

## Supporting Information

### Mapping the protein-binding sites for iridium(III)-based CO-releasing 5 molecules

Marco Caterino<sup>‡</sup>, Ariel A. Petruk<sup>†</sup>, Alessandro Vergara<sup>‡, #</sup>, Giarita Ferraro<sup>‡</sup>, Fabio Doctorovich<sup>†</sup>,  
Dario A. Estrin<sup>†</sup>, Antonello Merlino<sup>‡, #, \*</sup>

10 <sup>‡</sup>Department of Chemical Sciences, University of Naples Federico II, Complesso Universitario di Monte Sant'Angelo, Via Cintia, I-80126, Napoli, Italy.  
Fax: +39081674090; Tel: +39081674276; E-mail: antonello.merlino@unina.it

<sup>#</sup>Departamento de Química Inorgánica, Analítica y Química Física/INQUIMAE-CONICET, University of Buenos Aires, Ciudad Universitaria, Pab. 2,  
C1428EHA Buenos Aires, Argentina

<sup>\*</sup>CNR Institute of Biostructures and Bioimages, Via Mezzocannone 16, Napoli, Italy.

15

20

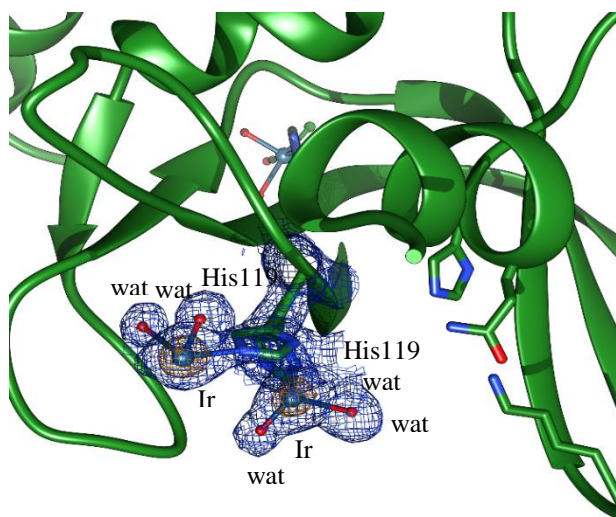


Figure S1. Details for the IrCl<sub>5</sub>CO<sub>2</sub><sup>-</sup> binding site close to His119 of molecule A from crystal 1. 2Fo-Fc electron density map is contoured at 1.5  $\sigma$  (blue) and 2.5 (orange) level.

