Supporting Information

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

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Figure S1. ESI-MS spectra obtained from HPLC peak I of the reaction between kiteplatin and glutathione. Spectrum of positive doubly-charged ion [C₃₂H₆₀N₁₀O₁₂S₂Pt₂]²⁺: a) experimental, b) calculated isotopic distribution. ESI-MS spectrum of negative ion [C₃₂H₅₇N₁₀O₁₂S₂Pt₂]⁻: c) experimental, d) calculated isotopic distribution.
Figure S2. $^1$H 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\textsubscript{22}H\textsubscript{43}N\textsubscript{7}O\textsubscript{6}Pt\textsubscript{2}S]\textsuperscript{2+}: a) experimental, b) calculated isotopic distribution. ESI-MS spectrum of negative ion [C\textsubscript{23}H\textsubscript{41}N\textsubscript{7}O\textsubscript{8}Pt\textsubscript{2}S]\textsuperscript{−}: c) experimental, d) calculated isotopic distribution.

Figure S4. ESI-MS spectrum of positive doubly-charged ion [C\textsubscript{22}H\textsubscript{43}N\textsubscript{7}Na\textsubscript{2}O\textsubscript{7}Pt\textsubscript{2}S]\textsuperscript{2+} obtained from HPLC peak III of the reaction between kiteplatin and glutathione: a) experimental, b) calculated isotopic distribution.
Figure S5. $^1$H 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. $^1$H 1D (top) and 2D COSY (bottom) spectra of kiteplatin-cysteine adduct recorded in D$_2$O. * 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 $[\text{C}_{11}\text{H}_{25}\text{ClN}_{3}\text{O}_{2}\text{PtS}]^{2+}$: a) experimental, b) calculated isotopic distribution. The negative ion $[\text{C}_{11}\text{H}_{24}\text{Cl}_{3}\text{N}_{3}\text{O}_{2}\text{PtS}]^{-}$: c) experimental, d) calculated isotopic distribution.
Figure S10. $^1$H 1D (top) and 2D COSY (bottom) spectra of kiteplatin-methionine adduct recorded in D$_2$O. * indicates residual solvent peak.