Electronic Supplementary Information for Dalton Transactions

Nickel binding to histone H4:

Maria Antonietta Zoroddu,[a*] Massimiliano Peana,[a] Serenella Medici,[a] Luigi Casella,[b] Enrico Monzani[b] and Max Costa[c]

[a*]*Department of Chemistry & Pharmacy Faculty, University of Sassari, via Vienna 2, 07100 Sassari, Italy*

[b]*Department of Chemistry,University of Pavia, Italy*

[c] *Department of Environmental Medicine and Kaplan Comprehensive Cancer Center, New York University School of Medicine, New York, USA*

1)- Dependence of the intensity of the CD bands in a high affinity single binding equilibrium

The present treatment follows a similar analysis of binding equilibrium carried out by a spectrophotometric method [1].

In the presence of a single association between histone H4 (H) and Ni^{2+} the distribution of the species in solution is described by the binding constant and the following equations:

$$H + Ni^{2+} \underset{}{\overset{K_B}{\rightleftharpoons}} H - Ni^{2+} \qquad K_B = \frac{\left[H - Ni^{2+}\right]}{\left[H\right]\cdot\left[Ni^{2+}\right]}$$

$[H]_0 = [H\text{-}Ni^{2+}] + [H]$

$[Ni^{2+}]_0 = [H\text{-}Ni^{2+}] + [Ni^{2+}]$

where $[H]$, $[Ni^{2+}]$ $[H\text{-}Ni^{2+}]$ are the actual concentrations of free H4, nickel(II) and their complex, respectively. $[H]_0$ and $[Ni^{2+}]_0$ are the total (free plus bound) concentrations of H4 and nickel(II). The dependence of $[H\text{-}Ni^{2+}]$, $[H]$ and $[Ni^{2+}]$ as a function of $[H]_0$, $[Ni^{2+}]_0$ and K_B can be obtained by solving the equations system. The variation in CD intensity depends directly on the fraction of H bound to Ni^{2+} according to the equation:

$$\Delta I = \Delta I_\infty \times \frac{\left[H - Ni^{2+}\right]}{\left[H\right]_0}$$

Thus, at each addition of nickel(II) the total intensity is given by:

$$I = \Delta I + I_0$$

The introduction of the equation for $[H\text{-}Ni^{2+}]$, obtained from the equation system, gives the final equation that reports the observed absorbance variation as a function of K_B, $[H]_0$, $[Ni^{2+}]_0$ and ΔI_∞:

$$I = \frac{\Delta I_\infty}{2\cdot\left[Ni^{2+}\right]_0\cdot K_B}\cdot\left\{K_B\cdot\left(\left[Ni^{2+}\right]_0 + \left[H\right]_0\right) + 1 - \sqrt{K_B^2\cdot\left(\left[Ni^{2+}\right]_0 - \left[H\right]_0\right)^2 + 2\cdot K_B\cdot\left(\left[Ni^{2+}\right]_0 + \left[H\right]_0\right) + 1}\right\} + I_0$$

[1] E. Monzani, B. Bonafè, A. Fallarini, C. Redaelli, L. Casella, L. Minchiotti, M. Galliano. Biochim. Biophys. Acta, 1547, 302-312 (2001).

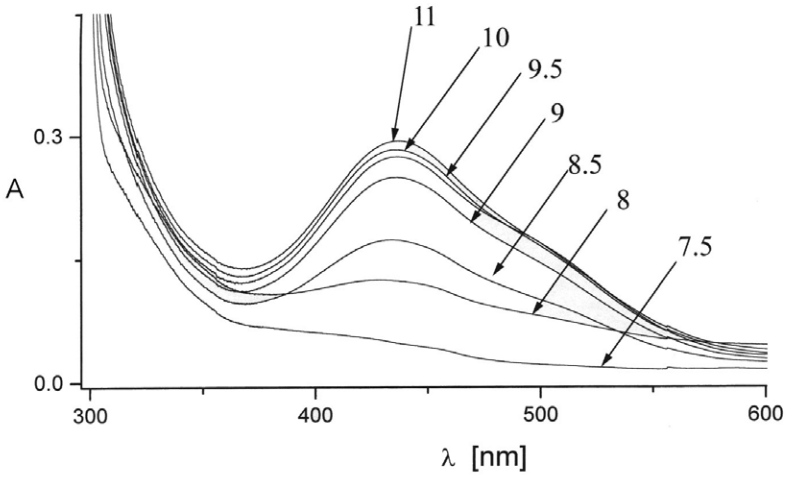

Fig. 1S pH dependence of the UV–Vis spectra for the complex between H4 tail and Ni^{II} in a 1:1 molar ratio. The figures shown on the curves give the pH values.