

Electronic Supporting Information (ESI)

**Metal Ions Binding to the RecA Intein from *Mycobacterium tuberculosis***

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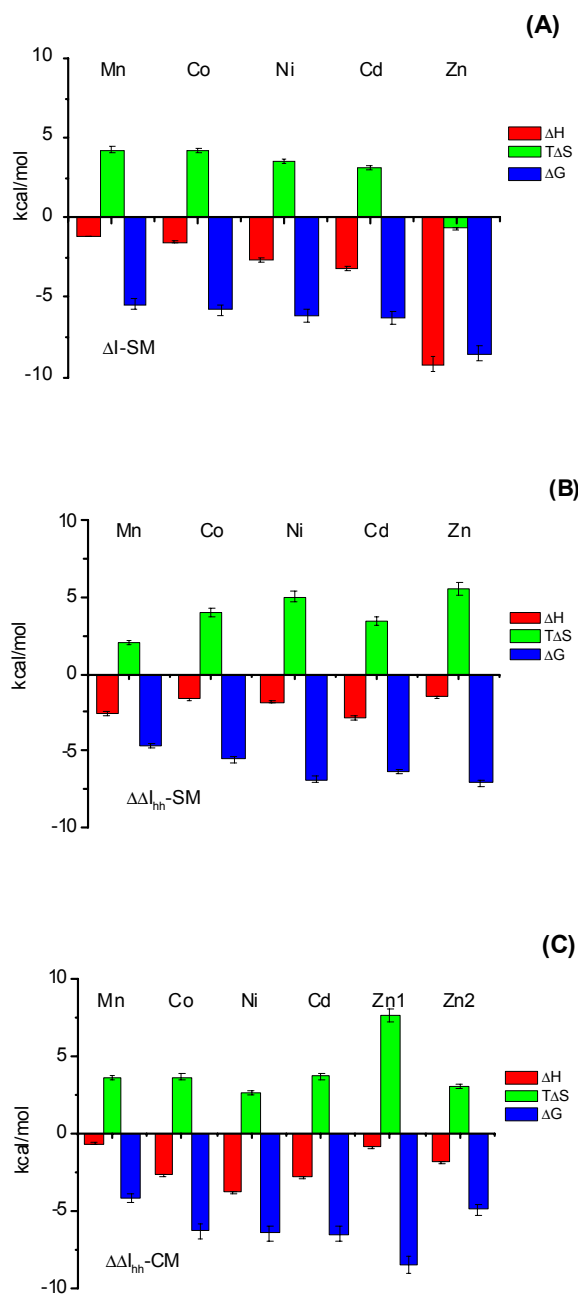


Fig. S1. Thermodynamic values from ITC titration ( $\Delta H_{ITC}$ ,  $T\Delta S_{ITC}$  and  $\Delta G_{ITC}$ ) in Tris buffer. A.  $\Delta I$ -SM; B.  $\Delta\Delta I_{hh}$ -SM; C.  $\Delta\Delta I_{hh}$ -CM

Table S1. Equilibrium dialysis of 20  $\mu\text{M}$   $\Delta\Delta\text{I}_{\text{hh}}$ -CM and  $\Delta\Delta\text{I}_{\text{hh}}$ -SM against  $\text{Zn}^{2+}$ .

| Sample: $\Delta\Delta\text{I}_{\text{hh}}$ -CM |                      | 1            | 2    | 3    |
|--|----------------------|--------------|------|------|
| $\text{Zn}^{2+}$ in dialysis buffer            | ( $\mu\text{M}$ )    | 0            | 10   | 20   |
| $\text{Zn}^{2+}$ detected in protein           | ( $\mu\text{g/ml}$ ) | undetectable | 2.38 | 2.56 |
| $\text{Zn}^{2+}$ detected in protein           | ( $\mu\text{M}$ )    | undetectable | 36.4 | 39.1 |
| Number of zinc in each protein                 |                      | 0            | 1.82 | 1.96 |
| Sample: $\Delta\Delta\text{I}_{\text{hh}}$ -SM |                      | 1            | 2    | 3    |
| $\text{Zn}^{2+}$ in dialysis buffer            | ( $\mu\text{M}$ )    | 0            | 10   | 20   |
| $\text{Zn}^{2+}$ detected in protein           | ( $\mu\text{g/ml}$ ) | undetectable | 1.24 | 1.38 |
| $\text{Zn}^{2+}$ detected in protein           | ( $\mu\text{M}$ )    | undetectable | 19.4 | 21.2 |
| Number of zinc in each protein                 |                      | 0            | 0.95 | 1.06 |

\* Equilibrium dialysis were carried out on 20  $\mu\text{M}$  protein samples against dialysis buffer with zinc concentration of 0, 10 and 20  $\mu\text{M}$ , respectively, for 48 hours. Zinc concentrations on protein were calculated by subtracting the zinc concentration measured out of the dialysis tube from that in the tube.

Table S2. Dynamic light scattering analysis of intein in the absence and presence zinc ion

|                           | $R_h$ (nm)  |             | MW-R (kDa)  |             |
|---------------------------|-------------|-------------|-------------|-------------|
|                           | $- Zn^{2+}$ | $+ Zn^{2+}$ | $- Zn^{2+}$ | $+ Zn^{2+}$ |
| $\Delta I$ -SM            | 2.0         | 2.6         | 17          | 35          |
| $\Delta\Delta I_{hh}$ -SM | 2.0         | 2.5         | 16          | 31          |
| $\Delta\Delta I_{hh}$ -CM | 2.0         | 2.5         | 16          | 31          |

$R_h$ : hydrodynamic radii

MW-R: apparent molecular mass

The measurement was performed in tris buffer. The hydrodynamic radius  $R_h$  was converted from translational diffusion coefficient  $D$  through the Stokes - Einstein equation. The apparent molecular masses were calculated from hydrodynamic radius  $R_h$  using Dynamics V6.2 software.

The small error of apparent molecular mass relative to the real molecular mass may be due to the protein particles shape.