

Copyright WILEY-VCH Verlag GmbH, D-69451 Weinheim, 2000.

Supporting Information for:

**First Crystal Structure of a Medicinally Relevant Gold Protein Complex:
Unexpected Binding of $[\text{Au}(\text{PEt}_3)]^+$ to Histidine**

Juan Zou, Paul Taylor, Jacqueline Dornan, Stephen P. Robinson, Malcolm D.

Walkinshaw*, Peter J. Sadler*

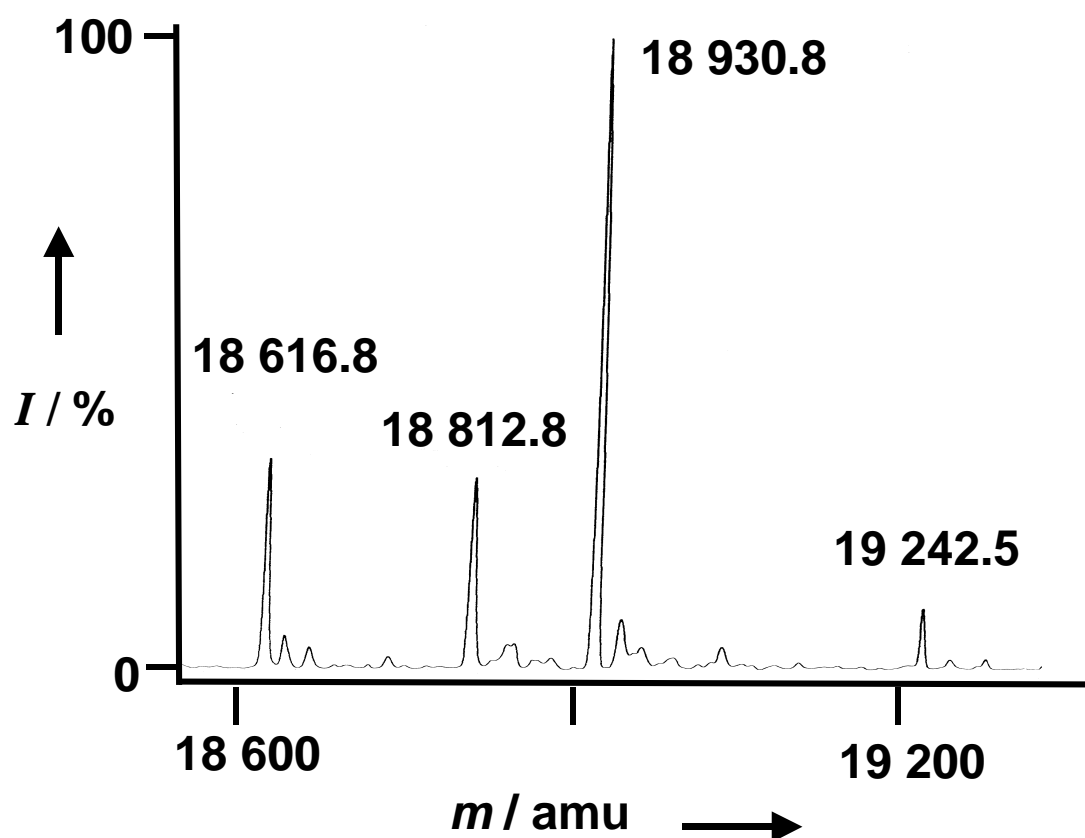


Figure S1. LC-ESI-MS of Cyp-3 (13.5 μM) after incubation with **1** (95 μM) for 5 d at 291 K. The peaks correspond to Cyp-3 + Au (18618.8 amu, theoretical mass: 18615.5 Da); Cyp-3 + 2Au (18812.8 amu, theoretical mass: 18812.4 Da); Cyp-3 + Au + $\{\text{AuPEt}_3\}$ (18930.8 amu, theoretical mass: 18930.6 Da); Cyp-3 + Au + 2 $\{\text{AuPEt}_3\}$ (19242.5 amu, theoretical mass: 19245.7 Da).

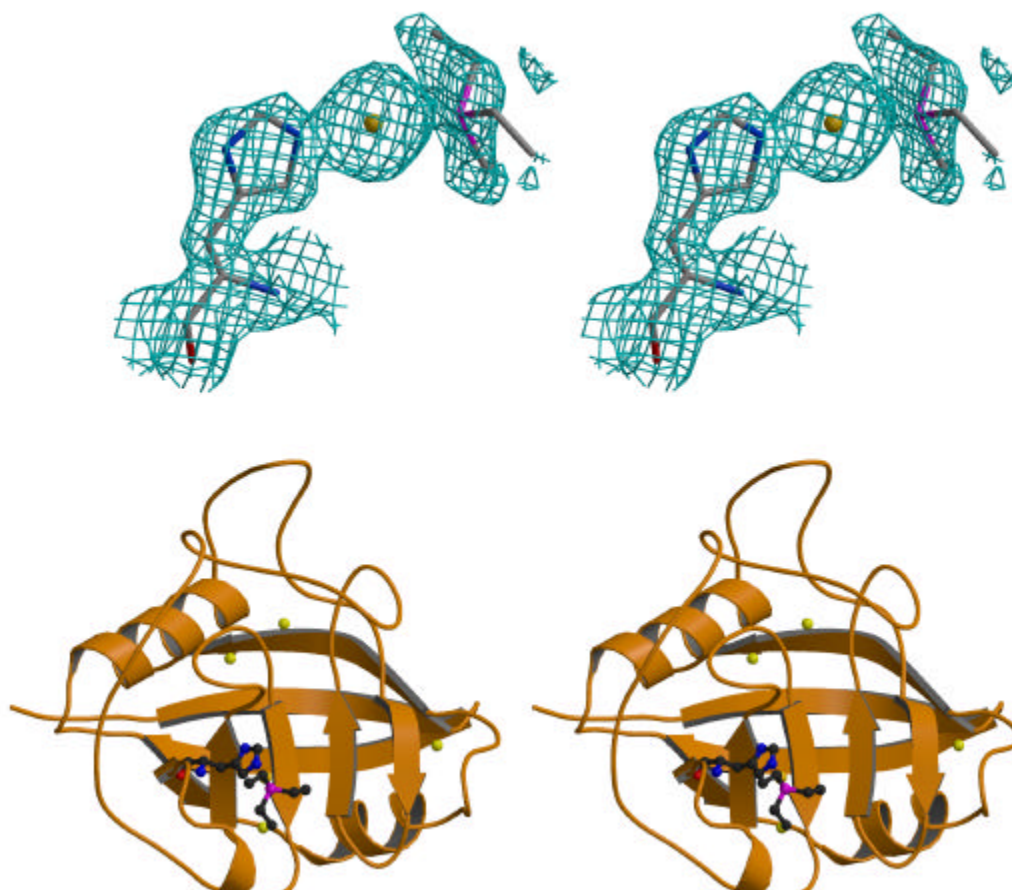


Figure S2. A colour version of Figure 3. **Top:** Stereo view of the gold binding site in Cyp-3. **Bottom:** Stereo view of Cyp-3 after reaction with **1** showing the S atoms of the 4 Cys residues (yellow balls: top left Cys40, top right Cys168, bottom left Cys122, bottom right Cys163), and $\{\text{AuPEt}_3\}^+$ bound to N ϵ 2 of His133 (N blue, Au orange, P purple).

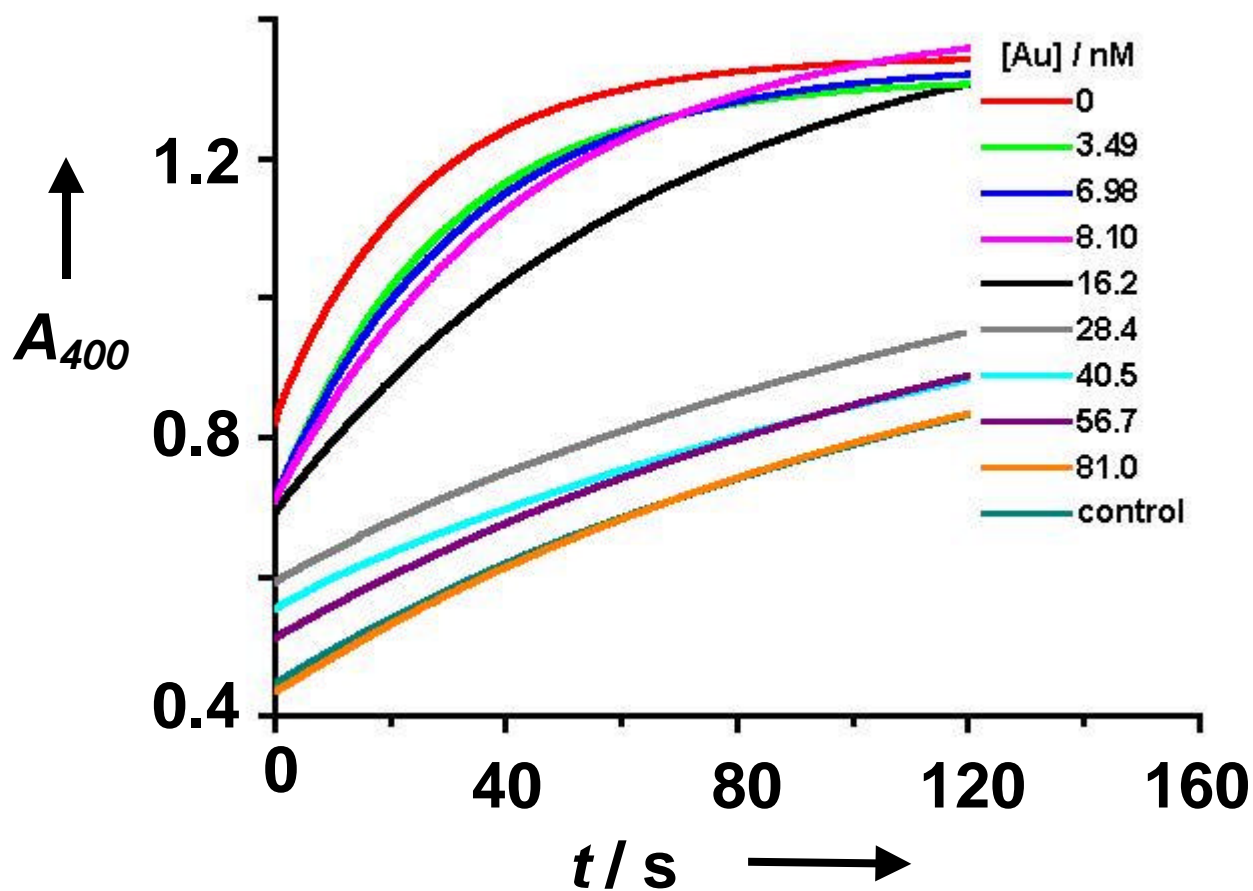


Figure S3. Plots of absorbance (400 nm) versus time for assay of the PPIase activity of Cyp-3 (8.1 nM) as described in ref. 11. The curves show the decrease in activity with increase in concentration of **1** from 0, 3.49, 6.98, 8.10, 16.2, 28.4, 40.5, 56.7 to 81.0 nM.