

Supporting Information

Unique Reactivity of Kiteplatin with S-donor Biomolecules and Nucleotides.

Emanuele Petruzzella,^{a,b} Nicola Margiotta,^b Giovanni Natile^b and James D. Hoeschele^a.

^a Chemistry Department, Eastern Michigan University, Ypsilanti, MI 48197, USA

Tel: +17344876681; email: jhoesche@emich.edu

^b Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Via E. Orabona 4, 70125

Bari, Italy

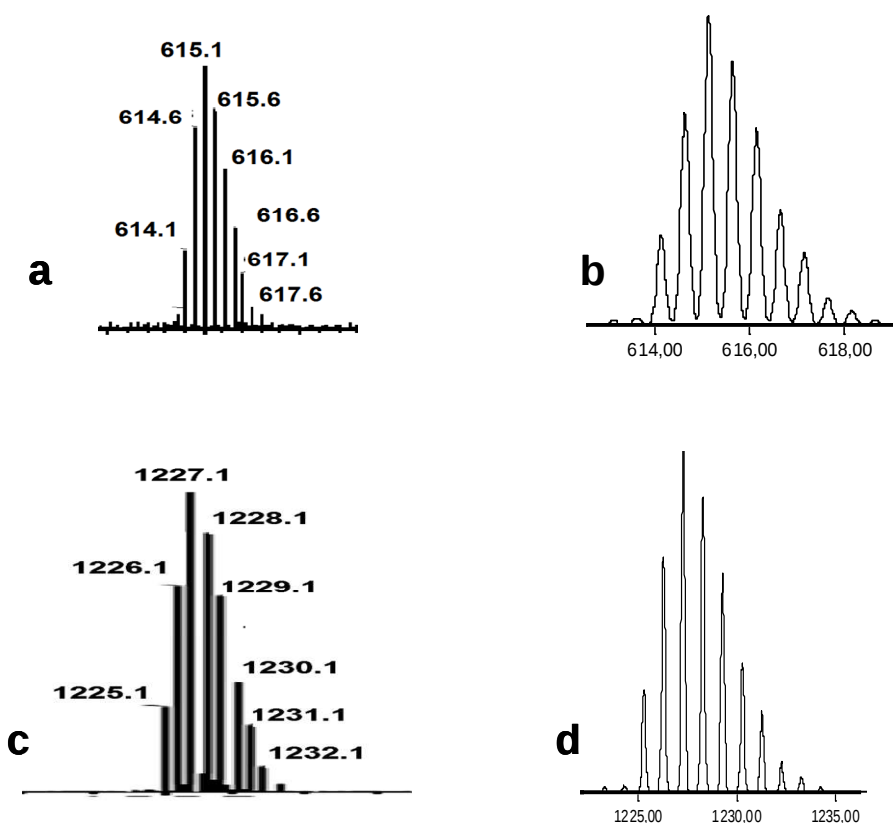


Figure S1. ESI-MS spectra obtained from HPLC peak I of the reaction between kiteplatin and glutathione. Spectrum of positive doubly-charged ion $[C_{32}H_{60}N_{10}O_{12}S_2Pt_2]^{2+}$: a) experimental, b) calculated isotopic distribution. ESI-MS spectrum of negative ion $[C_{32}H_{57}N_{10}O_{12}S_2Pt_2]^-$: c) experimental, d) calculated isotopic distribution.

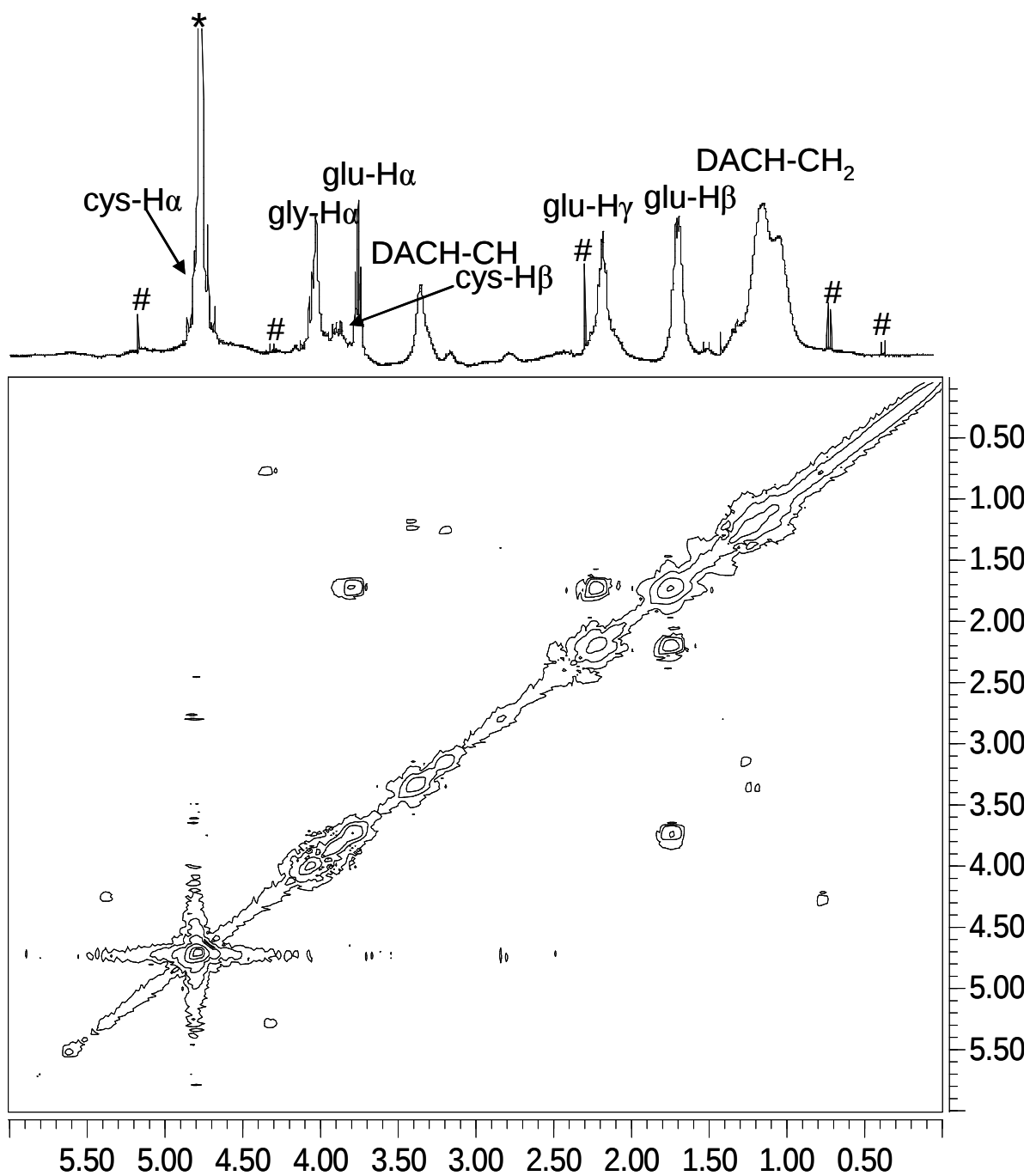


Figure S2. ^1H 1D (top) and 2D COSY (bottom) spectra of kiteplatin-glutathione adduct **I** with proton assignments. # indicates signals belonging to impurities present in the sample. * indicates residual solvent peak.

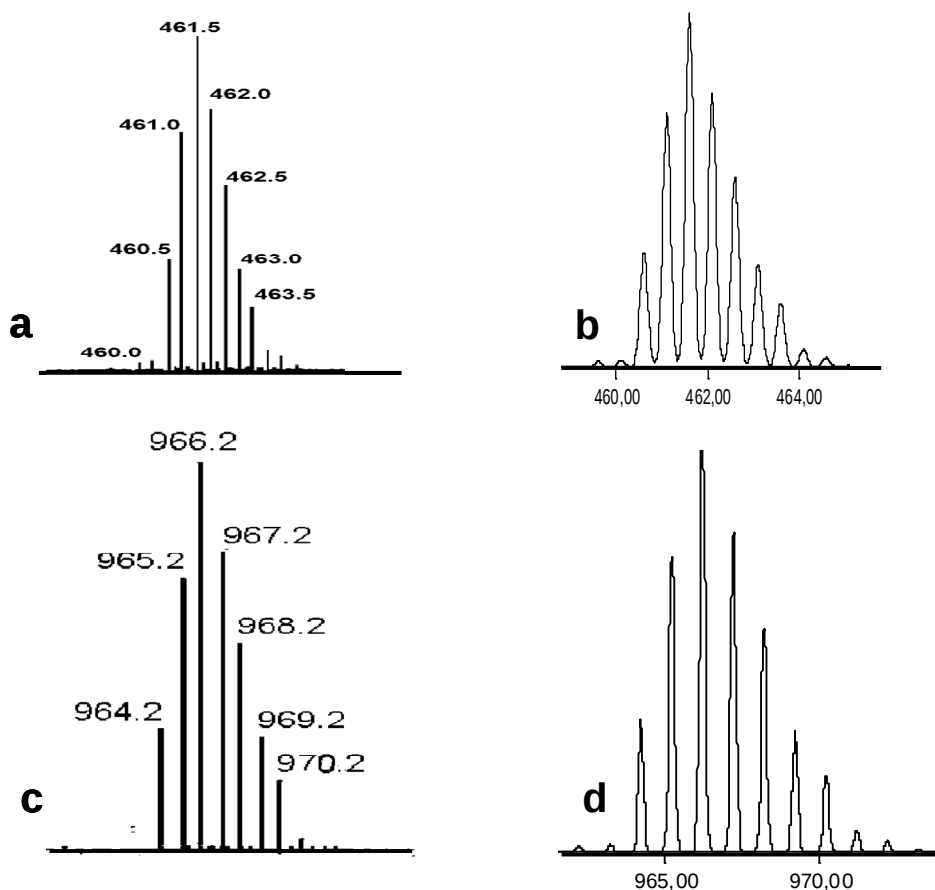


Figure S3. ESI-MS spectrum obtained from HPLC peak **II** of the reaction between kiteplatin and glutathione. Spectrum of positive doubly-charged ion $[C_{22}H_{43}N_7O_6Pt_2S]^{2+}$: a) experimental, b) calculated isotopic distribution. ESI-MS spectrum of negative ion $[C_{23}H_{41}N_7O_8Pt_2S]^-$: c) experimental, d) calculated isotopic distribution.

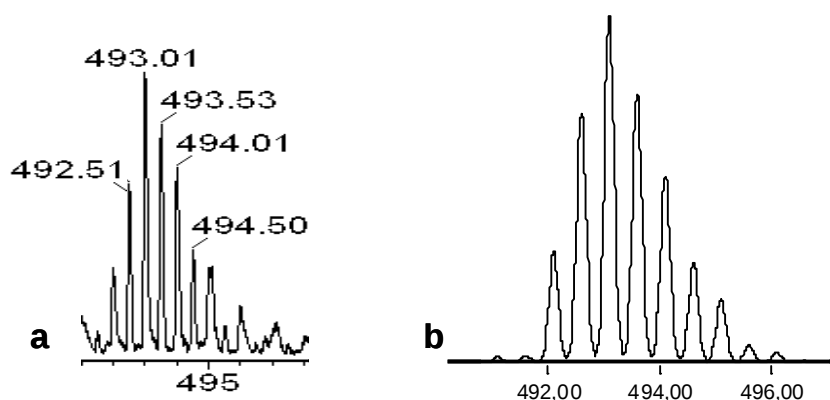


Figure S4. ESI-MS spectrum of positive doubly-charged ion $[C_{22}H_{43}N_7Na_2O_7Pt_2S]^{2+}$ obtained from HPLC peak **III** of the reaction between kiteplatin and glutathione: a) experimental, b) calculated isotopic distribution.

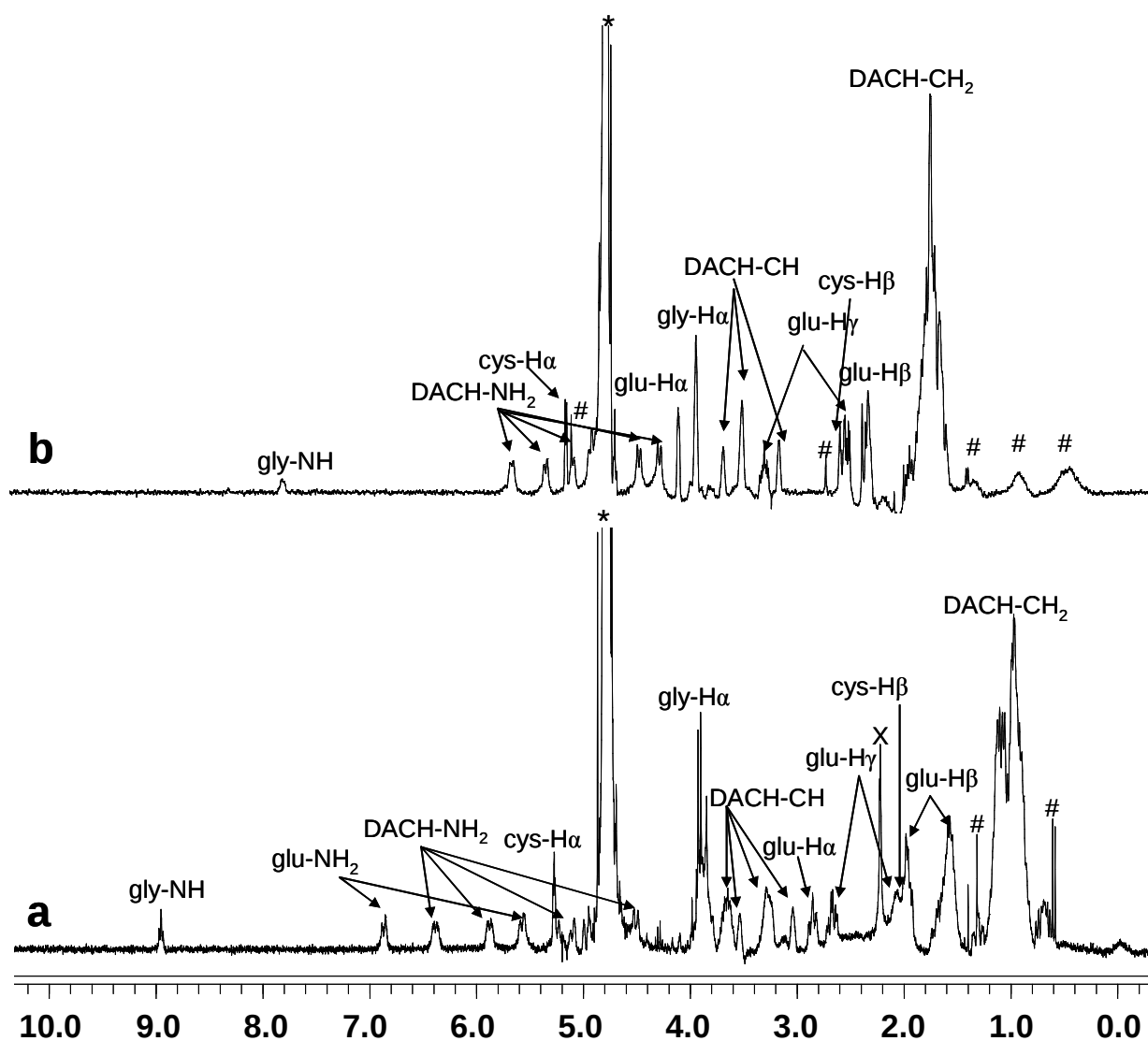


Figure S₅. ^1H NMR spectra of kiteplatin-glutathione adducts **II** (a) and **III** (b) with proton assignments. # indicate signals belonging to impurities present in the sample. * indicates residual solvent peak.

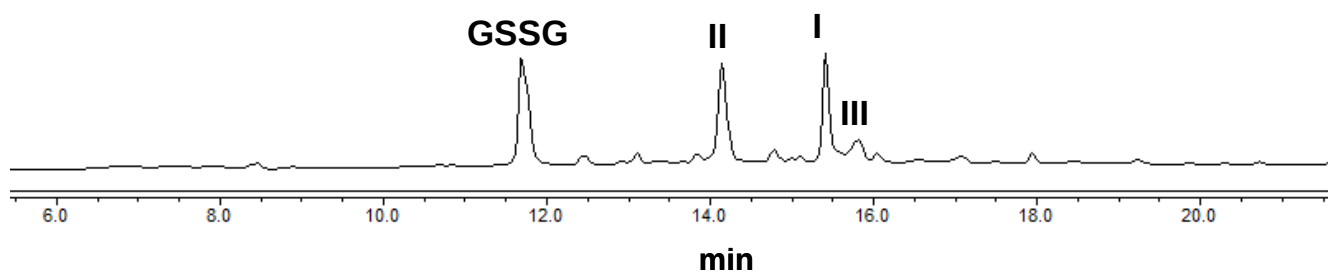


Figure S₆. HPLC chromatogram of the reaction between kiteplatin and GSSG after 1 day at 37 °C. Also in this case adduct **II** redissolved in water generating adduct **III**.

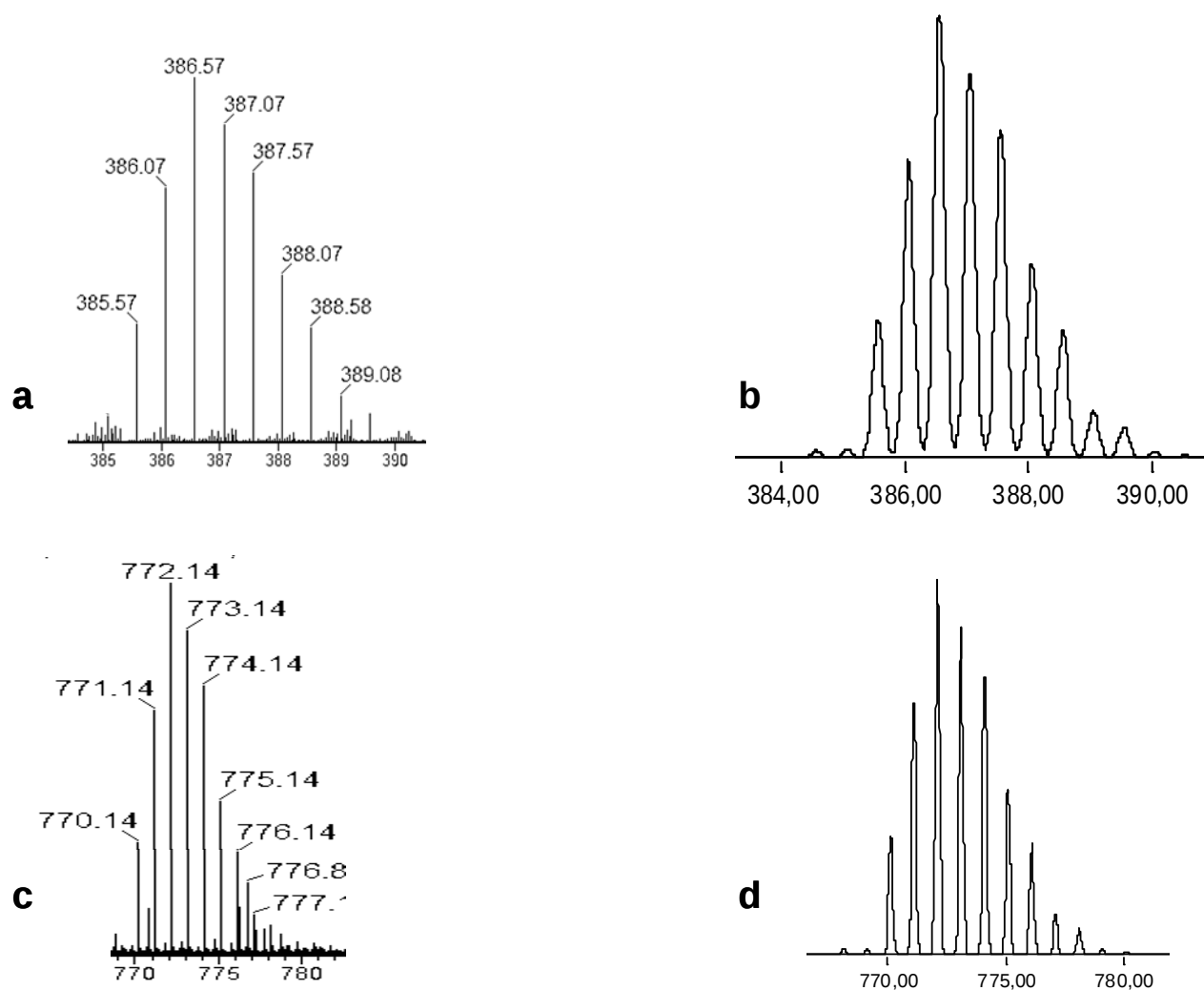


Figure S7. ESI-MS spectrum of the major product of the reaction between kiteplatin and cysteine. The positive doubly-charged ion, $[C_{15}H_{34}ClN_5O_2SPt_2]^{2+}$: a) experimental, b) calculated isotopic distribution. The positive mono charged ion $[C_{15}H_{33}ClN_5O_2SPt_2]^+$: a) experimental, b) calculated isotopic distribution.

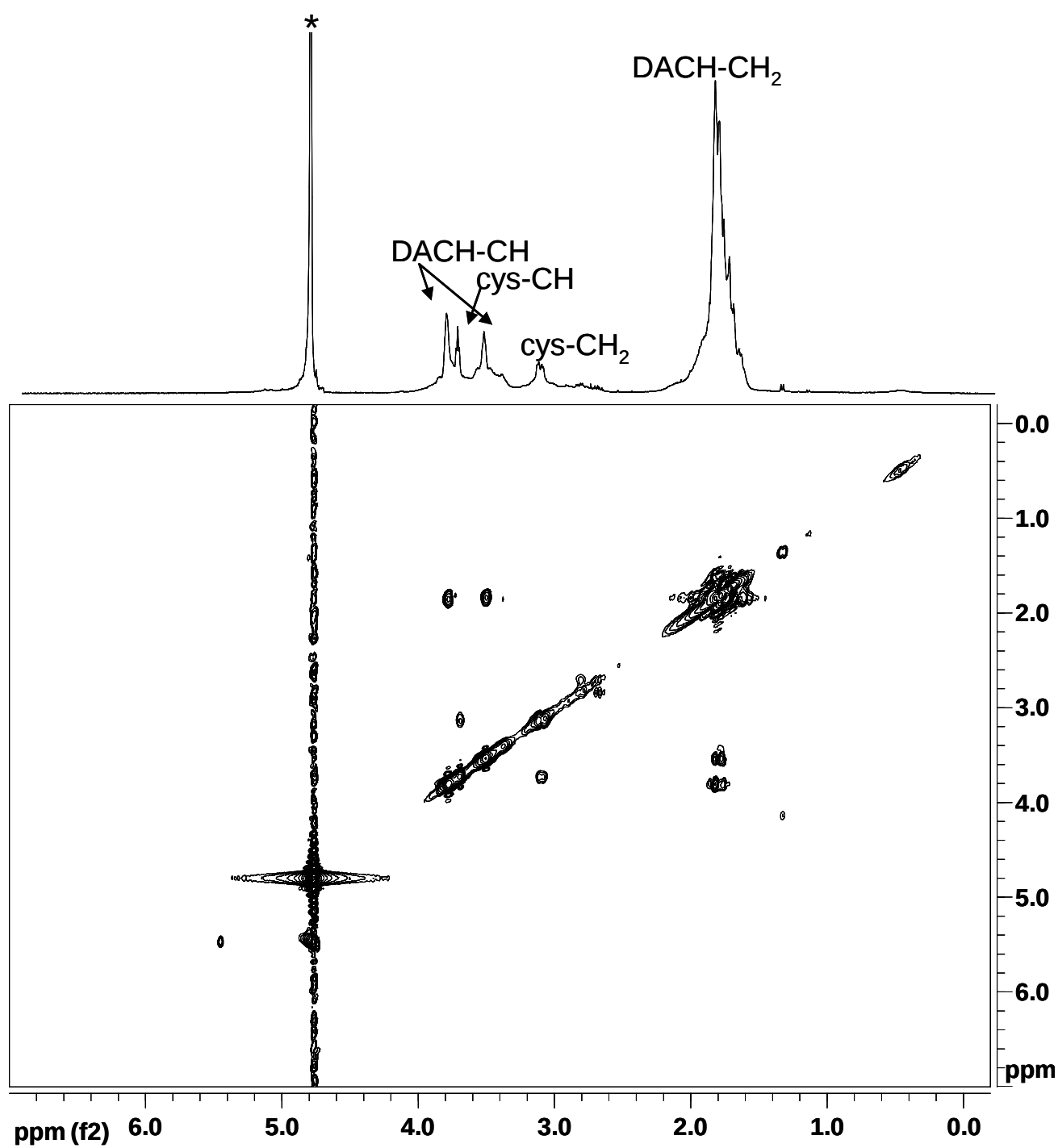


Figure S₈. ¹H 1D (top) and 2D COSY (bottom) spectra of kiteplatin-cysteine adduct recorded in D₂O. * indicates residual solvent peak.

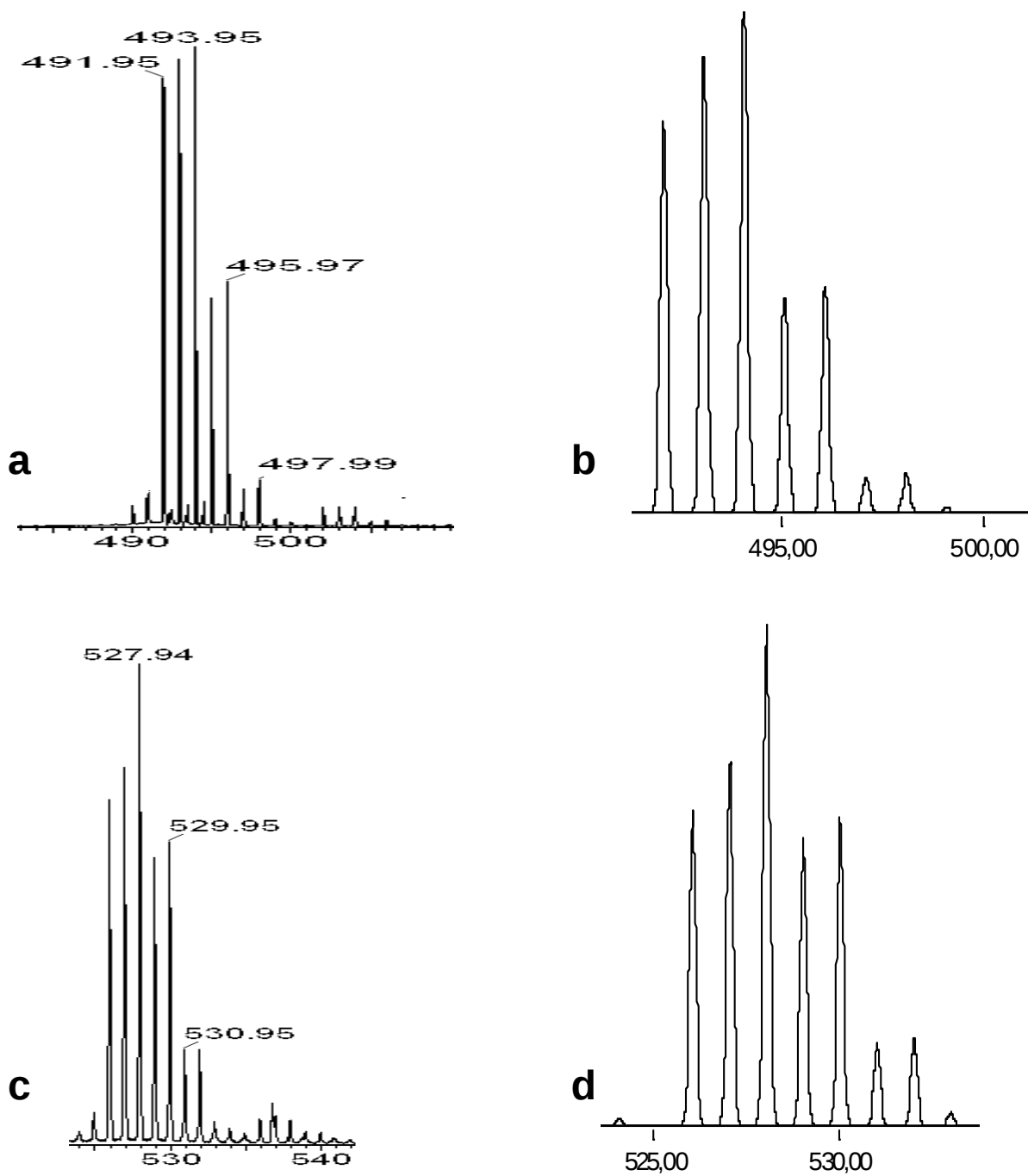


Figure S9. ESI-MS spectra of the major product of the reaction between kiteplatin and methione. The positive doubly charged ion $[C_{11}H_{25}ClN_3O_2PtS]^{2+}$: a) experimental, b) calculated isotopic distribution. The negative ion $[C_{11}H_{24}Cl_3N_3O_2PtS]^-$: c) experimental, d) calculated isotopic distribution.

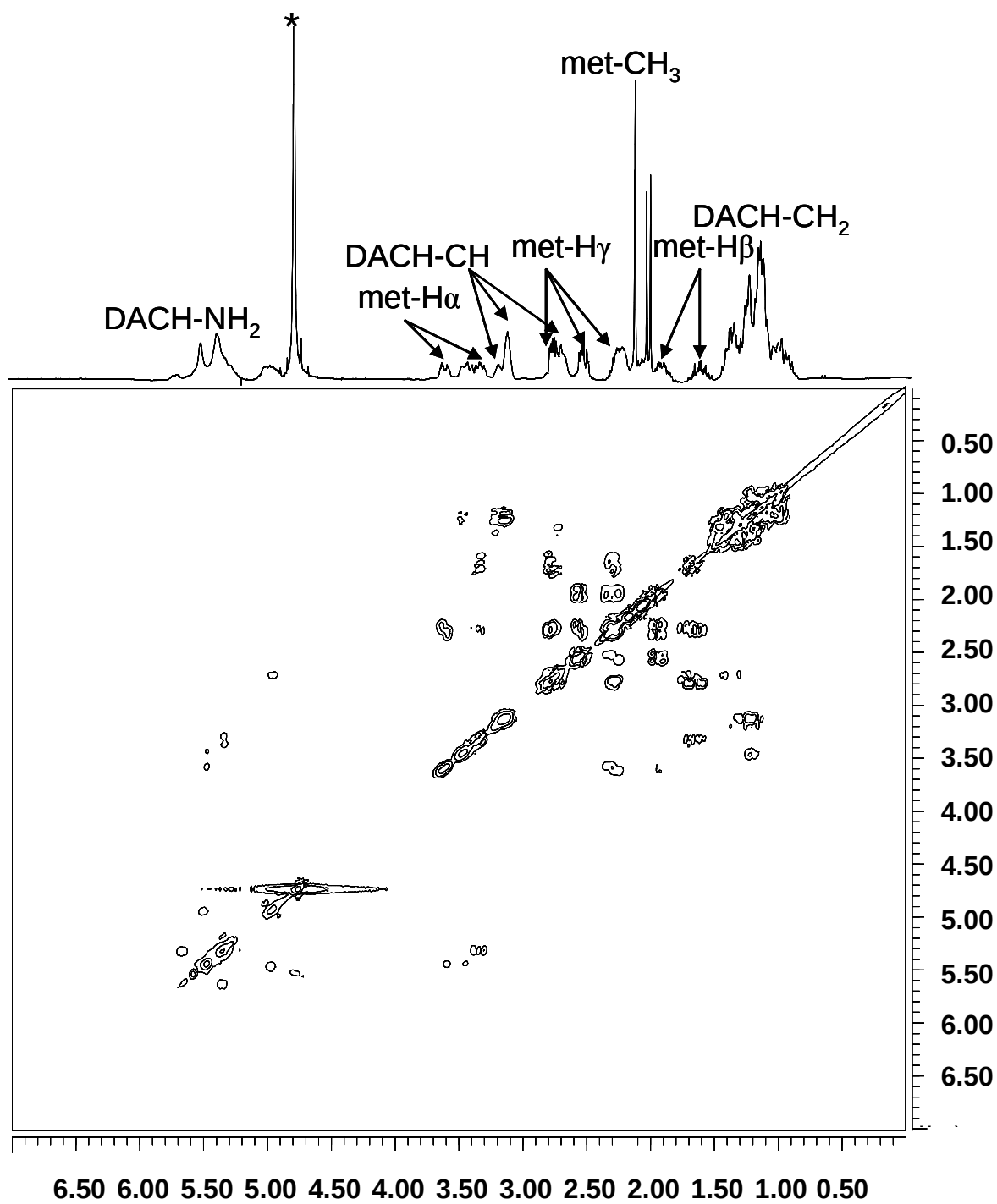


Figure S₁₀. ^1H 1D (top) and 2D COSY (bottom) spectra of kiteplatin-methione adduct recorded in D_2O . * indicates residual solvent peak.