BIOINFORMATION

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Supplementary material:

Table 1: Surflex score of active compound

S.No	Compounds	CScore score[a]	Crash score[b]	Polar score[c]	G score[d]	PMF score[e]	D score[f]	Chem score[g]	No. of hydrogen bonds
1.	Quercetin	5.95	-0.79	5.90	-109.38	-32.24	-95.13	-24.43	6
2.	Chlorogenic acid	5.66	-1.97	5.89	-135.54	-78.77	-127.01	-22.47	5
3.	5,7-dimethoxycoumarin	4.46	-0.66	3.17	-83.86	-35.99	-54.88	-17.67	5
4.	Caffeic acid	4.44	-1.20	5.33	--111.6	-51.47	-53.77	-18.23	4
5.	Kaempferol	3.87	-1.32	2.66	-70.07	-69.40	-95.20	-21.76	5
6.	p-Coumaric acid	3.81	-1.01	3.02	-72.41	-11.99	-82.9	-23.39	6
7.	Protocatechuic acid	2.95	-0.50	2.54	-64.54	-35.55	-127.5	-13.78	5

[a] CScore is a consensus scoring which uses multiple types of scoring functions to rank the affinity of ligands
[b] Crash-score revealing the inappropriate penetration into the binding site.
[C] Polar region of the ligand.
[d] G-score showing hydrogen bonding, complex (ligand-protein), and internal (ligand-ligand) energies.
[e] PMF-score indicating the Helmholtz free energies of interactions for protein-ligand atom pairs (Potential of Mean Force, PMF).
[f] D-score for charge and van der Waals interactions between the protein and the ligand.
[g] Chem-score points for hydrogen bonding, lipophilic contact, and rotational entropy, along with an intercept term.

Table 2: Molecular properties and drug likeness of active compounds

S.No	Compounds	PubChem CID	Molecular Weight[g/mol]	LogP (Octanol-water partition coefficient value)	H-Bond Donor	H-Bond Acceptor
1.	Quercetin	5280343	302.2	1.5	5	7
2.	Chlorogenic Acid	1794427	354.3	0.4	6	9
3.	5,7-dimethoxycoumarin	2775	206.1	1.9	0	4
4.	Caffeic acid	4652	180.1	1.2	3	4
5.	Kaempferol	5280863	286.2	1.9	4	6
6.	p-Coumaric acid	637542	164.1	1.5	2	3
7.	Protocatechuic acid	72	154.1	1.1	3	4

Table 3: ADMET Predicted profile for active compound

(a) Absorption							
Models	**Quercetin**	**Chlorogenic acid**	**5,7-dimethoxycoumarin**	**Caffeic acid**	**Kaempferol**	**p-Coumaric acid**	**Protocatechuic acid**
Blood-Brain barrier	BBB+	BBB+	BBB+	BBB+	BBB+	BBB+	BBB+
Human Intestinal Absorption	HIA+	HIA+	HIA+	HIA+	HIA+	HIA+	HIA+
Caco-2 Permeability	Caco2+	Caco2+	Caco2+	Caco2+	Caco2+	Caco2+	Caco2+
P-glycoprotein Inhibitor	NI	NI	NI	NI	NI	NI	NI
Renal Organic Cation Transporter	NI	NI	NI	NI	NI	NI	NI
(b) Metabolism							
CYP450 2C9 Substrate	NS	NS	NS	NS	NS	NS	NS
CYP450 2D6 Substrate	NS	NS	NS	NS	NS	NS	NS
CYP450 3A4	NS	NS	NS	NS	NS	NS	NS

Substrate								
CYP450 Inhibitor	1A2	NI	NI	NI	NI	NI	NI	NI

Table 3: (contd.) ADMET Predicted profile for active compounds

CYP450 Inhibitor	2C9	NI	NI	NI	NI	NI	NI	NI
CYP450 Inhibitor	2D6	NI	NI	NI	NI	NI	NI	NI
CYP450 Inhibitor	2C19	NI	NI	NI	NI	NI	NI	NI
CYP450 Inhibitor	3A4	NI	NI	NI	NI	NI	NI	NI
(c) Toxicity								
AMES Toxicity		NT	NT	NT	NT	NT	NT	NT
Carcinogens		NC	NC	NC	NC	NC	NC	NC

NI – Non-inhibitor; NS – Non-substrate; NT – Non-toxic; NC – Non-carcinogen