

Supplementary materials

Table S1. Representative enzymes from each family of the metallo-hydrolase-like MBL-fold protein superfamily reported by Daiyasu et al (2001) [1], Bebrone (2007) [5], and Palzkill (2013) [11].

Member of Metallo-hydrolase-Like MBL-Fold Protein Superfamily	Protein Name	Organism	Accession	
			Genbank Accession Number	PDB ID
B1 MBL	BcII	<i>Bacillus cereus</i>	-	1BMC
	CcrA	<i>Bacteroides fragilis</i>	-	1ZNB
	IMP-1	<i>Pseudomonas aeruginosa</i>	-	1DD6
	BlaB	<i>Chryseobacterium meningoseptica</i>	-	1M2X
	SPM-1	<i>Pseudomonas aeruginosa</i>	-	2FHX
	NDM-1	<i>Klebsiella pneumonia</i>	-	3ZR9
	VIM-1	<i>Pseudomonas aeruginosa</i>	-	5N5G
	GIM-1	<i>Pseudomonas aeruginosa</i>	-	2YNT
	DIM-1	<i>Pseudomonas stutzeri</i>	-	4WD6
	TMB-1	<i>Achromobacter xylobacter</i>	-	5MMD
B2 MBL	CphA	<i>Aeromonas hydrophila</i>	-	1X8G
	Sfh-1	<i>Serratia fonticola</i>	-	3SD9
B3 MBL	L1	<i>Stenotrophomonas maltophilia</i>	-	1SML
	FEZ-1	<i>Legionella gormannii</i>	-	1K07
	BJP-1	<i>Bradyrhizobium japonicum</i>	-	3LVZ
	AIM-1	<i>Pseudomonas aeruginosa</i>	-	4AWY
	SMB-1	<i>Serratia marcescens</i>	-	3VPE
	GOB-18	<i>Elizabethkingia meningoseptica</i>	-	5K0W
Glyoxalase II (GLXII)	GloB	<i>Salmonella enterica</i> subsp. <i>enterica</i> serovar <i>typhimurium</i>	-	2QED
	YcbL	<i>Salmonella enterica</i>	-	2XF4
N-acyl-L-homoserine lactonase (AHL)	AiiA	<i>Bacillus thuringiensis</i>	-	2A7M
Flavodiiron proteins	ROO	<i>Desulfovibrio gigas</i>	-	1E5D
Cleavage and polyadenylation specificity factors	CPSF-73	<i>Homo sapiens</i>	-	2I7V
Arylsulfatase	SdsA1	<i>Pseudomonas aeruginosa</i>	-	2CG3
5'-exonuclease	Exo1	<i>Homo sapiens</i>	NP_666226.1	-
Ribonuclease	Tm	<i>Thermotoga maritima</i>	-	1WW1

Member of Metallo-hydrolase-Like MBL-Fold Protein Superfamily	Protein Name	Organism	Accession	
			Genbank Accession Number	PDB ID
Cyclic nucleotide phosphodiesterase	ZipD	<i>Escherichia coli</i>	-	2CBN
Insecticide hydrolase	MPH	<i>Pseudomonas</i> sp WBC-3	-	4LE6
Proteins required for natural transformation competence	ComA	<i>Neisseria gonorrhoeae</i>	P51973	-
Choline-binding protein	CbpE	<i>Streptococcus pneumoniae</i>	-	1WRA

Table S2. Comparison of enzyme kinetics data of several B3 MBLs and GLXIIs towards ampicillin and SLG respectively.

B3 MBL	K_M (mM)	k_{cat} (s ⁻¹)	k_{cat}/K_M (mM ⁻¹ s ⁻¹)
L1 [57]	3.0×10^{-1}	580	1.9×10^3
AIM-1 [58]	4.1×10^{-2}	594	1.4×10^3
FEZ-1 [59]	> 5	> 5.5	1.1×10
GLXII	K_M (mM)	k_{cat} (s ⁻¹)	k_{cat}/K_M (mM ⁻¹ s ⁻¹)
GloB [26]	2.95×10^{-1}	209.9	7.1×10^2
YcbL [35]	5.0×10^{-1}	0.9	1.8
<i>A. thaliana</i> GLXII [25]	3.91×10^{-1}	129	3.3×10^2

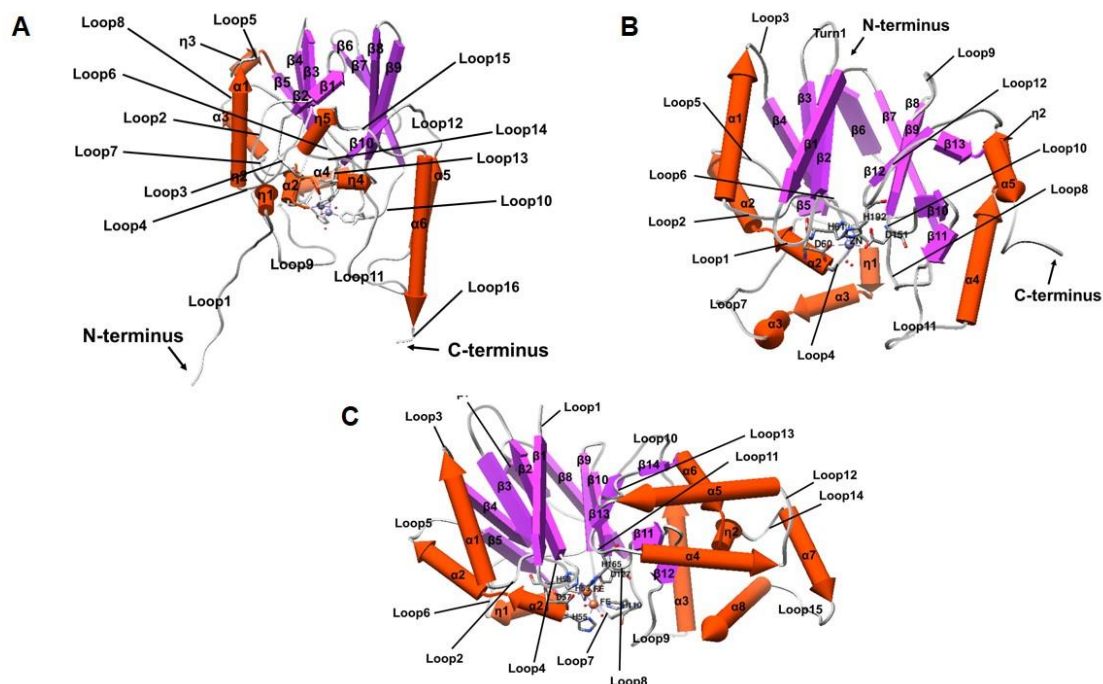


Figure S1. Crystal structure of (A) L1 MBL (PDB ID: 1SML, chain A), (B) YcbL (PDB ID: 2XF4, chain A) and (C) GloB (PDB ID: 2QED, chain A) with labelled secondary structure elements.