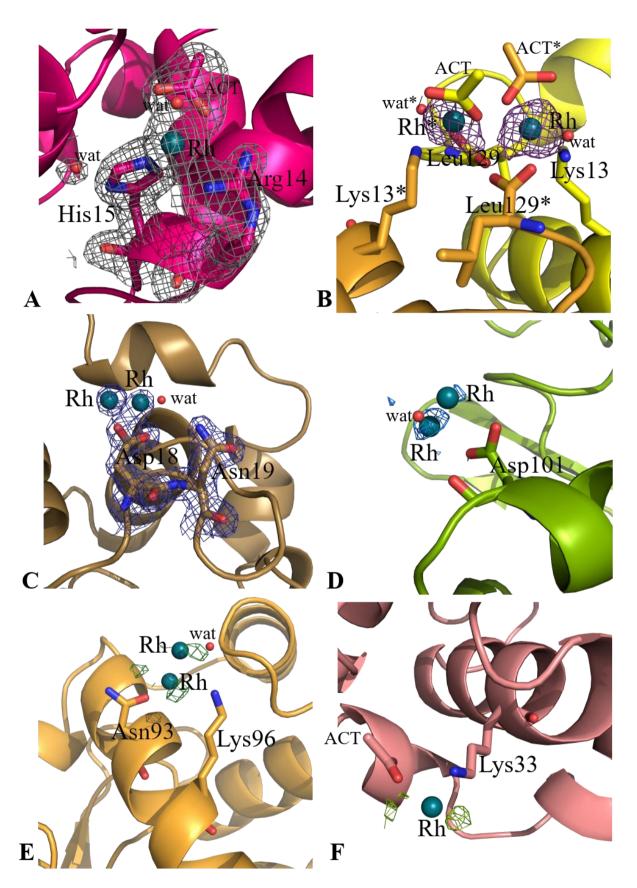
## Article

## Unusual Structural Features in the Adduct of Dirhodium Tetraacetate with Lysozyme

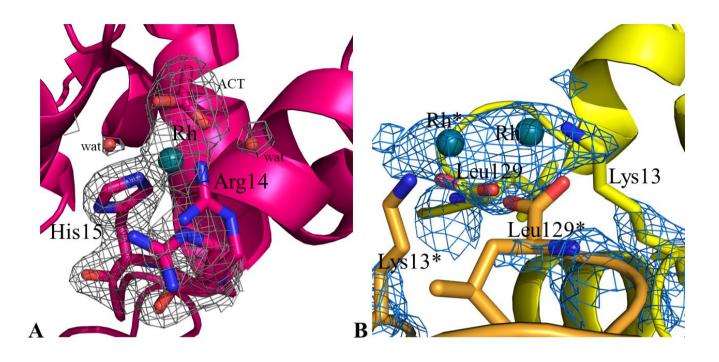
Domenico Loreto 1, Giarita Ferraro 2 and Antonello Merlino 1,\*

- Department of Chemical Sciences, University of Naples Federico II, 80126 Napoli, Italy; domenico.loreto@unina.it
- Department of Chemistry "Ugo Schiff", University of Florence, via della Lastruccia, 3-13, 50019 Sesto Fiorentino, Florence, Italy; giarita.ferraro@unifi.it
- \* Correspondence: antonello.merlino@unina.it

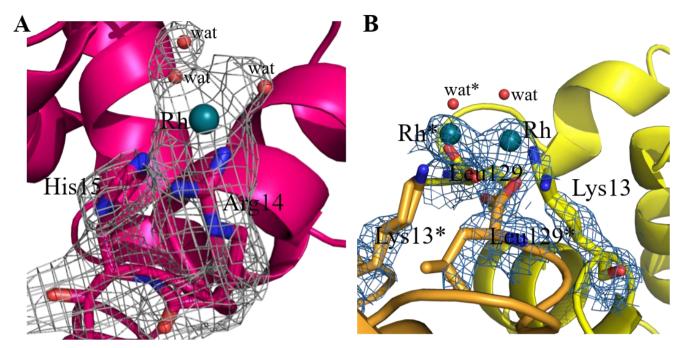
## Supporting information



**Figure S1.** Examples of anomalous difference electron density maps at the Rh binding sites close to side chains of Arg14 and His15 (**A**), close to the C-terminal tail (**B**), close to side chain of Asp18 (**C**), Asp101 (**D**), Asn93 and Lys96 (**E**) and of Lys33 (**F**) in the structures of Rh/HEWL adducts here reported. Maps are contoured at 3.0  $\sigma$  in panels A and B and at 2.0  $\sigma$  in the other panels.



**Figure S2.** Details of Rh binding sites close to the side chains of Arg14 and His15 (**A**) and close to the C-terminal tail and the side chain of Lys13 (**B**) in Crystal 5. 2Fo-Fc electron density maps are contoured at 1.0  $\sigma$ . \* refers to atoms from symmetry related molecules.



**Figure S3.** Details of Rh binding sites close to the side chains of Arg14 and His15 (**A**) and close to the C-terminal tail and the side chain of Lys13 (**B**) in Crystal 6. 2Fo-Fc electron density maps are contoured at  $1.0 \, \sigma$ .

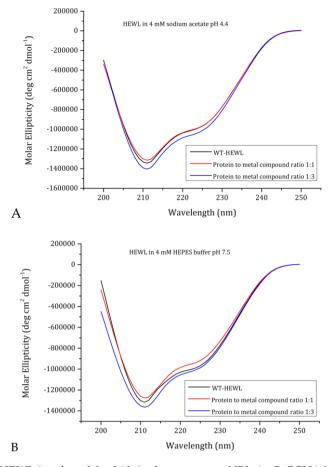
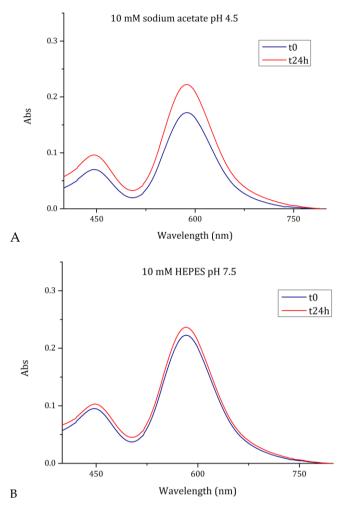


Figure S4. CD spectra of HEWL incubated for 24 h in the presence of  $[Rh_2(\mu-O_2CCH_3)_4]$  at different protein to metal compound ratios in (A) 4 mM sodium acetate buffer pH 4.4 and (B) 4 mM HEPES buffer pH 7.5.



**Figure S5.** UV-Vis spectra of [Rh<sub>2</sub>( $\mu$ -O<sub>2</sub>CCH<sub>3</sub>)<sub>4</sub>] in (**A**) 10 mM sodium acetate buffer at pH 4.5 and (**B**) 10 mM HEPES pH 7.5