Supplementary Information

Identification of dual human acetylcholinesterase and butyrylcholinesterase inhibitors through pharmacophore-based virtual screening, molecular docking and molecular dynamics simulation studies

Poonam Yadav & Shivani Jaiswal*
Institute of Pharmaceutical Research, GLA University, Mathura 281 406, India
E-mail: shivani.rs.phe16@iitbhu.ac.in, shivanijaiswal.2010@rediffmail.com

Received 4 January 2025; accepted (revised) 22 January 2025

Table of Contents

Table S1. Results of various parameters calculated during GH scoring.

S. No.	Parameter	AChE	BuChE
1	Total molecules in database (D)	380	400
2	Total number of actives in the database (A)	47	69
3	Total hits (Ht)	29	55
4	Active hits (Ha)	25	48
5	%Yield of actives[(Ha/Ht) ×100]	86.2069	87.27273
6	Enrichment factor (E) [(Ha×D)/(Ht×A)	6.969919	5.059289
7	False positives (Ht-Ha)	4	7
8	Goodness of hit score	0.77953	0.828458

Table S2 Estimated ligand-protein complex binding energy, average RMSD, and RMSF for 100-ns MD simulations.

Compound	**Avg RMSD (Å)**	**Avg RMSF (Å)**	**Binding energies (Kcal/mol)**
ZINC000329492445	1.32±0.21	0.91±0.56	-82.57
ZINC000001693021	1.38±0.09	0.95±0.69	-81.42
ZINC000257331938	1.59±0.38	0.93±0.62	-77.46

Table S3. Estimated ligand-protein complex binding energy, average RMSD, and RMSF for 100-ns MD simulations.

Compound	**Avg RMSD (Å)**	**Avg RMSF (Å)**	**Binding energies (Kcal/mol)**
ZINC000329492445	2.48±0.51	0.91±0.41	-78.86
ZINC000001693021	0.29±0.09	0.76±0.35	-76.99
ZINC000257331938	1.60±0.28	0.93±0.60	-68.47

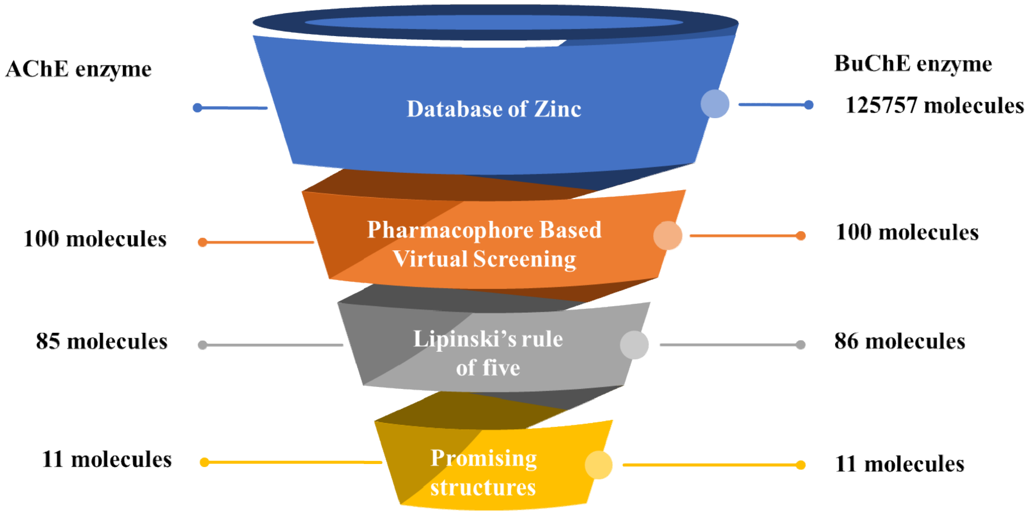

Figure S1: Virtual screening analysis.

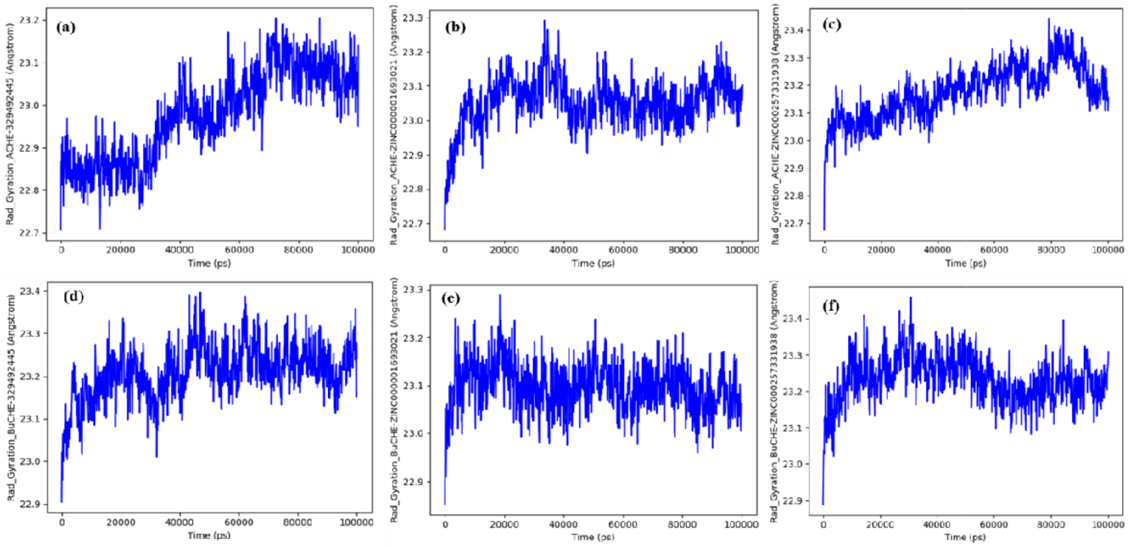

Figure S2: rGYR with AChE enzyme: (a) **ZINC000329492445**, (b) **ZINC000001693021**, and (c) **ZINC000257331938**; **rGYR with BuChE enzyme**: (d) **ZINC000329492445**, (e) **ZINC000001693021**, and (f) **ZINC000257331938**.