

Computational investigation into *Parinari curatellifolia* flavonoids as lead hepatoprotective therapeutics

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SUPPLEMENTARY DATA

Supplementary Table 1: Phytochemical constituent of *P. curatellifolia* extracts

Phytochemical	Crude methanolic extract	Flavonoid rich extract
Alkaloids	+	-
Anthraquinones	-	-
Cardenolides	+	-
Flavonoids	+	+
Phlobatannins	+	-
Saponins	+	-
Steroids	+	-
Tannins	+	-
Terpenoids	+	-

(+)Present(-) Absent

Supplementary Table 2(a-l):

Prediction of Activity Spectra for Substances (PASS) bioactivity prediction for *Parinari curatellifolia* flavonoids

Table 1a

3-Methyl quercetin (3-MQ)	P _A	P _I
CYP1A inducer	0.924	0.002
Antimutagenic	0.960	0.001
Peroxidase inhibitor	0.948	0.002
Hepatoprotective	0.739	0.006
Chemoprotective	0.755	0.005
Antioxidant	0.867	0.005
Free radical scavenger	0.864	0.002

Table 1b

Apigenin	P _A	P _I
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Membrane integrity agonist	0.967	0.002
Antimutagenic	0.926	0.002
CYP1A inducer	0.907	0.002
Histamine release inhibitor	0.791	0.003
Antioxidant	0.740	0.004
Free radical scavenger	0.719	0.004

Table 1c

Baicalein	P_A	P_I
Anaphylatoxin receptor antagonist	0.965	0.002
Peroxidase inhibitor	0.961	0.003
Membrane integrity agonist	0.945	0.004
CYP1A inducer	0.899	0.004
Antimutagenic	0.886	0.002
Apoptosis agonist	0.881	0.005
Antioxidant	0.881	0.003
Antineoplastic	0.789	0.013
Free radical scavenger	0.705	0.004
Histamine release inhibitor	0.705	0.004

Table 1d

Chrysin	P_A	P_I
Membrane integrity agonist	0.965	0.003
Membrane permeability inhibitor	0.946	0.002
Aldehyde oxidase inhibitor	0.933	0.003
Peroxidase inhibitor	0.922	0.002
CYP1A inducer	0.916	0.002
Antimutagenic	0.915	0.002
Antioxidant	0.717	0.004
Histamine release inhibitor	0.705	0.004

Table 1e

Genistein	P_A	P_I
Membrane integrity agonist	0.913	0.008
Xenobiotic-transporting ATPase inhibitor	0.896	0.002
Antimutagenic	0.874	0.003
Peroxidase inhibitor	0.841	0.004
Lipid metabolism regulator	0.833	0.005
Anaphylatoxin	0.801	0.004
Antioxidant	0.781	0.004

Table 1f

Isorhamnetin	P_A	P_I
Membrane integrity agonist	0.965	0.003
CYP1A inducer	0.963	0.001
Antimutagenic	0.961	0.001
Peroxidase inhibitor	0.955	0.001
Aldehyde oxidase inhibitor	0.912	0.004
NOS2 expression inhibitor	0.895	0.001
Free radical scavenger	0.886	0.002
Lipid peroxidase inhibitor	0.841	0.003
Antineoplastic	0.804	0.011
Chemoprotective	0.772	0.004

Hepatoprotectant	0.740	0.006
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Table 1g

Kaempferol	P_A	P_I
Membrane integrity agonist	0.974	0.002
Membrane permeability inhibitor	0.965	0.001
Peroxidase inhibitor	0.956	0.001
Antimutagenic	0.948	0.001
CYP1A inducer	0.944	0.002
Xenobiotic-transporting ATPase inhibitor	0.890	0.002
Antibiotic	0.864	0.003
Free radical scavenger	0.774	0.003
Antioxidant	0.929	0.003
Anticarcinogenic	0.720	0.008

Table 1h

Myricetin	P_A	P_I
Membrane integrity agonist	0.968	0.002
Antimutagenic	0.963	0.001
CYP1A inducer	0.926	0.001
Membrane permeability inhibitor	0.959	0.002
Antioxidant	0.929	0.003
Anaphylatoxin	0.919	0.003
apoptosis agonist	0.915	0.004
Xenobiotic-transporting ATPase inhibitor	0.905	0.002
Free radical scavenger	0.837	0.002
Antineoplastic	0.842	0.000
Lipid peroxidase inhibitor	0.836	0.003

Table 1i

Pinocembrin	P_A	P_I
Membrane integrity agonist	0.962	0.003
Membrane permeability inhibitor	0.850	0.005
Antimutagenic	0.842	0.003
Lipid peroxidase inhibitor	0.802	0.003
Antioxidant	0.792	0.003
Apoptosis agonist	0.751	0.04
Free radical scavenger	0.750	0.003
Antineoplastic	0.748	0.019
Hepatoprotectant	0.713	0.007

Table 1j

Quercetin	P_A	P_I
Membrane permeability inhibitor	0.962	0.002
Peroxidase inhibitor	0.962	0.001
Antimutagenic	0.961	0.001
CYP1A inducer	0.959	0.001
Apoptosis agonist	0.895	0.004
Aldehyde oxidase inhibitor	0.894	0.004
Anaphylatoxin	0.875	0.005
Free radical scavenger	0.816	0.002
Antineoplastic	0.799	0.012
Anticarcinogenic	0.761	0.007
Chemopreventive	0.717	0.006
Hepatoprotectant	0.706	0.007
Anti-inflammatory	0.704	0.015

Table 1k

Silibinin	P_A	P_I
Free radical scavenger	0.956	0.001
Membrane integrity agonist	0.957	0.003
Hepatoprotectant	0.939	0.002
APOA1 expression enhancer	0.936	0.002
TP53 expression enhancer	0.914	0.005
Lipid protein Inhibitor	0.909	0.003
Antioxidant	0.859	0.003
HIF1 expression inhibitor	0.857	0.008
HM0X1 expression inhibitor	0.844	0.003

Table 1l

Tricetin	P_A	P_I
Membrane integrity agonist	0.960	0.003
Membrane permeability inhibitor	0.949	0.002
Antimutagenic	0.947	0.001
Peroxidase inhibitor	0.942	0.002
CYP1A inducer	0.938	0.002
Aldehyde oxidase inhibitor	0.932	0.003
Apoptosis agonist	0.893	0.004
Antineoplastic	0.833	0.008
Xenobiotic-transporting ATPase inhibitor	0.804	0.003
Free radical scavenger	0.770	0.003
Lipid peroxidase inhibitor	0.763	0.004