

Supplementary Information

Selenenylsulfide covalent-directed chemistry for the detection of sulfhydryl groups using a diselenide fluorescent probe

*Chunqiu Ma, Jichao Xu, Xiaolu Wang, Xuewen Wang, Lei Zhang, Su Jing**

School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China.

**Corresponding author. Email: sjing@njtech.edu.cn.*

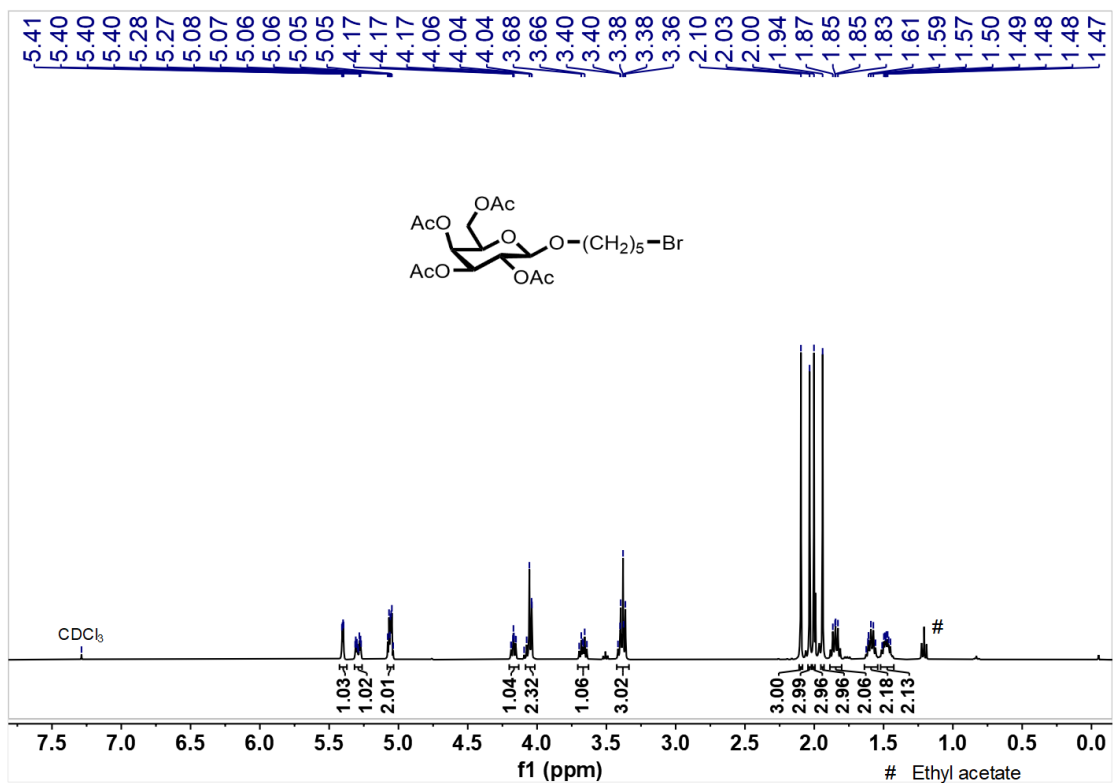


Fig. S1. ¹H NMR spectrum of compound 2.

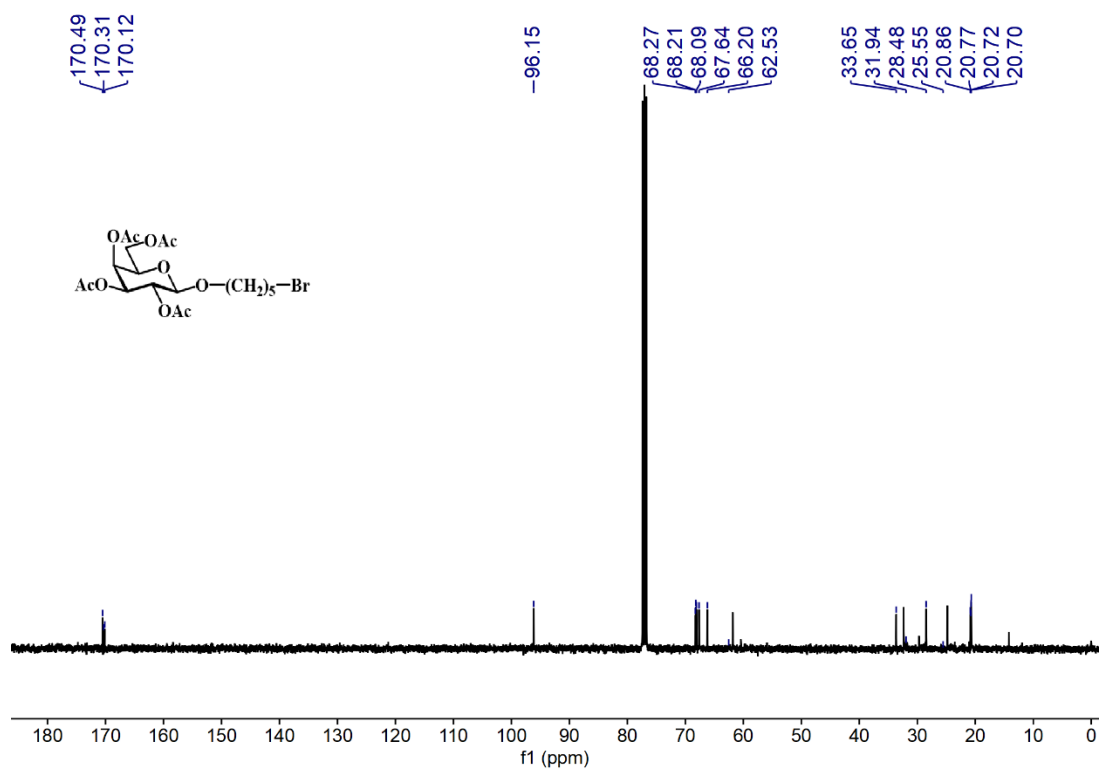


Fig. S2. ¹³C NMR and spectrum of compound 2.

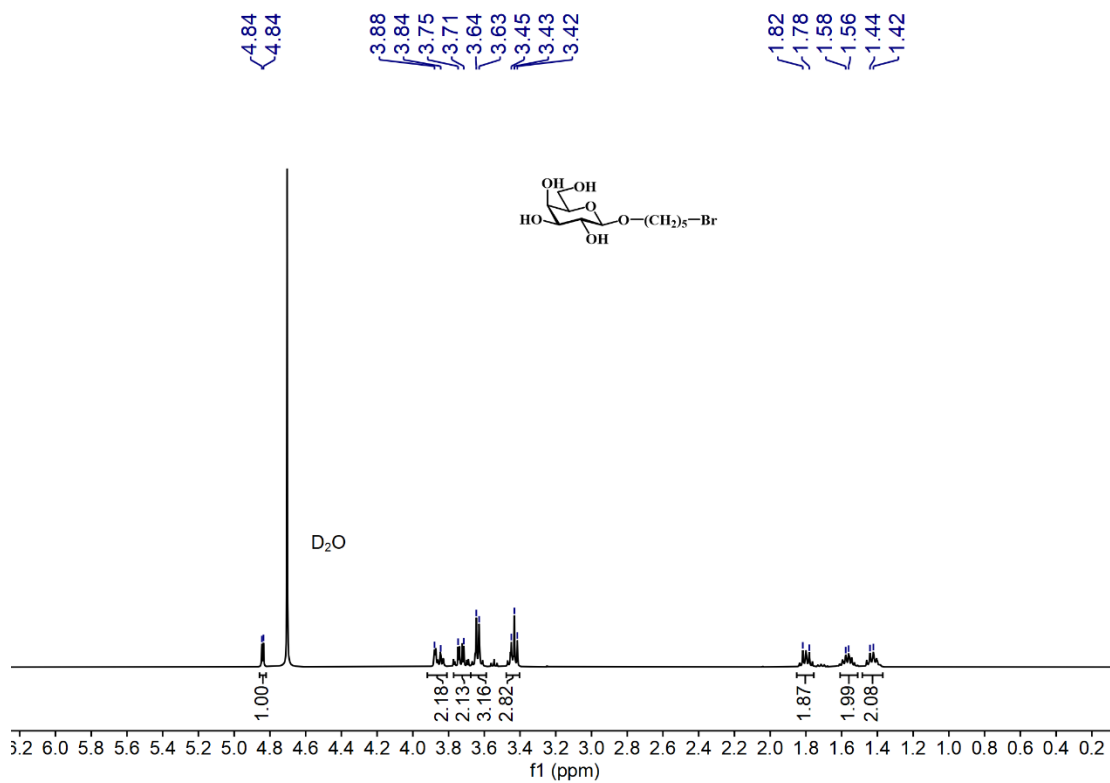


Fig. S3. $^1\text{H NMR}$ spectrum of compound 3.

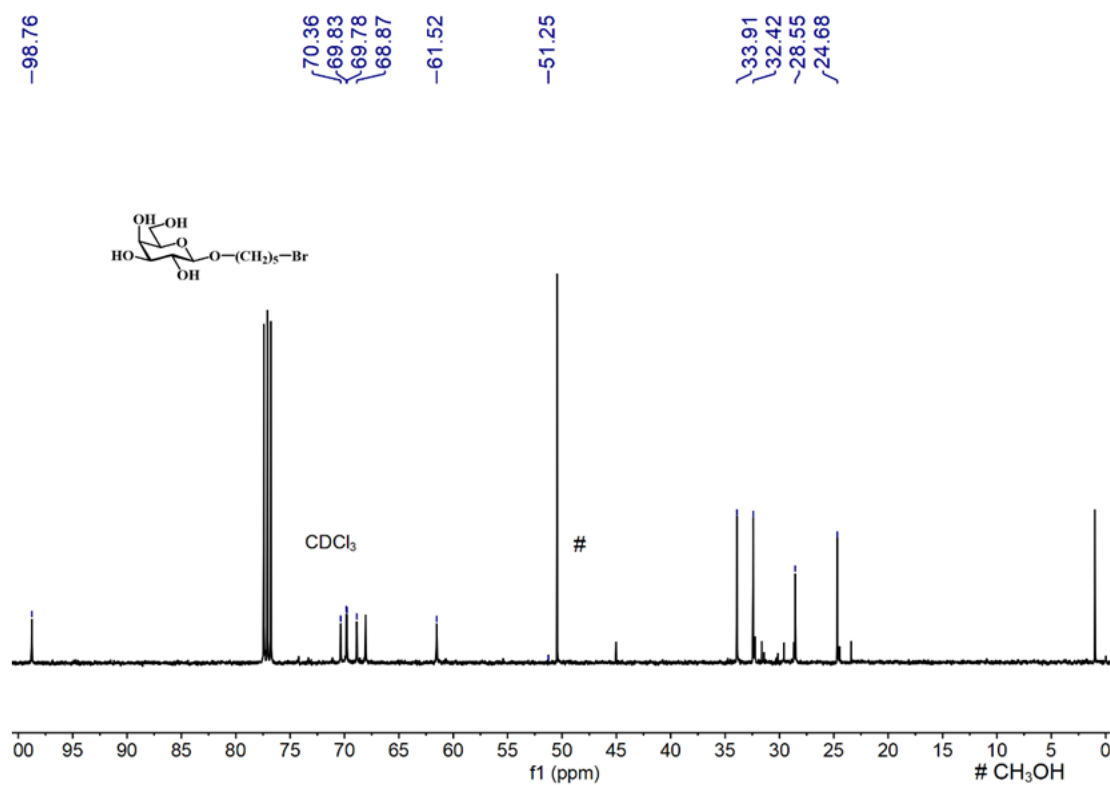


Fig. S4. $^{13}\text{C NMR}$ and spectrum of compound 3.

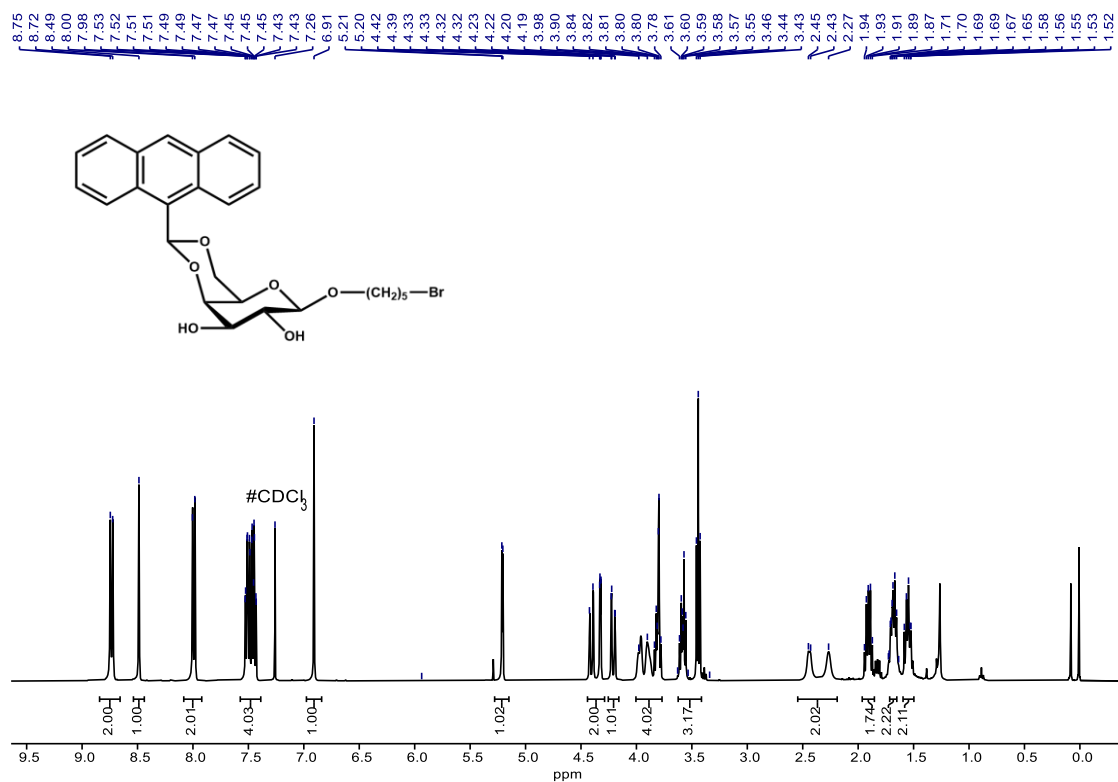


Fig. S5. ¹H NMR spectrum of compound 4.

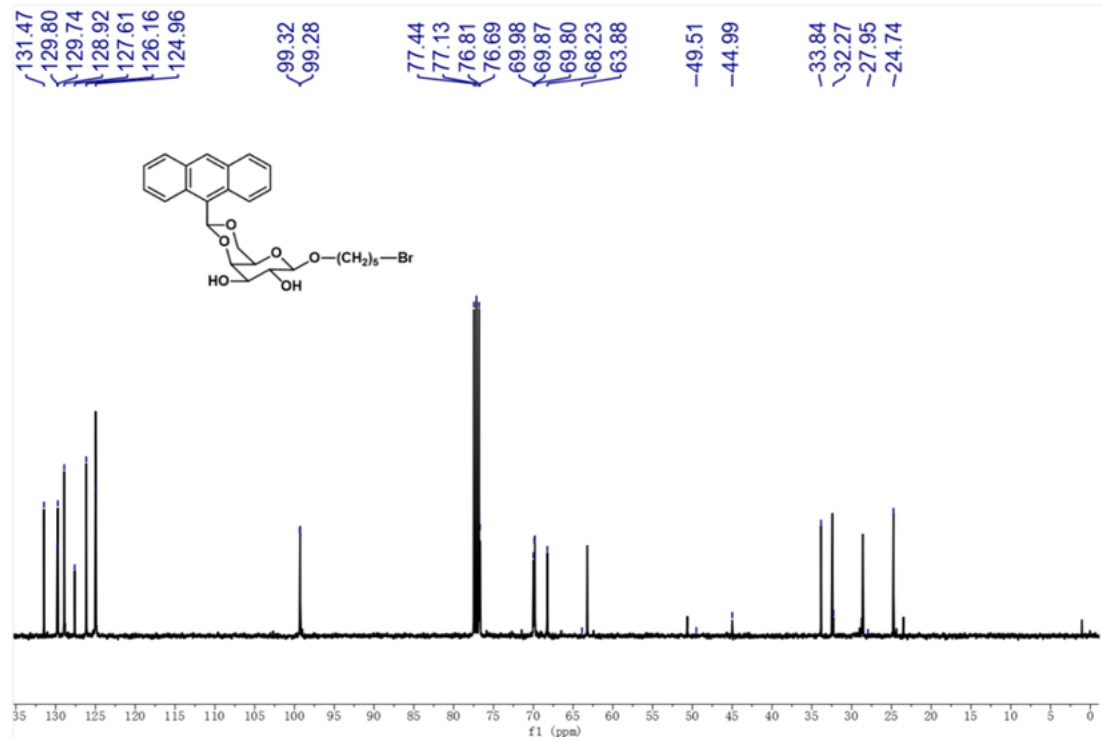


Fig. S6. ¹³C NMR and spectrum of compound 4.

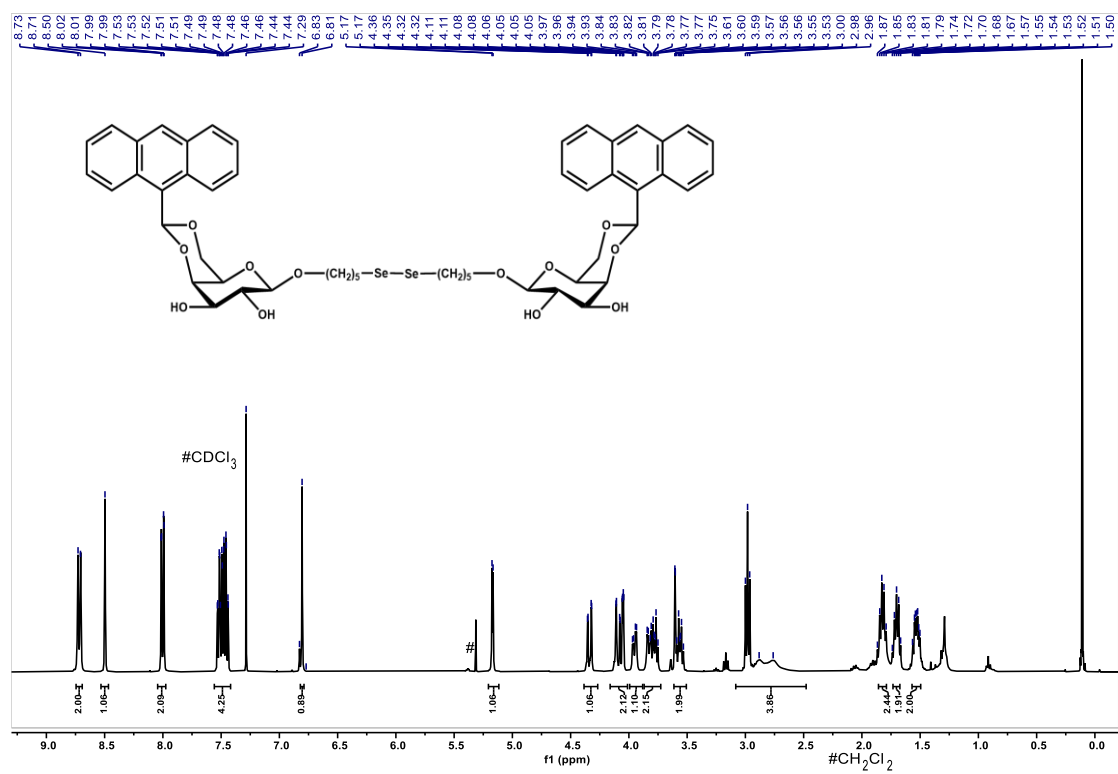


Fig. S7. ¹H NMR spectrum of compound 5.

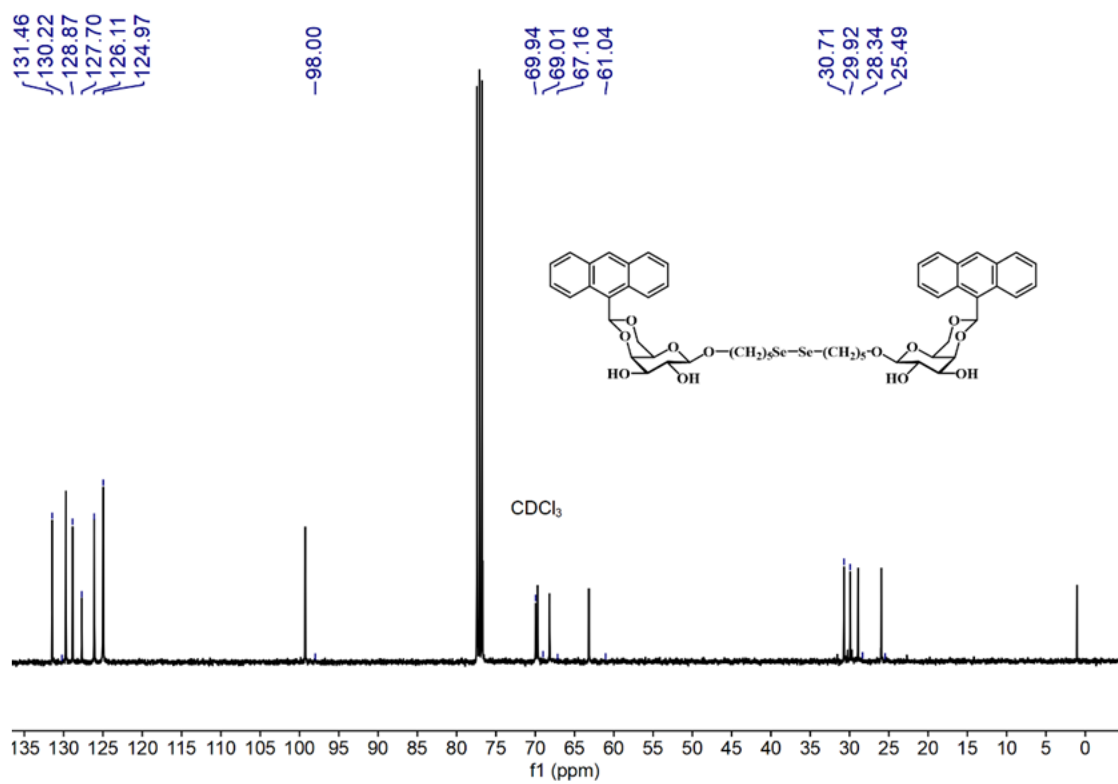


Fig. S8. ¹³C NMR spectrum of compound 5.

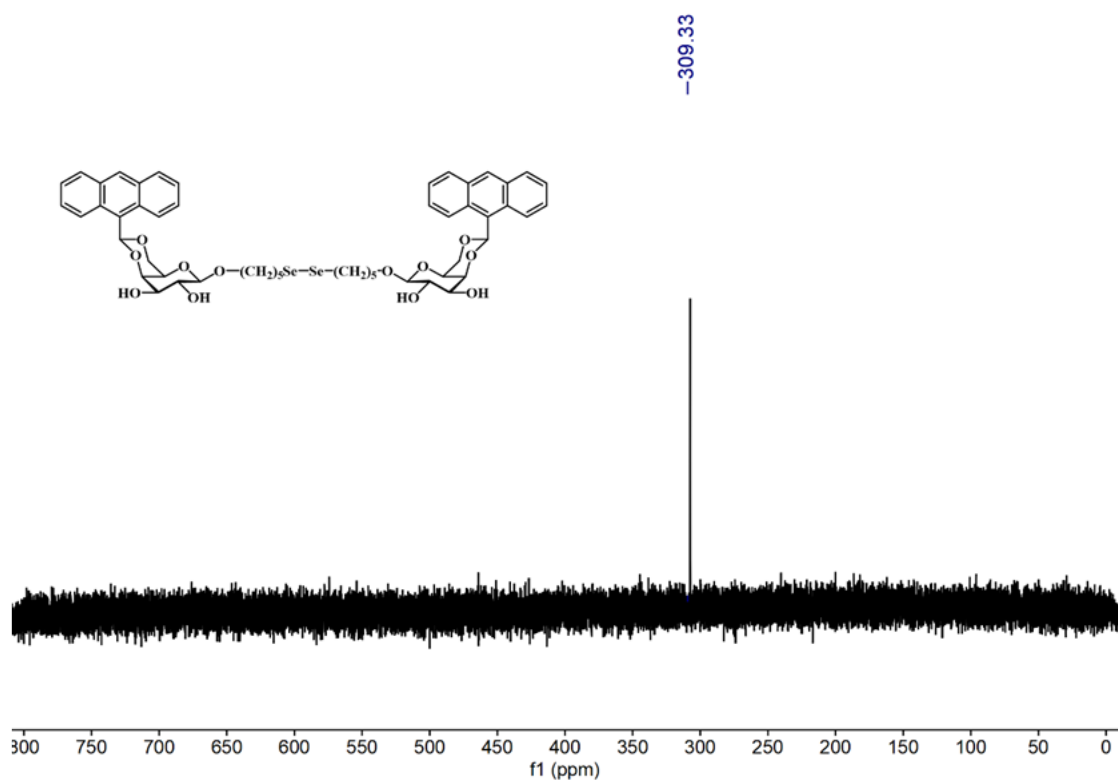


Fig. S9. ^{77}Se NMR spectrum of compound **5**.

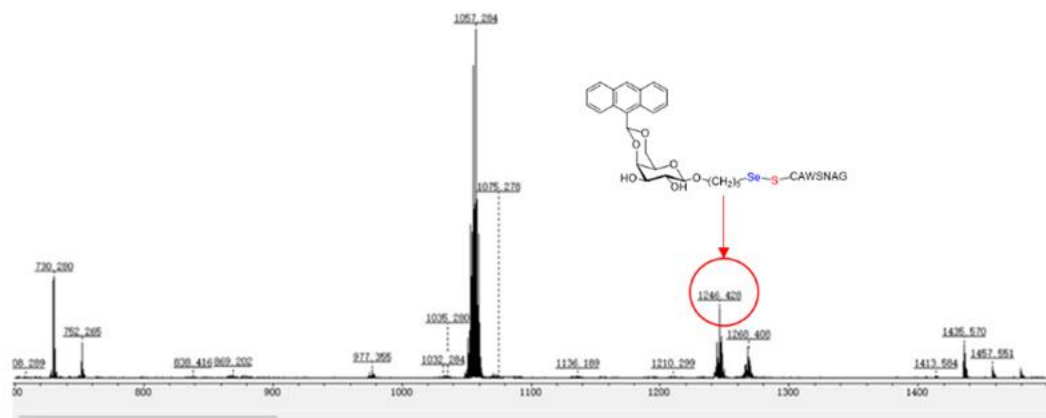


Fig. S10. MALDI-TOF-MS mass spectrum of compound **5** + peptide (CAWSNAG).

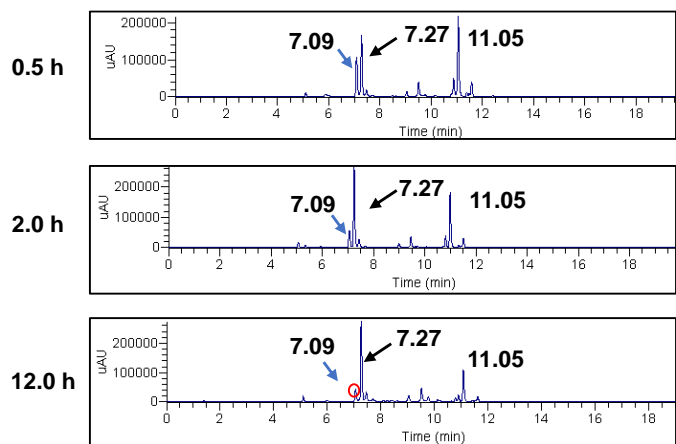
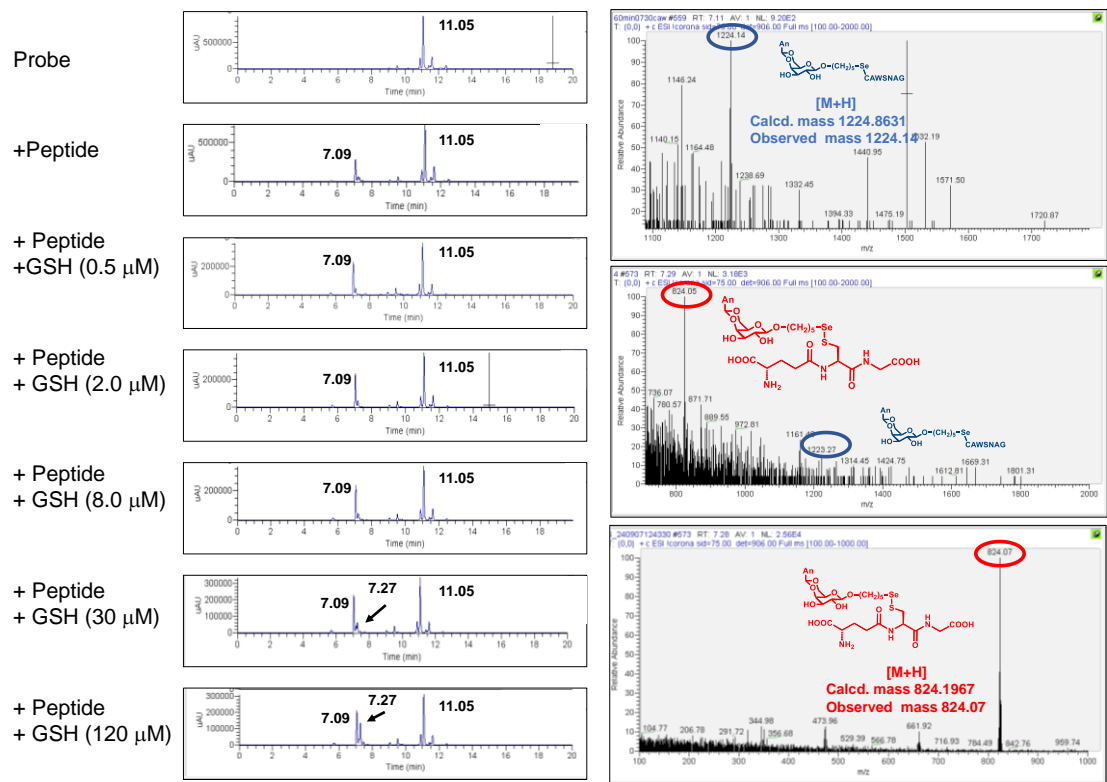


Fig. S12. LC-MS analysis of the probe-peptide conjugate in the presence of reduced glutathione (1.0 mM) after different times.

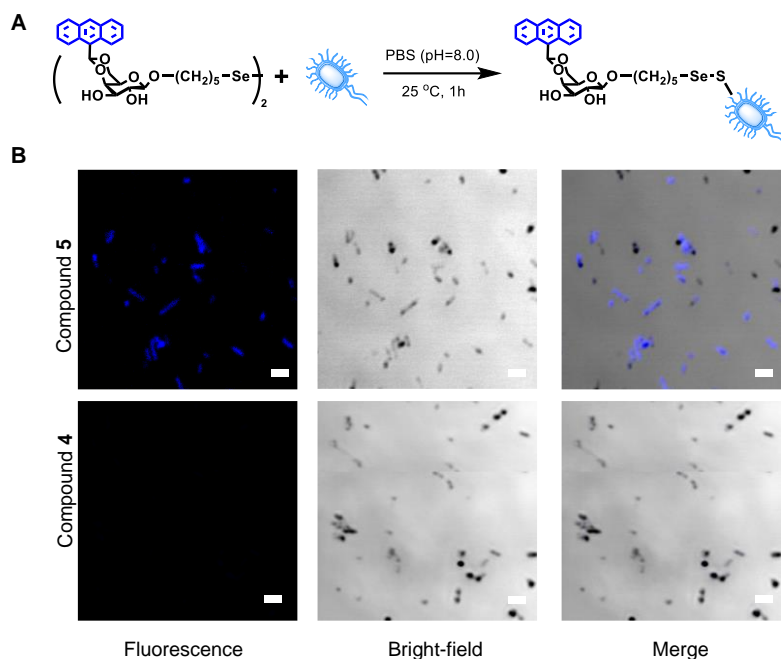


Fig. S13. (A) Schematic diagram of the reaction routine for labelling *E. coli* with the probe **5**. (B) Fluorescence confocal images of *E. coli* labelled with probe **5**. Scale bar, 5 μm .

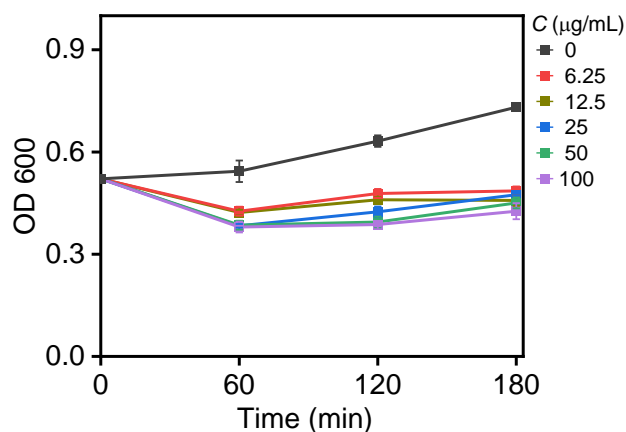


Fig. S14. Effects of varying concentrations of compound **5** on the growth of *E. coli*.

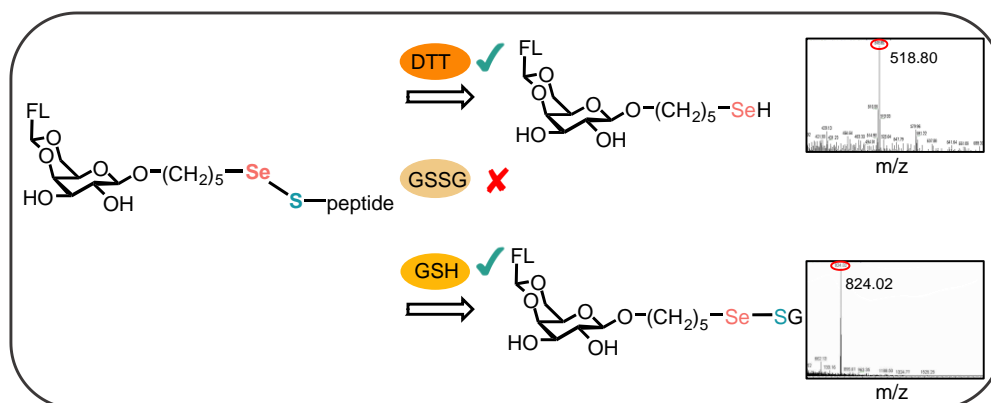


Fig. S15. The effect of reducing sulfhydryl-containing compounds, GSH and DTT, on the conjugation of probe-peptide via Se-S covalent chemistry.