Antimicrobial activity of the Auranofin analogue bearing acetylcysteine in place of thiosugar against *Staphylococcus* strains. An experimental and theoretical investigation

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Characterization of AF-AcCys

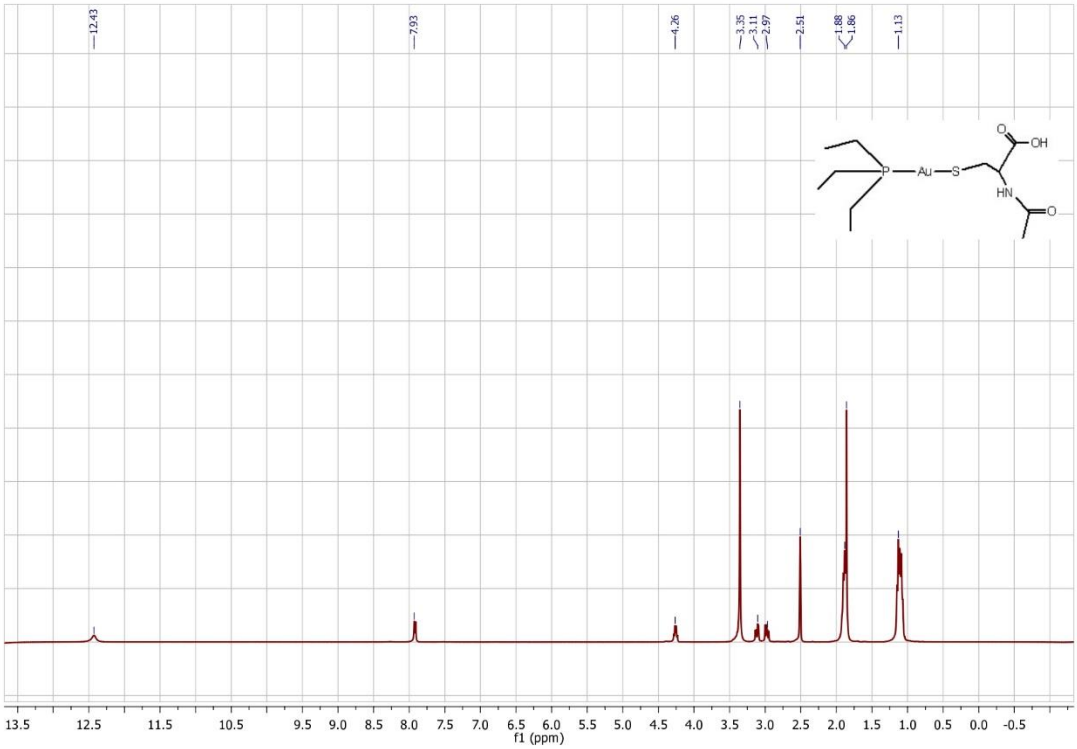

Figure S1: ^{1}HNMR (400 MHz; DMSO-d_6).

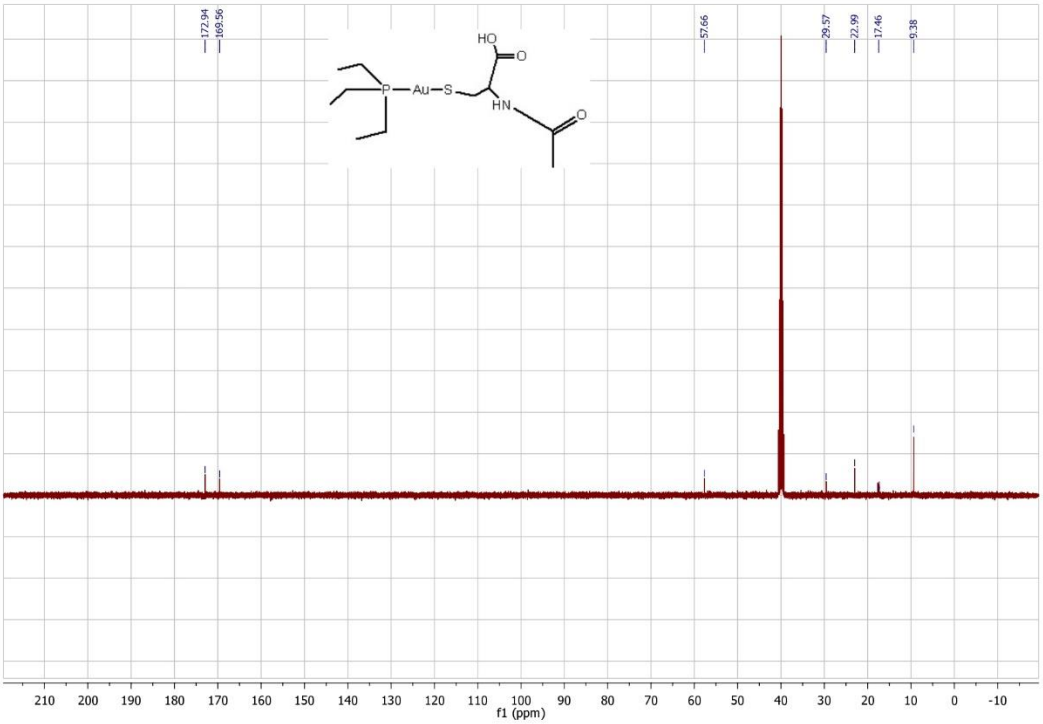

Figure S2: $^{13}C\{^{1}H\}$NMR (100 MHz; DMSO-d_6).

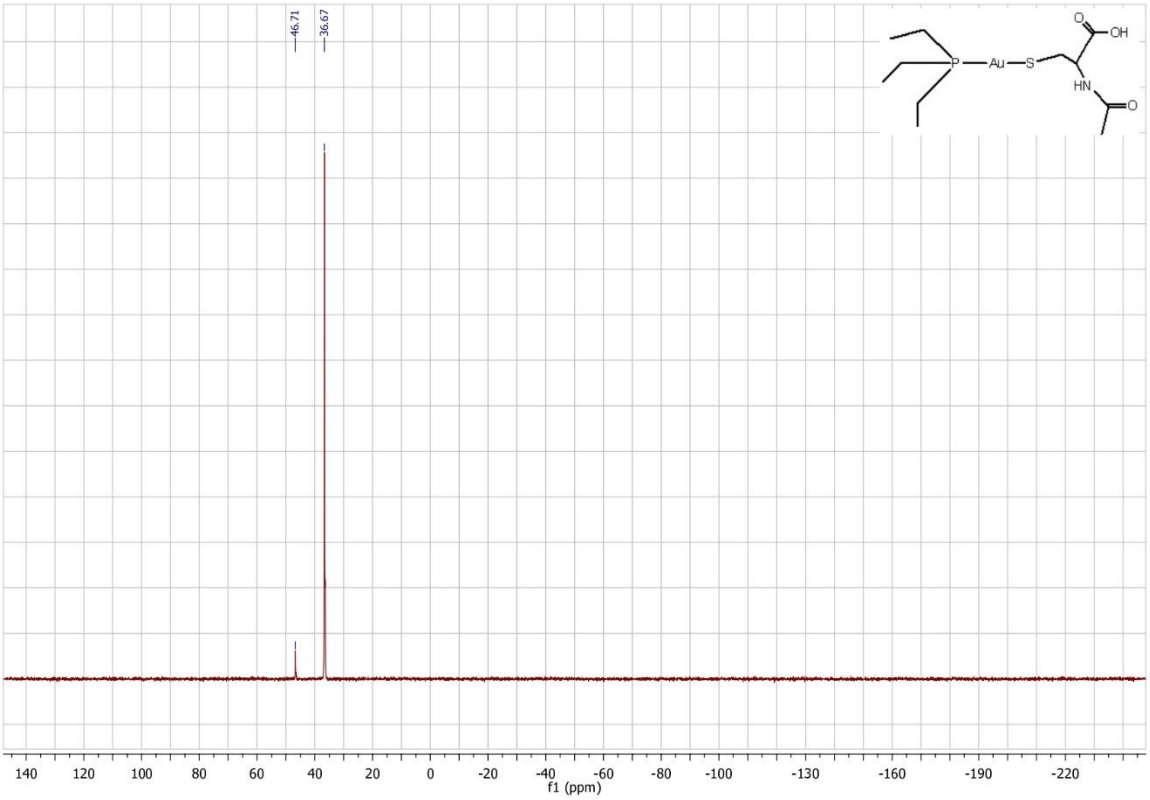

Figure S3: $^{31}P\{^{1}H\}$NMR (160 MHz; DMSO-d_6).

Stability studies of AF-AcCys and Auranofin

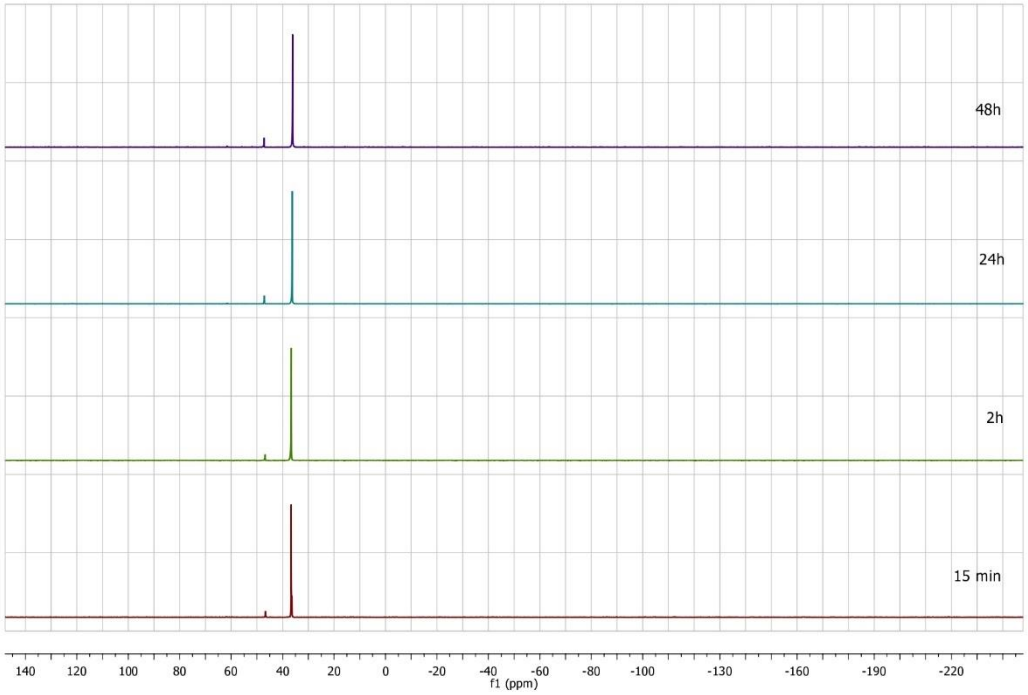

Figure S4: Stability study of AF-AcCys; $^{31}P\{^{1}H\}$NMR (160 MHz; DMSO-d_6/D_2O 1:1) δ = *46.48; 36.66*.

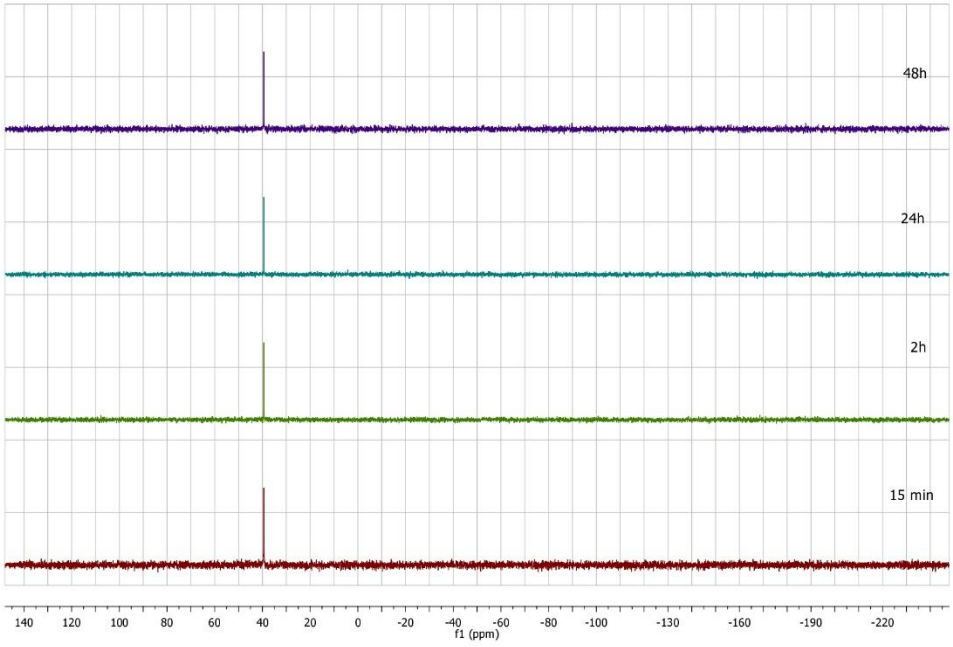

Figure S5: Stability study of Auranofin; $^{31}P\{^{1}H\}$NMR (160 MHz; DMSO-d_6/D_2O 2:1) δ = 39.45.

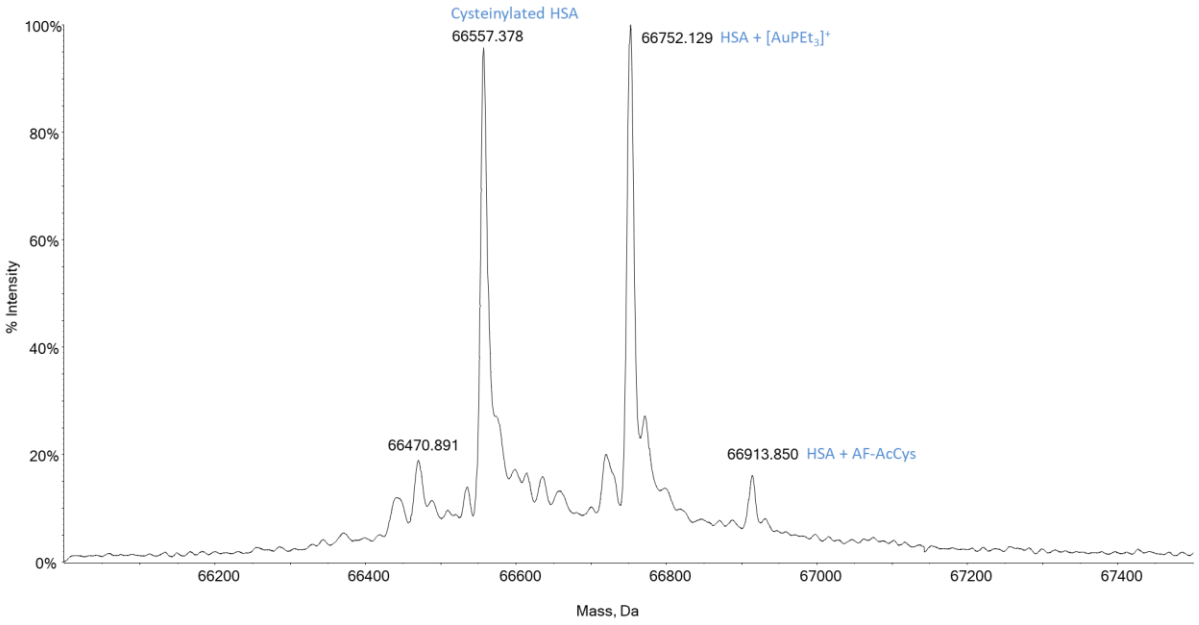

Figure S6. Deconvoluted ESI mass spectrum for HSA $5 \cdot 10^{-6}$ M incubated with AF-AcCys (1:2 ratio) for 24 h at 37 °C in ammonium acetate solution 20 mM, pH=6.8.

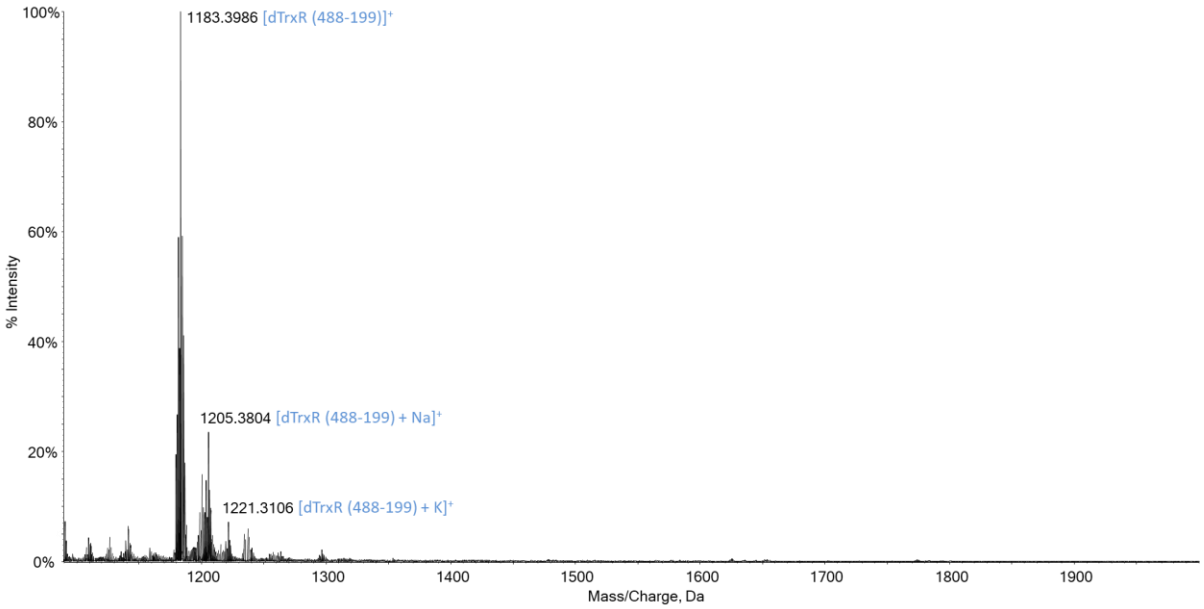

Figure S7. ESI mass spectrum of dTrxR(488–499) 10^{-6} M in water.

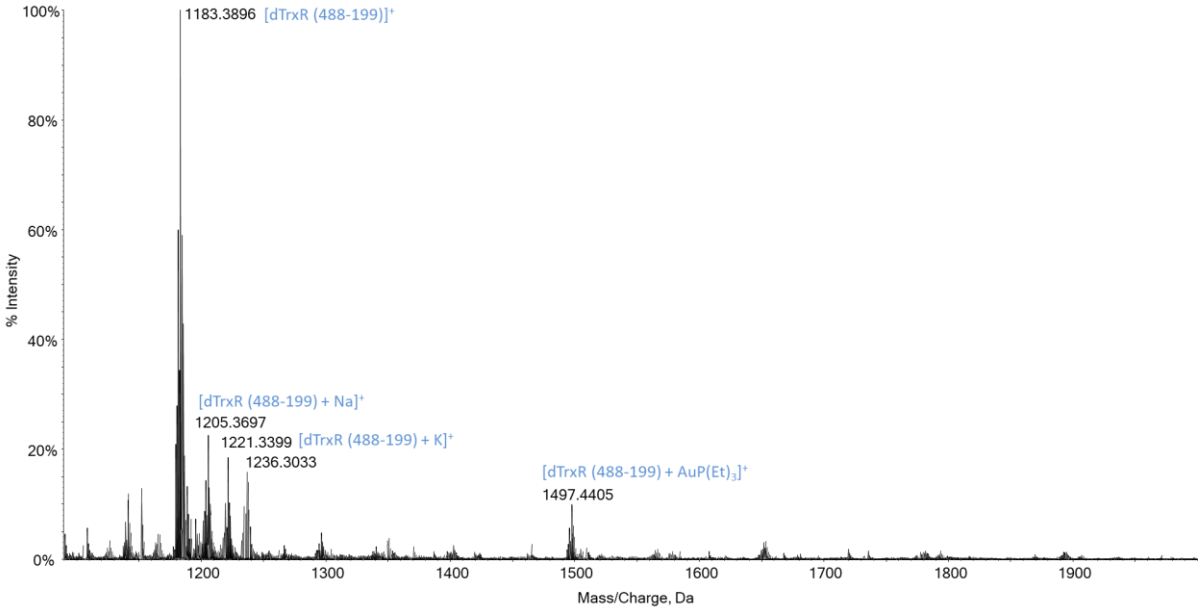

Figure S8. ESI mass spectrum of dTrxR(488–499) 10^{-6} M incubated with AF-AcCys (1:2 ratio) for 30 min at 37 °C in water.

Table S1. Mulliken charges distribution in AF and AF-AcCys. All values in a.u.

Fragment or atom	Mulliken charges	
	AF	AF-AcCys
Au	+0.14	+0.16
P	+0.17	+0.17
PEt_3	+0.37	+0.34
S	-0.51	-0.56
Thiosugar/AcCys	-0.51	-0.50