Electronic Supplementary Material (ESI) for RSC Advances.

Ligand based pharmacophore modelling and integrated computational approaches in the quest of small molecule inhibitor against hCA IX

S.No	SMILES

1	CC(NC1=NN=C(S(=O)(N)=O)S1)=O
3	O=C(/C=C/C1=C(OC)C=C(OC)C=C1OC)/C=C/C2=CC=C(S(N)(=O)=O)C=C2
4	O=S(C(C=C1)=CC=C1N(N=N2)CC2CCC(C=C3)=CC=C3C4=CC=NC=C4)(N)=O
5	O=S(C1=CC=C(N2C=C(C3=CC=CC=C3)N=N2)C=C1)(N)=O
6	CC1=C(NC(NCC2=CC(S(=O)(N)=O)=CC=C2)=O)OC3=CC=CC=C13
7	O=S(C1=CC=CC(CNC(NC2=CC3=CC(Br)=CC=C3O2)=O)=C1)(N)=O
8	NS(C1=CC=C(NC(NC2=NC(C)=C(C)N=C2C)=O)C=C1)(=O)=O
9	CN1C[C@@H]2[C@@H](C[C@@H]([C@]2(C(=O)O)NC(=O)CS(=O)(=O)N)O)C(=C1)C(=O)N
10	C1=CC(=C(C=C1C/C(=N\O)/C(=O)NCCS(=O)(=O)N)Br)O
11	O=C([Se]CC#C)CC(C1=C2C=CC(OC)=C1)=C(C)N2C(C3=CC=C(Cl)C=C3)=O
12	FC(F)(F)C1=CC=CC(NC2=C(C([Se]CC#C)=O)C=CC=C2)=C1

Ligand ID	ZINC ID	Docking score	RMSD	Amino acid interaction
V1	Zinc00151360	-6.47	0.841	HIS 94, ZN 301
V2	Zinc00342043	-6.80	0.916	THR 199, ASN 62, SER 65, ZN 301
V3	Zinc70666499	-7.10	0.950	ARG 18, ZN 301

Table S1. Active Compounds used in the pharmacophore validation.

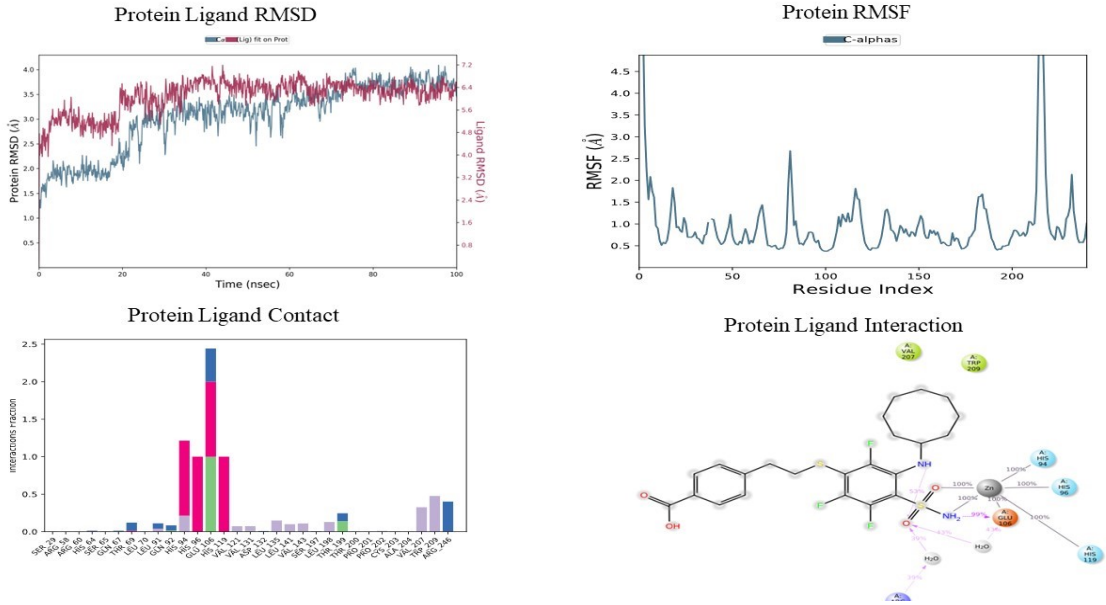

Figure S1. Molecular dynamics simulation data of the Apoprotein.

V4	Zinc02420638	-5.97	0.761	THR 199, HIS 94
V5	Zinc18137077	-5.89	0.929	GLN 92, ZN 301
V6	Zinc01767896	-5.80	0.593	ASN 62, GLN 92
V7	Zinc03844670	-7.19	0.881	THR 199, HIS 94, ZN 301
V8	Zinc13532309	-5.58	0.957	VAL 121, ZN 301
V9	Zinc03845641	-6.09	0.606	GLN 92, ASN 62
V10	Zinc01704331	-5.60	0.957	HIS 94, ZN 301
V11	Zinc00536677	-6.11	0.906	ASN 62, HIS 94
V12	Zinc01505327	-6.38	0.770	HIS 94
V13	Zinc00003955	-7.08	0.835	ZN 301
V14	Zinc38440019	-6.87	0.818	GLN 92, GLN 67, ZN 301
V15	Zinc04994155	-6.03	0.936	HIS 96, ZN 301
V16	Zinc0049817	-6.28	0.886	HIS 94, ZN 301
V17	Zinc04701335	-7.18	0.631	THR 199, ZN 301
V18	Zinc11689965	-7.71	0.704	HIS 94, THR 199, SER 197, ZN 301
V19	Zinc72324703	-7.22	0.404	THR 199, ARG 60, ZN 301
V20	Zinc04180215	-5.65	0.498	HIS 94, ARG 18, ZN 301
V21	Zinc68572305	-6.04	0.917	ASN 62, ZN 301
V22	Zinc19703228	-6.57	0.830	VAL 121, ZN 301
V23	Zinc19732669	-5.96	0.954	HIS 94, GLN 92, ASN 62
V24	Zinc03847982	-5.85	0.920	GLN 92, ZN 301
V25	Zinc12620605	-6.34	0.956	THR 199, GLN 92, ASN 62
V26	Zinc00518929	-7.05	0.795	LEU 198, THR 199, ZN 301
V27	Zinc02168937	-6.44	0.576	LEU 91, THR 199, ZN 301
V28	Zinc03846889	-6.74	0.933	THR 199, ZN 301
V29	Zinc04261842	-6.64	0.769	THR 199, HIS 94, ZN 301
V30	Zinc04504454	-6.43	0.764	HIS 94, ZN 301
V31	Zinc01675744	-6.39	0.855	ASN 62
V32	Zinc20112806	-6.87	0.967	GLN 92, ZN 301
V33	Zinc13544730	-6.64	0.551	THR 199, ZN 301
V34	Zinc13406180	-8.07	0.737	GLN 92, ZN 301
V35	Zinc09419065	-8.05	0.895	ZN 301, HIS 96, THR 199
V36	Zinc25315630	-6.96	0.567	ZN 301, HIS 94
V37	Zinc04528652	-6.89	0.922	THR 199, ZN 301
V38	Zinc68581601	-6.06	0.494	ASN 62, THR 199, ZN 301
V39	Zinc14658109	-7.01	0.796	HIS 94
V40	Zinc03844579	-6.90	0.769	HIS 94, VAL 121, ZN 301
V41	Zinc03844582	-6.92	0.767	THR 199, THR 69, ZN 301
V42	Zinc70666213	-6.40	0.950	ASN 244, HIS 94
V43	Zinc04267306	-7.13	0.928	HIS 94, ZN 301

Standard	Acetazolamide	-5.96		HIS 94, ASN 62, THR 200, ZN 301

Table S2. Lead compounds generated from Zinc database with its ZINC ID, RMSD value, Binding score, and Amino acid residue.