Supplementary materials

For

Eriodictyol: a review of its pharmacological activities and molecular mechanisms related to ischemic stroke

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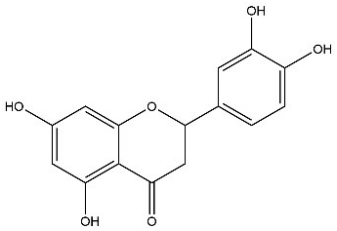
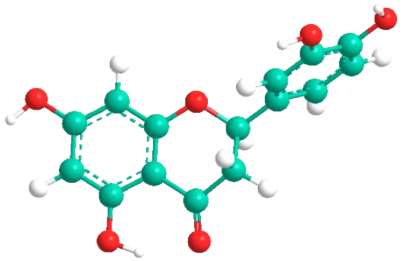
Supplementary Table 1 Physicochemical properties and ADMET systematic evaluation results for Eriodictyol and relevant metabolites. Mw, molecular weight; Log S, aquesous solubility optimal: -4 < Log S < 0.5 log mol/ L; Log P, distribution coefficient P, optimal: 0 < Log P < 3; Log D, physiological pH 7.4, optimal: 1 < Log D < 3; Het, heteroatoms, 1 < Het < 15; fChar, Formal charge, -4 < fChar < 4; Rot, rotatable bonds, 0 < Rot < 11; MaxRing, atoms in the biggest ring, optimal: 0 < MaxRing < 18; HD, hydrogen bond donors, 0 < HD < 7; TPSA, topological polar surface area, optimal: 0 < TPSA < 140; F, 30 % bioavailability; HIA, human intestinal absorption; VD, volume distribution, optimal: 0.04 < VD < 20 L/kg; $T_{1/2}$, terminal elimination half-life; CL, clearance; $T_{1/2}$, terminal elimination half-life; H-HT, human hepatotoxicity; DILI, drug induced liver injury.

The data are obtained from the website: https://admetmesh.scbdd.com/, http://www.chemspider.com/, https://www.chemicalbook.com/, https://www.chemsrc.com/.

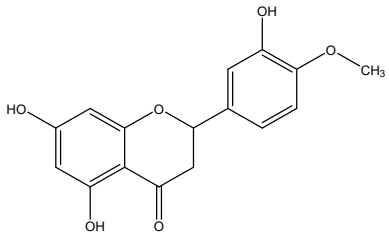
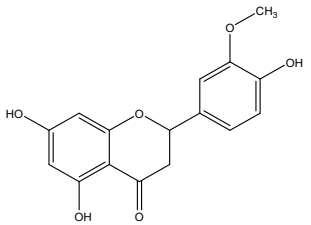
Name	Eriodictyol
2D Structure	

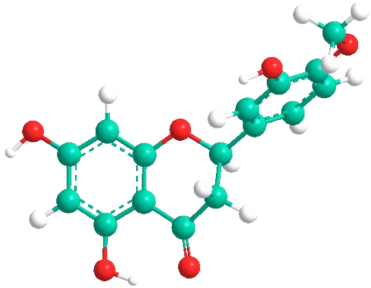
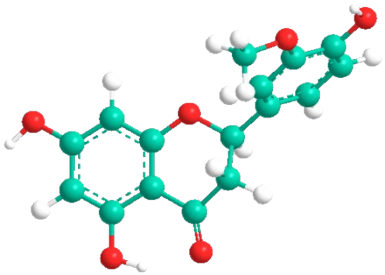
3D Structure	
Cas number	552-58-9
Canonical SMILES	C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC(=C(C=C3)O)O
IUPAC name	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydrochromen-4-one[1]
Molecular Formula	$C_{15}H_{12}O_6$
Mw	288.25
Melting point	238-239 °C[2]
Boiling point	625.2 ± 55.0 °C (Predicted)
Density	1.586 ± 0.06 g/cm^3 (Predicted)
Storage	2-8 °C
Form	Powder
Pka	7.49 ± 0.40 (Predicted)
Color	Colorless[2]
Stability	Hygroscopic
UV spectra	UVmax (methanol): 286 nm[3]
TPSA	107.220
Log S	-3.827 mol/L
Log P	2.118
Log D	2.307
fChar	0

Number of HBA	6
Number of HBD	4
Number of Rot	1
Number of Het	6
MaxRing	10
Number of Rig	18
Number of HD	4
HIA	---
PPB	93.320 %
$F_{30\%}$	+++
VD (L/ kg)	0.561
CL (mL/ min /kg)	19.889
$T_{1/2}$ (h)	0.856
H-HT	--
DILI	+++

Supplementary Table 2 Physicochemical properties and ADMET systematic evaluation results for Homoeriodictyol and Hesperetin and relevant metabolites. Mw, molecular weight; Log S, aquesous solubility optimal: -4 < Log S < 0.5 log mol/ L; Log P, distribution coefficient P, optimal: 0 < Log P < 3; Log D, physiological pH 7.4, optimal: 1 < Log D < 3; Het, heteroatoms, 1 < Het < 15; fChar, Formal charge, -4 < fChar < 4; Rot, rotatable bonds, 0 < Rot < 11; MaxRing, atoms in the biggest ring, optimal: 0 < MaxRing < 18; HD, hydrogen bond donors, 0 < HD < 7; TPSA, topological polar surface area, optimal: 0 < TPSA < 140; F, 30 % bioavailability; HIA, human intestinal absorption; VD, volume distribution, optimal: 0.04 < VD < 20 L/kg; $T_{1/2}$, terminal elimination half-life; CL, clearance; $T_{1/2}$, terminal elimination half-life; H-HT, human hepatotoxicity; DILI, drug induced liver injury.

The data are obtained from the website: https://admetmesh.scbdd.com/, http://www.chemspider.com/, https://www.chemicalbook.com/, https://www.chemsrc.com/.

Name	Hesperetin	Homoeriodictyol
2D Structure		

3D Structure		
Cas number	520-33-2	446-71-9
Canonical SMILES	COC1=C(C=C(C=C1)C2CC(=O)C3=C(C=C(C=C3O2)O)O)O	COC1=C(C=CC(=C1)C2CC(=O)C3=C(C=C(C=C3O2)O)O)O
IUPAC name	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-2,3-dihydrochromen-4-one	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydrochromen-4-one
Molecular Formula	$C_{16}H_{14}O_6$	$C_{16}H_{14}O_6$
Mw	302.28	302.28
Melting point	230-232 °C[4]	225-227 ºC (dec.)
Boiling point Density	586.2±50.0 °C (760 mmHg) 1.5±0.1 g/cm3	583.8 ºC (760mmHg) 1.458g/cm^3
Storage Form	2-8 °C Needle like crystallization[4]	2-8 °C Powder
Pka	7.49 ± 0.40 (Predicted)	7.49 ± 0.40 (Predicted)
Color	Yellow[4]	White[5]
Stability	-	-
UV spectra	254 nm[4]	254 nm[5]
TPSA	96.22	96.22
Log S	-3.975 mol/L	-3.956 mol/L
Log P	2.473	2.476
Log D	2.6	2.579

fChar	0	0
Number of HBA	6	6
Number of HBD	3	3
Number of Rot	2	2
Number of Het	6	6
MaxRing	10	10
Number of Rig	18	18
Number of HD	3	3
HIA	0.014	0.014
PPB	95.30 %	95.42 %
$F_{30\%}$	0.98	0.98
VD (L/ kg)	0.673	0.68
CL (mL/ min /kg)	15.68	15.839
$T_{1/2}$ (h)	0.773	0.782
H-HT	0.112	0.11
DILI	0.895	0.888

References

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2. W. Wu, C. Z. Wang, X. Li, X. R. Li, Q. M. Xu and S. L. Yang, Chemical constituents of antitumor active fraction of Lysimachia clethroides, *Chinese Traditional and Herbal Drugs*, 2011, **42**, 38-41.
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