

**SUPPLEMENTARY TABLE S6**  
**DOCKING RESULTS**

Sl.NO	CHEMBLID	Promising candidates (Drug bank)	Interacting residues	XP GScore	glide energy
1	CHEMBL1234613	Nadide	Lys125,Arg132,Lys163,Phe176,Val178	-8.257	-61.723
2	CHEMBL1200507	Iodixanol	Ala152,Arg155,Glu159,Arg162,Lys163,Gly164,His165	-8.175	-71.448
3	CHEMBL556	Deferoxamine	Glu159,Arg160,His165,Asp171,Ala172,Glu173	-6.895	-56.603
4	CHEMBL1200455	Iohexol	Ser156,Glu159,Lys163,His165	-6.802	-46.204
5	CHEMBL118013	GXZAKQFASANPDR-UHFFFAOYSA-N *	Ala152,Ser156,Glu159,His165	-7.21	-44.421
6	CHEMBL449317	Hesperidin	Ala131,Arg162,Val178,Asn179,Arg186	-6.739	-41.925
7	CHEMBL370143	Paromomycin	Arg155,Glu159,Arg162,Lys163,His165,	-7.629	-44.795
8	CHEMBL376923	Butirosin	Glu159,Arg162,Lys163,Asn179	-6.901	-46.131
9	CHEMBL1200570	Meglumine	Ser156,Glu159,His165	-6.397	-29.118
10	CHEMBL372795	Streptomycin	Ala152,Arg155,Glu159,Arg162	-6.476	-34.015
11	CHEMBL1384	Kanamycin	Glu159,His165,Ser156,Glu181	-6.375	-38.892
12	CHEMBL1950576	Dihydrostreptomycin	Arg155,Glu159,His165	-6.097	-38.487
13	CHEMBL1201194	UCSJYZPVAKXKNQ-ZCTIVXDHSA-N*	Arg155,Glu159,His165	-5.98	-27.833
14	CHEMBL296588	Pepstatin A	Arg155,Glu159,Arg162,His165,Gln167	-5.808	-42.838
15	CHEMBL1725	Iopromide	Arg155,Glu159,Ser156,Arg162,Lys163,His165	-5.767	-37.938
16	CHEMBL511565	Ovoflavin*	Asn179,Arg186,Leu188,Lys190	-5.755	-32.374
17	CHEMBL52	Nordihydroguaiaretic acid	Ala131,Arg132,Val178,Leu188	-5.652	-33.604
18	CHEMBL184618	Framycetin	Glu159,Lys163,His165	-7.803	-44.122
19	CHEMBL1730	Cefotaxime	Arg155,Ser156,Glu159,Arg162,His165	-5.64	-34.025
20	CHEMBL221572	Ribostamycin	Glu159	-6.296	-30.981
21	CHEMBL1296	Cefotiam	Arg155,Ser156,Glu159,Arg160,Arg162,His165	-5.675	-39.908
22	CHEMBL65433	Imidurea	Ser156,Glu159,Arg162,Lys163,His165	-5.798	-41.825
23	CHEMBL1200614	Ioversol	Ser156,Glu159,Lys163,His165	-5.461	-40.157
24	CHEMBL1909452	Apramycin	Ser156,Glu159,Glu181	-5.833	-48.724
25	CHEMBL3754093	PGBHMTALBBVCIT-UFTIIHCESA-N*	Ser156,Glu159,Lys163,His165	-7.954	-46.362
26	CHEMBL58	Mitoxantrone	Ala152,Glu159,Arg162,Lys163	-5.358	-41.405
27	CHEMBL2105769	Protoveratrine A	Glu159,Glu167	-5.304	-31.097
28	CHEMBL487417	Vitexin	Ser156,Glu159,Lys163,His165	-5.312	-31.753
29	CHEMBL182	Ganciclovir	Ala152,Ser156,Lys165,	-5.248	-26.692
30	CHEMBL1679	Leucovorin	Ala131,Arg162,Arg186,Leu188,Lys190	-5.128	-46.501
31	CHEMBL195892	Gentamicin C1	Ala152,Ser156,Glu159	-5.192	-44.989
32	CHEMBL44354	Ceftazidime	Lys125,Arg132,Lys190	-5.192	-44.989