Computational screening of promising beta-secretase 1 inhibitors through multi-step molecular docking and molecular dynamics simulations - pharmacoinformatics approach

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Supplementary data

Table S1. Binding energy and inhibitory activity of standard BACE1 inhibitors

Molecule	Binding energy	IC_{50} (nM)
AZD3293	-9.00	0.60
AZD3839	-9.10	4.80
CNP520	-7.00	11.00
E2609	-9.30	5.00
JNJ54861911	-7.90	1.10
LY2886721	-8.30	20.30
MK8931	-8.50	13.00
RG7129	-8.40	2.00
TAK070	-8.70	Not reported

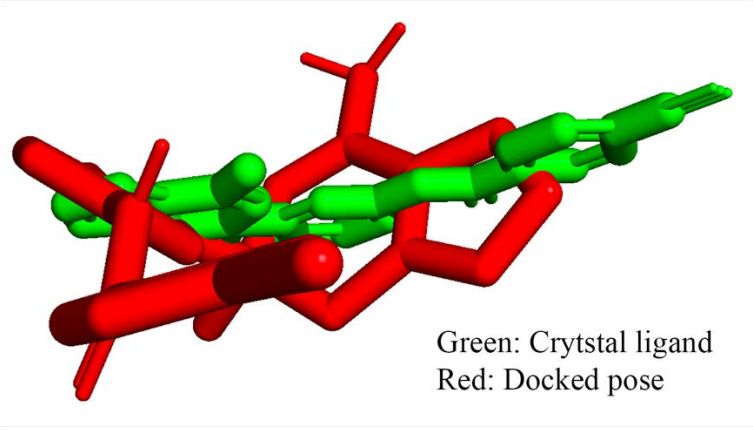

Figure S1. Superimpose of co-crystal ligand and best docked pose of M7D.

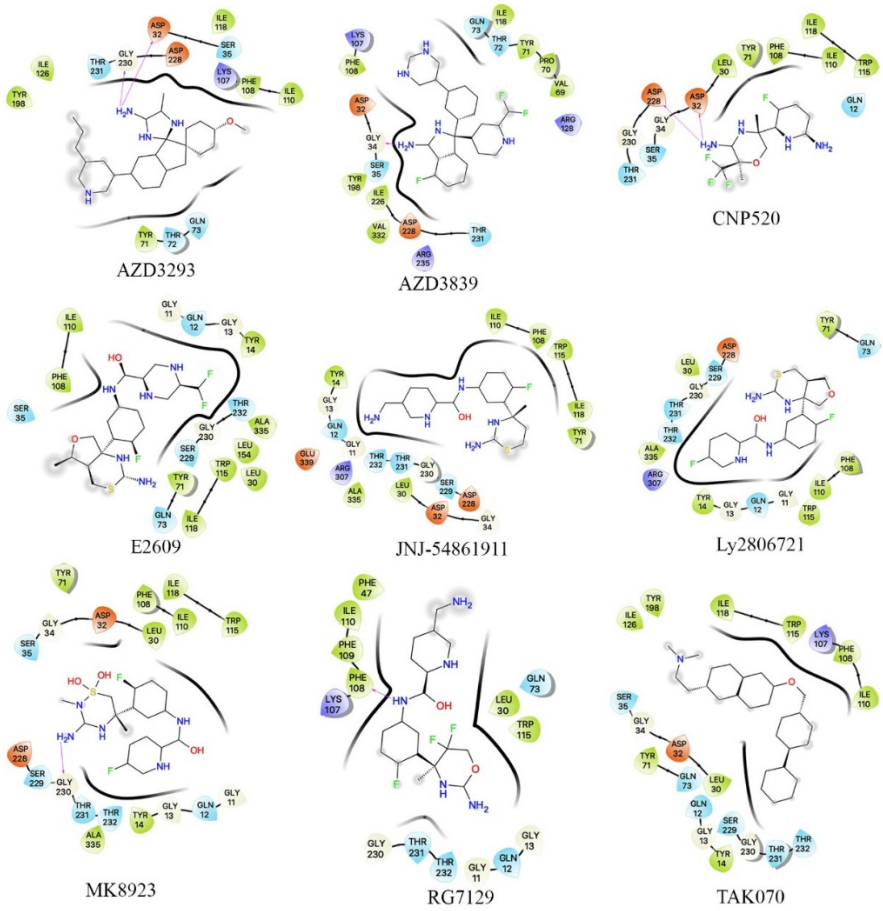

Figure S2. Two-dimensional binding interaction of standard BACE1 inhibitors

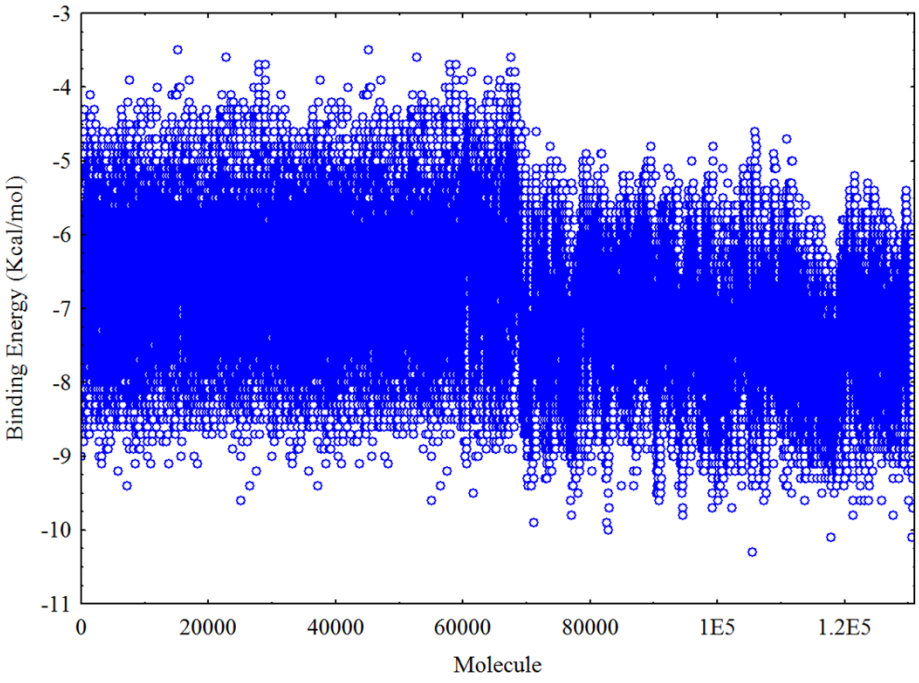

Figure S3. Binding energy distribution of molecules from CNS-Asinex database