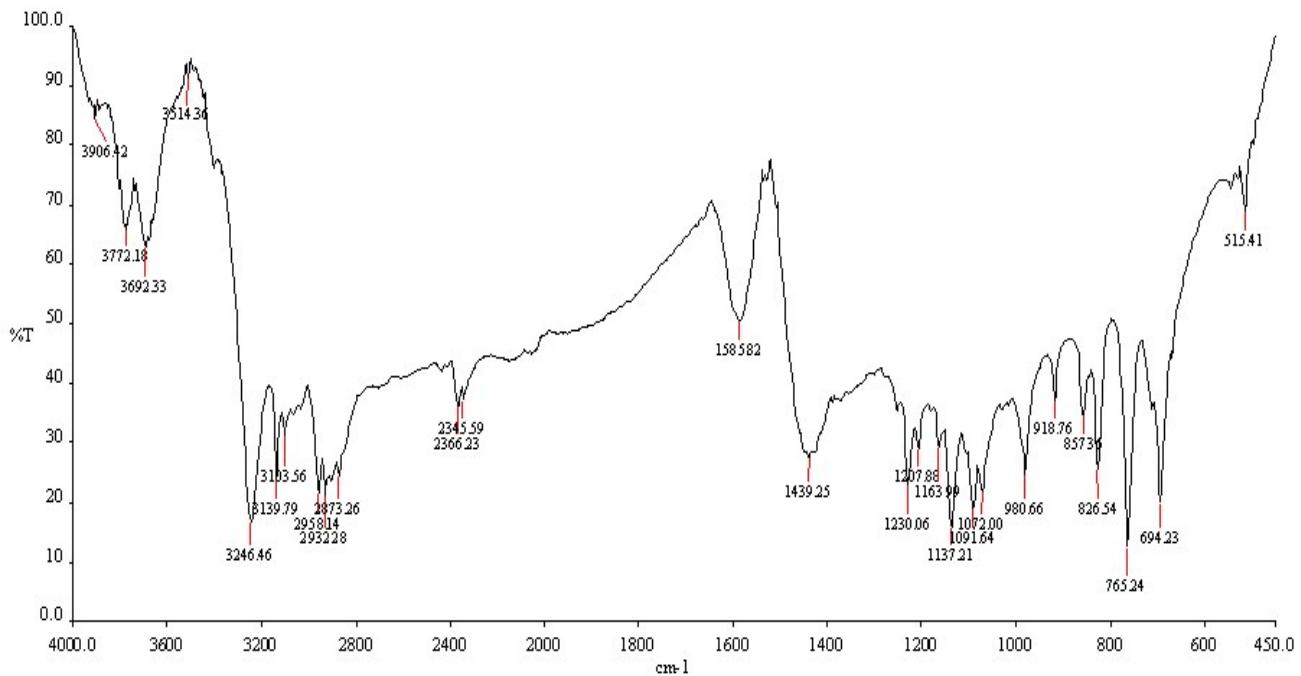


Figure S10. FT-IR Spectrum of 1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butane-2-thiol (4b)

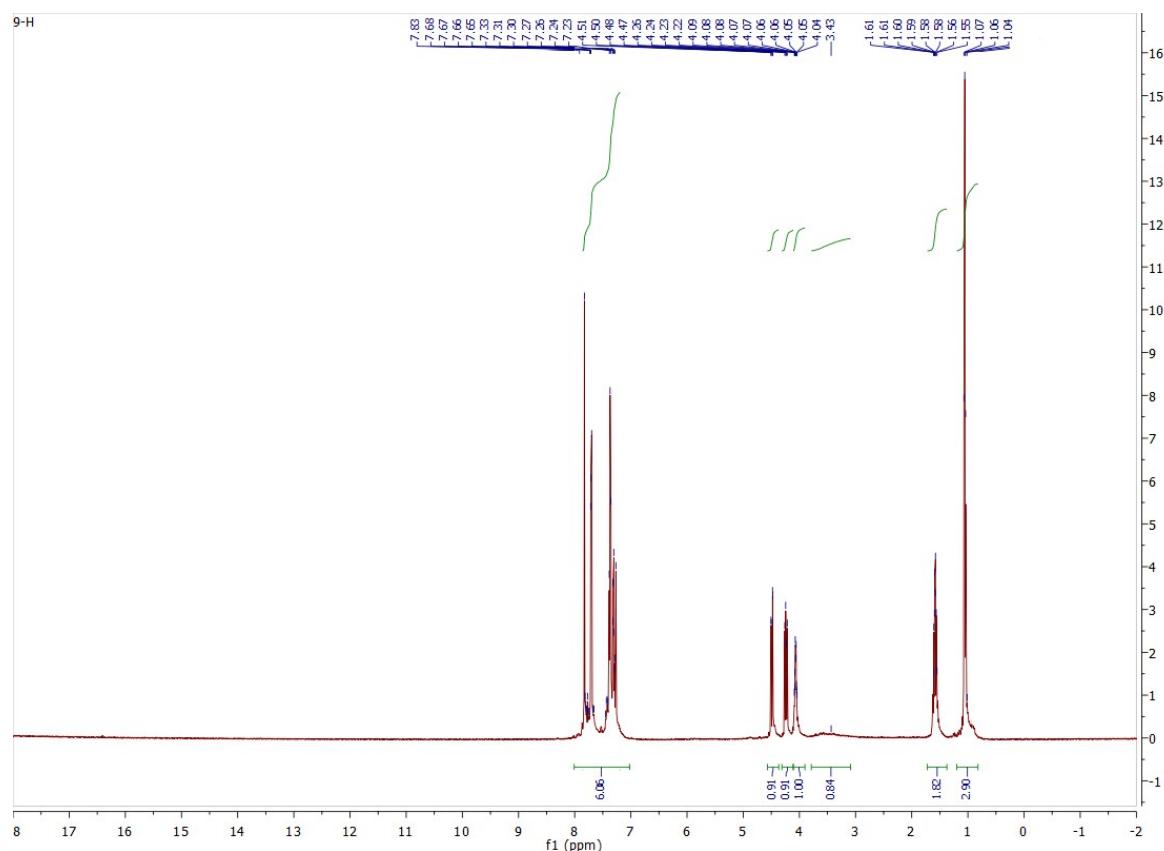


Figure S11. ¹H NMR Spectrum of 1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butane-2-thiol (4b)

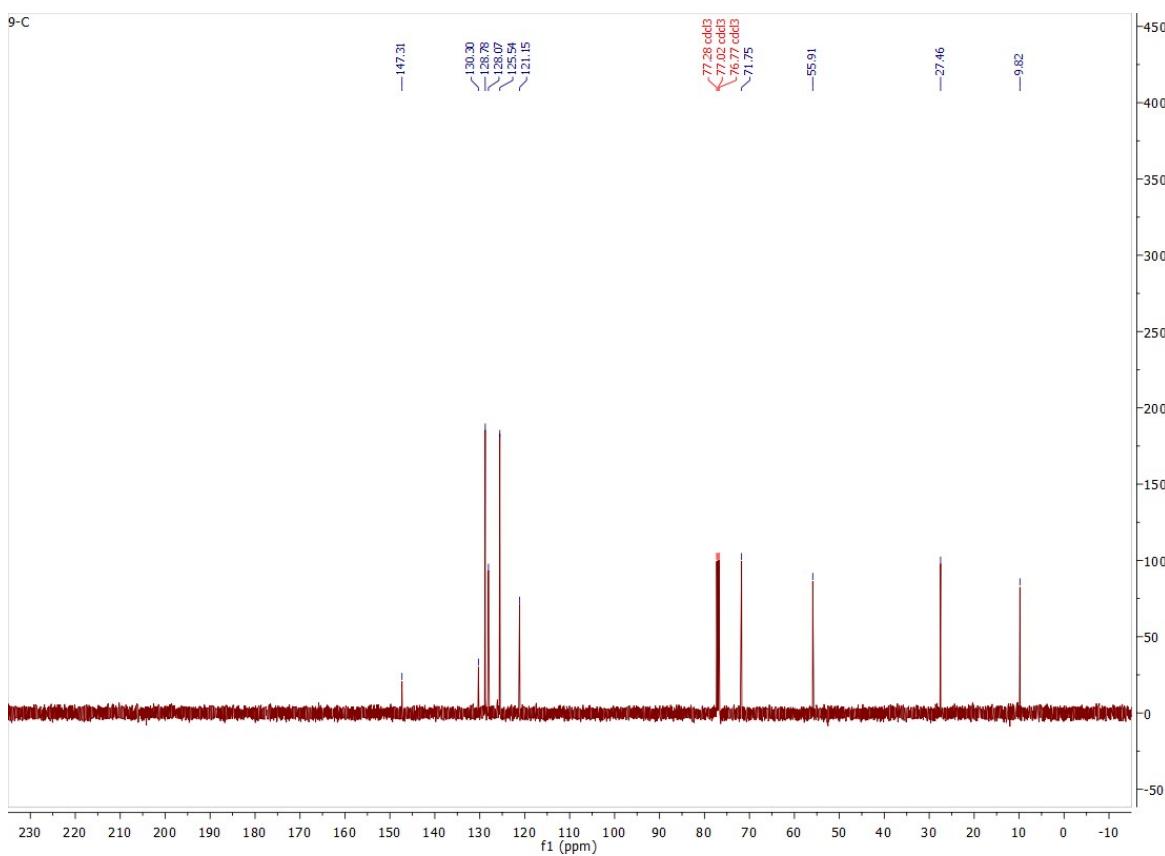


Figure S12. ^{13}C NMR Spectrum of 1-(4-phenyl-1*H*-1,2,3-triazol-1-yl)butane-2-thiol (**4b**)

1-Isopropoxy-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (5b)

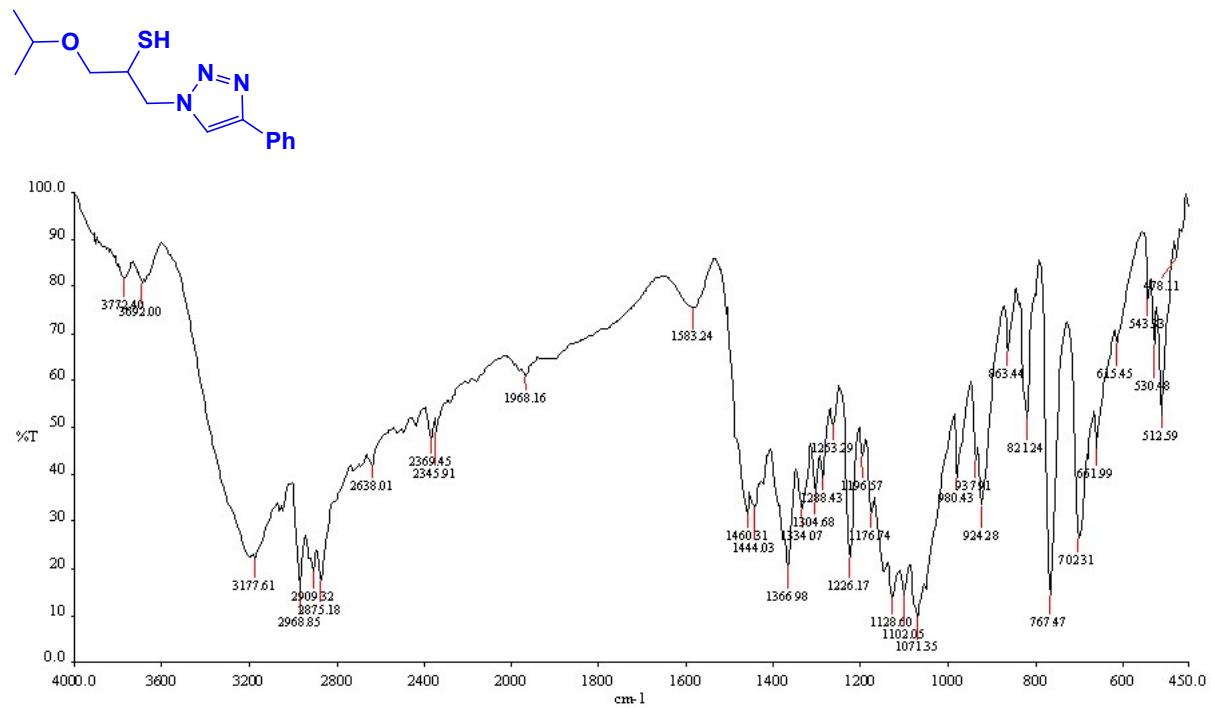


Figure S13. FT-IR Spectrum of 1-isopropoxy-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (**5b**)

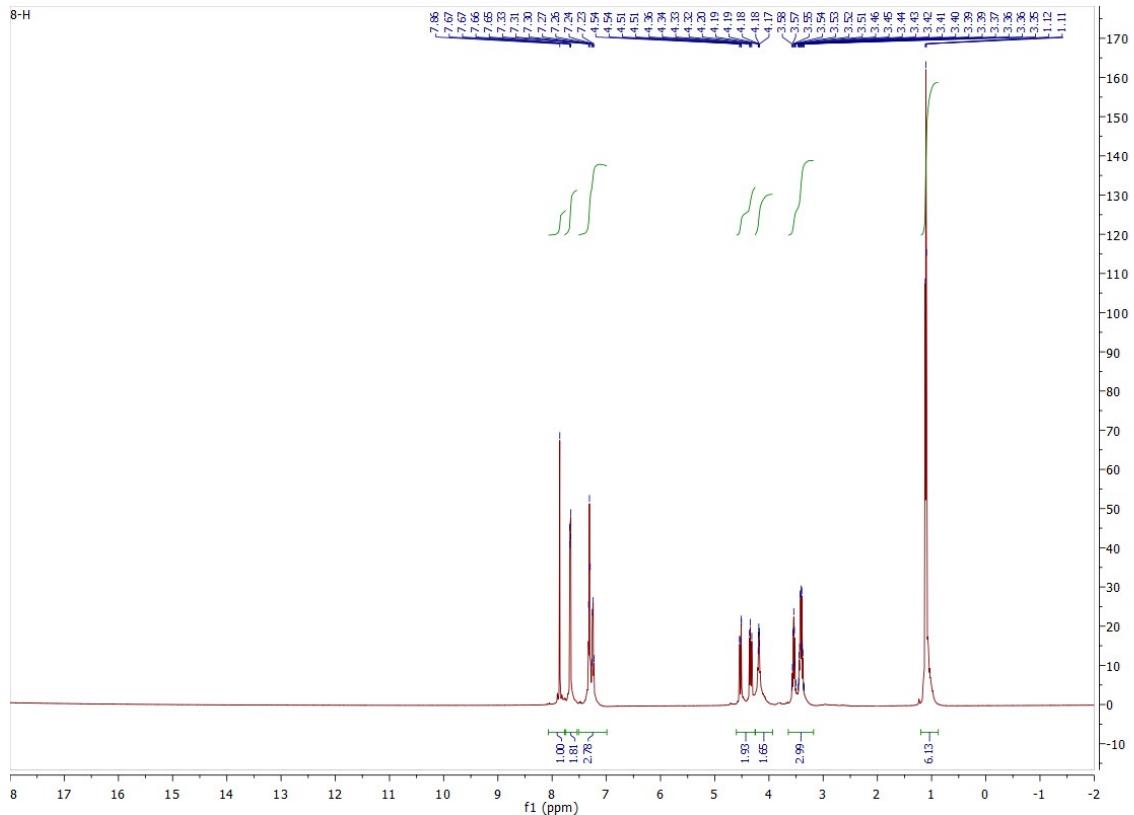


Figure S14. ^1H NMR Spectrum of 1-isopropoxy-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (**5b**)

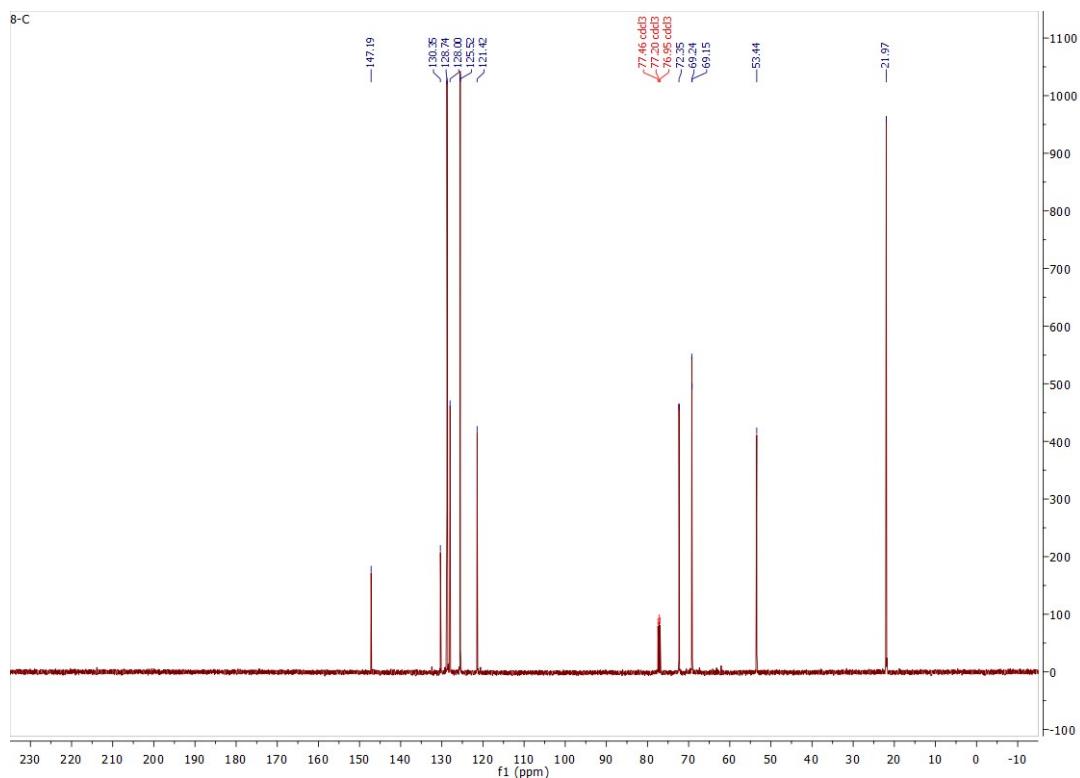


Figure S15. ^{13}C NMR Spectrum of 1-isopropoxy-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (**5b**)

*2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)cyclohexane-1-thiol (6b)*

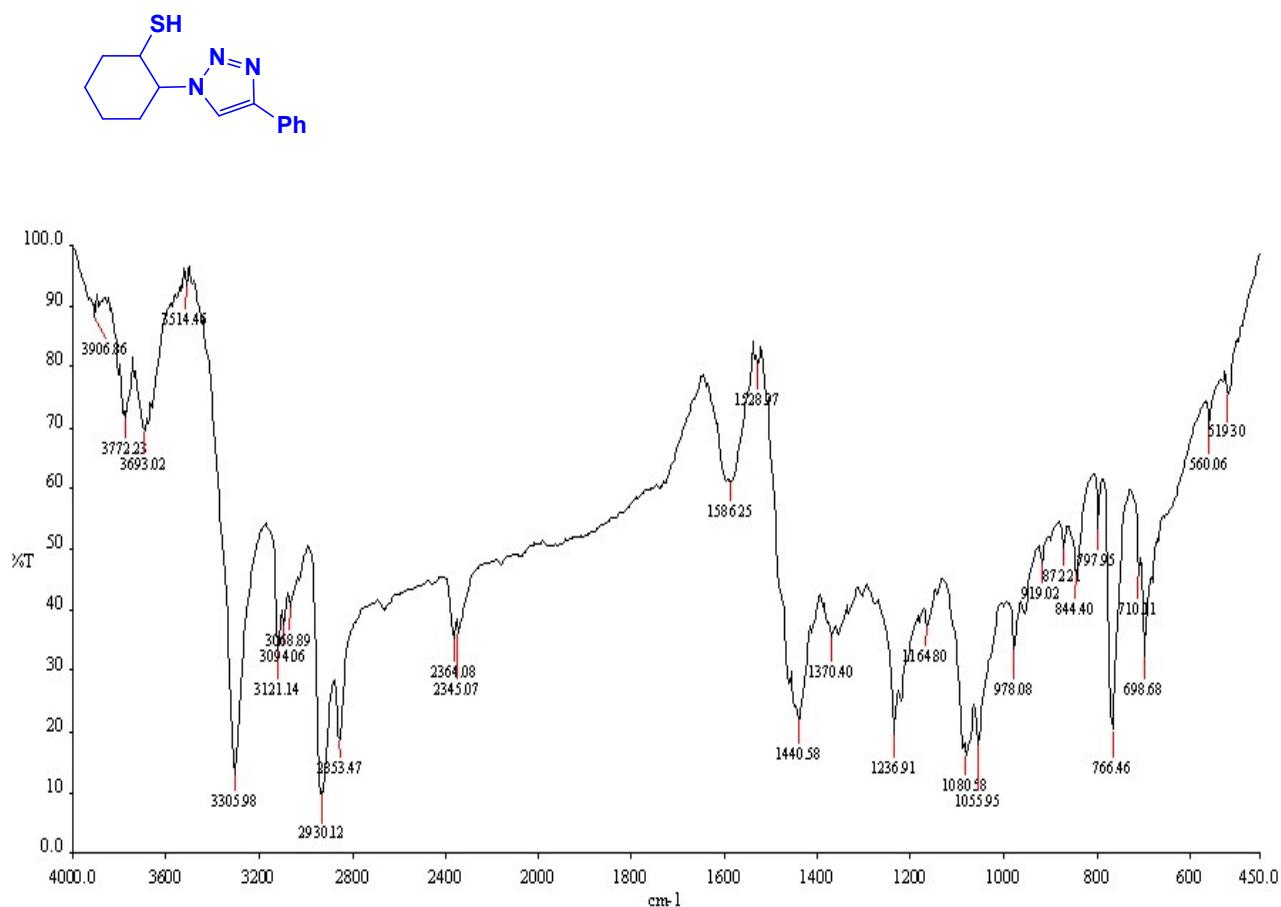


Figure S16. FT-IR Spectrum of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)cyclohexane-1-thiol (6b)

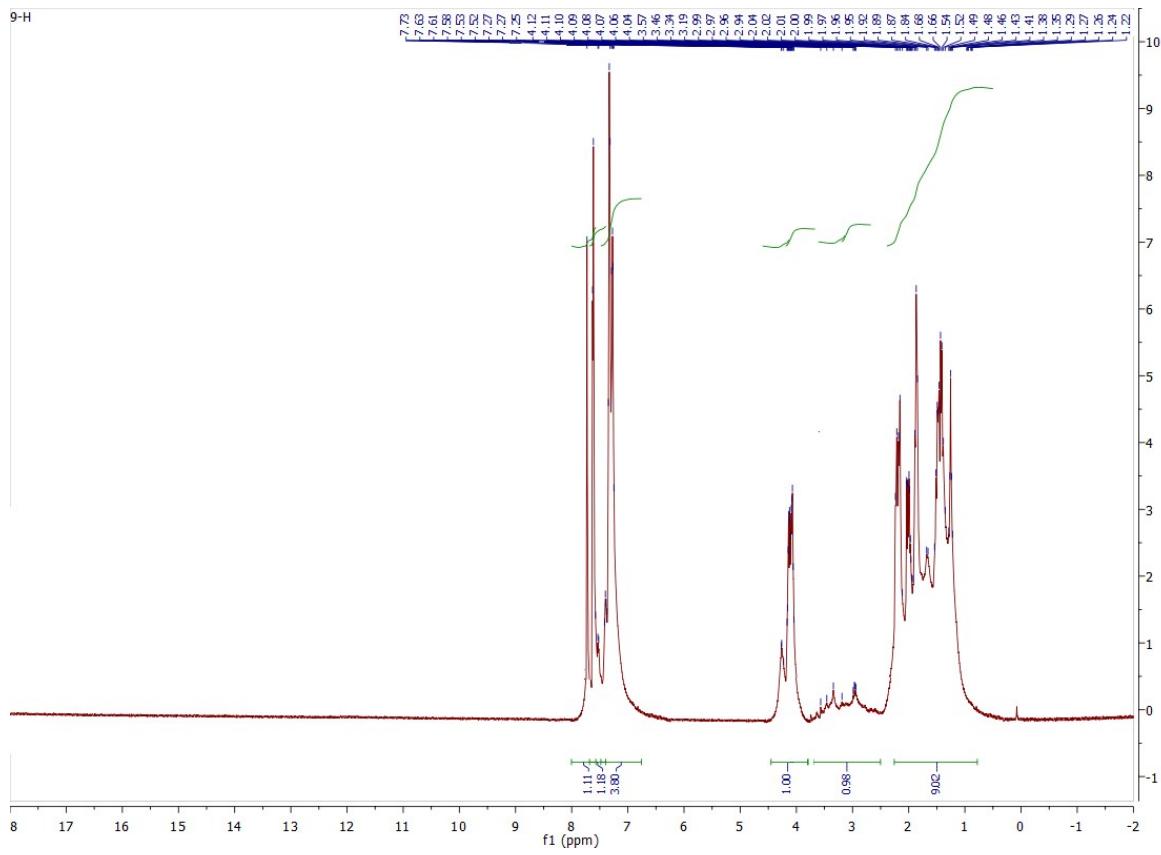


Figure S17. ^1H NMR Spectrum of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)cyclohexane-1-thiol (6b)

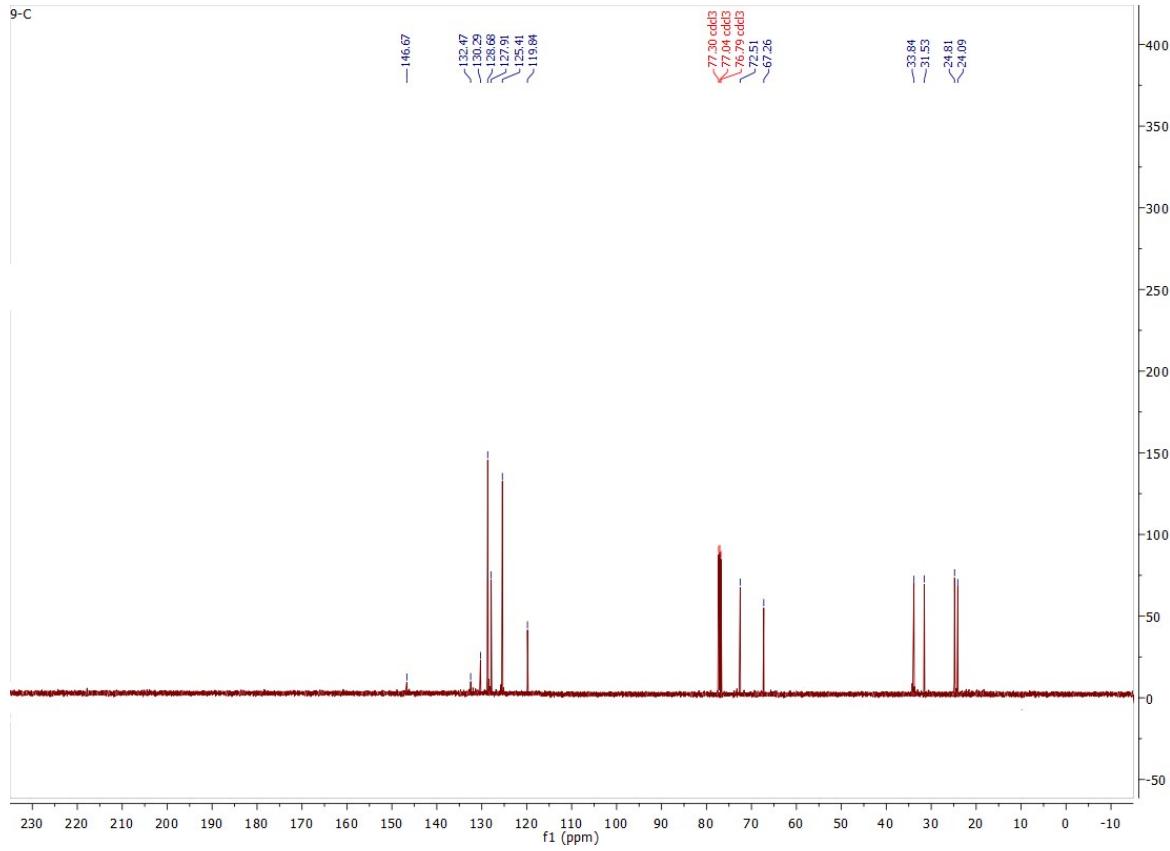


Figure S18. ^{13}C NMR Spectrum of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)cyclohexane-1-thiol (6b)

*1-(Allyloxy)-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (7b)*

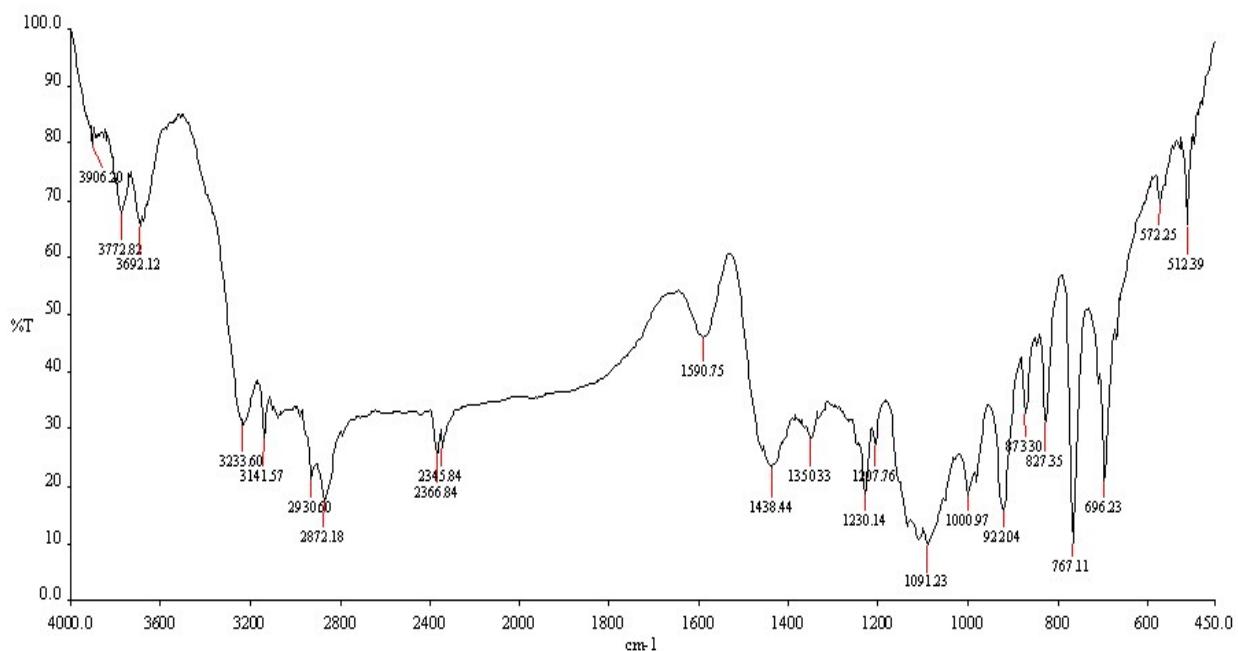
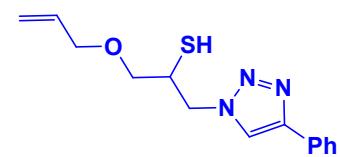


Figure S19. FT-IR Spectrum of *1-(allyloxy)-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol* (7b)

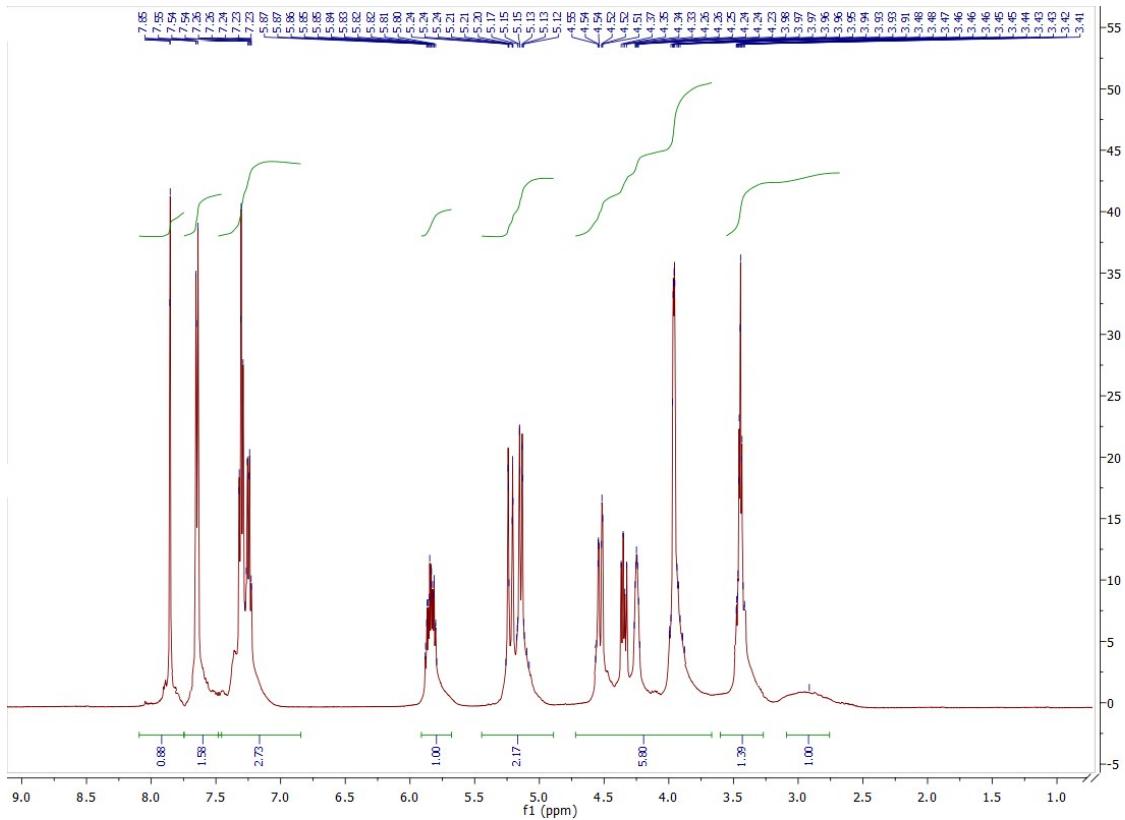


Figure S20. ^1H NMR Spectrum of 1-(allyloxy)-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (7b)

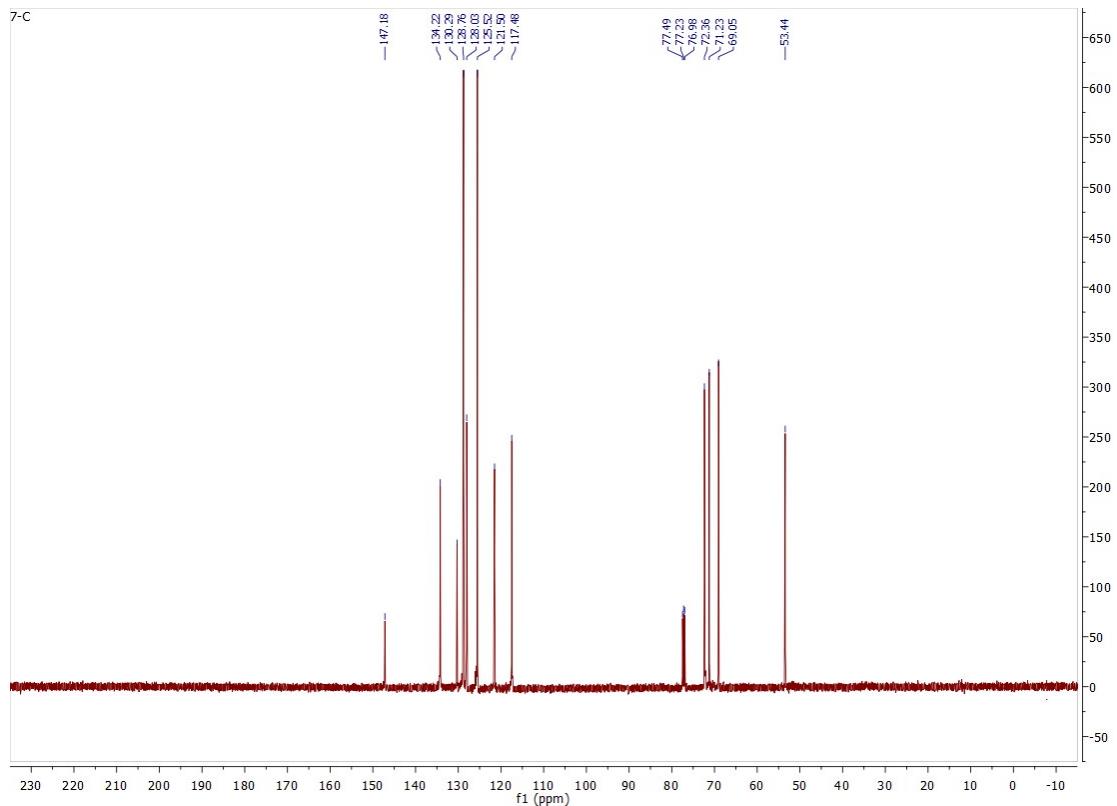


Figure S21. ^{13}C NMR Spectrum of 1-(allyloxy)-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propane-2-thiol (7b)

*2-Mercapto-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl methacrylate (8b)*

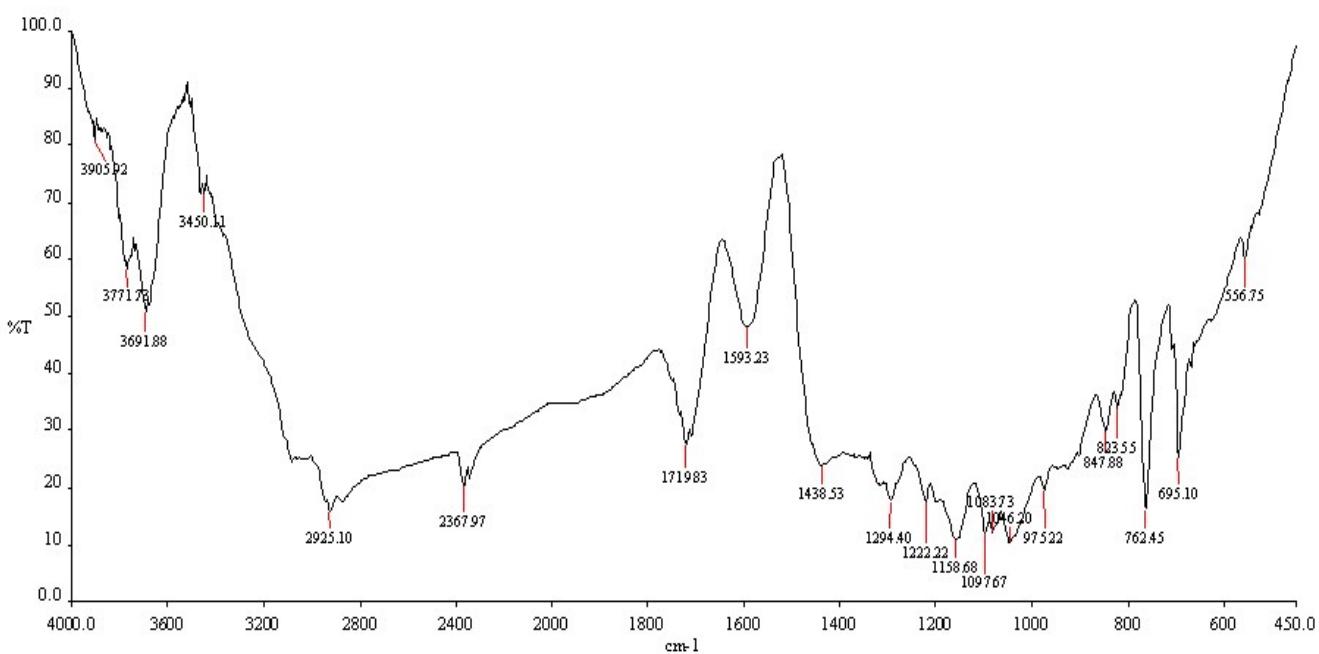
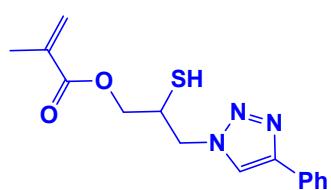


Figure S22. FT-IR Spectrum of 2-mercaptopropyl methacrylate (8b)

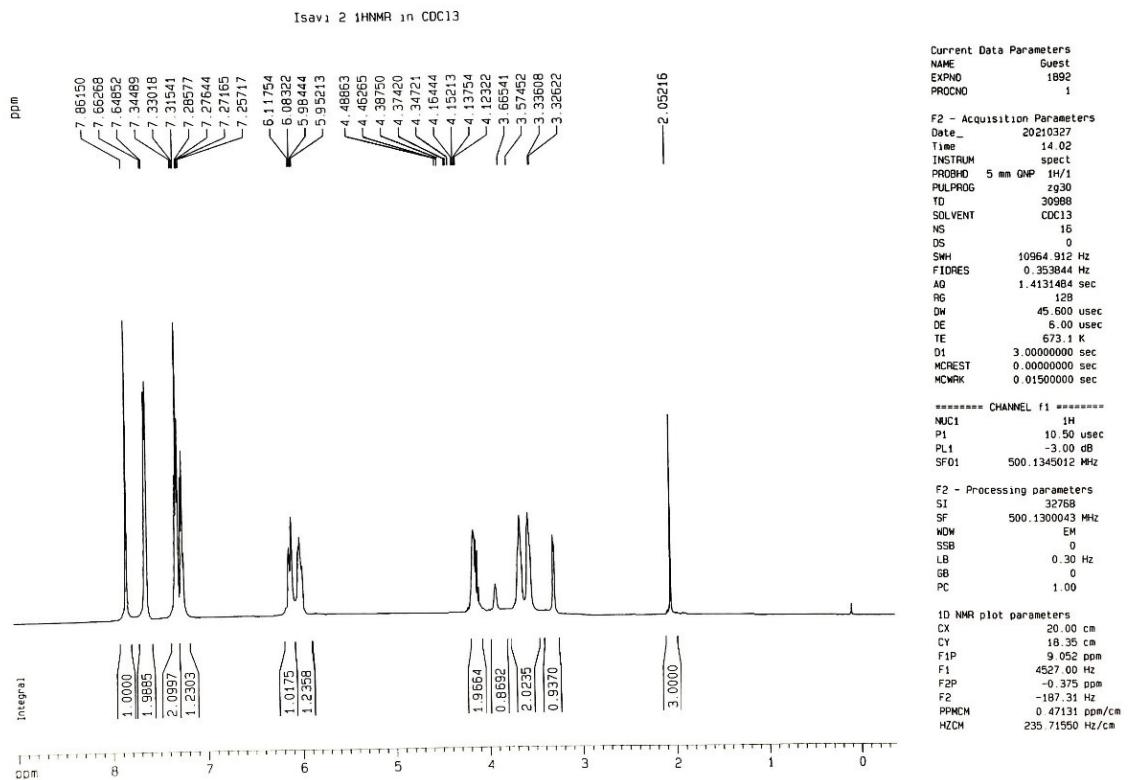


Figure S23. ^1H NMR Spectrum of 2-mercaptopropanoic acid 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl methacrylate (**8b**)

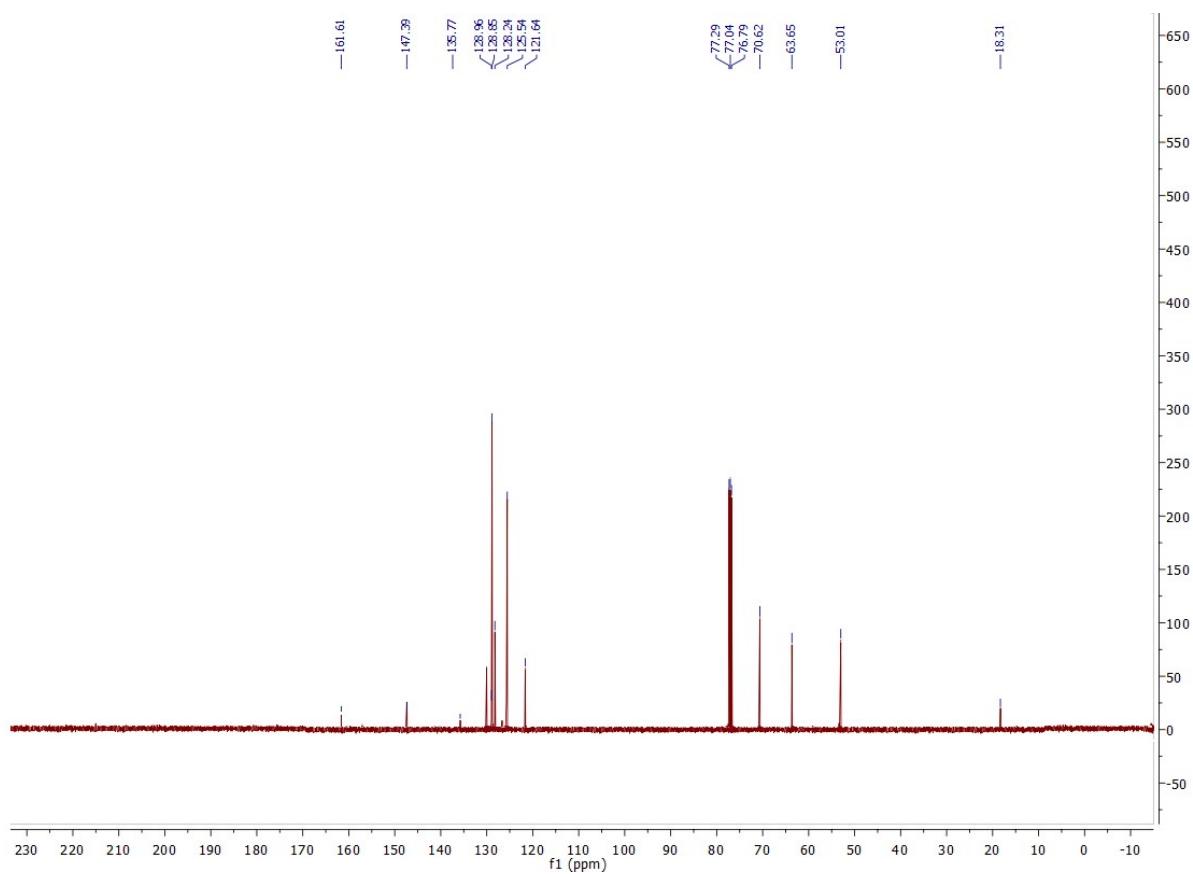
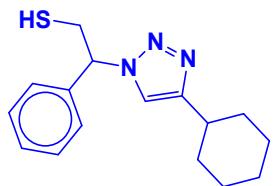


Figure S24. ^{13}C NMR Spectrum of 2-mercaptopro-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propyl methacrylate (**8b**)

2-(4-Cyclohexyl-1*H*-1,2,3-triazol-1-yl)-2-phenylethane-1-thiol (9b**)**



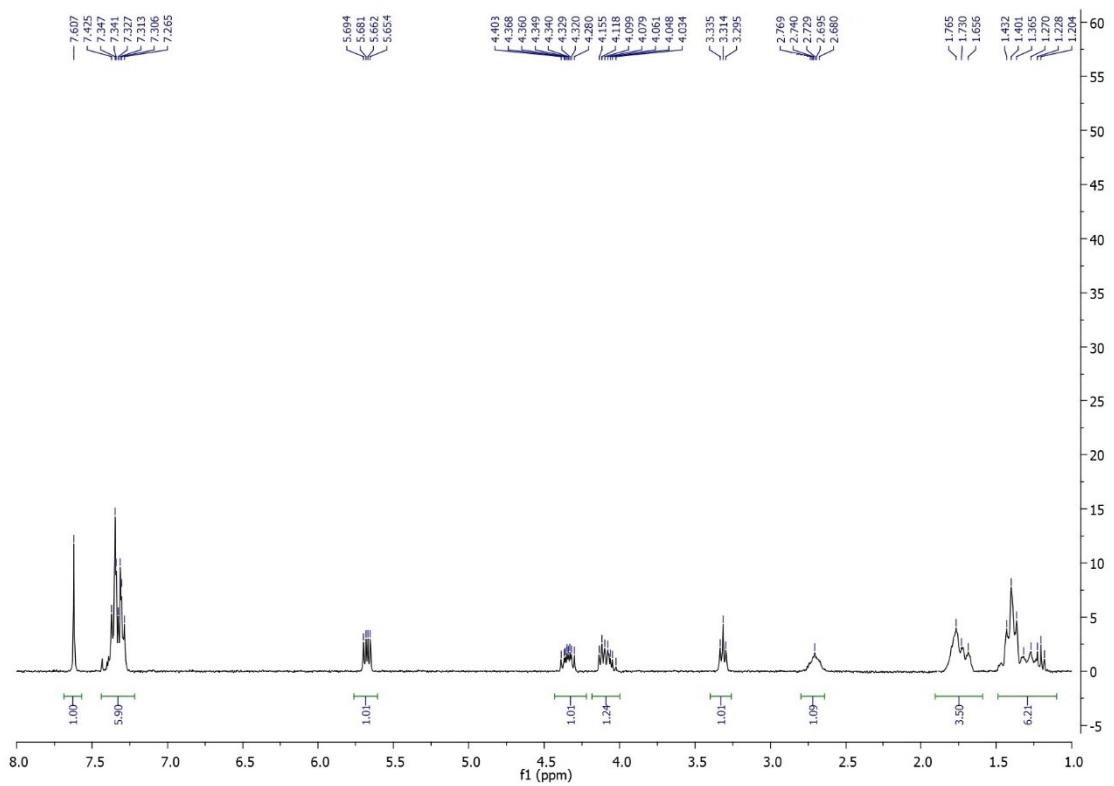


Figure S25. ^1H NMR Spectrum of 2-(4-cyclohexyl-1*H*-1,2,3-triazol-1-yl)-2-phenylethane-1-thiol (**9b**)

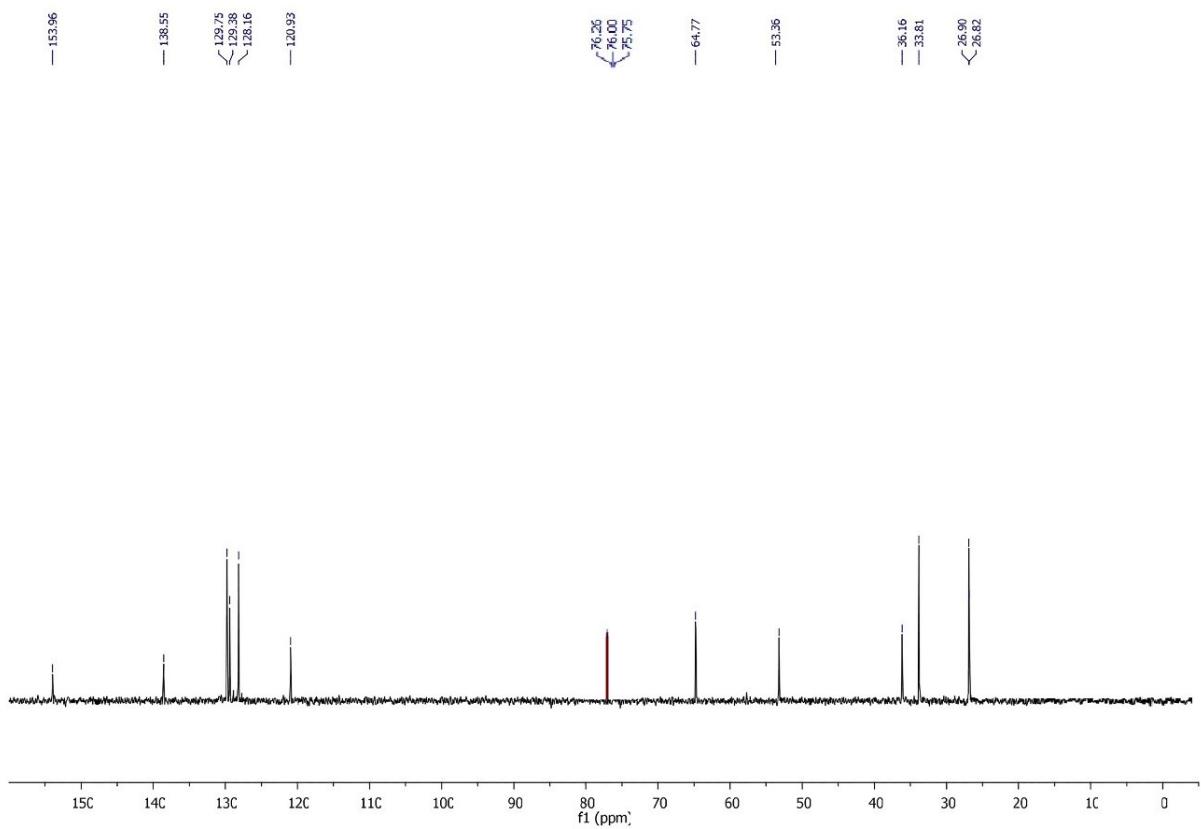
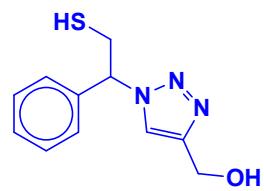


Figure S26. ^{13}C NMR Spectrum of 2-(4-cyclohexyl-1*H*-1,2,3-triazol-1-yl)-2-phenylethane-1-thiol (**9b**)

(*1*-(2-Mercapto-1-phenylethyl)-1*H*-1,2,3-triazol-4-yl)methanol (**10b**)



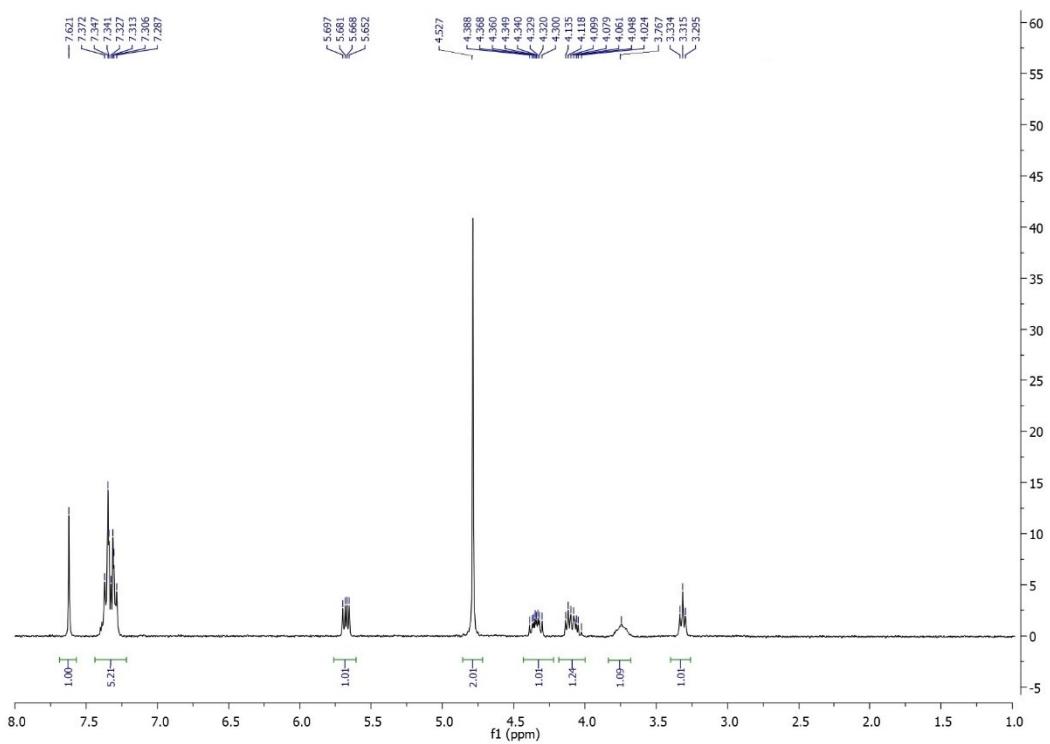


Figure S27. ¹H NMR Spectrum of (1-(2-mercaptopro-1-phenylethyl)-1*H*-1,2,3-triazol-4-yl)methanol (**10b**)

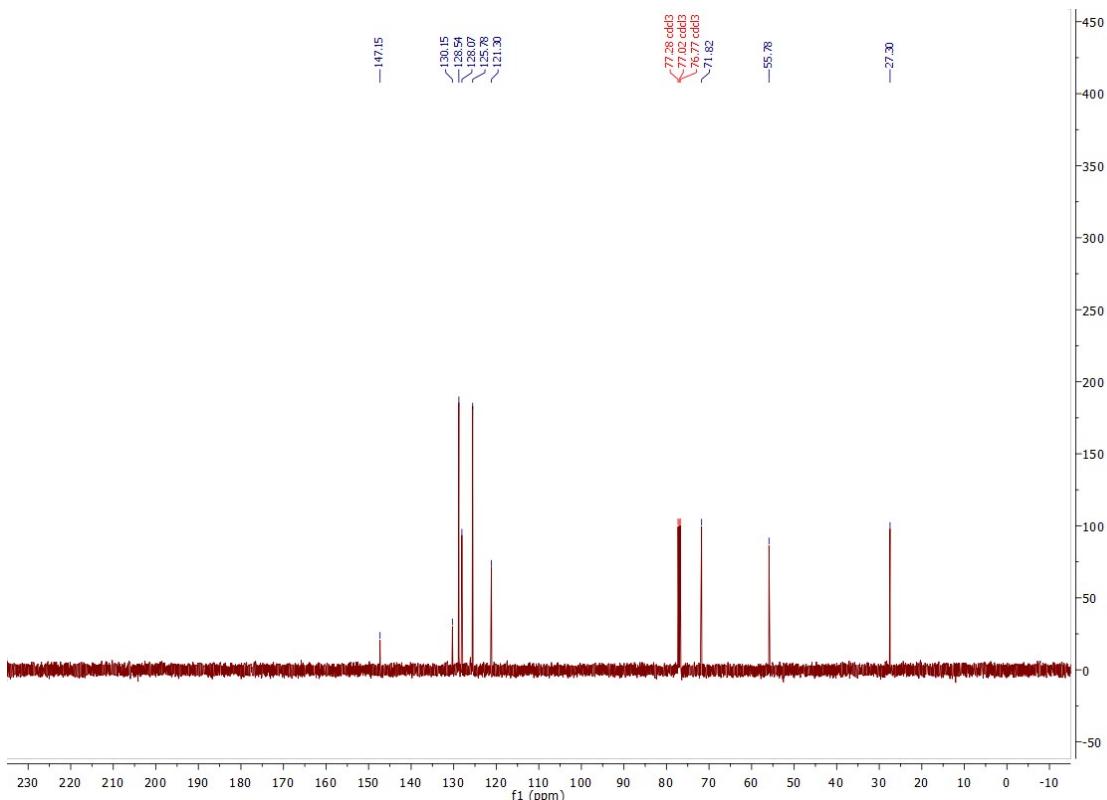


Figure S28. ¹³C NMR Spectrum of (1-(2-mercaptopro-1-phenylethyl)-1*H*-1,2,3-triazol-4-yl)methanol (**10b**)

2-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-2-phenylethane-1-thiol (11b)

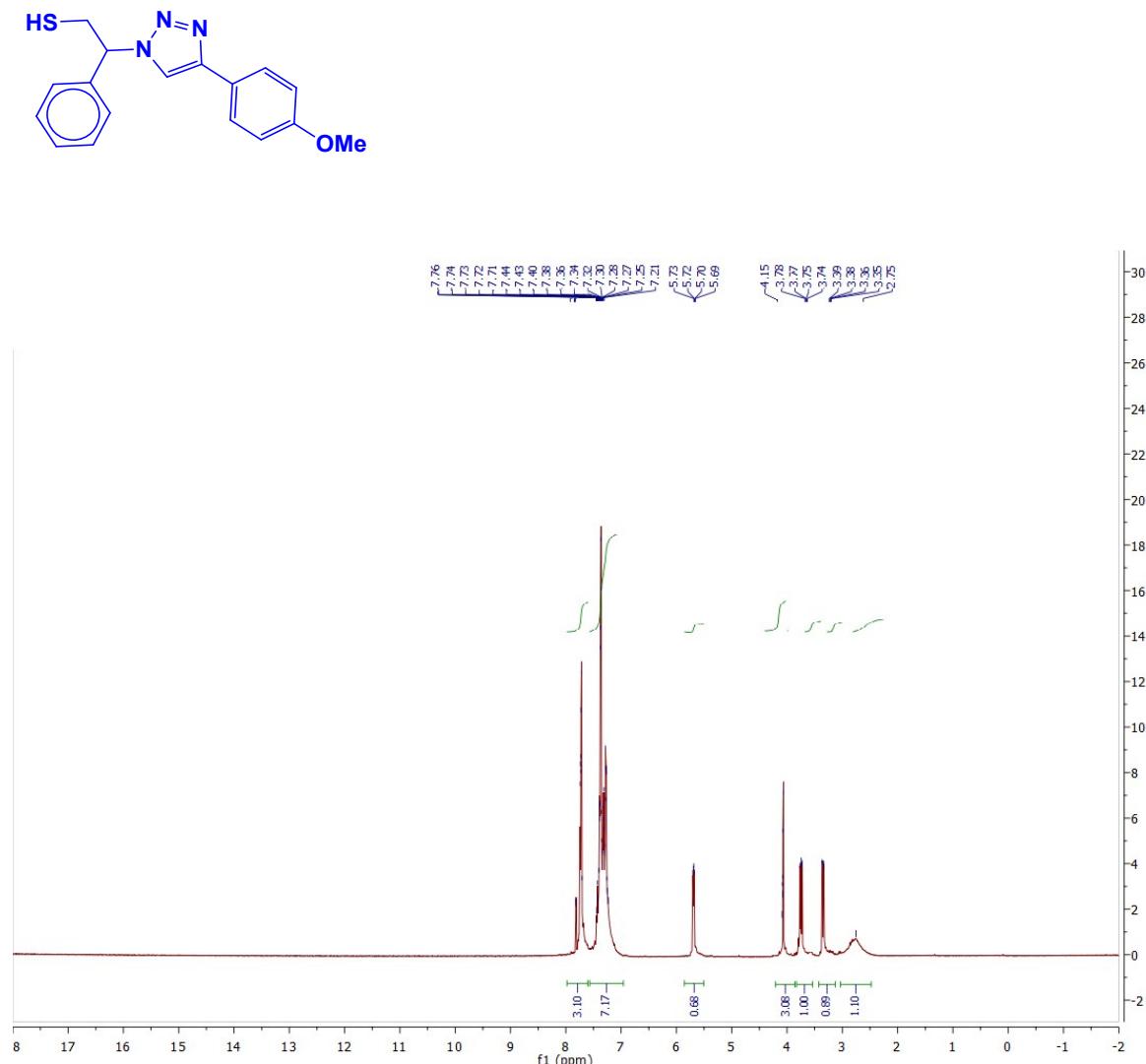


Figure S29. ¹H NMR Spectrum of 2-(4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-2-phenylethane-1-thiol (11b)

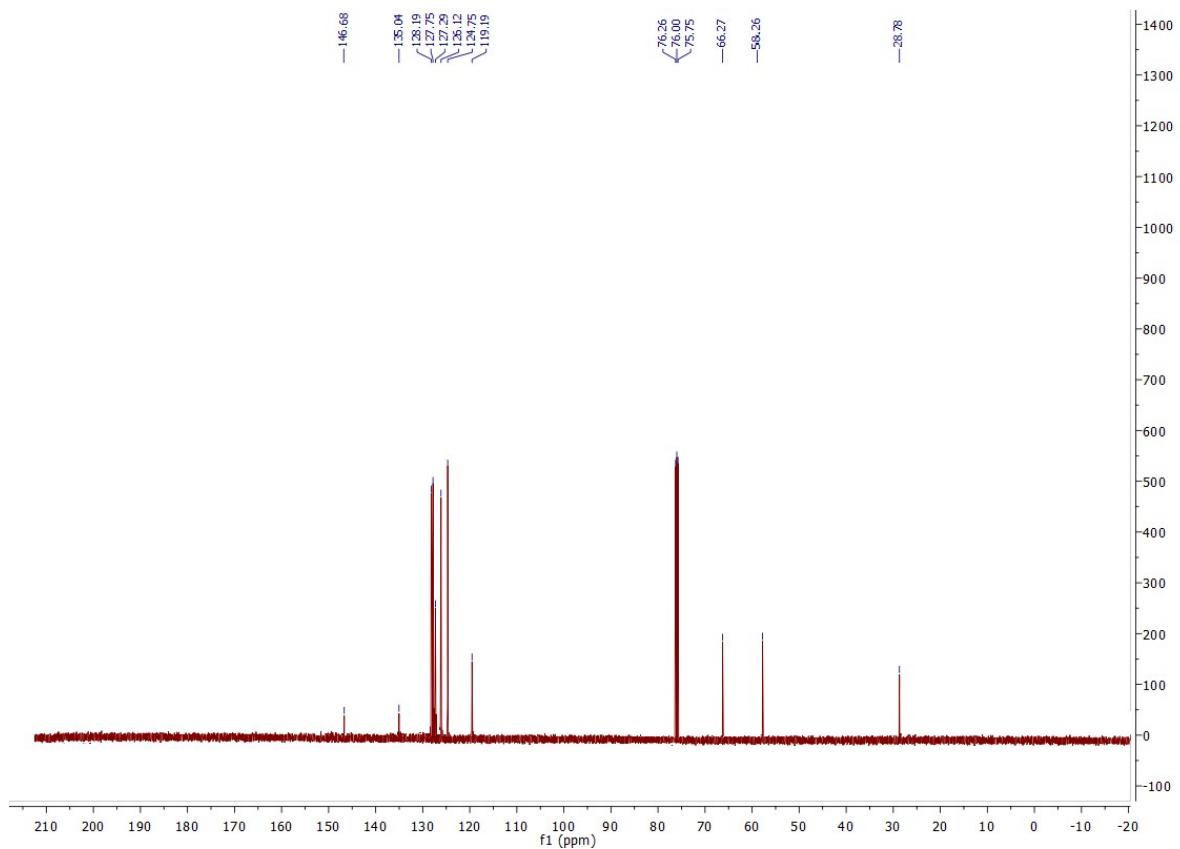


Figure S30. ¹³C NMR Spectrum of 2-(4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-2-phenylethane-1-thiol (11b)

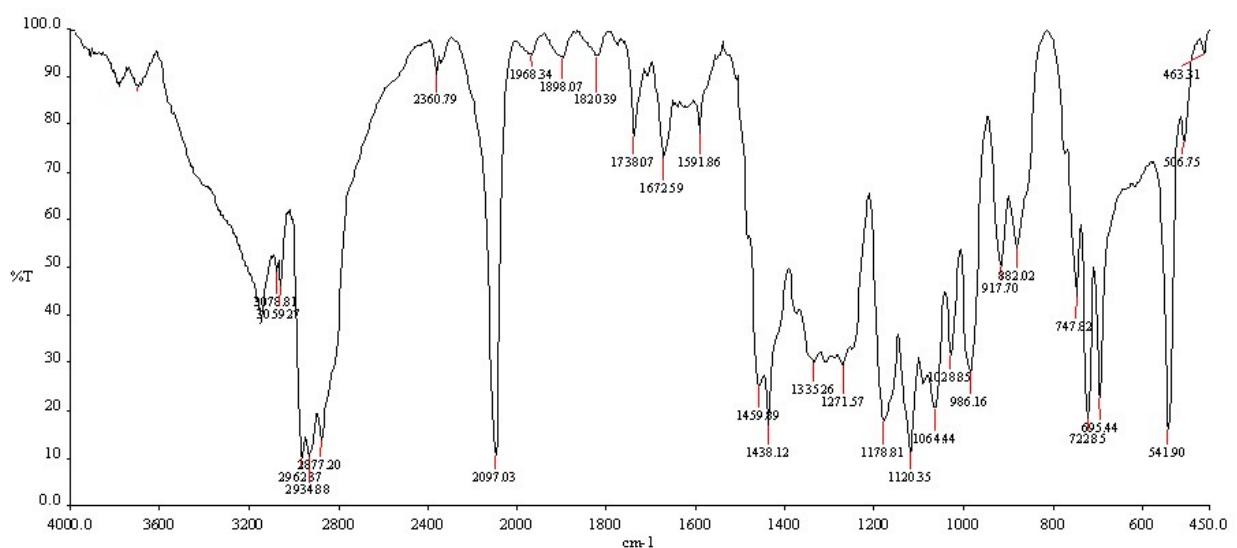


Figure S31. FT-IR Spectrum of 2-azido-2-phenylethanethiol intermediate