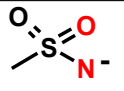
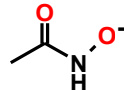
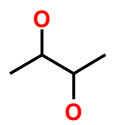
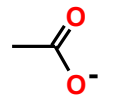
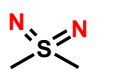
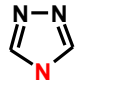
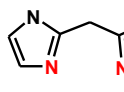

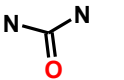



Supplementary Material

MetLigDB: a web-based database for the identification of chemical groups to design metalloprotein inhibitors

Hwanho Choi, ¹Hongsuk Kang, ²and Hwangseo Park

Table S1. A list of representative ligand moieties for Zn²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

ligand group	ligand name	protein(s)	coordination geometry
	sulfoamide	carbonic anhydrase 2	tetrahedral trigonal bipyramidal
	hydroxamate	matrix metalloproteinase histone acetylase thermolysin	trigonal bipyramidal
	butane-2,3-diol	6-pyruvoyltetrahydropterin synthase golgi alpha-mannosidase II 2-C-methyl-D-erythritol 2,4-clycodiphosphate synthase glucose-6-phosphate isomerase	trigonal bipyramidal
	carboxylate	carboxypeptidase A aryldialkylphosphatase alcohol dehydrogenase thioredoxin-disulfide reductase peptidyl-dipeptidase A N-acyl-D-amino-acid deacylase leukotriene-A4 hydrolase peptide deformylase peptidyl-dipeptidase A succinyl-diaminopimelate desuccinylase	tetrahedral trigonal bipyramidal
	sulfodiimine	carboxypeptidase A matrilysin	tetrahedral
	1,2,4-triazole	carbonate dehydratase	tetrahedral
	diimidazolymethane	trypsin thrombin	trigonal bipyramidal
	2-(1 <i>H</i> -imidazol-2-yl)-phenol	trypsin	trigonal bipyramidal
	urea	carboxypeptidase A	tetrahedral
	thiolate	carboxypeptidase A	tetrahedral

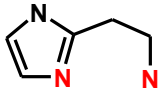
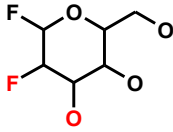
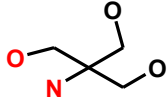
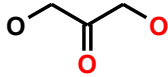
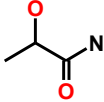

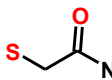
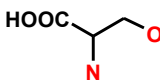
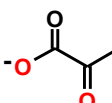
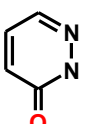
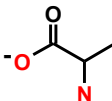
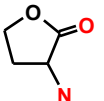
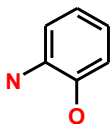
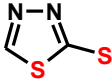
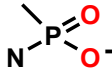
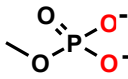
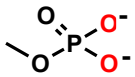
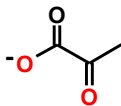
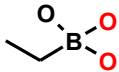
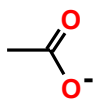
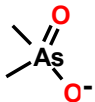
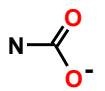
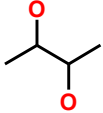
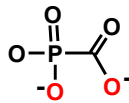
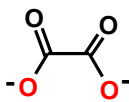
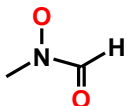
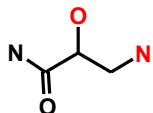
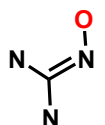
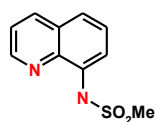
	2-(1 <i>H</i> -imidazol-2-yl)-ethylamine	histidinol dehydrogenase	octahedral
	2-deoxy-2-fluorohexopyranosyl fluoride	mannosyl-oligosaccharide 1,3-1,6- α -mannosidase	trigonal bipyramidal
	2-amino-2-hydroxymethylpropane-1,3-diol	mannan endo-1,4- β -mannosidase	trigonal bipyramidal
	dihydroxyacetone	L-rhamnulose-1-phosphate aldolase	trigonal bipyramidal
	2-hydroxypropionamide	aminopeptidase	trigonal bipyramidal
	imidazole	trypsin immunoglobulin tax1-binding protein 3	tetrahedral
	2-mercaptoacetamide	thermolysin neprilysin	trigonal bipyramidal
	2-amino-3-hydroxypropionic acid	4-hydroxythreonine-4-phosphate dehydrogenase	trigonal bipyramidal
	2-oxopropanoate	2-isopropylmalate synthase	square pyramidal
	2 <i>H</i> -pyridazin-3-one	phosphodiesterase 4D	octahedral
	2-aminopropanoate	transcriptional regulator, HTH_3 family	octahedral
	homoserine lactone	AIIA-like protein	octahedral
	2-aminophenol	ranasmurfin	trigonal bipyramidal
	[1,3,4]thiadiazole-2-thiol	stromelysin 1	octahedral
	phosphoramidate	stromelysin	tetrahedral
	phosphonate	carboxypeptidase A N-formylmethionylaminoacyl-tRNA deformylase	tetrahedral

Table S2. A list of representative ligand moieties for Mn²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

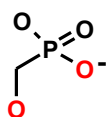
ligand group	ligand name	protein(s)	coordination geometry
	phosphate	pyruvate kinase type II site-specific deoxyribonuclease dethiobiotin synthase phosphotransferases dimethylallyltranstransferase	trigonal bipyramidal tetrahedral
	2-oxopropanoate	isocitrate dehydrogenase pyruvate kinase fumarylacetoacetase sialic acid synthase	tetrahedral octahedral
	boronate	arginase	trigonal bipyramidal
	carboxylate	Xaa-Pro aminopeptidase glucose-7-phosphate isomerase classical-complement-pathway C3/C5 convertase glucose-7-phosphate isomerase	trigonal bipyramidal square pyramidal
	cacodylate	cholesterol oxidase	tetrahedral
	carbamate	urease	trigonal bipyramidal
	butane-2,3-diol	xylose isomerase D-psicose 3-epimerase ω-amidase	trigonal bipyramidal octahedral
	phosphonoformate	glutathione transferase	trigonal bipyramidal
	oxalate	oxalate decarboxylase phosphoenolpyruvate carboxykinase	octahedral square pyramidal
	<i>N</i> -hydroxy- <i>N</i> -methylformamide	1-deoxy-D-xylulose-5-phosphate reductoisomerase	trigonal bipyramidal
	3-amino-2-hydroxypropionamide	methionine aminopeptidase-2	octahedral
	<i>N</i> -hydroxyguanidine	arginase	tetrahedral



N-(quinolin-8-yl)methanesulfonamide

methionyl aminopeptidase

tetrahedral



hydroxyphosphonate

glyoxalase

trigonal bipyramidal

Table S3. A list of representative ligand moieties for $\text{Fe}^{2+}/\text{Fe}^{3+}$ ions in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

ligand group	ligand name	protein(s)	coordination geometry
	2-oxopropanoate	factor inhibiting hif-1 alpha deacetoxycephalosporin-C synthase oxidoreductase phytanoyl-CoA dioxygenase leucocyanidin oxygenase alkylated DNA repair protein alkB peptide-aspartate β -dioxygenase	trigonal bipyramidal
	carboxylate	hydroxyquinol 1,2-dioxygenase ribonucleoside-diphosphate reductase asparagine oxygenase	octahedral
	phosphate	O-sialoglycoprotein endopeptidase family II pyrophosphatase	square pyramidal tetrahedral
	thiolate	isopenicillin N synthase cysteine dioxygenase	tetrahedral
	sulfide	deacetoxycephalosporin C synthase	tetrahedral
	thiazolidin-5-ylmethanol	isopenicillin N synthase	trigonal bipyramidal
	3-mercapto-N-(2-methylsulfanylethyl)propionamide	isopenicillin N synthase	trigonal bipyramidal
	2-(1-hydroxyethylidene)cyclohexanone	4-hydroxyphenylpyruvate dioxygenase	square pyramidal
	2-hydroxybenzamide	hypoxia-Inducible Factor Prolyl Hydroxylase (PHD2)	square pyramidal
	butane-2,3-diol	nitrobenzene dioxygenase	tetrahedral

Table S4. A list of representative ligand moieties for Mg²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

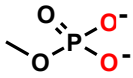
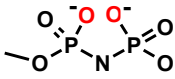
ligand group	ligand name	protein(s)	coordination geometry
	phosphate	phosphoenolpyruvate carboxykinase adenylate cyclase ADP-ribosylation factor 1 glucose-1-phosphate cytidylyltransferase small G protein RAB3A DNA-directed DNA polymerase large gamma subunit of initiation factor eIF2	tetrahedral square pyramidal octahedral
	phosphoamino-phosphate	RAB11B, member RAS oncogene family translation initiation factor 2 gamma	tetrahedral square pyramidal

Table S5. A list of representative ligand moieties for Ni²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.


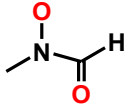
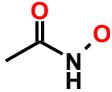
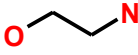
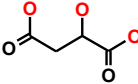
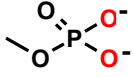
ligand group	ligand name	protein(s)	coordination geometry
	carboxylate	urease	trigonal bipyramidal
	<i>N</i> -hydroxy- <i>N</i> -methylformamide	formylmethionine deformylase	trigonal bipyramidal
	hydroxamate	formylmethionine deformylase peptide deformylase	trigonal bipyramidal
	2-aminoethanol	1-aminocyclopropane-1-carboxylate synthase	trigonal bipyramidal
	2-hydroxysuccinate	HpNikR, helix-helix family of transcriptional regulators	octahedral
	phosphate	ferric hydroxamate uptake receptor	tetrahedral

Table S6. A list of representative ligand moieties for Cu²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

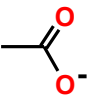
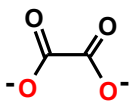
ligand group	ligand name	protein(s)	coordination geometry
	carboxylate	galactose oxidase bacterial YhcH protein	octahedral
	oxalate	lactoferrin	square pyramidal

Table S7. A list of representative ligand moieties for Co²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

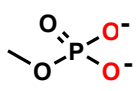
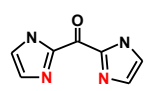
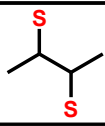
ligand group	ligand name	protein(s)	coordination geometry
	phosphate	N-formylmethionylaminoacyl-tRNA deformylase	tetrahedral
	bis-(1 <i>H</i> -imidazol-2-yl)- methanone	trypsin	tetrahedral

Table S8. A list of representative ligand moieties for Mo²⁺ ion in metalloproteins. Indicated in red are the atoms coordinated to the metal ion.

ligand group	ligand name	protein(s)	coordination geometry
	butane-2,3-dithiol	nitrate reductase	square pyramidal