

Supplementary materials

Table S1. The root-mean-square deviation (RMSD) for CYP1A2, 2C9, and 3A4.

CYP isoform	RMSD
1A2	0.413931
2C9	0.020090
3A4	1.454134

Table S2 The total scores of CYP isoforms-ligands molecular docking

CYP isoform	Probe ¹	Dihydrotanshinone	Tanshinone I	Cryptotanshinone	Tanshinone IIA
1A2	8.1835	8.7425	8.6532	5.9218	6.4312
2C9	5.0936	3.5947	5.0060	2.6552	4.0515
3A4	16.4210	4.4355	3.8878	6.1238	4.9618

¹ α -Naphthoflavone, sulfaphenazole, and ketoconazole are probes for CYP 1A2, 2C9, and 3A4, respectively.