

**Table 18.** Multiple docking scores of the best lead and the best docked existing inhibitors with selected human MMPs

S.No.	Therapeutic target	Lead 1			Best Co-crystal ligand / inhibitor		
		RRD (kcal/mol)	QPLD (kcal/mol)	IFD (kcal/mol)	RRD (kcal/mol)	QPLD (kcal/mol)	IFD (kcal/mol)
1	MMP-1	-11.169	-10.452	-10.594	-9.394	-9.367	-10.067
2	MMP-2	-13.827	-12.206	-13.982	-8.637	-9.047	-8.917
3	MMP-3	-14.128	-14.754	-14.564	-12.857	-13.588	-13.191
4	MMP-7	-11.182	-12.155	-7.576	-9.136	-9.290	-7.333
5	MMP-9	-12.936	-13.425	-13.212	-11.567	-11.878	-11.526
6	MMP-10	-14.87	-12.038	-13.182	-6.259	-6.372	-7.312
7	MMP-11	-9.698	-9.077	-10.181	-2.572	-7.606	-7.366
8	MMP-12	-12.160	-12.158	-11.311	-10.275	-7.908	-9.828
9	MMP-13	-15.185	-15.479	-14.392	-10.320	-12.343	-11.891
10	MMP-14	-8.711	-8.773	-8.577	-6.092	-6.021	-5.892

**Table 19.** QPLD interactions of the best docked existing inhibitors and the best lead with selected human MMPs

S.No.	MMP	Crystal ligand / existing ligand bonded interactions	Crystal ligand / existing ligand non bonded interactions	Lead bonded interactions	Lead non bonded interactions
1.	MMP-1	R04 (G179, L181, A182, Y210, E219, P238, Y240, Zn275)	R04 (G178, N180, H183, A184, E209, V215, H218, H222, H228, Y237, S239)	Lead 1 (G179, L181, E209, Y210, P238, Y240, Zn275)	Lead 1 (G178, N180, A182, R214, V215, H218, E219, H228, Y237, S239, T241)