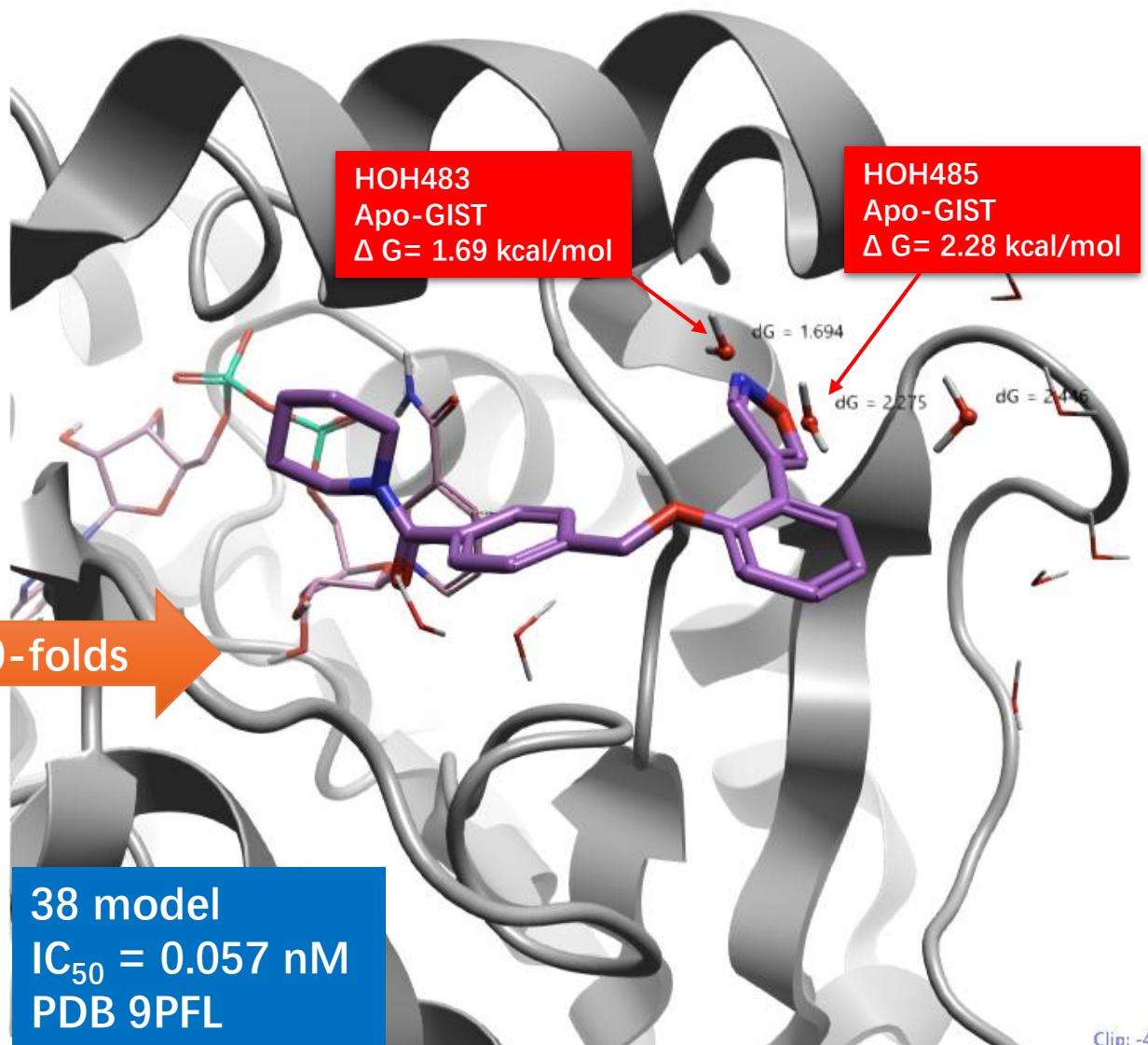


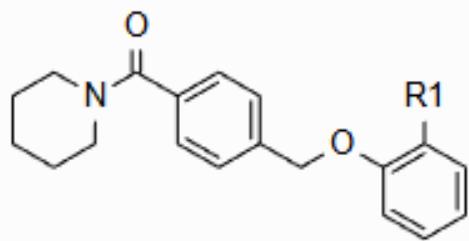
$$\Delta\Delta G_{\text{bind}}^{\text{Exp}} = -3.62 \text{ kcal/mol}$$



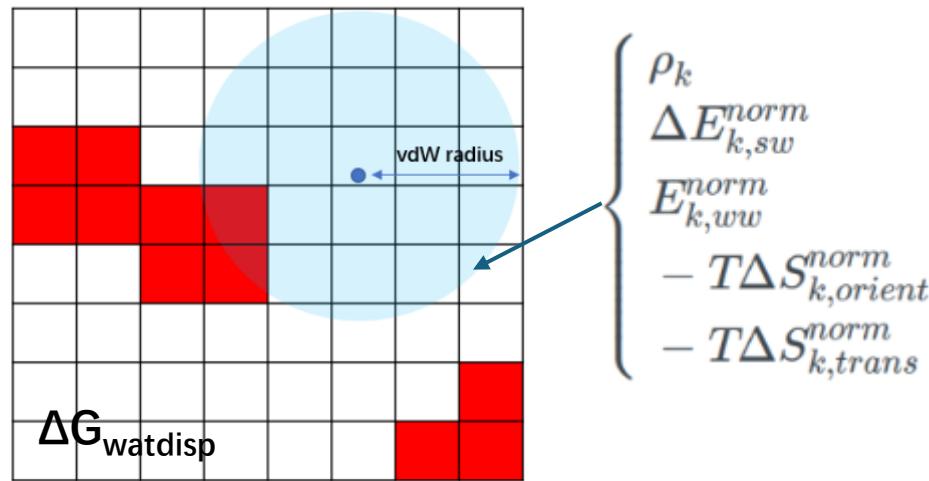
$$\Delta\Delta G_{\text{watdisp}} = -3.70 \text{ kcal/mol}$$

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Clip: -40.2A



Compound	R ₁	15-PGDH IC ₅₀ (nM)
4	-Br	26
38		0.057



$$V = \{v_i | v_i \in \text{ligand}\} \dots (7)$$

$$\Delta G_{watdisp} = \alpha \times \text{vol} \times \sum_{v_i \in V} G_{GIST}(v_i) \dots (8)$$

GNINA Docking scores for compounds 4 and 38, along with $\Delta G_{watdisp}$.

Compound	4	38
gauss_1	122.46680	149.03520
gauss_2	1420.47168	1643.15222
repulsion	5.23956	6.98573
hydrophobic	94.15118	101.49037
non_dir_h_bond	1.99749	2.97978
Affinity (kcal/mol)	-9.53	-10.23
CNNaffinity	6.77	7.39
$\Delta G_{watdisp}$ (kcal/mol)	-18.144	-21.846
Affinity-Corr (kcal/mol)	-9.53	-13.93
Exp ΔG (kcal/mol)	-10.34	-13.96

$$\Delta G_{bind}^{docking-GIST-corr} = \Delta G_{bind}^{docking} + \Delta G_{watdisp}$$

$$\Delta \Delta G_{bind}^{docking-GIST-corr} = \Delta \Delta G_{bind}^{docking} + \Delta \Delta G_{watdisp}$$

$$\Delta \Delta G_{bind}^{docking-GIST-corr} = -0.70 + (-3.70) = -4.40 \text{ kcal/mol}$$

$$\Delta \Delta G_{bind}^{Exp} = -3.62 \text{ kcal/mol}$$

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