Supplementary material-1

Validation of Zn++ complex homology model:

In the homology model, coordinates of Zn^{+2} atoms and water in active site were mimicked from the crystal structure of template **Figure** 1a&1b. The distances measured between the atom-pairs with compare with template 1P42 are given **table**1&2. These validate our protocol for addition of metal ion and water molecule to proteins.

Figure 1a

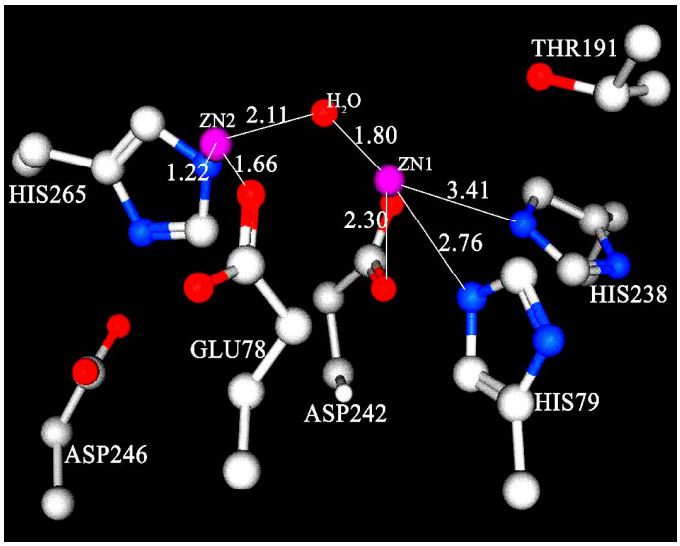

Figure 1b

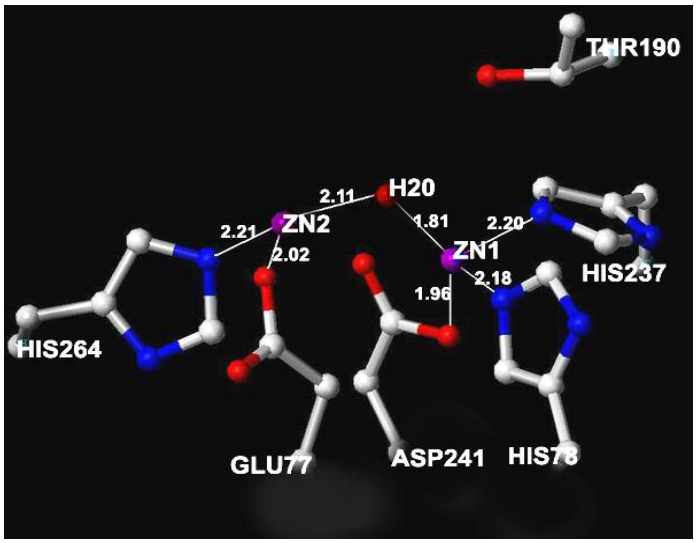

Table-1

Atom1	Atom2	Distance (Å)	
		Crystal structure-1P42 (Template)	EcLpxC Homology Model
Zn1	NE2(His79)	2.08	2.76
Zn1	NE2(His238)	2.17	3.41
Zn1	OD1(Asp242)	1.99	2.30
Zn1	O(H2O)	1.80	1.80
Zn2	O(H2O)	2.11	2.11
Zn2	OE2(Glu78)	1.98	1.66
Zn2	NE2(His265)	2.07	1.22

Table-2

Atom1	Atom2	Distance (Å)	
		Crystal structure-1P42 (Template)	PaLpxC Homology Model
Zn1	NE2(His78)	2.08	2.18
Zn1	NE2(His237)	2.17	2.2
Zn1	OD1(Asp241)	1.99	1.959
Zn1	O(H2O)	1.80	1.804
Zn2	O(H2O)	2.11	2.105
Zn2	OE2(Glu77)	1.98	2.02
Zn2	NE2(His264)	2.07	2.21