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Identification of potential AChE inhibitors through combined machine-learning and structure-based design approaches

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Supplementary Data

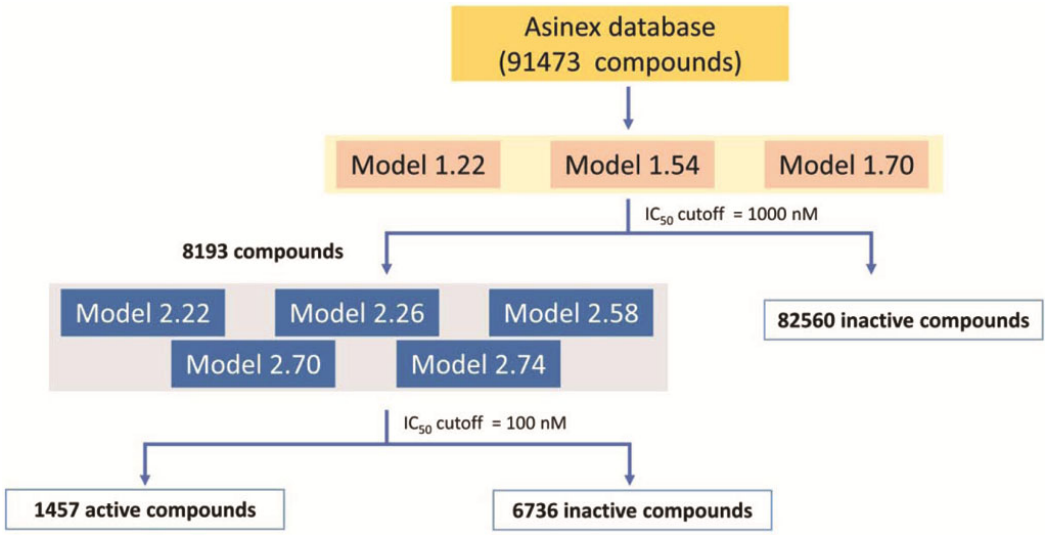

Fig. S1 — ML-based screening of the Asinex compounds to identify potential AChE inhibitors

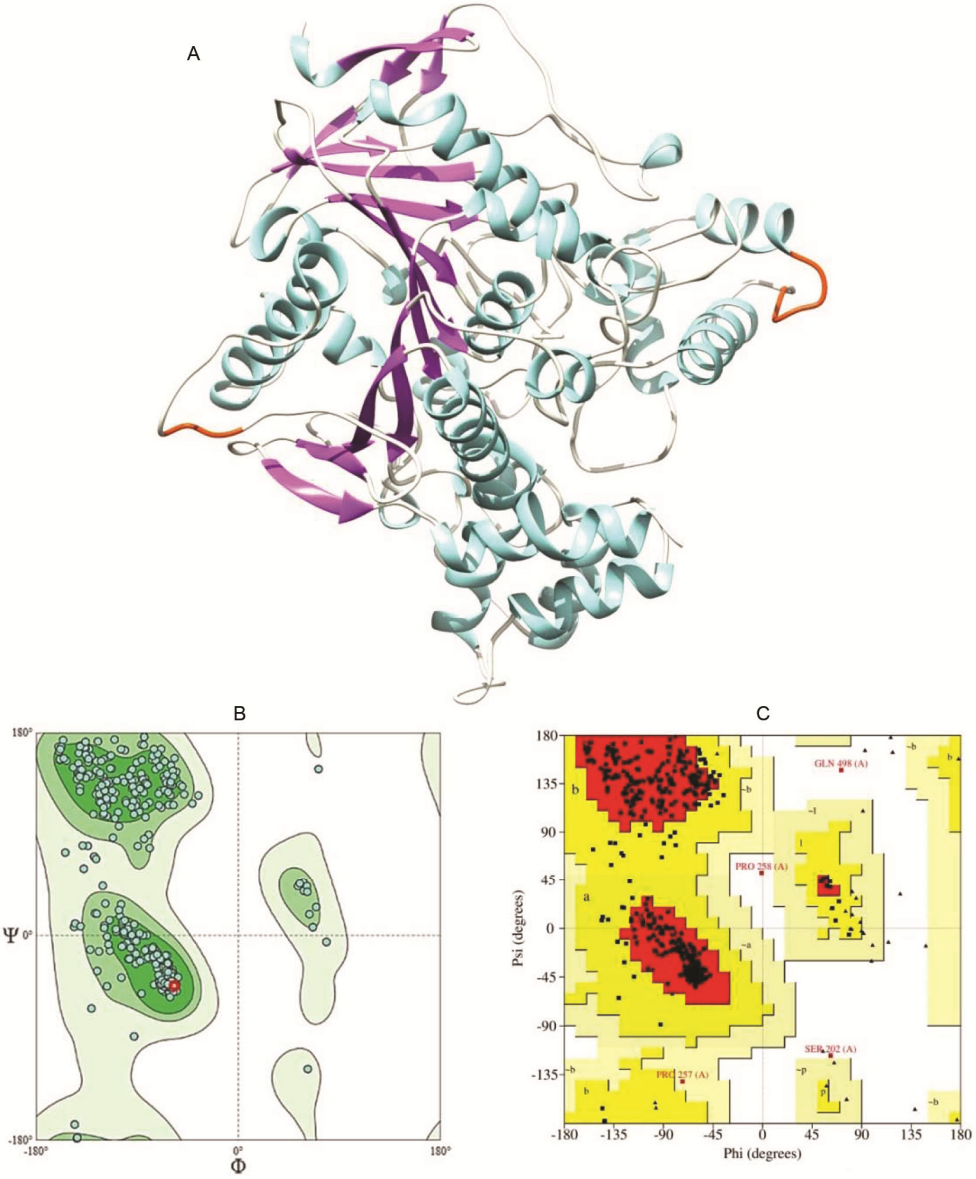

Fig. S2 — (A) Homology model of Human AChE enzyme with the constructed loops indicated in orange colour; (B and C) Ramachandran plot of the developed homology model obtained from PROCHECK and RAMPAGE, respectively

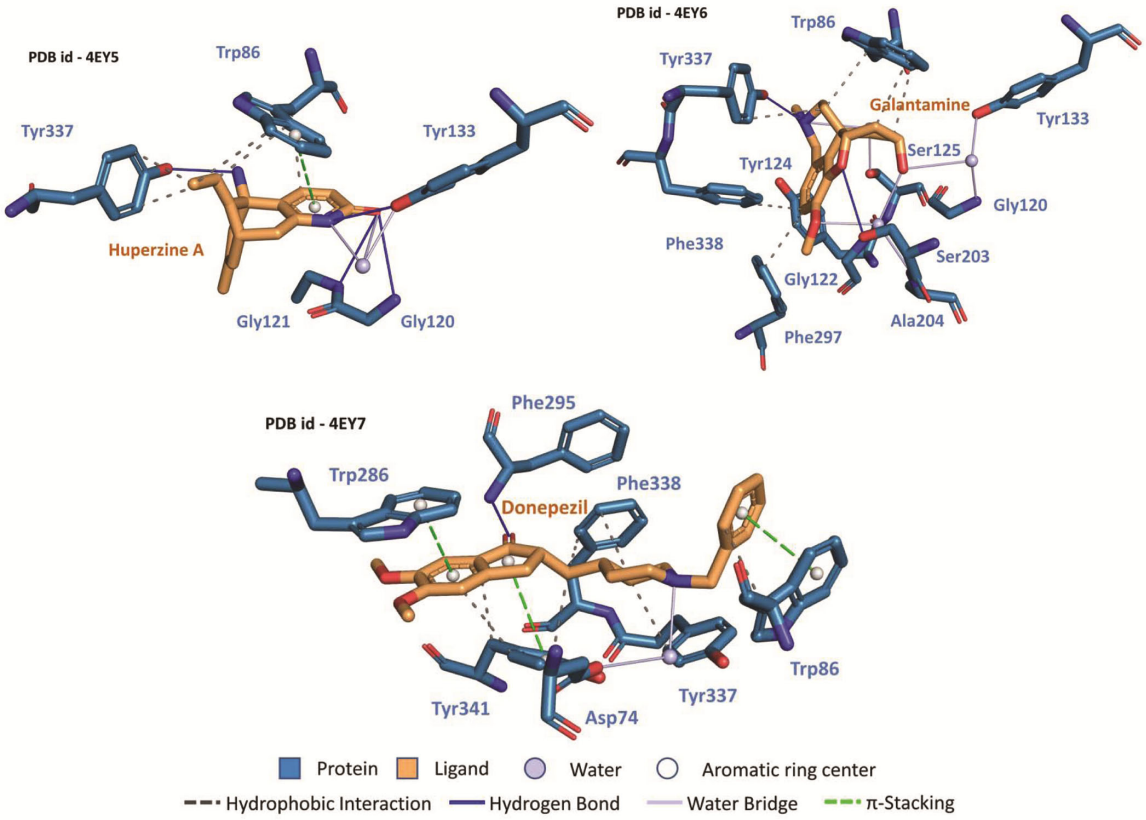

Fig. S3 — 3D interaction of Huperzine A, Galantamine and Donepezil with active site residues of AChE enzyme

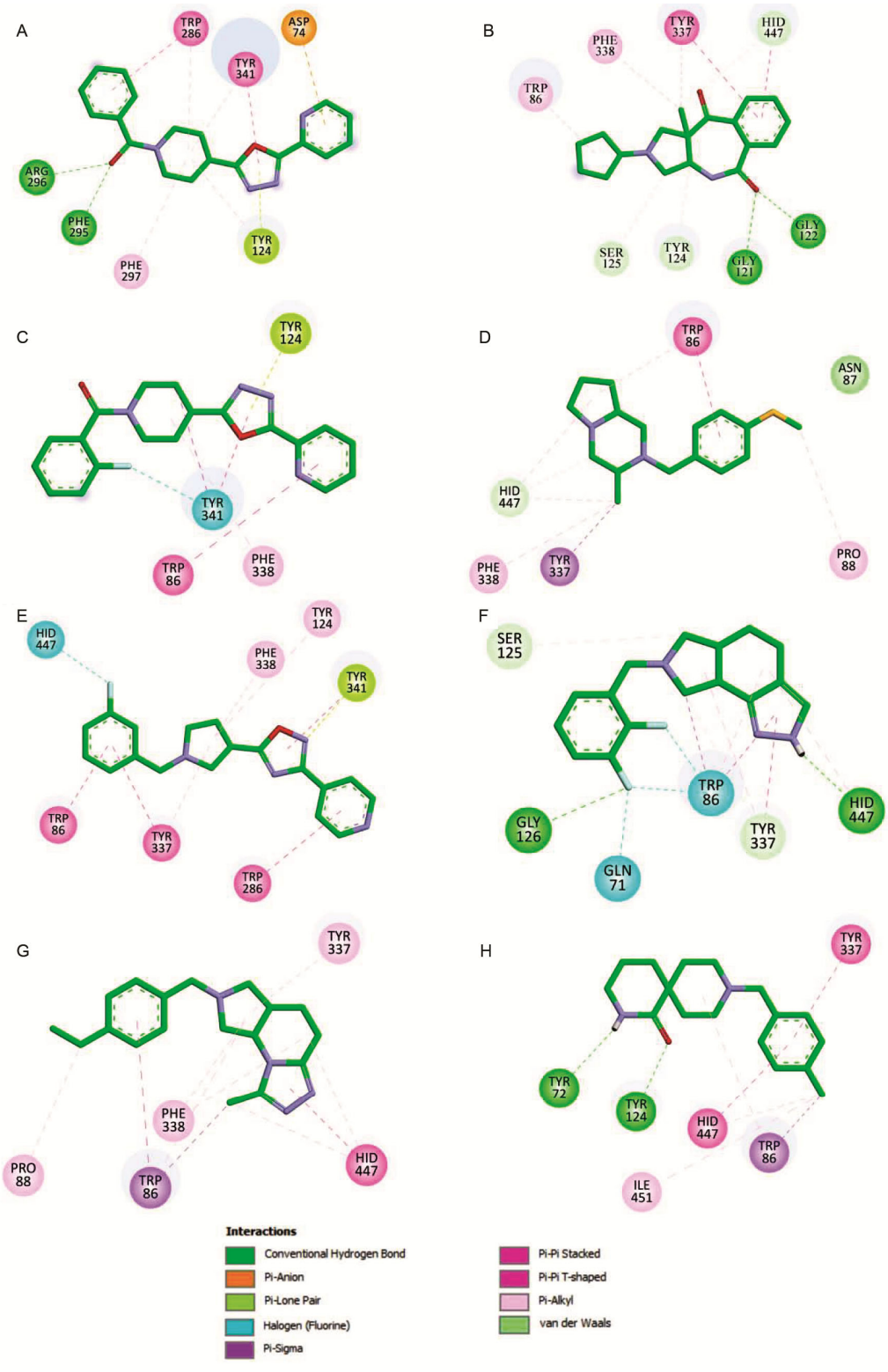

Fig. S4 — 2D interaction diagram of the AChE inhibitors with active site residues of AChE enzyme: (A) AOP19760577; (B) ART22341446; (C) AOP19760615; (D) AAM13201183; (E) LMG19707967; (F) ART21232619; (G) ART21295754; and (H) LMG16204648

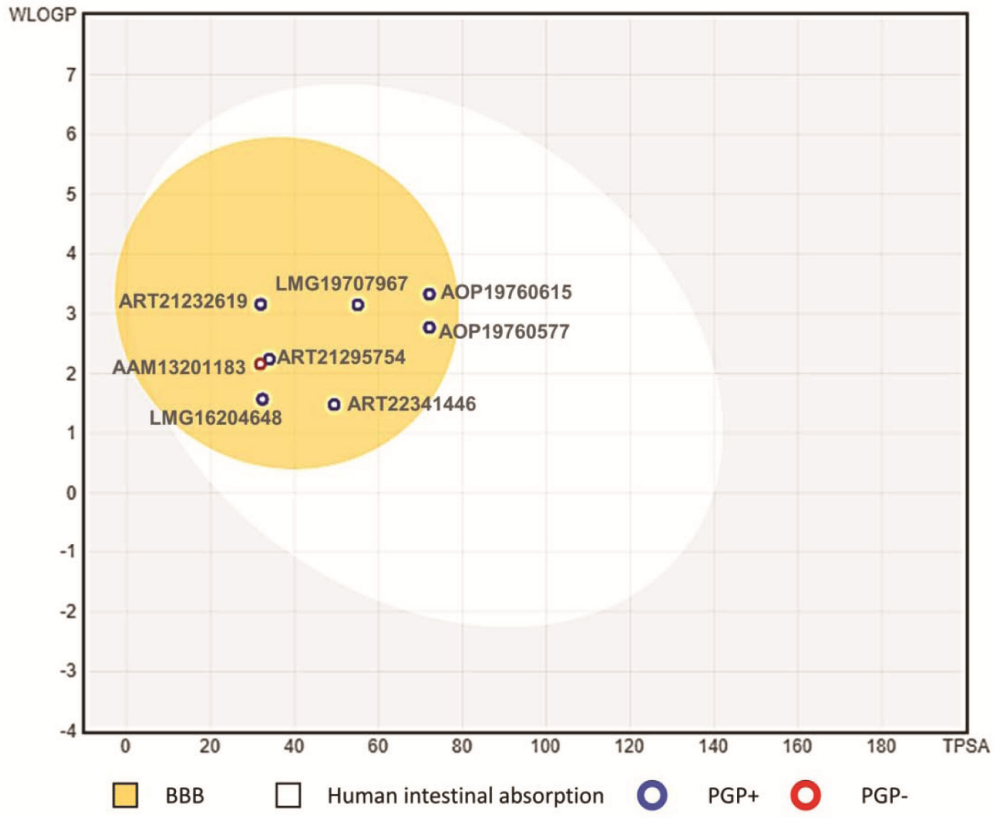

Fig. S5 — BOILED-Egg diagram of the AChE inhibitors

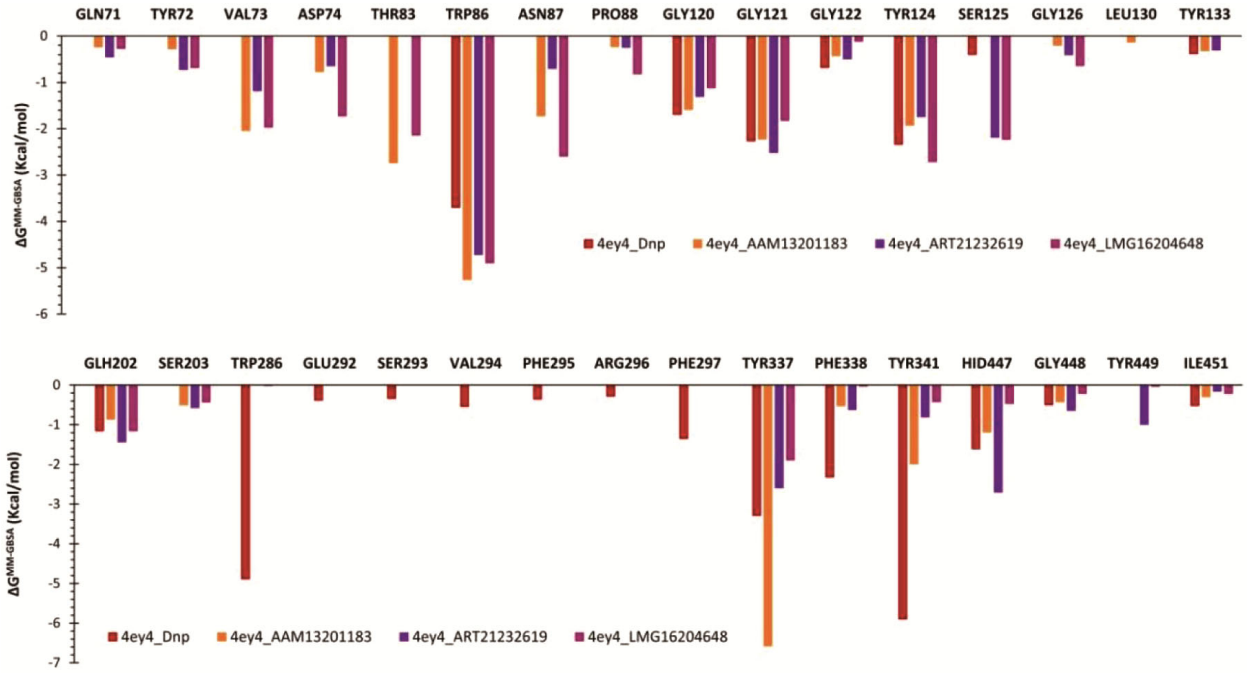

Fig. S6 — The per-residue interaction of various ligands with AChE obtained through MM-GBSA