Chasing ChEs-MAO B Multi-targeting 4-Aminomethyl-7-Benzyloxy-2*H*-Chromen-2-ones

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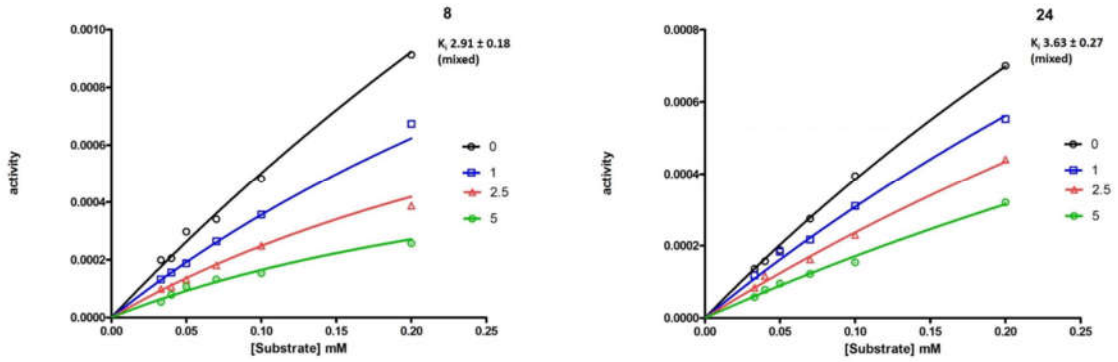

Figure S1. eeAChE enzyme kinetics (Michaelis-Menten curves) for compounds **8** (left) and **24** (right).

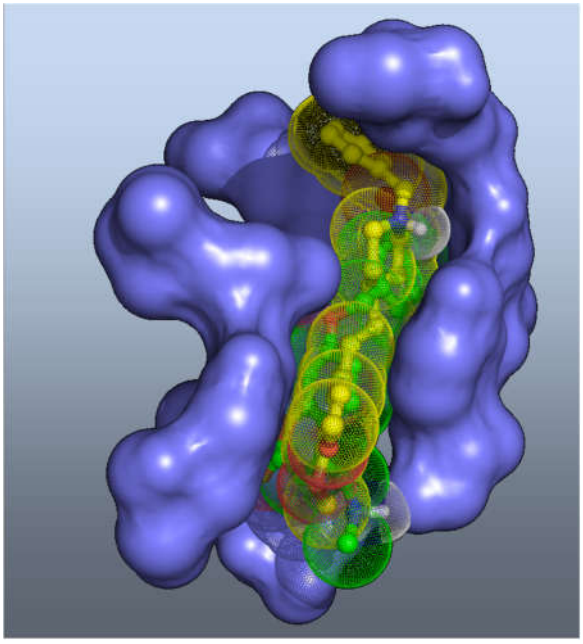

Figure S2. Ball and stick model showing the superimposition of the binding poses of donepezil (yellow) and compound **8** (green) within human AChE (PDB code 6OW4).

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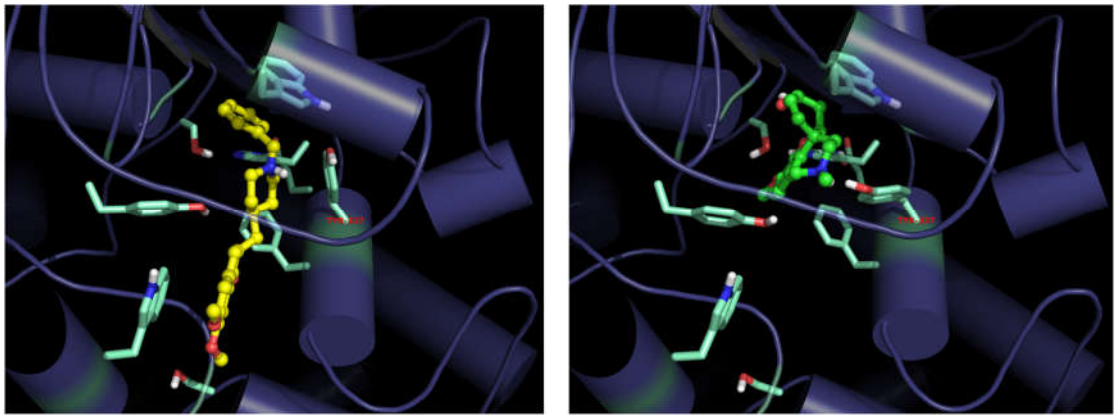

Figure S3. Different rotamers for mid-gorge Tyr337 (cyan) in the crystal structures of hAChE complexed with donepezil (yellow; PDB code 6OW4) and galantamine (green; PDB entry 4EY6) employed in docking simulations. Other key residues, showing no shift between the two models, are shown in cyan.

Table S1. hAChE docking data for compounds **8**, **24** as compared to donepezil.

entry	FEB[a]	Population[b]	Efficacy[c]	CSA[d]
8	-11.62	59/250	0.505	352.99
24	-12.71	26/250	0.489	393.89
donepezil	-10.86	55/250	0.388	442.44

[a] Free energy of binding (kcal/mol) as estimated by the AutoDock scoring function.
[b] Frequency of the selected cluster.
[c] Ligand efficacy calculated measured as the absolute FEB value divided by the number of heavy atoms.
[d] Contact surface area in $Å^2$.