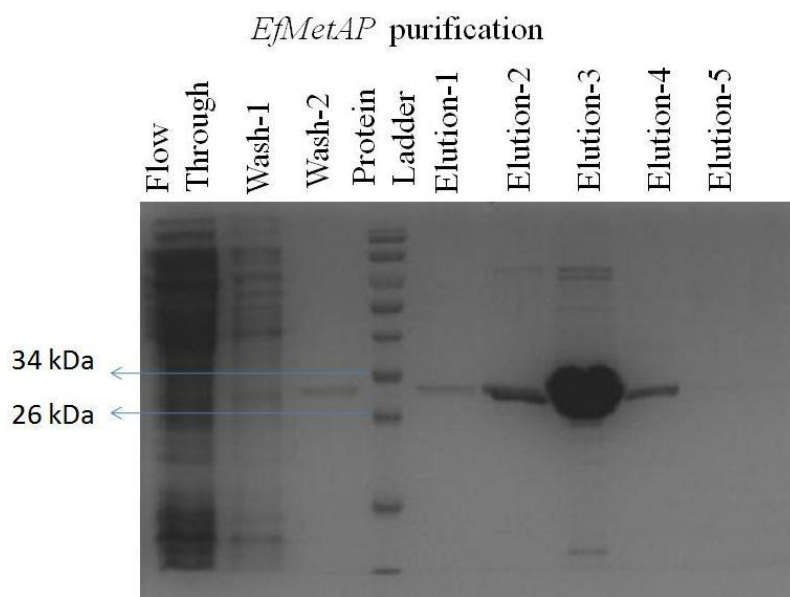


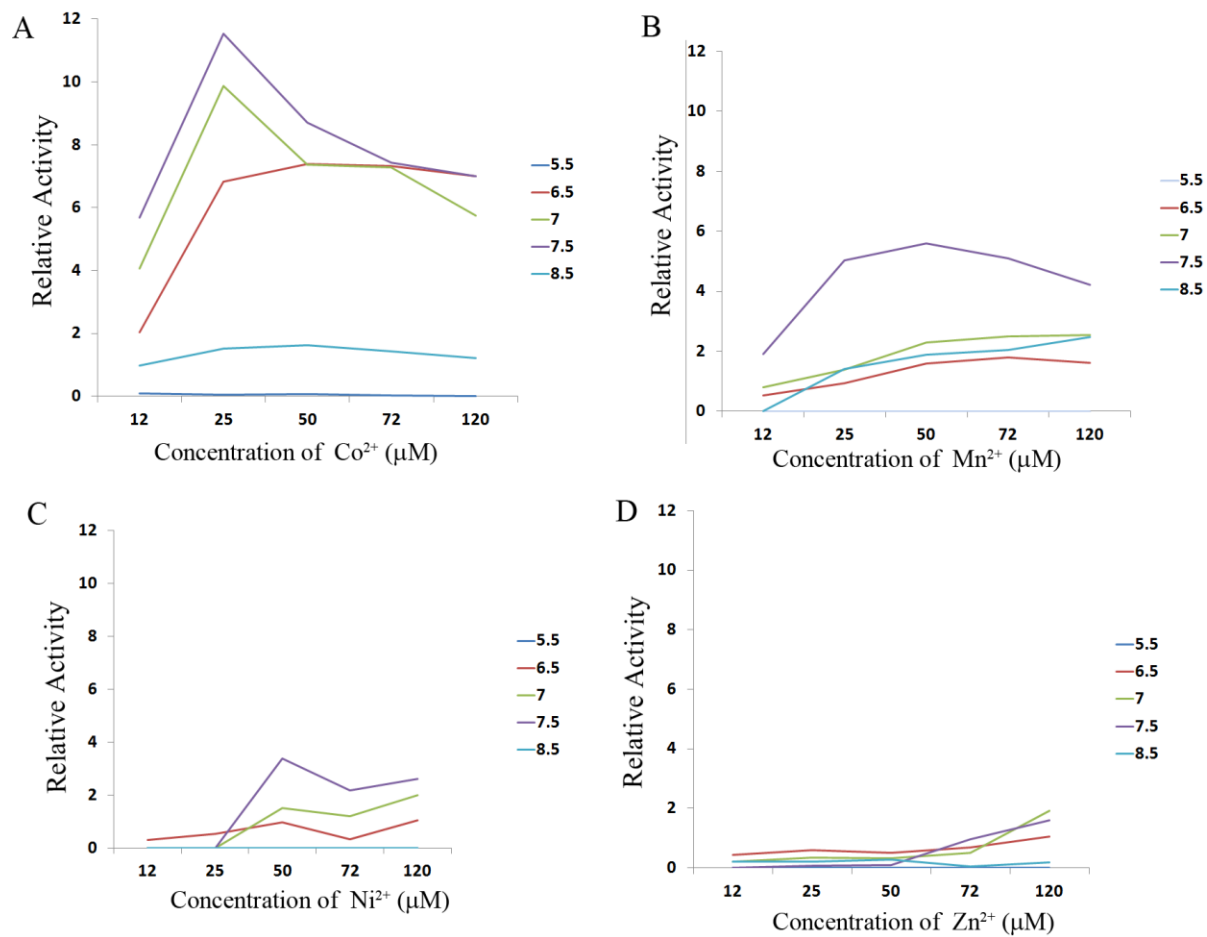
## Supplementary material:

**Purification of *EfMetAP*:** C-terminus penta-his tagged 30 KDa *EfMetAP* was expressed and purified from BL21 (DE3) *E. coli* strain. More than 95% pure protein was obtained from the single nickel affinity column judged by coomassie blue-stained SDS-polyacrylamide gel.

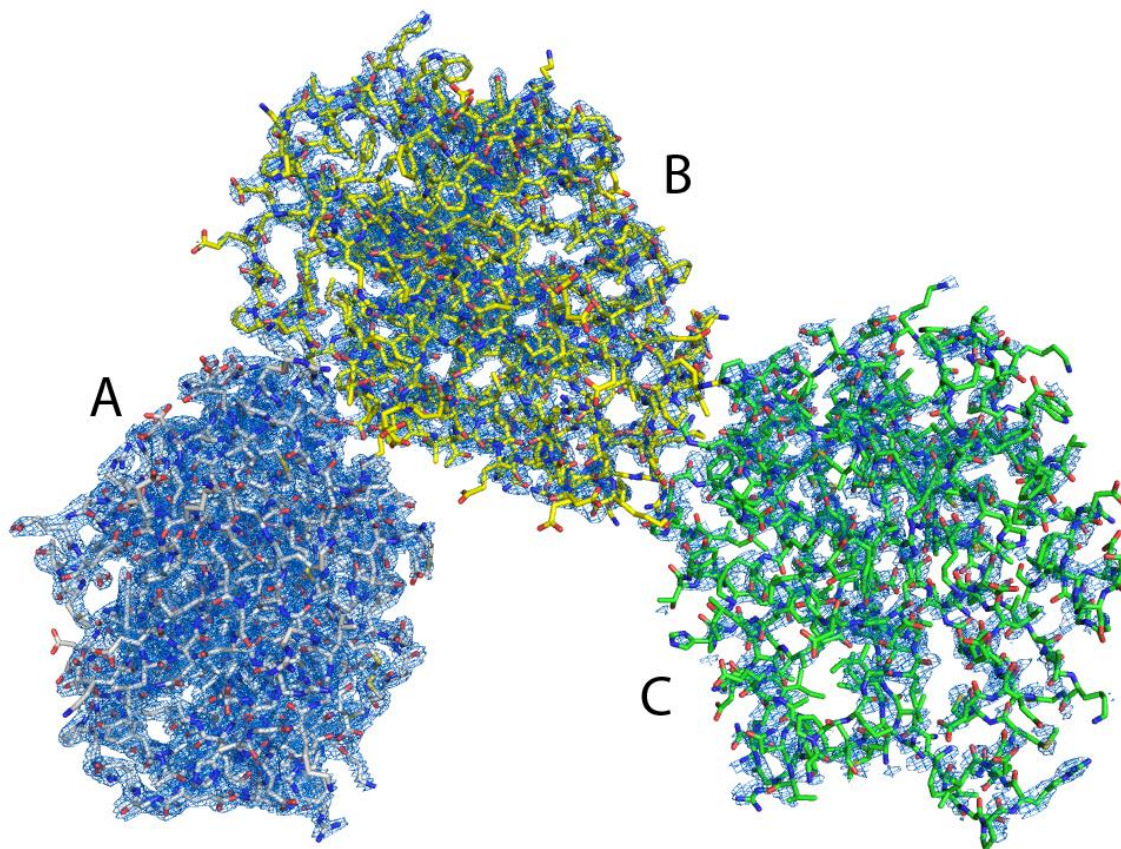


**Supplementary Figure 1.** Purification of PolyHis-tagged *EfMetAP* (~30 kDa).

### Buffer pH Vs Metal ions variation



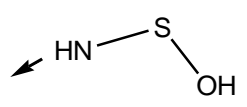
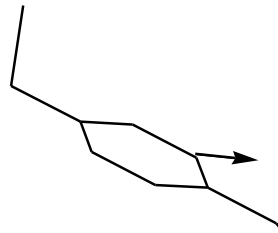
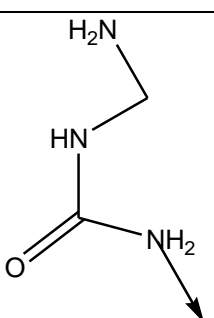
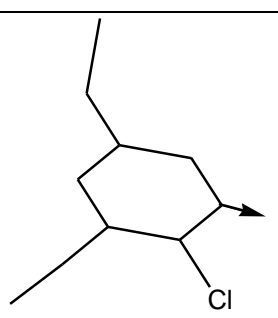
Supplementary Figure 2. Activity of *EfmMetAP* with pH and Metal ions variation

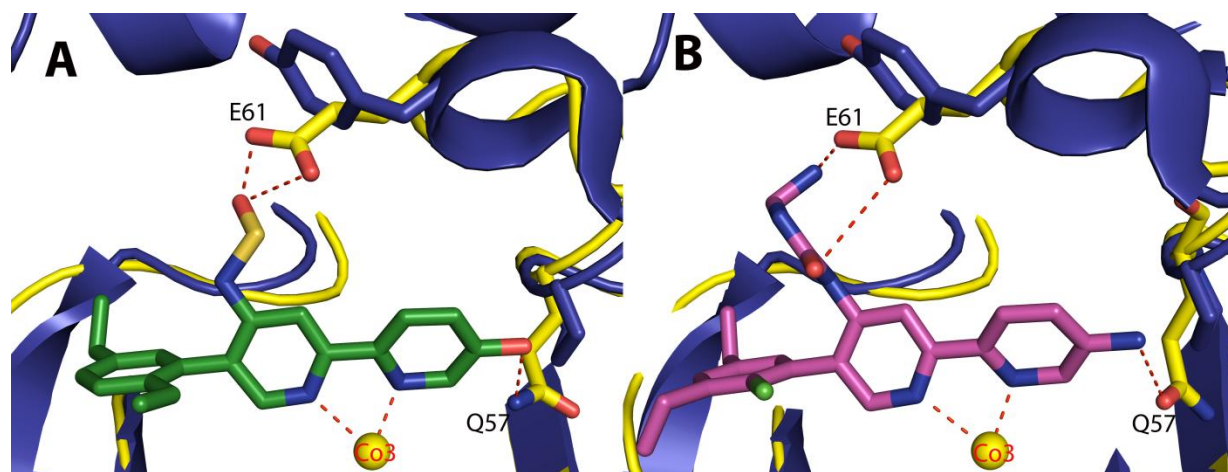


**Supplementary Figure 3.** Crystal structure of *EfMetAP* at 2.3 Å with three molecules in the asymmetric unit ( $2F_o-2F_c$  electron density contoured at  $1.5\sigma$ ). Molecule A, B and C represented by white, yellow and green sticks respectively. Good density was observed for all residues in molecules A and B while parts of the molecule C could not be traced.

## Virtual Screening

Virtual screening of 126 bipyridine derivatives was carried against *EfmetAP* and *HsMetAp* to find out microbes specific inhibitor. Two molecules have good hit against *EfMetAP*.

Compound Id	R1	R2	R3	R4	Binding energy with <i>EfMetAP</i> (kcal/mol)	Binding energy with <i>HsMetAP</i> (kcal/mol)
1	OH	H			-8.0	-7.2
2	NH2	H			-8.1	-7.0



**Supplementary Figure 4.** possible binding mode of bipyridine derivatives with *EfMetAP*.

Yellow cartoon represent *EfMetAP*, while blue cartoon represents *HsMetAP*. (A) Interaction of compound 1 and (B) compound 2 with *EfMetAP*.

