

**Figure S1.** Binding affinity of Cd-(21) with Cd<sup>2+</sup> by ITC assay.

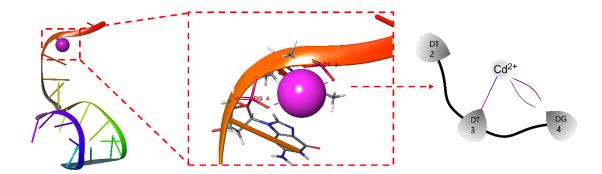


Figure S2. 2D and 3D molecular docking illustrations between Cd<sup>2+</sup> and Cd-(21).