

Molecular Docking Results (Boltz-2)

Predicted affinity between candidate ligands and hub proteins

Protein (Hub Genes)

AKT1	NA	6.62	5.69	5.77	NA	6.06	6.04	NA	5.45	NA	5.77	5.14	5.79	5.26	NA
MTOR	6.74	7.38	6.56	6.31	6.39	6.12	5.42	5.28	5.61	5.82	5.53	6.16	5.41	5.17	4.70
PIK3CA	6.60	5.88	6.37	5.80	5.88	6.63	6.20	5.93	6.12	5.86	5.43	6.21	5.74	5.84	4.95
ENO1	6.59	6.00	7.46	7.13	6.44	6.22	6.42	6.59	6.01	5.80	5.91	5.92	5.48	5.37	5.03
SLC27A5	7.24	7.00	6.39	6.73	6.65	5.84	6.22	6.14	6.35	6.10	6.73	5.84	5.97	6.24	4.82

pIC50 (higher is better)

