## **Supporting Information**

## **Organometallic Glutathione S-transferase Inhibitors**

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Figure S1. Coplanarity of the bipyridine unit in the crystal of 1b (images produced using Mercury CCDC 3.6).



**Figure S2.** Intermolecular parallel-displaced  $\pi$ - $\pi$  stacking interactions between the bipyridine ligands in the crystal of **1b** (centroid-centroid distance 3.955 Å, distance between the two bipyridine planes 3.543 Å, image produced using Mercury CCDC 3.6.



**Figure S3.** Complex **1b** crystallized as a racemic mixture of the two enantiomers (*R*<sub>os</sub> and *S*<sub>os</sub>) owing to the chirality of the metal atoms (image produced using Mercury CCDC 3.6).



**Figure S4**. Hydrogen bonding interactions in the network of **1b** between the chloride anion (acting as a bifurcated acceptor) with the CH<sub>3</sub>OH and CHCl<sub>3</sub> solvents (image produced using Mercury CCDC 3.6).

**Table S1.** Parameters of intramolecular H-bonding interactions in the network of complex 1b (contact D-<br/>H $\cdots$ A corresponds to O-H $\cdots$ Cl<sup>-</sup> and C-H $\cdots$ Cl<sup>-</sup>).

<i>D</i> -H…A	Distance, Å			Angle
interaction	D-H	H <i>A</i>	<i>D</i> A	<i>D</i> -H… <i>A</i> , °
O-H…Cl <sup>-</sup>	0.840	2.384	3.027	133.81
C-H…Cl <sup>.</sup>	0.996	2.364	3.353	171.98



Figure S5. <sup>1</sup>H NMR spectra of 1a and 1b recorded in DMSO-d<sub>6</sub>.







**Figure S7**. Inhibition curves of **1a**, **1b**, **2a** and **2b** on GST P1-1. The activity of GST P1-1 was assayed in the presence of increasing concentrations of inhibitor.



**Figure S8.** IC<sub>50</sub> values (μM) determined for RAPTA-C, OAPTA-C, EA-H, ligands **L1** and **L2**, and complexes **1a**, **1b**, **2a** and **2b** towards human ovarian cancer A2780 and A2780cisR (cisplatin sensitive and resistant), immortalized and human embryonic kidney HEK-293 cells in a cell proliferation inhibition assay. Values are

given as the mean  $\pm$  SD.