Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - top scores docking

Adriana de Oliveira Fernandes, Valéria Vieira Moura Paixão, Yria Jaine Andrade Santos, Eduardo Borba Alves, Ricardo Pereira Rodrigues, Daniela Aparecida Chagas-Paula, Aurélia Santos Faraoni, Rosana Casoti, Marcus Vinicius de Aragão Batista, Marcel Bermudez, Silvio Santana Dolabella and Tiago Branquinho Oliveira

Table S3. The 20 best ligands for each receptor based on their ChemPLP indexes. The scores showed here refer to the arithmetic mean of the score for the 10 runs of each ligand, along with their SD values.

Ligands	FabZ	FabI
2-(4-Methoxyphenyl)-1-benzopyran-4-one	52.78 ± 0.51	-
3,6-Dimethoxy-2-phenyl-1-benzopyran-4-one	47.82 ± 0.65	-
3,7-Dimethoxy-2-phenyl-1-benzopyran-4-one	51.45 ± 0.34	-
3′,4′,7-Trihydroxyisoflavan	59.98 ± 0.99	-
4-*O*-Methylequol	65.09 ± 0.39	-
5-Hydroxy-4′,7-dimethoxyflavanone	49.10 ± 2.09	-
6-Methoxy-2-(2-methoxyphenyl)-1-benzopyran-4-one	51.57 ± 0.63	-
6′-Hydroxy-*O*-desmethylangolensin	64.53 ± 4.50	-
6′-Hydroxyangolensin	64.32 ± 2.89	-
7-Methoxy-2-(2-methoxyphenyl)-1-benzopyran-4-one	50.60 ± 2.90	-
7-Methoxy-2-(4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	58.03 ± 0.25	-
7-Methoxy-5-methyl-2-phenyl-1-benzopyran-4-one	53.71 ± 0.37	-
8-Methoxy-2-(2-methoxyphenyl9-1-benzopyran-4-one	33.80 ± 4.41	-
Angolensin	70.84 ± 2.15	-
Butein	70.00 ± 1.08	-
Epicatechin-3′-glucuronide	37.58 ± 5.29	-
Irisolidone	48.05 ± 0.55	-
Malvidin 3-*O*-glucoside	-29.98 ± 64.93	-
Naringin	40.14 ± 4.03	-
Peruvianoside I	6.44 ± 16.11	-
Quercetin-3′-glucuronide	40.38 ± 2.31	-
(-)-Epicatechin	-	43.88 ± 1.96
(+)-Catechin	-	38.45 ± 2.01
3′-O-Methylcatechin	-	41.30 ± 2.06
3′-O-Methylequol	-	51.77 ± 3.23
3′,4′,5,7-Tetrahydroxyisoflavanone	-	55.99 ± 3.47
3′,4′,7-Trihydroxyisoflavanone	-	54.71 ± 2.85
5-Hydroxy-3,6,7,2′,4′,5′-hexamethoxyflavone	-	28.13 ± 5.97
5,6,7,4′-Tetrahydroxyisoflavone	-	49.11 ± 3.08
5,7,2′-Trihydroxy-3,6,4′,5′-tetramethoxyflavone	-	44.27 ± 1.19
5,7,8,3′,4′-Pentahydroxyisoflavone	-	44.14 ± 1.34
5,7,8,4′-Tetrahydroxyisoflavone	-	46.98 ± 0.78

Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - top scores docking

Ligands	FabZ	FabI
6,7,3′,4′-Tetrahydroxyisoflavone	-	47.47 ± 1.99
7,8,3′,4′-Tetrahydroxyisoflavone	-	51.91 ± 0.66
Butin	-	53.93 ± 0.88
Cis-4-hydroxyequol	-	54.96 ± 0.70
Cyanidin	-	62.44 ± 1.02
Delphinidin 3-*O*-glucoside	-	-7.53 ± 22.39
Dihydrodaidzein 7-*O*-glucuronide	-	57.21 ± 3.72
Epicatechin 5-*O*-β-D-glucopyranoside-3-benzoate	-	0.09 ± 18.72
Equol 4′-*O*-glucuronide	-	47.45 ± 10.66
Formononetin	-	52.72 ± 2.34
Malvidin 3-*O*-arabnoside	-	-11.20 ± 44.85
Malvidin 3-*O*-glucoside	-	-7.18 ± 38.71
O-Desmethylangolensin	-	75.34 ± 3.21
Stevenin	-	37.48 ± 1.30
Tectoridin	-	29.07 ± 7.34