

Supplementary material:

E_{score} , is defined by the following energy terms:

$$E_{score} = E_{inter} + E_{intra}$$

Where E_{inter} is the ligand-protein interaction energy:

$$E_{inter} = \sum_{i \in ligand} \sum_{j \in protein} \left[E_{PLP}(r_{ij}) + 332.0 \frac{q_i q_j}{4r_{ij}^2} \right]$$

The E_{PLP} term is a piecewise linear potential. The second term describes the electrostatic interactions between charged atoms.

Table 1: The Docking Results

Name	Interaction energy between the ligand and protein (Arbitrary unit)	HBond Energy (Arbitrary unit)
Phloretin	-84.35	-10.83
Quercetin	-83.19	-5.74
Chloramphenicol	-73.61	-4.51
Naringenin	-79.19	-5.55
Tetracycline	-106.66	-0.29
Pongachalcone I	-69.05	-3.12