Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary material

Molecular modeling studies of 1,2,4-triazine derivatives as novel h-DAAO inhibitors by 3D-QSAR, docking and dynamics simulations

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Table 1S Uni-column statistics of the training and test sets for the 3D-QSAR model study

Data set	Inhibitory potency	Average	Maximum	Minimum	Standard Deviation	Sum
Training	pIC_{50}	6.717	7.398	4.000	0.704	208.236
Test	pIC_{50}	6.153	7.301	4.398	1.138	36.917

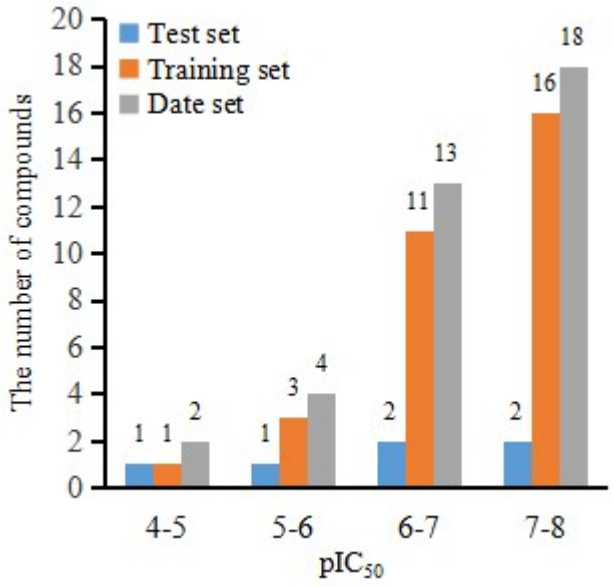

Fig. 1S Histogram of biological data distribution statistics in the 3D-QSAR analysis

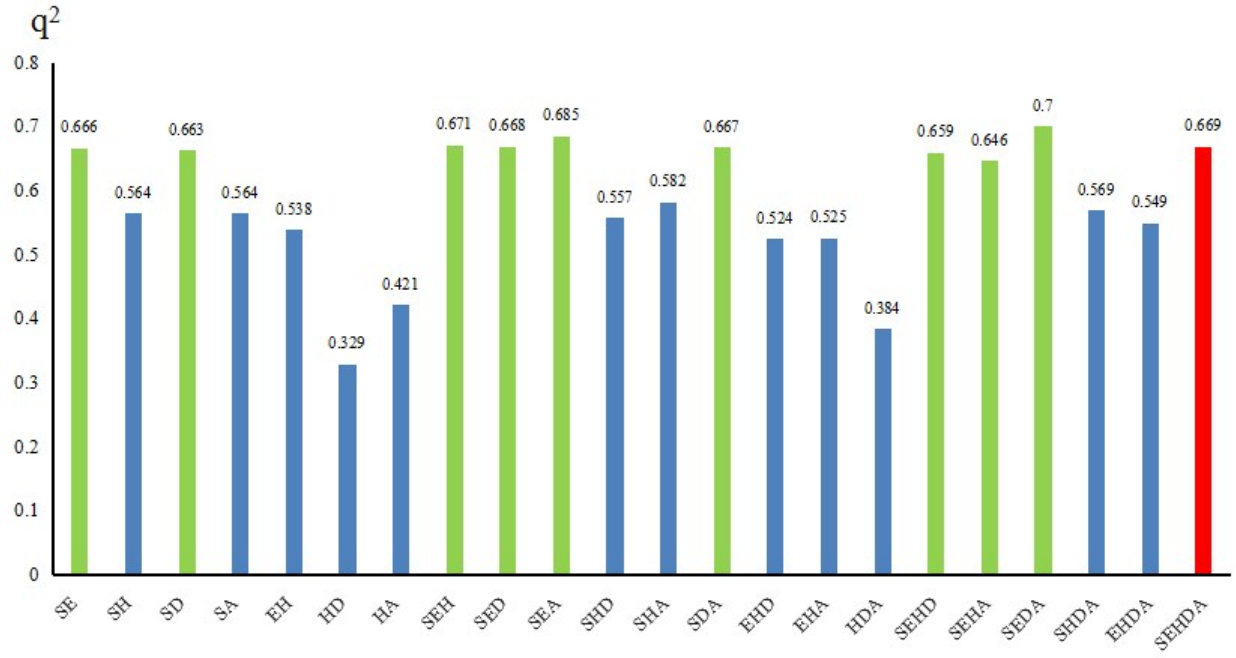

Fig. 2S Efficient color histogram indexing for the q^2 values of probable field combinations in CoMSIA analysis. (green: combinations with higher q^2 values, red: the best field combination).

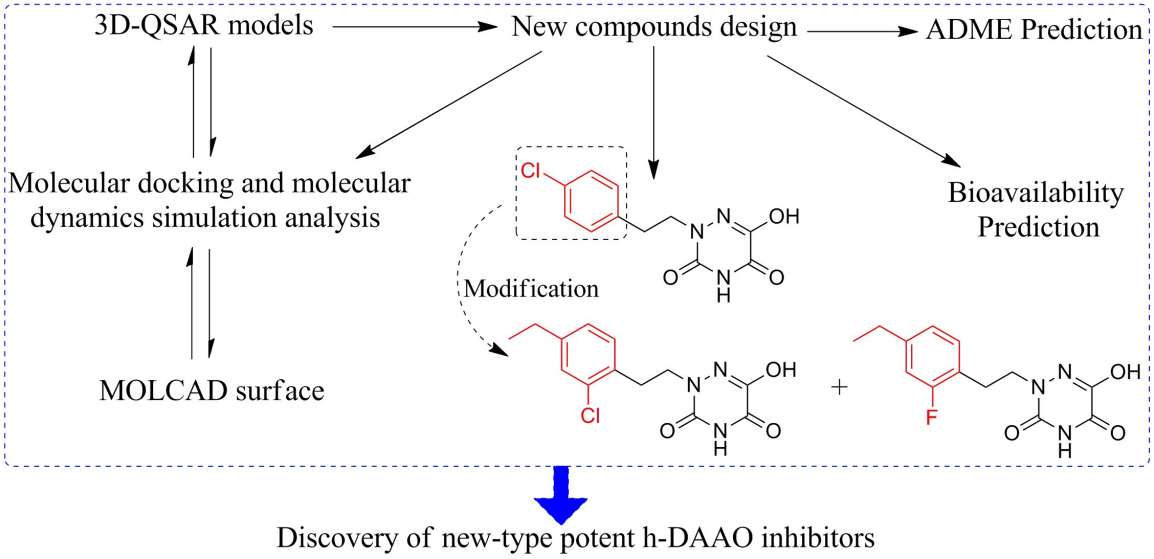

Fig. 3S Basic flowchart of research programme.

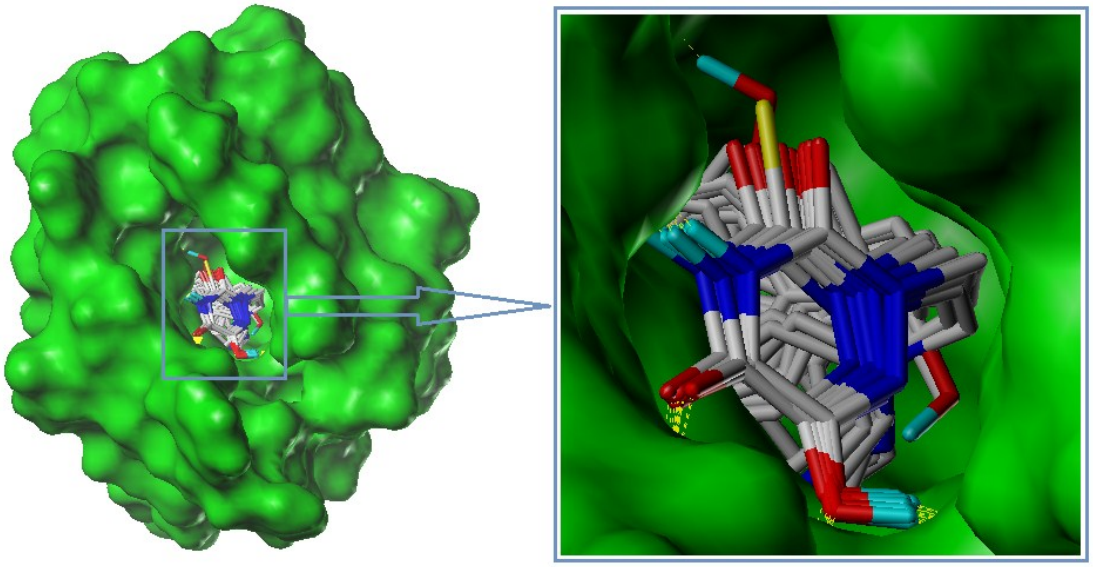

Fig. 4S Docking results of all compounds and surface of the binding site. (yellow lines: hydrogen bonds)

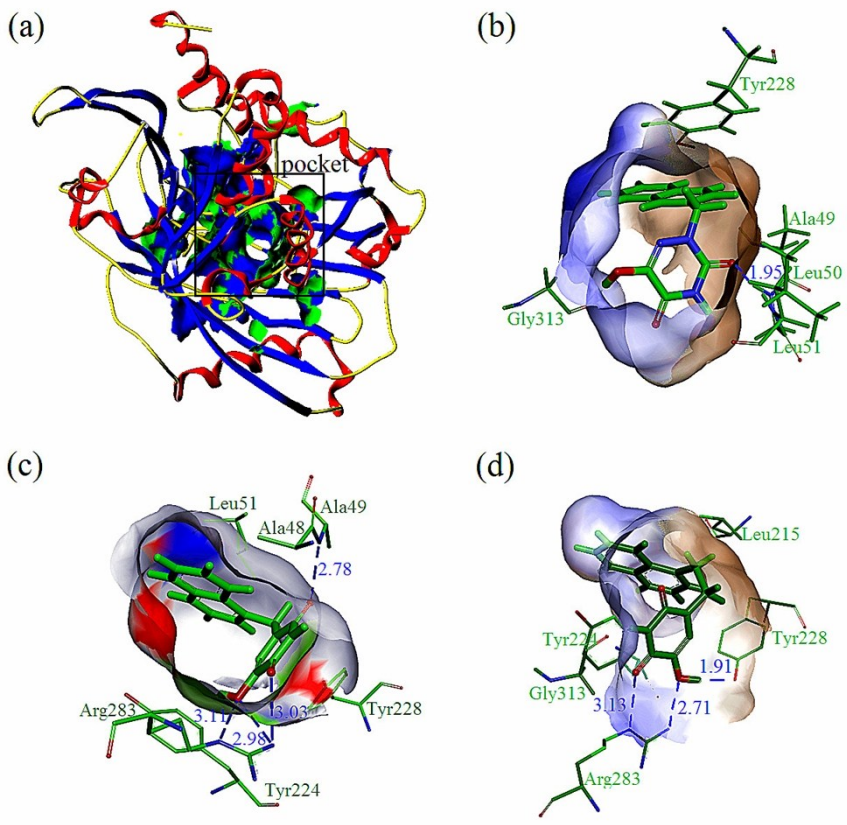

Fig. 5S The binding pocket (a), docking results and surface of compound **4** (b), **5** (c) and **6** (d). (blue lines: hydrogen bonds)

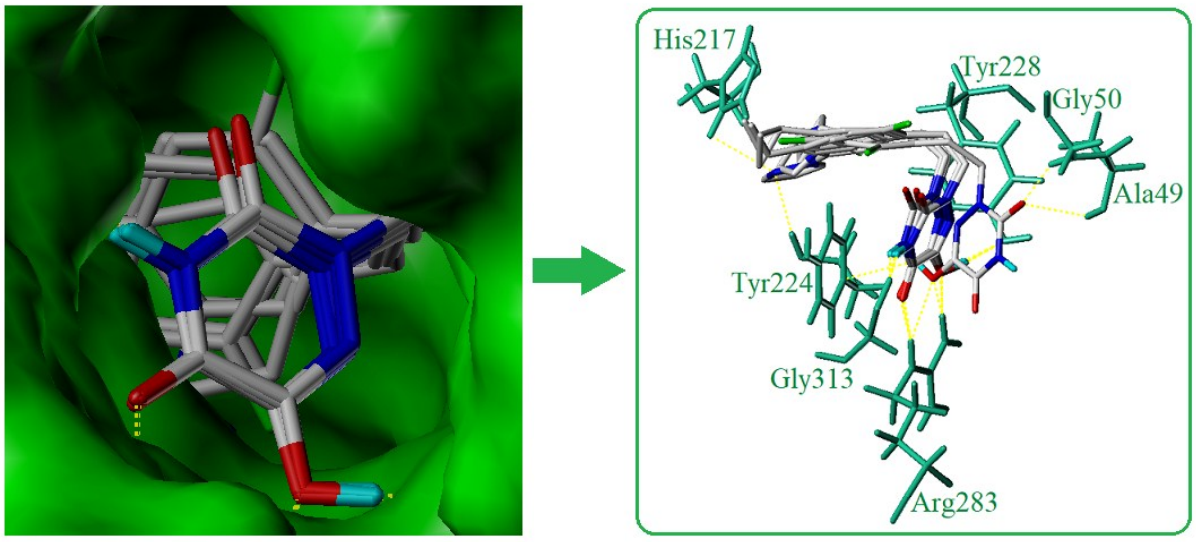

Fig. 6S Docking results of all designed compounds into the binding site of protein 3W4K. (yellow lines: hydrogen bonds)

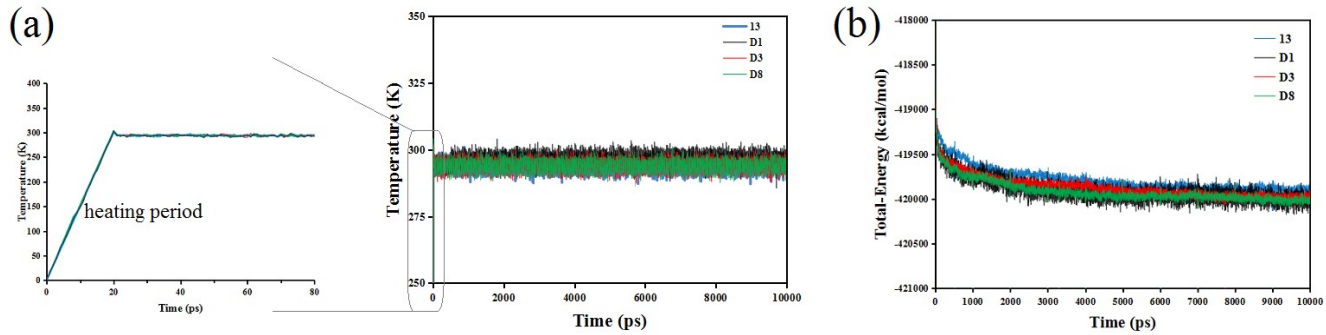

Fig. 7S The total-energy (a) and temperature (b) of the inhibitor-protein complexes versus dynamics time.

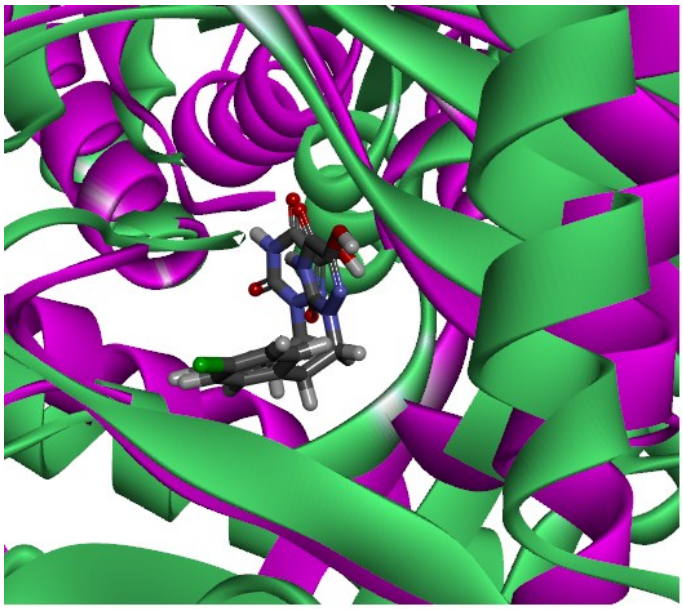

Fig. 8S Structural comparison between original structure (purple) and dynamics equilibrium structure (green) of 13-3W4K.

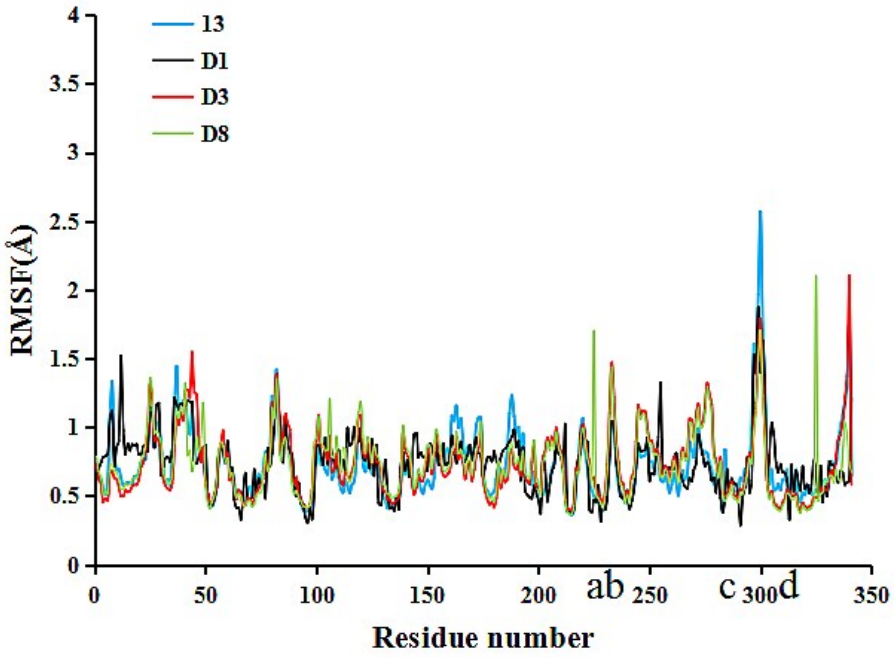

Fig. 9S Root-mean-square fluctuation (RMSF) the ligand-3W4K complexes versus residue number. (a: Tyr224; b: Tyr228; c: Arg283; d: Gly313)

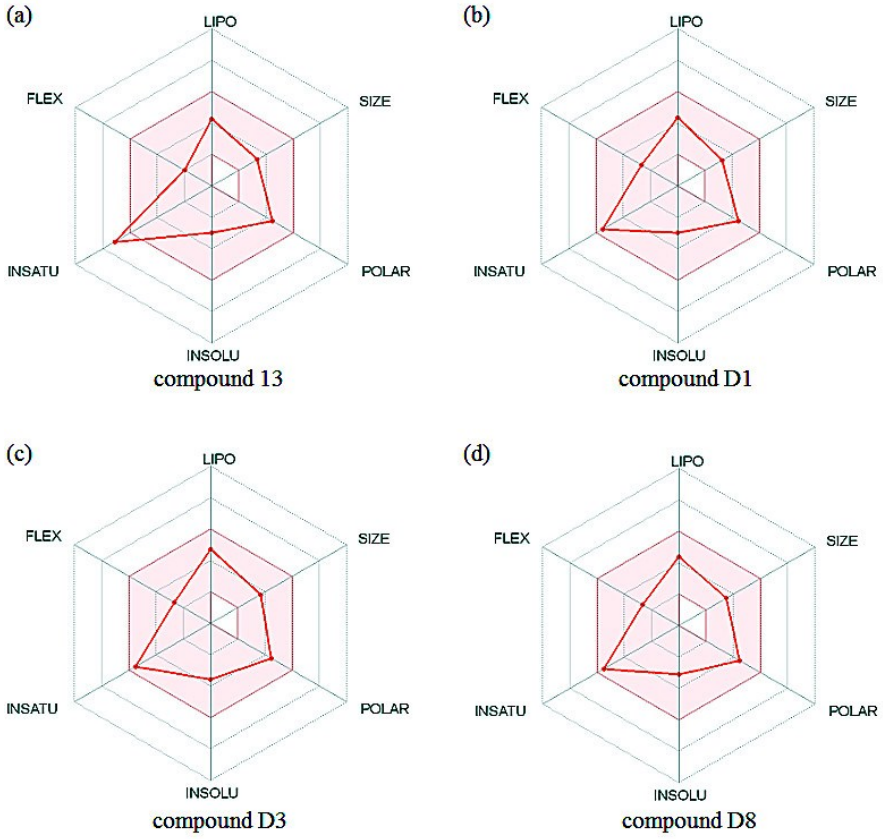

Fig. 10S The bioavailability radars for compounds 13 (a), D1 (b), D3 (c) and D8 (d).

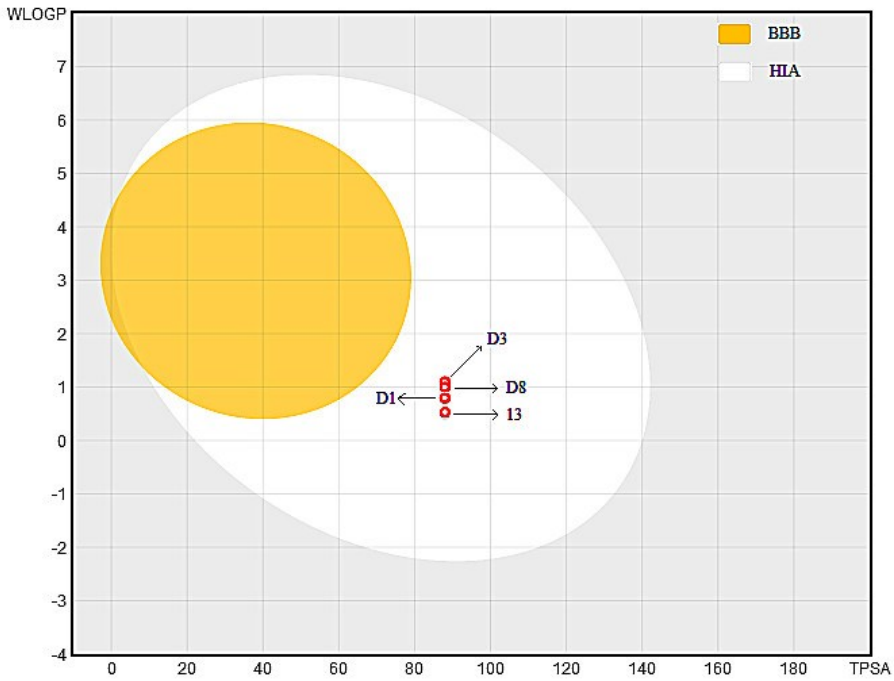

Fig. 11S The BOILED-Egg model for intuitive assessment of HIV and BBB through the position of the representative compounds.