SUPPLEMENTARY INFORMATION CC-COM-0202013-041045

Zinc Finger Peptide Cleavage By a Dinuclear Platinum Compound.

John B. Mangrum, Ibrahim Zgani, Samantha D Tsotsoros, Yun Qu and Nicholas P. Farrell.

Experimental Details. Platinum compounds and zinc finger starting materials were prepared as previously.^{1,2}

For mass spectrometry experiments, initial 1mM reaction mixtures were made in water at $37^{\circ}C$ and pH 7.0 adjusted using ammonium hydroxide, then H₂O/MeOH (6/94) aliquots of approx. 10 μ M used for spraying. Experimental procedure in general followed published protocol.³ The reaction solution was not adjusted for pH during the reaction.

NMR Spectroscopy. NMR experiments also followed published procedure and were conducted at 1 mM concentration (1:1) in 5% $D_2O/95\%$ H₂O.²

For HSQC { 1 H, 15 N} NMR Spectroscopy the spectra were recorded at 37 °C on a Bruker AVANCE III 600 MHz spectrometer (1 H, 600.1 MHz; 15 N, 60.8 MHz) fitted with a pulsed field gradient module and 5mm inverse quadruple resonance (QXI) probe. The 1 H NMR chemical shifts were internally referenced to TSP, the 15 N chemical shifts externally referenced to 15 NH₄NO₃. The two-dimensional [1 H, 15 N] HSQC spectra were recorded in phase sensitive mode using Echo/Antiecho-TPPI gradient selection. A total of 1024 points were acquired in the 1 H dimension and 96 complex points in the 15 N dimension with 128 transients. 1 mM platinum complex was allowed to react with 1 equiv of ZF in 5% D₂O / 95% H₂O, and the reaction was followed by HSQC spectroscopy. 20 two-dimensional spectra were obtained at hourly intervals which can determine the half-life of the reaction by the integration of 15 NH₃ peaks.

- 1. M.E. Oehlsen, Y. Qu and N. Farrell, *Inorg. Chem.* 2003, **42**, 5498; M.E. Oehlsen, A. Hegmans, Y. Qu and N. Farrell, *J. Biol. Inorg. Chem.* 2005, **10**, 433 and references therein.
- 2. A.I. Anzellotti, Q. Liu, M.J. Bloemink, J.N. Scarsdale and N. Farrell, *Chemistry and Biology*, 2006, **13**, 539.
- 3. Q.A. dePaula, J.B. Mangrum and N.P. Farrell, J. Inorg. Biochem. 2009, 103, 1347.

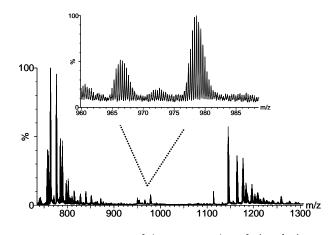


Figure S1. ESI-MS of the 1:1 complex of I (1,1/t,t) with intact zinc finger. The noncovalent association of ZF and Pt compound is shown in the inset at 978 m/z.

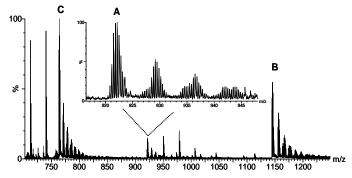


Figure S2. Incubation of 1,1/c,c, II, with ZF after 4hours. Peak denoted (A) represents loss of Zn and subsequent loss of NH_3 and Cl on the platinum compound. B is free, intact ZF.