

## Identification of novel selective MMP-9 inhibitors as potential anti-metastatic lead using structure based hierarchical virtual screening and molecular dynamics simulation

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**Table S1: Calculated RESP Charges for His - Zn(II) complex**

HID (CAT domain)		HID (CAT domain)		HID (CAT domain)	
Atom	Charge	Atom	Charge	Atom	Charge
N	-1.05555	N	-0.80392	N	-0.98842
H	0.84327	H	0.63871	H	0.80561
CA	0.36146	CA	0.39884	CA	0.25551
HA	0.10971	HA	0.03234	HA	0.0445
CB	-0.73514	CB	-0.72359	CB	-0.68113
HB2	0.24212	HB2	0.24035	HB2	0.23238
HB3	0.22404	HB3	0.27046	HB3	0.21388
CG	0.36067	CG	0.21643	CG	0.4846
CD2	-0.24686	ND1	-0.04145	ND1	-0.39717
HD2	0.17737	HD1	0.29007	HD1	0.37764
ND1	-0.25241	CE1	-0.05153	CE1	0.20781
HD1	0.36303	HE1	0.19955	HE1	0.15988
CE1	-0.01336	NE2	-0.36632	NE2	-0.48685
HE1	0.19486	CD2	-0.04857	CD2	-0.12165
NE2	-0.21706	HD2	0.11117	HD2	0.09435
C	0.50234	C	0.39475	C	0.45107
O	-0.49696	O	-0.44885	O	-0.41546
		Zn	0.91792		
		OW	-0.68999		
		HW1	0.45008		
		HW2	0.41545		