

## **Interactions of oxaliplatin with the cytoplasmic thiol containing ligand glutathione**

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Figure S1: A comparison between the experimentally determined isotopic patterns of the assigned species in Table 1 (panels A) and their corresponding theoretically modeled isotopic patterns (panels B) in Gaussian profile mode at a resolution of 1500 using the Qual Browser version 2.0 software by Thermo Electron Corporation.

Figure S2: A comparison between the experimentally determined isotopic cluster at  $m/z$  615 observed in Figure 6 as obtained due to the isolation and fragmentation of the entire isotopic envelope of the ion  $[\text{GSH} + \text{OxPt} + \text{H}]^+$  (panels A) and the theoretically modeled pattern of the proposed  $[\text{GSH} - \text{H} + \text{Pt}(\text{dach})]^+$  ion (panels B).

Table S1: Electronic energies, Zero-Point Vibrational Energies, Thermal Energies, Entropies and relative free energies for species calculated at B3LYP/LANL2DZ. Italicized values are for PCM calculations in a water solvent.