Supplementary material

Table S1: Molecular docking parameters for the interaction of ligands with NDM-1

Donor atom	Acceptor atom	Distance (Å)	Type of interaction	Docking energy, ΔG (kcal mol^{-1})	Binding affinity, K_d (M^{-1})
Meropenem (Control)					
Zn	Asp124:OD1	2.65268	Electrostatic	-7.9	6.2×10^5
Gln123:HN	Lig:O	1.83673	Hydrogen Bond		
Asn220:HD21	Lig:O	1.74830	Hydrogen Bond		
His189:CE1	Lig:O	3.59611	Hydrogen Bond		
His250	Lig:C	4.45873	Hydrophobic (Pi-Alkyl)		
Compound 1					
Gln123:HN	Lig:O	2.23140	Hydrogen Bond	-5.7	1.5×10^4
Lig:H	Asp124:OD2	2.67619	Hydrogen Bond		
Trp93	Lig	4.84540	Hydrophobic (Pi-Pi T-shaped)		
Lig	Val73	4.90669	Hydrophobic (Alkyl)		
Lig:C	Val73	4.16146	Hydrophobic (Alkyl)		
Phe70	Lig:C	5.23287	Hydrophobic (Pi-Alkyl)		
Trp93	Lig	5.22239	Hydrophobic (Pi-Alkyl)		
			Hydrophobic (Pi-Alkyl)		
Compound 2					
Lig:H	His120:NE2	2.68764	Hydrogen Bond	-6.0	2.5×10^4
Lig:H	Asp124:OD1	2.55858	Hydrogen Bond		
Asp124:OD2	Lig	3.86467	Electrostatic (Pi-Anion)		
Lig:C	Val73	4.40664	Hydrophobic (Alkyl)		
Compound 3					
Lig:H	His250:NE2	2.40288	Hydrogen Bond	-6.0	2.5×10^4
Lig:H	His120:NE2	2.81175	Hydrogen Bond		
Lig:H	His189:NE2	2.30996	Hydrogen Bond		
Asp124:OD2	Lig	3.79230	Electrostatic (Pi-Anion)		
Lig:H	His250	2.79062	Hydrogen Bond (Pi-Donor)		
Lig:C	Leu65	5.15741	Hydrophobic (Alkyl)		
Trp93	Lig	4.84339	Hydrophobic (Pi-Alkyl)		
Trp93	Lig:C	5.18681	Hydrophobic (Pi-Alkyl)		
Lig	Cys208	5.48747	Hydrophobic (Pi-Alkyl)		
			Hydrophobic (Pi-Alkyl)		
Compound 4					
Lig:H	His120:NE2	2.59981	Hydrogen Bond	-6.2	3.5×10^4
Lig:H	Asp124:OD1	2.60945	Hydrogen Bond		

Asp124:OD2 Trp93 Lig:C Trp93 Lig	Lig Lig Leu65 Lig:C Cys208	3.78924 4.89358 5.18009 5.14392 5.49731	Electrostatic (Pi-Anion) Hydrophobic (Pi-Pi T-shaped) Hydrophobic (Alkyl) Hydrophobic (Pi-Alkyl) Hydrophobic (Pi-Alkyl)		
Compound 5					
Lig:H Lig:H Lig:H His189:CE1 Asp124:OD2 Lig:Cl N Lig:C Lig	His250:NE2 His120:NE2 His189:NE2 Lig:O Lig His250 Val73 Val73	2.37525 2.85780 2.77597 3.56765 3.88985 3.79463 4.27020 5.37177	Hydrogen Bond Hydrogen Bond Hydrogen Bond Carbon Hydrogen Bond Electrostatic (Pi-Anion) Hydrophobic (Pi-Sigma) Hydrophobic (Alkyl) Hydrophobic (Pi-Alkyl)	-6.2	3.5×10^4

Table S2: Molecular docking parameters for the interaction of ligands with CTX-M-15.

Donor atom	**Acceptor atom**	**Distance (Å)**	**Type of interaction**	**Docking energy, Δ*G* (kcal mol^{-1})**	**Binding affinity, K_d (M^{-1})**
Avibactam (control)					
Asn104:HD22 Lys234:HZ1 Lig:H	Lig:O Lig:O Thr216:O	2.61748 2.51108 2.78293	Hydrogen Bond Hydrogen Bond Hydrogen Bond	-6.8	9.7×10^4
Compound 1					
Ser70:HG Asn132:HD22 Asn170:HD22	Lig:O Lig:O Lig:O	2.95585 1.86264 2.86371	Hydrogen Bond Hydrogen Bond Hydrogen Bond	-6.7	8.2×10^4
Compound 2					
Ser70:HG Ser130:HG Asn132:HD22 Lig:H Lig:H Tyr105 Tyr105	Lig:O Lig:O Lig:O Asn132:OD1 Glu166:OE2 Lig Lig:C	2.85091 2.38463 1.86294 2.13260 3.06227 4.10881 4.28344	Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrophobic (Pi-Alkyl) Hydrophobic (Pi-Alkyl)	-6.5	5.8×10^4
Compound 3					
Ser70:HG	Lig:O Lig:O	2.91922 1.89778	Hydrogen Bond Hydrogen Bond	-6.5	5.8×10^4

Asn132:HD22 Asn170:HD22 Lig:H Lig:H	Lig:O Ser130:O Asn132:OD1	2.85566 2.39515 2.63829	Hydrogen Bond Hydrogen Bond Hydrogen Bond		
Compound 4					
Lys73:HZ3 Ser130:HG Asn132:HD22 Asn170:HD22 Lig:H	Lig:O Lig:O Lig:O Lig:O Asn132:OD1	2.95838 2.25025 1.89371 2.85984 2.31038	Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrogen Bond	-6.8	9.7×10^4
Compound 5					
Ser130:HG Asn132:HD22 Asn170:HD22 Lig:H Lig:H	Lig:O Lig:O Lig:O Ser130:O Asn132:OD1	2.26789 1.82750 2.85047 2.33443 2.65272	Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrogen Bond	-6.7	8.2×10^4

Table S3: Molecular docking parameters for the interaction of ligands with OXA-48

Donor atom	Acceptor atom	Distance (Å)	Type of interaction	Docking energy, ΔG (kcal mol^{-1})	Binding affinity, K_d (M^{-1})
Imipenem (control)					
Arg250:HH22	Lig:O	1.774	Hydrogen Bond	-6.1	2.9×10^4
Lig:H	Ser70:OG	1.827	Hydrogen Bond		
Lig:H	Thr209:OG1	2.263	Hydrogen Bond		
Lig:HN	Lys116:O	2.315	Hydrogen Bond		
Lig:H	Thr209:OG1	2.377	Hydrogen Bond		
Lig:H	Tyr211:O	2.325	Hydrogen Bond		
Compound 1					
Tyr211:HN	Lig:O	2.447	Hydrogen Bond	-6.3	4.1×10^4
Val120:CG2	Lig	3.779	Hydrophobic (Pi-Sigma)		
Lig:C	Ile102	5.133	Hydrophobic (Alkyl)		
Tyr211	Lig:C	5.279	Hydrophobic (Pi-Alkyl)		
Compound 2					
Trp105:HE1	Lig:O	2.316	Hydrogen Bond	-6.3	4.1×10^4
Arg250:HH12	Lig:O	2.999	Hydrogen Bond		
Arg250:HH22	Lig:O	1.750	Hydrogen Bond		
Compound 3					
Tyr211:HN	Lig:O	2.513	Hydrogen Bond	-6.2	3.5×10^4
Lig:H	Tyr211:O	2.955	Hydrogen Bond		
Val120:CG2	Lig	3.845	Hydrophobic (Pi-Sigma)		
Lig:C	Ile102	5.058	Hydrophobic (Alkyl)		
Tyr211	Lig:C	5.272	Hydrophobic (Pi-Alkyl)		
Lig	Leu158	5.443	Hydrophobic (Pi-Alkyl)		
Compound 4					
Tyr211:HN	Lig:O	2.909	Hydrogen Bond	-6.4	4.9×10^4
Arg250:HH12	Lig:O	1.885	Hydrogen Bond		
Lig:H	Thr209:OG1	2.300	Hydrogen Bond		
Tyr211	Lig	5.802	Hydrophobic (Pi-Pi T-shaped)		
Tyr211	Lig	5.532			
Tyr211	Lig:Cl	5.205	Hydrophobic (Pi-Pi T-shaped)		
Lig	Leu247	5.026	Hydrophobic (Pi-Alkyl)		
			Hydrophobic (Pi-Alkyl)		
Compound 5					

Tyr211:HN	Lig:O	2.614	Hydrogen Bond		
Arg214:HE	Lig:O	2.339	Hydrogen Bond		
Tyr211	Lig	5.366	Hydrophobic (Pi-Pi T-shaped)		
Lig:C	Ile102	5.150			
Lig:Cl	Ile102	5.063	Hydrophobic (Alkyl)	-6.2	3.5×10^4
Tyr211	Lig:C	5.077	Hydrophobic (Alkyl)		
Lig	Val120	4.999	Hydrophobic (Pi-Alkyl)		
Lig	Leu158	5.247	Hydrophobic (Pi-Alkyl)		
			Hydrophobic (Pi-Alkyl)		