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Article

Hierarchical Virtual Screening and Binding Free Energy Prediction of Potential Modulators of Aedes Aegypti Odorant-Binding Protein 1

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SUPPLEMENTARY MATERIAL

Table S1. 2D chemical structure of prioritized compounds from pharmacophore and docking-based virtual screening

Table S2. Training and test set employed in pharmacophore model construction and validation

Figure S1. RMSD representation of best poses from GOLD score functions. Red stick: crystallographic ligand; Blue stick: ChemPLP (RMDS: 0.703 A^2); Yellow line: GoldSCORE (RMSD: 2.92 A^2); Magenta line: ChemSCORE (RMSD: 8.10 A^2); Green line: ASP (RMSD: 8.24 A^2).

Table S1. 2D chemical structure of prioritized compounds from pharmacophore and docking-based virtual screening.

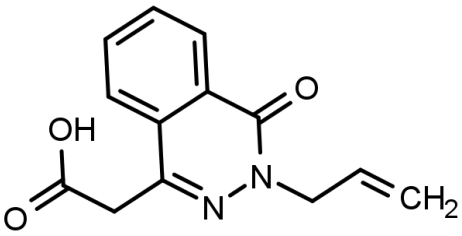
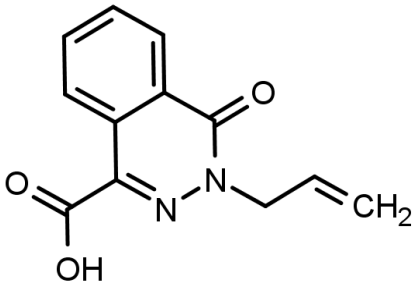
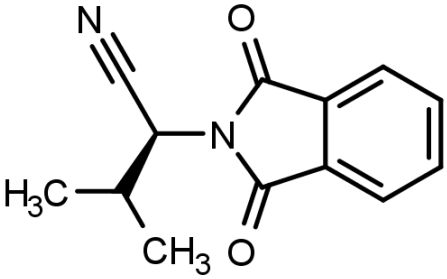
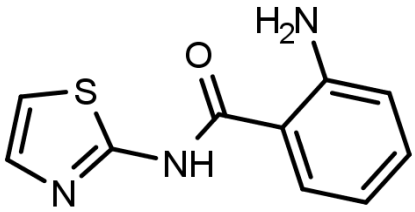
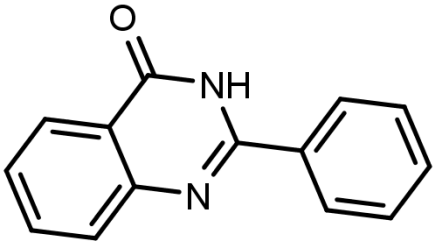
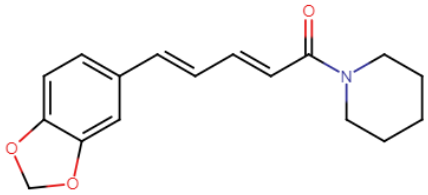
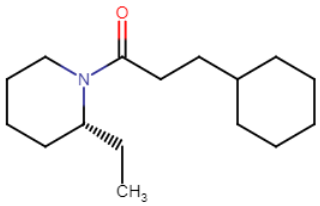
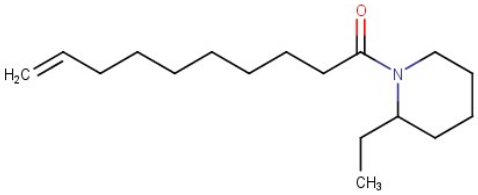
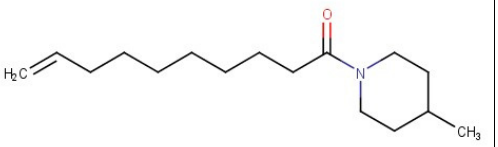
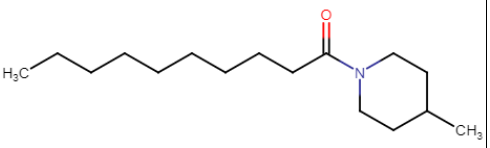
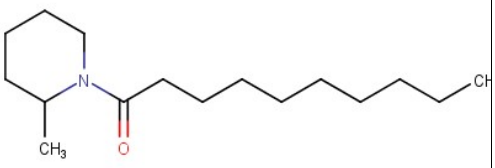
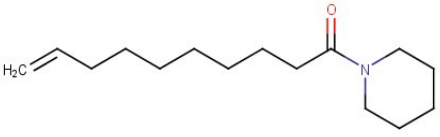
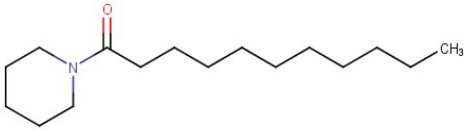
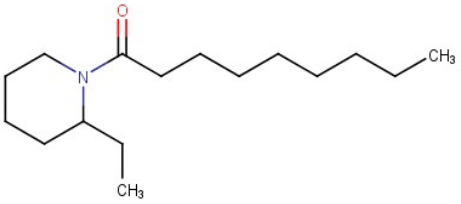
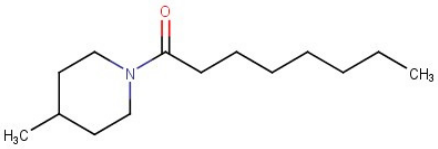
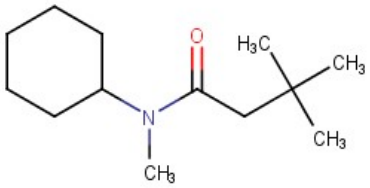
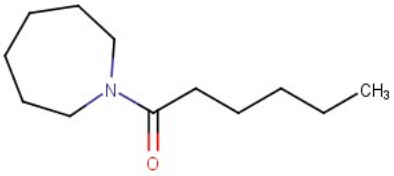
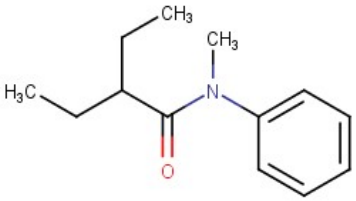
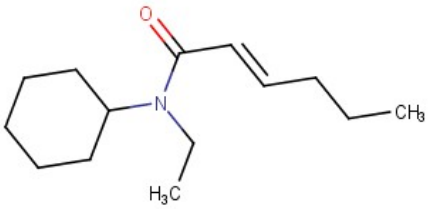
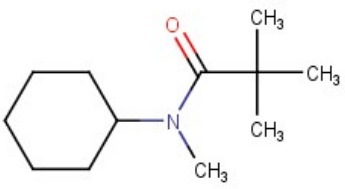
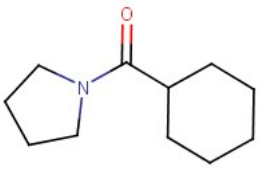
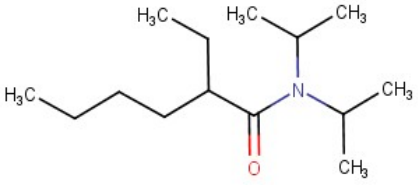
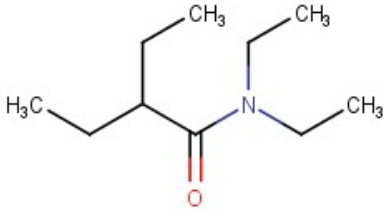
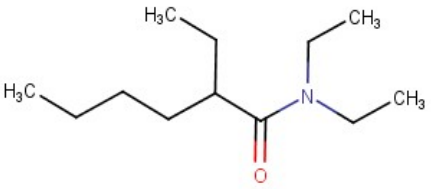
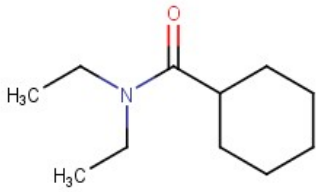
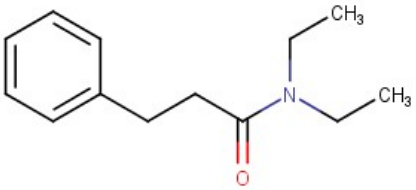
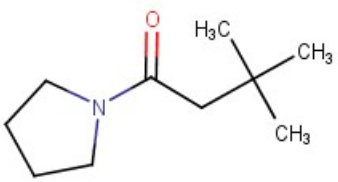
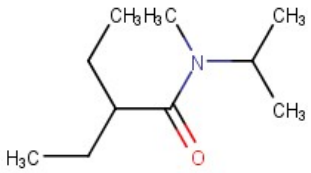
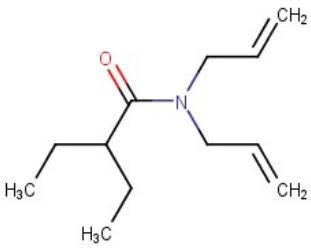
ZINC Code	Chemical sketch	IUPAC name
ZINC62702141		2-[4-Oxo-3-(prop-2-en-1-yl)-3,4-dihydrophthalazin-1-yl]acetic acid
ZINC10483047		4-Oxo-3-(prop-2-en-1-yl)-3,4-dihydrophthalazine-1-carboxylic acid
ZINC71773878		(2*S*)-2-(1,3-Dioxo-2,3-dihydro-1H-isoindol-2-yl)-3-methylbutanenitrile
ZINC380698		2-Amino-*N*-(1,3-thiazol-2-yl)benzamide
ZINC17917305		2-Phenyl-3,4-dihydroquinazolin-4-one

Table S2. Training and test set employed in pharmacophore model construction and validation.

Compound	IUPAC name	2D structure	K_i (μM)
01	(2*E*,4*E*)-5-(2*H*-1,3-Benzodioxol-5-yl)-1-(piperidin-1-yl)penta-2,4-dien-1-one		0.46
02	3-Cyclohexyl-1-[(2*R*)-2-ethylpiperidin-1-yl]propan-1-one		1.24
03	1-(2-Ethylpiperidin-1-yl)dec-9-en-1-one		1.90
04	1-(4-Methylpiperidin-1-yl)dec-9-en-1-one		2.50
05	1-(4-Methylpiperidin-1-yl)decan-1-one		2.99
06	1-(2-Methylpiperidin-1-yl)decan-1-one		4.04
07	1-(Piperidin-1-yl)dec-9-en-1-one		4.79
08	1-(Piperidin-1-yl)undecan-1-one		5.28

09	1-(2-Ethylpiperidin-1-yl)nonan-1-one		6.05
10	1-(4-Methylpiperidin-1-yl)octan-1-one		9.05
11	*N*-Cyclohexyl-*N*-3,3-trimethylbutanamide		10.50
12	1-(Azepane-1-yl)hexan-1-one		17.59
13	2-Ethyl-*N*-methyl-*N*-phenylbutanamide		15.40
14	(3*E*)-*N*-Cyclohexyl-N-ethylhex-3-enamide		4.18
15	*N*-Cyclohexyl-*N*-2,2-trimethylpropanamide		46.31

16	1-Cyclohexanecarbonylpyrrolidine		19.90
17	2-Ethyl-*N*,*N*-bis(propan-2-yl)hexanamide		114.99
18	*N*,*N*-2-Triethylbutanamide		320.17
19	*N*,*N*-2-Triethylhexanamide		92.18
20	*N*,*N*-Diethylcyclohexanecarboxamide		27.37
21	*N*,*N*-Diethyl-3-phenylpropanamide		17.51
22	3,3-Dimethyl-1-(pyrrolidin-1-yl)butan-1-one		87.18

23	2-Ethyl-*N*-methyl-*N*-(propan-2-yl)butanamide		86.06
24	2-Ethyl-*N*,*N*-bis(prop-2-en-1-yl)butanamide		80.64

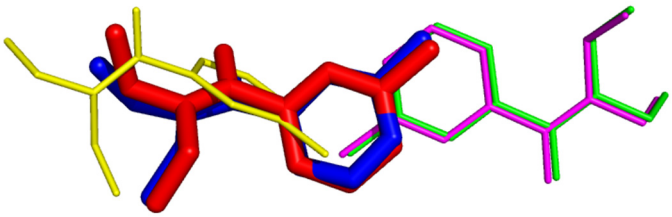


Figure S1. RMSD representation of best poses from GOLD score functions. Red stick: crystallographic ligand; Blue stick: ChemPLP (RMDS: 0.703 A^2); Yellow line: GoldSCORE (RMSD: 2.92 A^2); Magenta line: ChemSCORE (RMSD: 8.10 A^2); Green line: ASP (RMSD: 8.24 A^2).