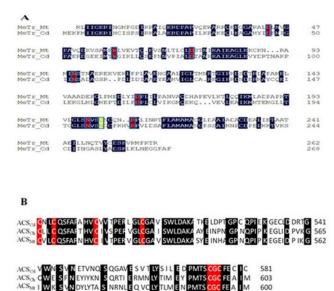
## **Supplementary Information**

**Figure S1** (**A**) Sequence alignment of MeTr<sub>Cd</sub> and MeTr<sub>Mt</sub>, completely conserved sequences labeled in black. Substrate binding residues were labeled in red and yellow.

(B) Partial sequence alignment of  $ACS_{Cd}$ ,  $ACS_{Ch}$  and  $ACS_{Mt}$ , completely conserved residues labeled in black. The residues of the metal center of A-cluster were labeled in red.



**Figure S2** Antibacterial activity for *Clostridium difficile* (strain: ATCC 43255 and ATCC 9689) by different chelators of A (8-hydroxyquinoline), B (2,2-dipyridyl) and C (1,10-phenanthroline) in different concentration, respectively. A paper disc containing 30 ng vancomycin was shown as positive control.



**Figure S3** (**A**) Ni X-ray absorption edge spectra of Ni-recombinant ACS<sub>Cd</sub>; (**B**) Ni-K edge EXAFS (left) and corresponding Fourier transform (right) for ACS<sub>Cd</sub> including fit with two nitrogen ligands, five sulfur ligands and one oxygen ligand for two Ni. All Ni-S distances were assumed to be identical to lower the number of fit parameters. The Ni-metal contributions, refined to 2.690 Å for Ni-Ni, 1.879 Å for Ni-N, 2.177 Å for Ni-S bond distance, respectively, result in the FT-peak at 3 Å due to the first shell phase shift correction applied.

