Supporting Information

Metallo-β-Lactamase Mediated Antimicrobial Resistance and Progress in Inhibitor Discovery

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Supplementary Table S1. Summary of discovered MBLs.

Acronym	Full name[a]	First report,		Variant no.	Intri./ acq.[c]	RefSeq accession no.
		Year	Species[b]			
Subclass B1						
BcII	Beta-lactamase II	1966	*B. cereus*	6	I	NG_047222
CcrA or CfiA	—	1990	*B. fragilis*	18	A	NG_050389
IMP	imipenemase	1991	*P. aeruginosa*	91	A	NG_049172
BlaB	—	1998	*E. meningoseptica*	37	I	NG_048691
VIM	Verona integron-encoded MBL	1999	*P. aeruginosa*	78	A	NG_050336
IND	—	1999	*C. indologenes*	16	I	NG_049224
EBR	*Empedobacter brevis* MBL	2002	*E. brevis*	4	I	NG_049078
SPM	Sao Paulo MBL	2002	*P. aeruginosa*	1	A	NG_050140
CGB	—	2002	*C. gleum*	1	I	NG_051689
MUS	—	2002	*M. odoratimimus*	2	I	NG_049324
TUS	—	2002	*M. odoratus*	1	I	NG_050315
JOHN	—	2003	*F. johnsoniae*	1	I	NG_049239
GIM	German imipenemase	2004	*P. aeruginosa*	2	A	NG_049143
SIM	Seoul imipenemase	2005	*A. baumannii*	2	A	NG_050131
SLB	—	2005	*S. livingstonensis*	1	I	NG_047545
SFB	—	2005	*S. frigidimarina*	1	I	NG_047544
KHM	Kyorin Health Science MBL	2008	*C. freundii*	1	A	NG_049240
NDM	New Delhi MBL	2008	*K. pneumonia*, *E. coli*	43	A	NG_049326
ALI	*Aliivibrio salmonicida* MBL	2008	*A. salmonicida*	2	I	NG_057427
DIM	Dutch imipenemase	2010	*P. stutzeri*	1	A	NG_049077
FIM	Florence imipenemase	2012	*P. aeruginosa*	1	A	NG_049091
TMB	Tripoli MBL	2012	*A. xylosoxidans*	2	I	NG_050313
PEDO-3	—	2015	*P. kyungheensis*	1	I	NG_049959
ANA	—	2015	*Anaeromyxobacter* spp.	1	—	NG_057424
MOC	—	2016	*M. odoratus*	1	—	NG_051495
GRD23	—	2016	—	1	A	NG_062239
SPN79	—	2016	—	1	—	NG_062234
HMB	Hamburg MBL	2017	*P. aeruginosa*	1	I	NG_052225
VarG	—	2017	*V. cholerae*	1	I	NG_057468
ECV	—	2017	*E. vietnamensis*	1	—	NG_059320
FIA	—	2017	*F. aestuarina*	1	—	NG_057437
MYO	—	2017	*M. odoratimimus*	1	A	NG_059325
MYX	—	2017	*M. xanthus*	1	—	NG_057453
ORR	—	2017	*O. rhinotracheale*	1	I	NG_059317
PST	—	2017	*P. stutzeri*	2	—	NG_057439
SHD	—	2017	*S. denitrificans*	1	—	NG_077967
SHN	—	2017	*S. denitrificans*	1	—	NG_059313

SPS	—	2017	*S. smaragdinae*	1	—	NG_059316
STA	—	2017	*S. aurantiaca*	1	—	NG_057419
TTU	—	2017	*T. turnerae*	1	—	NG_059314
ZOG	—	2017	*Z. galactanivorans*	1	—	NG_057434
AFM	*Alcaligenes faecalis* MBL	2018	*A. faecalis*	4	A	NG_063835
CAM	Central Alberta MBL	2019	*P. aeruginosa*	1	A	NG_065859
VMB	*Vibrio* MBL	2020	*V. alginolyticus*	1	A	NG_070758
VAM	*Vibrio alginolyticus* MBL	2021	*V. alginolyticus*	1	A	NG_076653
GMB	German MBL	2022	*C. freundii, S. marcescens*, *R. planticola*	1	A	NG_073463
CrxA	Carbapenem resistance protein of *Bacteroides xylanisolvens*	2022	*B. xylanisolvens*	1	A	QPIO01000015
WUS	—	2022	*M. albus*	1	—	NG_080791
Subclass B2						
CphA	Carbapenemase hydrolysing Aeromonas	1991	*A. hydrophila*	12	I	NG_050396
ImiS	—	1996	*A. veronii*	1	I	NG_050415
ImiH	—	2003	*A. hydrophila*	1	I	NG_050414
Sfh	—	2003	*S. fonticola*	1	I	NG_052115
PFM	*Pseudomonas fluorescens* MBL	2019	*P. synxantha*	3	A	NG_065936
CVI	*Chromobacterium violaceum* MBL	2020	*C. violaceum*	1	—	NG_067986
YEM	*Yersinia* MBL	2020	*Y. mollaretii*	1	—	NG_070759
BioF	Biofilter	2022	*Psuedomonas* spp.	1	—	NZ_JACOMR010000005
Subclass B3						
L1	—	1982	*S. maltophilia*	17	I	NG_047506
FEZ	—	2000	*L. gormanii*	1	I	NG_049090
GOB	Class B β-lactamase of *C. meningosepticum*	2000	*E. meningoseptica*	52	I	NG_049145
THIN-B	—	2001	*J. lividum*	1	I	NG_047549
MBL1b	—	2001	*C. crescentus*	1	I	NG_049292
CAU	—	2002	*C. vibrioides*	1	I	NG_048755
BJP	—	2006	*B. japonicum*	2	I	NG_048709
CAR	—	2008	*E. carotovora*	1	I	NG_048712
LRA	β-lactam resistance from Alaskan soil	2009	*J. lividum*	8	—	NG_047519
POM	*Pseudomonas otitidis* MBL	2011	*P. otitidis*	2	I	NG_049974
SMB	Serratia MBL	2011	*S. marcescens*	1	A	NG_050133
AIM	Adelaide imipenemase	2012	*P. aeruginosa*	2	A	NG_048689
EAM	—	2012	*E. aquimaris*	1	I	NG_062208
ECM	—	2012	*E. citreus*	1	I	NG_062207

EFM	—	2012	*E. flavus*	1	I	NG_062204
ELM	—	2012	*E. longus*	1	I	NG_062206
EVM	—	2012	*E. vulgaris*	1	I	NG_062205
PAM	*Pseudomonas alcaligenes* MBL	2013	*P. alcaligenes*	3	I	NG_076630
SPR	—	2014	*S. proteamaculans*	1	—	NG_052102
PEDO	—	2015	*P. roseu*, *P. borealis*	2	I	NG_049957
CPS	—	2015	*C. piscium*	1	I	NG_048587
ESP	—	2015	*E. tenax*	1	I	NG_049088
MSI	—	2015	*M. oculi*	1	I	NG_049323.2
SPG	—	2015	*Sphingomonas* spp.	1	I	NG_050139
Rm3	—	2016	—	1	—	NG_052128
GRD33	—	2016	—	1	I	NG_062238
CRD3	—	2016	—	1	I	NG_062235
DHT2	—	2016	*S. maltophilia*	1	I	NG_062233
ALG6	—	2016	—	1	I	NG_062236
ALG11	—	2016	—	1	—	NG_062237
PLN	*Pedobacter lusitanus*	2017	*P. lusitanus*	1	—	NG_055471
PNGM	Papua New Guinea MBL	2018	—	1	—	NG_065937
LMB	Linz MBL	2018	*E. cloacae*	1	A	NG_070744
B3SU1	—	2021	—	1	—	NG_076657
B3SU2	—	2021	—	1	—	NG_076658
SIE	*Sphingobium indicum* B3-E MBL	2021	*S. indicum*	1	—	NG_081773
NWM	—	2022	*P. aeruginosa*	1	—	NG_081702
PJM	*Pseudoxanthomonas japonensis* MBL	2022	*P. japonensis*	1	—	NG_080789

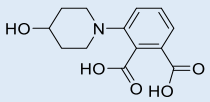
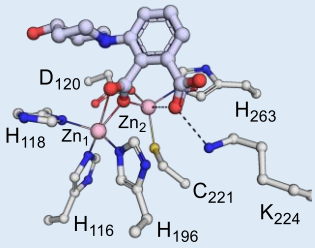
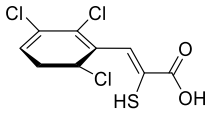
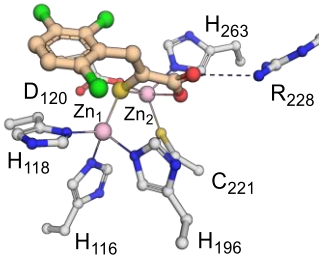
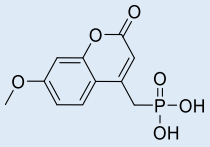
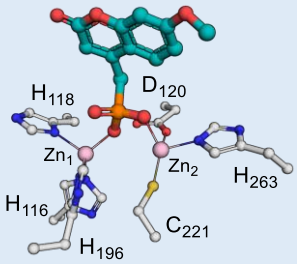
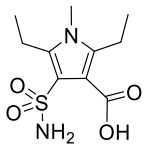
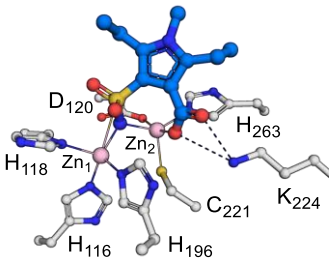
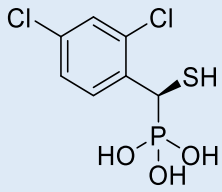
[a]MBL, metallo-β-lactamase.

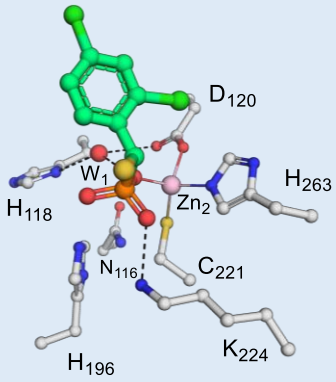
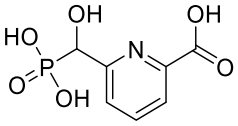
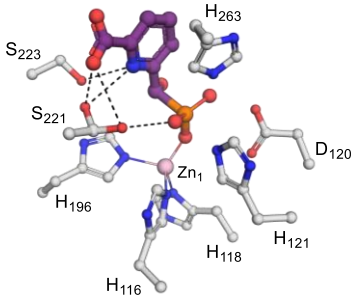
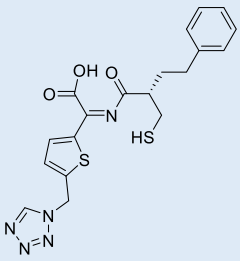
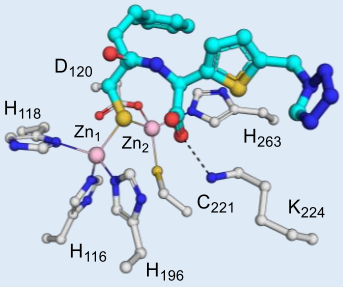
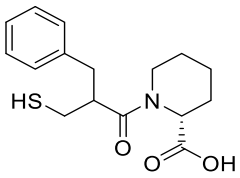
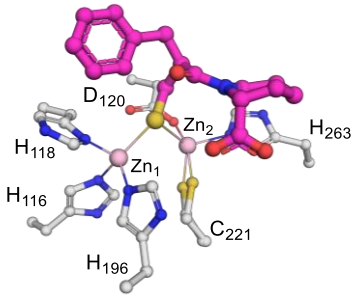
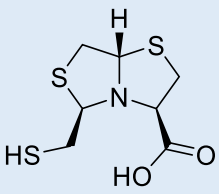
[b]Species: *A. baumannii, Acinetobacter baumannii*; *A. hydrophila, Aeromonas hydrophila*; *A. veronii, Aeromonas veronii*; *A. faecalis, Alcaligenes faecalis*; *A. salmonicida, Aliivibrio salmonicida*; *A. xylosoxidans, Achromobacter xylosoxidans*; *B. xylanisolvens, Bacteroides xylanisolvens*; *B. cereus, Bacillus cereus*; *B. fragilis, Bacteroides fragilis*; *B. japonicum, Bradyrhizobium japonicum*; *C. crescentus, Caulobacter crescentus*; *C. vibrioides, Caulobacter vibrioides*; *C. violaceum, Chromobacterium violaceum*; *C. gleum, Chryseobacterium gleum*; *C. indologenes, Chryseobacterium indologenes*; *C. piscium, Chryseobacterium piscium*; *C. freundii, Citrobacter freundii*; *E. meningoseptica, Elizabethkingia Meningoseptica*; *E. vietnamensis, Echinicola vietnamensis*; *E. brevis, Empedobacter brevis*; *E. cloacae, Enterobacter cloacae*; *E. tenax, Eristalis tenax*; *E. carotovora, Erwinia carotovora*; *E. aquimaris, Erythrobacter aquimaris*; *E. citreus, Erythrobacter citreus*; *E. flavus, Erythrobacter flavus*; *E. longus, Erythrobacter longus*; *E. vulgaris, Erythrobacter vulgaris*; *E. coli, Escherichia coli*; *F. aestuarina, Fibrella aestuarina*; *F. johnsoniae, Flavobacterium johnsoniae*; *J. lividum, Janthinobacterium lividum*; *K. pneumoniae, Klebsiella pneumoniae*; *L. gormanii, Legionella gormanii*; *M. oculi, Massilia*

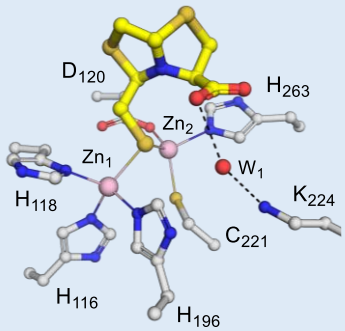
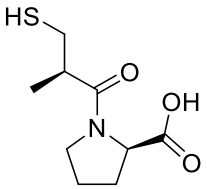
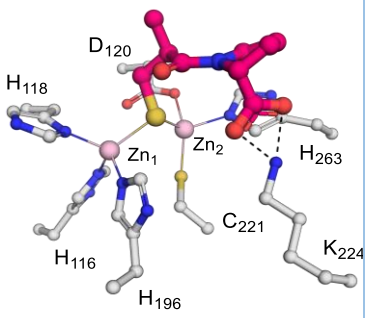
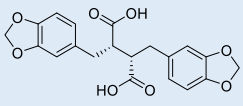
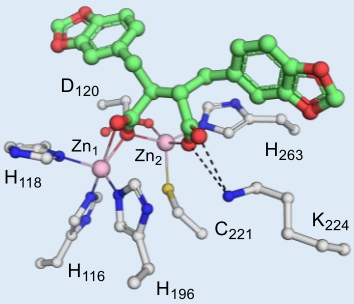
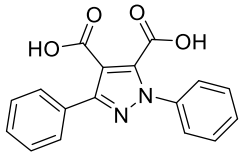
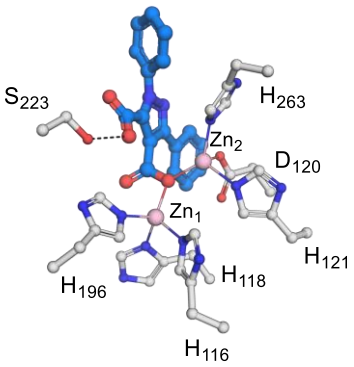
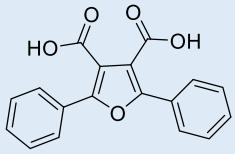
oculi; *M. albus, Myroides albus*; *M. odoratimimus, Myroides odoratimimus*; *M. odoratus, Myroides odoratus*; *M. xanthus, Myxococcus xanthus*; *O. rhinotracheale, Ornithobacterium rhinotracheale*; *P. borealis, Pedobacter borealis*; *P. kyungheensis, Pedobacter kyungheensis*; *P. lusitanus, Pedobacter lusitanus*; *P. roseu, Pedobacter roseu*; *P. aeruginosa, Pseudomonas aeruginosa*; *P. alcaligenes, Pseudomonas alcaligenes*; *P. otitidis, Pseudomonas otitidis*; *P. stutzeri, Pseudomonas stutzeri*; *P. synxantha, Pseudomonas synxantha*; *P. japonensis, Pseudoxanthomonas japonensis*; *R. planticola, Raoultella planticola*; *S. fonticola, Serratia fonticola*; *S. marcescens, Serratia marcescens*; *S. proteamaculans, Serratia proteamaculans*; *S. denitrificans, Shewanella denitrificans*; *S. frigidimarina, Shewanella frigidimarina*; *S. livingstonensis, Shewanella livingstonensis*; *S. indicum, Sphingobium indicum*; *S. smaragdinae, Spirochaeta smaragdinae*; *S. maltophilia, Stenotrophomonas maltophilia*; *S. aurantiaca, Stigmatella aurantiaca*; *T. turnerae, Teredinibacter turnerae*; *V. alginolyticus, Vibrio alginolyticus*; *V. cholerae, Vibrio cholerae*; *Y. mollaretii, Yersinia mollaretii*; *Z. galactanivorans, Zobellia galactanivorans*.

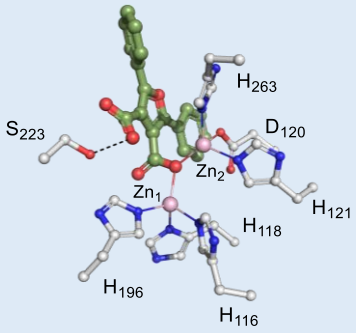
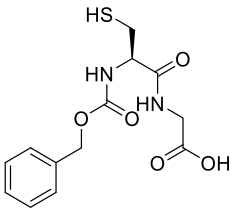
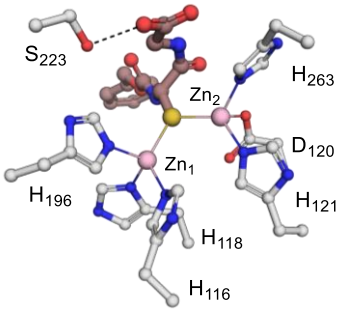
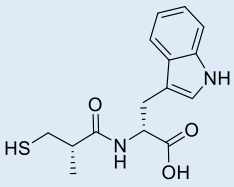
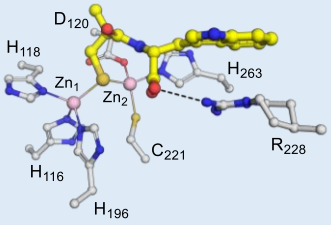
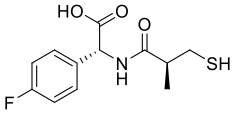
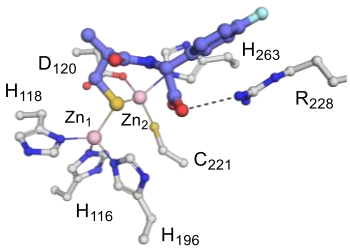
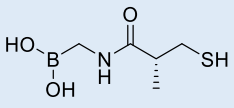
[c]Intr./acq., intrinsic to the species or acquired (not intrinsic to the species).

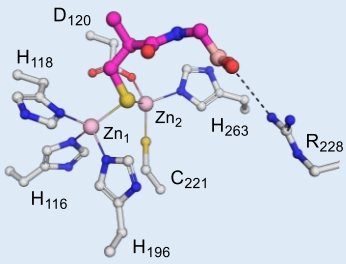
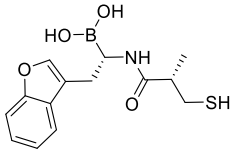
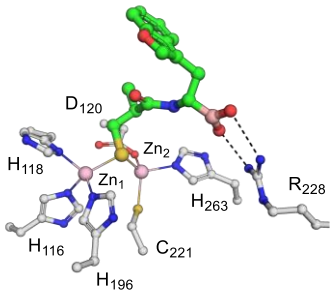
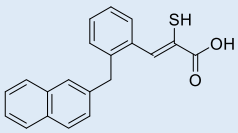
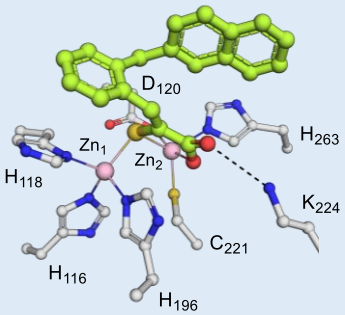
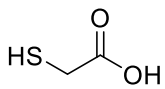
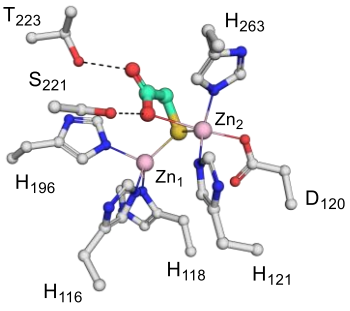
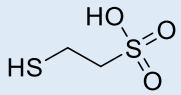
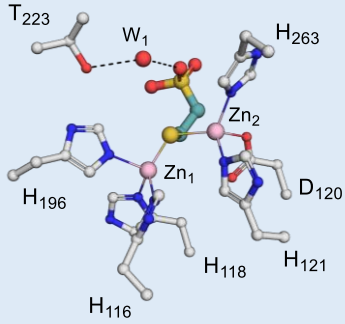
Supplementary Table S2. Inhibitor types and representative MBL inhibitors with inhibitory data and inhibition modes.

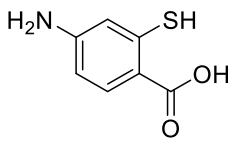
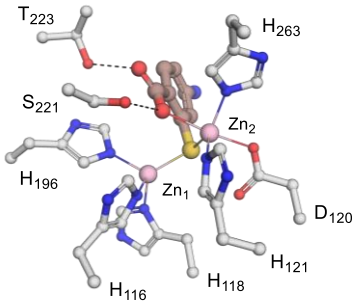
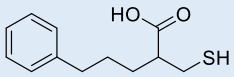
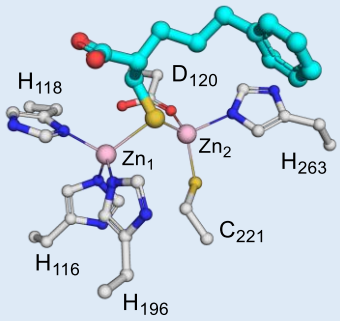
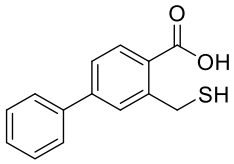
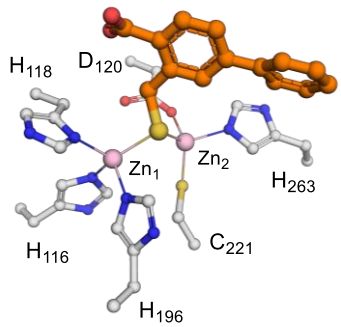
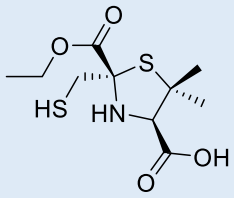
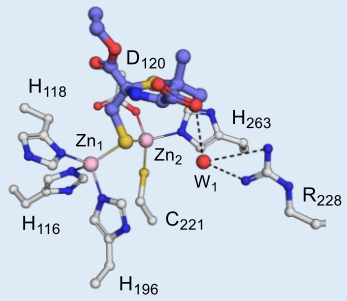
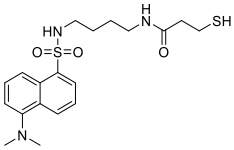
Type[a]	Chemical Structure	Inhibition Mode	Inhibitory Data	Ref.
Type I		B1 IMP-1 (PDB ID 3WXC) 	B1 IMP-1 IC_{50} = 2.7 μM	[S1]
Type I		B1 VIM-2 (PDB ID 4PVT) 	B1 NDM-1 IC_{50} = 1.05 μM B1 VIM-1 IC_{50} = 0.44 μM B1 VIM-2 IC_{50} = 0.30 μM B1 SPM-1 IC_{50} = 1.76 μM B1 IMP-1 IC_{50} = 0.00288 μM B1 BcII IC_{50} = 0.02 μM	[S2]
Type I (partly like Type III)		B1 NDM-1 (PDB ID 6D1B) 	B1 NDM-1 K_i = 123.7 μM B1 VIM-2 K_i = 2.1 μM	[S3]
Type I		B1 NDM-1 (PDB ID 6KZL) 	B1 NDM-1 K_i = 9.08 μM B1 VIM-2 K_i = 0.42 μM B1 IMP-1 K_i = 1.23 μM	[S4]
Type I		B2 CphA N220G (PDB ID 3IOG)	B1 VIM-4 K_i = 1 μM B2 CphA K_i = 5 μM B3 L1 K_i = 0.40 μM	[S5]

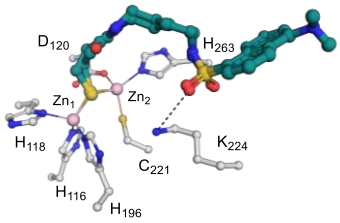
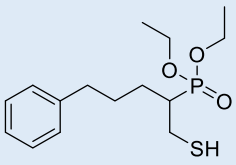
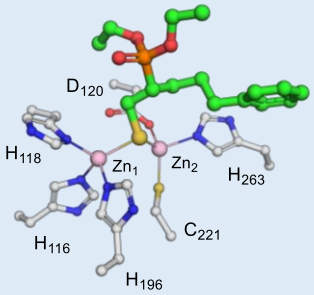
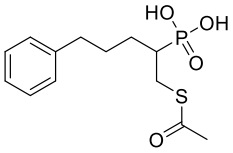
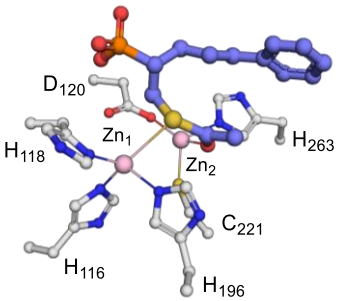
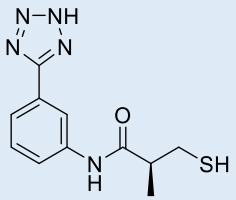
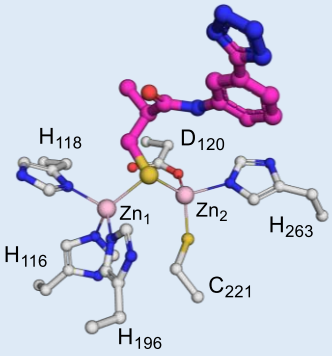
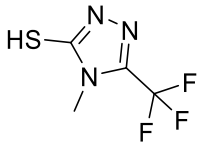
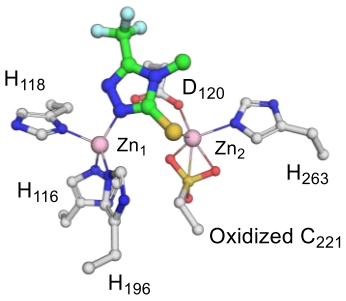
				
Type I (partly like Type III)		B3 L1 (PDB ID 5HH6) 	B1 NDM-1 K_i = 0.078 μM B1 VIM-2 K_i = 0.61 μM B1 IMP-1 K_i = 1.5 μM B3 L1 K_i = 0.4 μM	[S6]
Type I		B1 IMP-1 (PDB ID 1DD6) 	B1 IMP-1 IC_{50} = 0.09 μM	[S7]
Type I		B1 VIM-2 (PDB ID 5O7N) 	B1 NDM-1 IC_{50} = 0.7 μM B1 VIM-1 IC_{50} = 4.6 μM B1 IMP-7 IC_{50} = 0.9 μM	[S8]
Type I		B1 NDM-1 (PDB ID 4U4L)	B1 NDM-1 K_i = 7 μM B1 VIM-2 K_i = 2.9 μM B1 IMP-1 K_i = 8 μM B1 BcII K_i = 36 μM B2 Sfh-I K_i = 0.26 μM B3 L1 K_i = 12 μM B3 GOB-18 K_i = 41 μM	[S9]

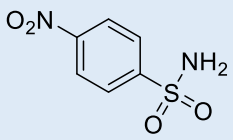
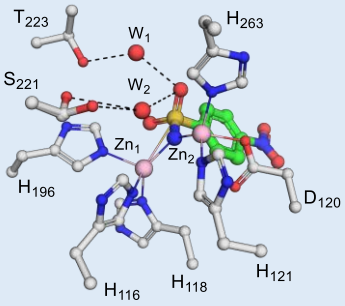
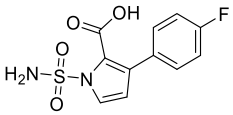
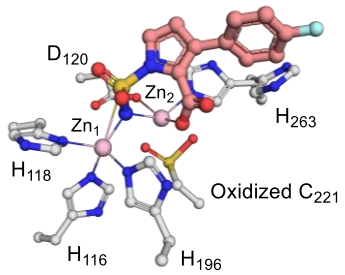
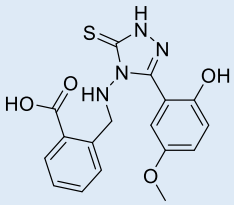
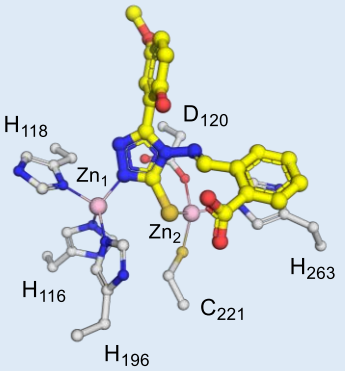
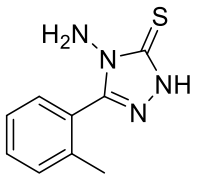
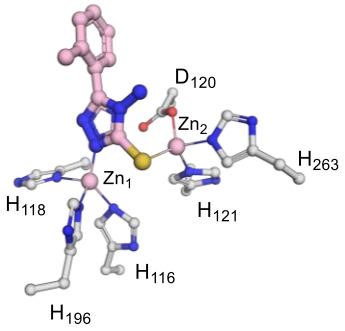
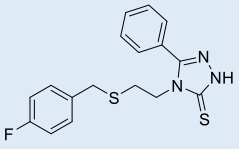
				
Type I		B1 IMP-1 (PDB ID 4C1G) 	B1 NDM-1 IC_{50} = 20.1 μM B1 VIM-2 IC_{50} = 0.072 μM B1 IMP-1 IC_{50} = 7.2 μM B1 SPM-1 IC_{50} = 261.8 μM B1 BcII IC_{50} = 10.7 μM	[S10]
Type I		B1 IMP-1 (PDB ID 1JJT) 	B1 IMP-1 IC_{50} = 0.009 μM	[S11]
Type I		B3 L1 (PDB ID 2GFJ) 	B3 L1 IC_{50} = 150 μM	[S12]
Type I		B3 L1 (PDB ID 2GFK)	B3 L1 IC_{50} = 30 μM	[S12]

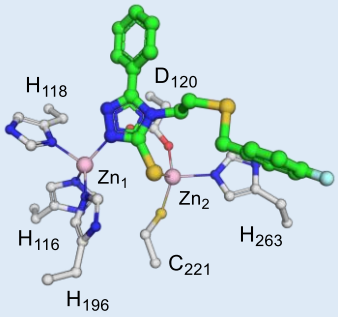
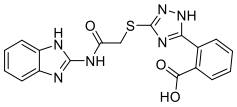
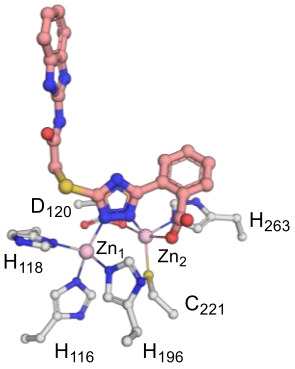
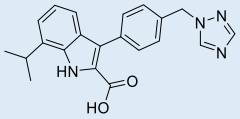
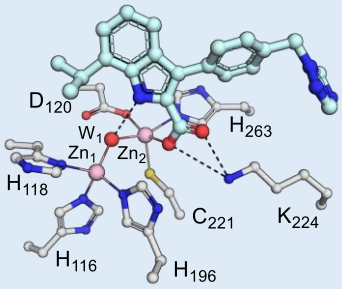
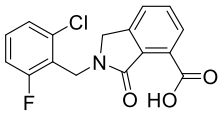
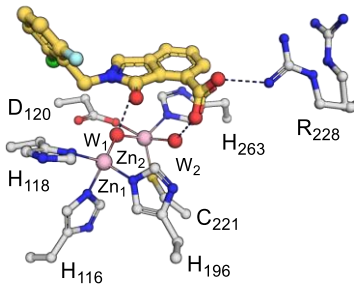
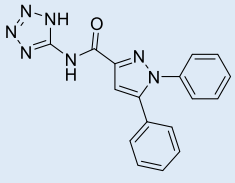
				
Type I		B3 L1 (PDB ID 2FU9) 	B3 BcII K_i = 42 μM	[S12]
Type I		B1 VIM-2 (PDB ID 5N4S) 	B1 NDM-1 IC_{50} = 24.81 μM B1 VIM-1 IC_{50} = 0.526 μM B1 VIM-2 IC_{50} = 0.055 μM B1 VIM-5 IC_{50} = 0.175 μM B1 IMP-1 IC_{50} = 0.041 μM B1 SPM-1 IC_{50} = 0.89 μM B1 BcII IC_{50} = 1.63 μM B2 CphA IC_{50} ~ 400 μM B3 L1 IC_{50} = 16.21 μM	[S13]
Type I		B1 VIM-2 (PDB ID 5Y6D) 	B1 NDM-1 IC_{50} = 5.59 μM B1 VIM-2 IC_{50} = 0.055 μM	[S14]
Type I		B1 VIM-2 (PDB ID 6J8R)	B1 NDM-1 IC_{50} = 67.13 μM B1 VIM-2 IC_{50} = 0.76 μM B3 GOB-18 IC_{50} = 2.23 μM	[S15]

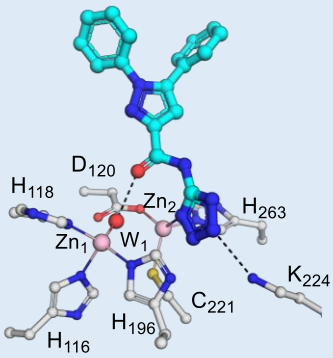
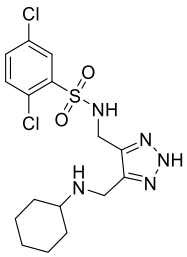
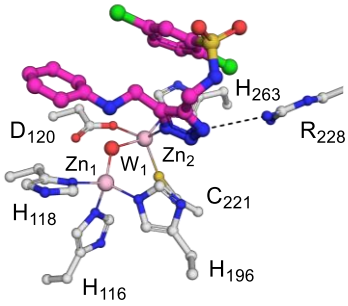
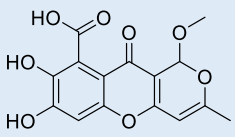
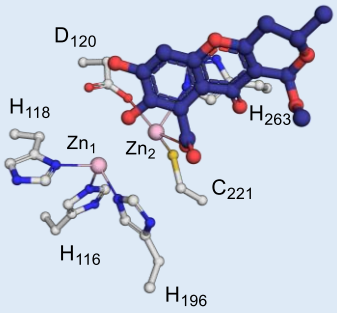
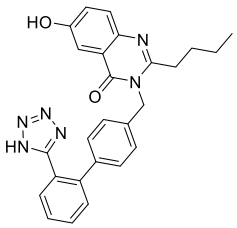
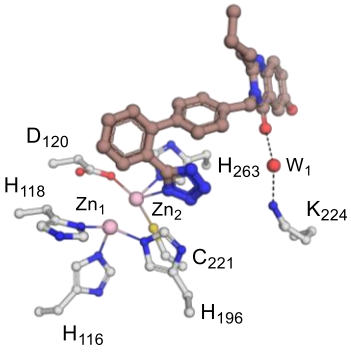
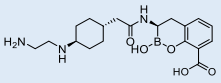
				
Type I		B1 VIM-2 (PDB ID 6JN6) 	B1 NDM-1 IC_{50} = 6.06 μM B1 VIM-2 IC_{50} = 0.07 μM B3 GOB-18 IC_{50} = 10.98 μM	[S15]
Type I		B1 BcII (PDB ID 6F2N) 	B1 NDM-1 IC_{50} = 1.1 μM B1 VIM-2 IC_{50} = 0.1 μM B1 IMP-1 IC_{50} = 0.08 μM B1 SPM-1 IC_{50} = 0.06 μM B1 BcII IC_{50} = 0.2 μM	[S16]
Type I		B3 SMB-1 (PDB ID 3VQZ) 	B3 SMB-1 K_i = 9.4 μM	[S17]
Type I		B3 SMB-1 (PDB ID 5AXR) 	B3 SMB-1 K_i = 184 μM	[S18]

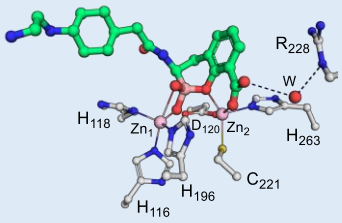
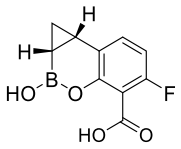
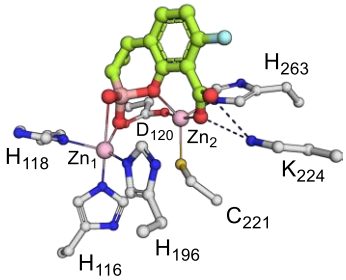
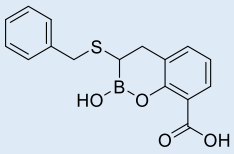
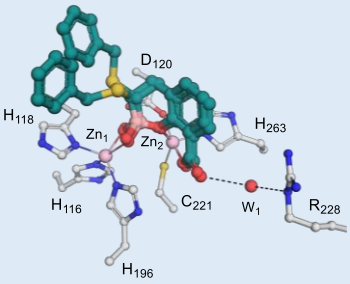
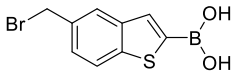
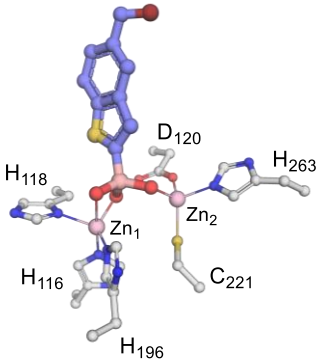
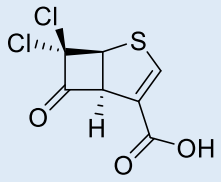
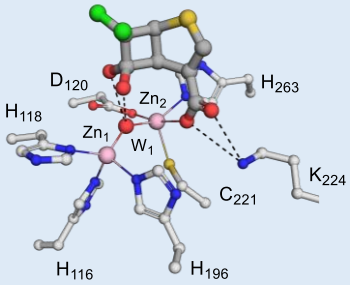
Type I		B3 SMB-1 (PDB ID 6K4X) 	B1 NDM-1 IC_{50} > 500 μM B1 VIM-2 IC_{50} = 42.1 μM B1 IMP-1 IC_{50} = 11.3 μM B3 SMB-1 IC_{50} = 0.22 μM B3 AIM-1 IC_{50} = 1.9 μM B3 L1 IC_{50} = 0.51 μM	[S19]
Type I		B1 VIM-2 (PDB ID 2YZ3) 	B1 VIM-2 K_i = 0.22 μM B1 IMP-1 K_i = 1.66 μM	[S20]
Type I		B1 VIM-2 (PDB ID 5K48) 	B1 NDM-1 IC_{50} = 5.59 μM B1 VIM-2 IC_{50} = 0.23 μM B1 IMP-1 IC_{50} = 0.23 μM	[S21]
Type I		B1 VIM-2 (PDB ID 6ZYN) 	B1 NDM-1 IC_{50} = 0.44 μM B1 VIM-2 IC_{50} = 0.75 μM B1 IMP-1 IC_{50} = 0.46 μM	[S22]
Type I		B1 IMP-1 (PDB ID 2DOO)	B1 IMP-1 K_i = 0.14 μM	[S23]

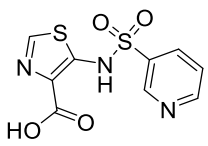
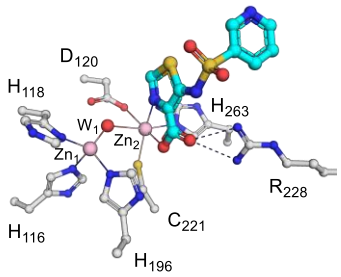
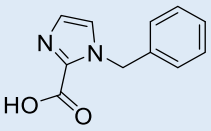
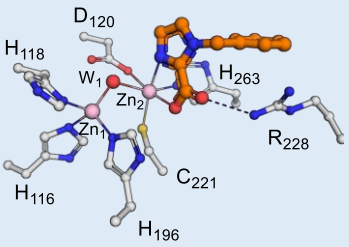
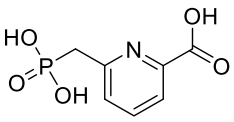
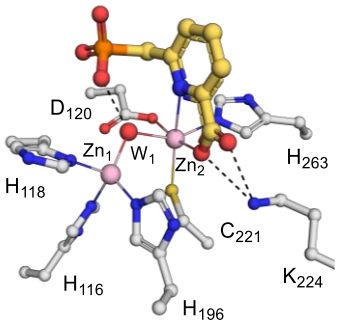
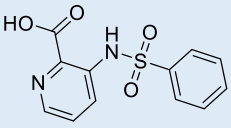
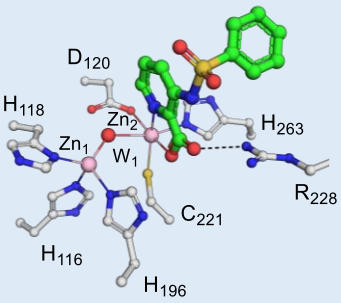
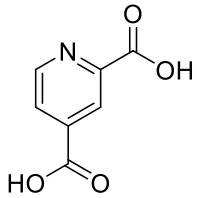
				
Type I		B1 VIM-2 (PDB ID 5MM9) 	B1 NDM-1 IC_{50} = 1.8 μM B1 VIM-2 IC_{50} = 0.38 μM B1 GIM-1 IC_{50} = 0.31 μM	[S24]
Type I		B1 VIM-2 (PDB ID 5NHZ) 	B1 NDM-1 IC_{50} = 1.8 μM B1 VIM-2 IC_{50} = 6.6 μM B1 GIM-1 IC_{50} = 26 μM	[S24]
Type I		B1 VIM-2 (PDB ID 7CJL) 	B1 VIM-2 IC_{50} = 0.044 μM B1 NDM-1 IC_{50} = 0.396 μM B1 IMP-1 IC_{50} = 0.71 μM	[S25]
Type I		B1 VIM-2 (PDB ID 5ACW) 	B1 VIM-2 IC_{50} = 232 μM	[S26]

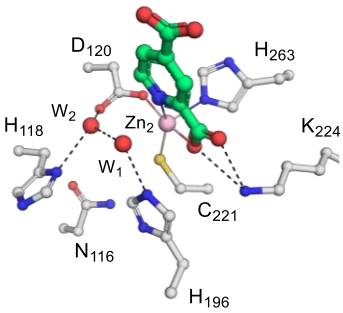
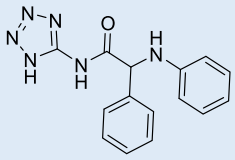
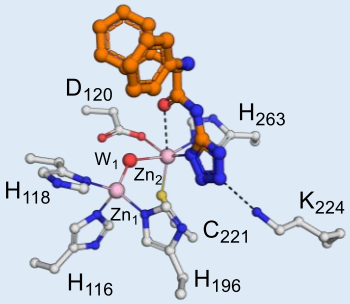
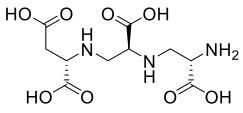
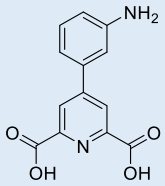
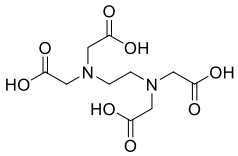
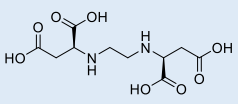
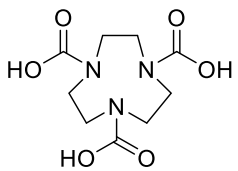
Type I		B3 BJP-1 (PDB ID 5WCM) 	B3 BJP-1 K_i = 100 μM	[S27]
Type I / **Type III**		B1 VIM-1 (PDB ID 7AYJ) 	B1 NDM-1 pIC_{50} = 8.1 B1 VIM-1 pIC_{50} = 6.9 B1 VIM-2 pIC_{50} = 7.7 B1 IMP-1 pIC_{50} = 9.2	[S28]
Type I		B1 VIM-2 (PDB ID 6YRP) 	B1 NDM-1 K_i = 27 μM B1 VIM-2 K_i = 0.7 μM B1 VIM-4 K_i = 0.5 μM B2 CphA K_i = 13 μM B3 L1 K_i = 9 μM	[S29]
Type I		B3 L1 (PDB ID 2HB9) 	-	[S12]
Type I		B1 VIM-2 (PDB ID 7OVF)	B1 NDM-1 K_i = 15.1 μM B1 VIM-1 K_i = 2.22 μM B1 VIM-2 K_i = 0.83 μM B1 VIM-4 K_i = 1.11 μM B1 IMP-1 K_i = 9.66 μM	[S30]

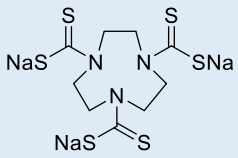
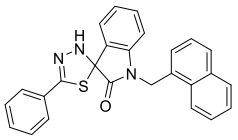
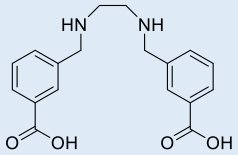
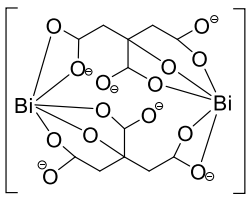
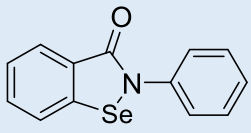
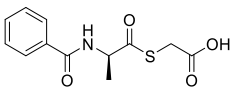
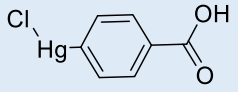
				
Type I		B1 VIM-2 (PDB ID 6KW1) 	B1 VIM-2 IC_{50} = 58.6 μM	[S31]
Type II (partly like Type IV)		B1 NDM-7 (PDB ID 7AEZ) 	B1 NDM-1 pIC_{50} = 9.2 B1 VIM-2 pIC_{50} = 8 B1 IMP-1 pIC_{50} = 7.7	[S32]
Type II		B1 VIM-2 (PDB ID 5LE1) 	B1 VIM-2 IC_{50} = 10.6 μM	[S33]
Type II		B1 NDM-1 (PDB ID 6MDU)	B1 NDM-1 K_i = 56 μM	[S34]

				
Type II		B1 VIM-2 (PDB ID 6TM9) 	B1 NDM-1 IC_{50} = 98 μM B1 VIM-2 IC_{50} = 0.23 μM	[S35]
Type II (like)		B1 CfiA (PDB ID 1HLK) 	B1 IMP-1 IC_{50} = 113 μM B1 CfiA IC_{50} = 256 μM	[S36]
Type II (like)		B1 CfiA (PDB ID 1A8T) 	B1 CfiA IC_{50} = 1.9 μM	[S37]
Type III	 VNRX-5133 (Phase III)	B1 VIM-2 (PDB ID 6SP7)	B1 NDM-1 IC_{50} = 0.19 μM B1 VIM-2 IC_{50} = 0.026 μM B1 IMP-1 IC_{50} = 39.8 μM	[S38]

				
Type III	 QPX-7728 (Phase I)	B1 NDM-1 (PDB ID 6V1M) 	B1 NDM-1 K_i = 0.032 μM B1 VIM-1 K_i = 0.008 μM B1 IMP-1 K_i = 0.22 μM	[S39]
Type III		B1 VIM-2 (PDB ID 6RPN) 	B1 NDM-1 pIC_{50} = 7.4 B1 VIM-1 pIC_{50} = 7.1 B1 VIM-2 pIC_{50} = 7.2 B1 IMP-1 pIC_{50} = 6.9 B2 CphA pIC_{50} = 6.3 B1 L1 pIC_{50} = 5.3	[S40]
Type III		B1 NDM-1 (PDB ID 6IBV) 	B1 NDM-1 K_i = 5.9 μM	[S41]
Type III		B1 SPM-1 (PDB ID 5NDB) 	B1 IMP-1 IC_{50} = 213 μM	[S42, 43]

Type IV	 ANT431	B1 VIM-2 (PDB ID 6HF5) 	B1 NDM-1 IC_{50} = 2.67 μM B1 VIM-1 IC_{50} > 200 μM B1 VIM-2 IC_{50} = 6.7 μM B1 IMP-1 IC_{50} = 54.0 μM	[S44]
Type IV		B1 VIM-2 (PDB ID 7CHV) 	B1 NDM-1 IC_{50} = 66.7 μM B1 VIM-2 IC_{50} = 0.45 μM B1 IMP-1 IC_{50} = 15.2 μM	[S45]
Type IV		B1 IMP-1 (PDB ID 5HH4) 	B1 NDM-1 K_i = 0.07 μM B1 VIM-2 K_i = 0.54 μM B1 IMP-1 K_i = 1.1 μM B3 L1 K_i = 0.5 μM	[S6]
Type IV		B1 VIM-2 (PDB ID 5MXQ) 	B1 NDM-1 IC_{50} = 49.9 μM B1 VIM-1 IC_{50} > 200 μM B1 VIM-2 IC_{50} = 1.9 μM B1 IMP-1 IC_{50} > 200 μM	[S44]
Type IV		B2 CphA (PDB ID 2GKL)	B2 CphA IC_{50} = 4.5 μM	[S46]

				
Type IV (partly like Type II)		B1 NDM-1 (PDB ID 6EFJ) 	B1 NDM-1 K_i = 477 μM	[S34]
Type V	 AMA	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 IC_{50} = 4.0 μM B1 VIM-2 IC_{50} = 9.6 μM	[S47]
Type V	 Dipicolinic Acid	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 IC_{50} = 0.08 μM B1 VIM-2 IC_{50} = 0.21 μM B1 IMP-1 IC_{50} = 0.24 μM	[S48]
Type V	 EDTA	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 IMP-1 IC_{50} = 27.9 μM	[S49]
Type V	 EDDS	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 IC_{50} = 0.18 μM B1 VIM-1 IC_{50} = 8 μM B1 SIM-1 IC_{50} = 9 μM	[S50]
Type V	 NOTA	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 K_i = 5.11 μM	[S51]

Type V		Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 K_i = 5.63 μM	[S51]
Type V	 SIT-Z5	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 IC_{50} = 6.6 μM	[S52]
Type V	 H2dedpa	Removing active site zinc ions or sequestering zinc ions in bacterial environment	B1 NDM-1 IC_{50} = 0.17 μM	[S53]
Type V	 CBS	Replacing active site zinc ions by one Bi(III) ion	B1 NDM-1 IC_{50} = 2.81 μM B1 VIM-2 IC_{50} = 3.55 μM B1 IMP-4 IC_{50} = 0.70 μM	[S54]
Type V	 Ebselen	Binding to NDM-1 by forming a S-Se bond with the residue C_{221} to destroy the active site	B1 NDM-1 K_i = 0.38 μM	[S55]
Type V	 SB214752	Inhibiting BcII by modifying the active site cysteine to destroy the active site	B1 BcII IC_{50} = 645 μM B3 L1 IC_{50} = 2 μM	[S56]
Type V	 *p*-CMB	Inhibiting NDM-1 by modifying the active site cysteine to destroy the active site	B1 NDM-1 IC_{50} = 9.0 μM	[S57]

[a] **Type I inhibitors**: replacing nucleophilic W_1 and W_2

Type II inhibitors: mimicking initial binding of intact β-lactams

Type III inhibitors: imitating the tetrahedral intermediates

Type IV inhibitors: simulating the binding of β-lactam anionic intermediates or hydrolysed products

Type V inhibitors: destructing active site metal binding

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