

Chemical analysis of *T. officinale* leaf extract using UPLC-TOF-MS negative ion mode (ESI-)

Compound	Adducts	Formula	m/z	Mass Error (ppm)
4-Methoxyphenoxyacetic acid	M-H ₂ O-H	C ₉ H ₁₀ O ₄	163.0396	-2.6145
p-coumaric acid	M-H	C ₉ H ₈ O ₃	163.0396	-2.9362
5,8-dihydroxycoumarin	M-H	C ₉ H ₆ O ₄	177.0187	-3.6158
6,7-Dihydroxycoumarin	M-H	C ₉ H ₆ O ₄	177.0187	-3.6158
5,7-Dihydroxycoumarin	M-H	C ₉ H ₆ O ₄	177.0187	-3.6158
Citric acid	M-H ₂ O-H, M-H	C ₆ H ₈ O ₇	191.0194	-1.9561
4-Methylesculetin	M-H	C ₁₀ H ₈ O ₄	191.0344	-2.7850
5,7-Dihydroxy-4-methylcoumarin	M-H	C ₁₀ H ₈ O ₄	191.0344	-2.7850
Quinic acid	M-H	C ₇ H ₁₂ O ₆	191.0560	-0.5738
Sinapinic acid	M-H ₂ O-H	C ₁₁ H ₁₂ O ₅	205.0503	-1.3059
Pro-Glu	M-H ₂ O-H	C ₁₀ H ₁₆ N ₂ O ₅	225.0876	-2.0003
Glu-pro	M-H ₂ O-H	C ₁₀ H ₁₆ N ₂ O ₅	225.0876	-2.0003
Taraxinic acid	M-H	C ₁₅ H ₁₈ O ₄	261.1133	0.4091
Pratol	M-H	C ₁₆ H ₁₂ O ₄	267.0662	-0.3047
6-Hydroxy-2'-methoxyflavone	M-H	C ₁₆ H ₁₂ O ₄	267.0662	-0.3047
2-O-(alpha-D-glucopyranosyl)-D-glyceric acid	M-H	C ₉ H ₁₆ O ₉	267.0721	-0.2615
2-(alpha-D-mannosyl)-D-glyceric acid	M-H	C ₉ H ₁₆ O ₉	267.0721	-0.2615
Luteolin	M-H	C ₁₅ H ₁₀ O ₆	285.0395	-3.3762
Chrysoeriol	M-H	C ₁₆ H ₁₂ O ₆	299.0548	-4.4455
Sorbifolin	M-H	C ₁₆ H ₁₂ O ₆	299.0548	-4.4455
Hispidulin	M-H	C ₁₆ H ₁₂ O ₆	299.0548	-4.4455
Rhamnocitrin	M-H	C ₁₆ H ₁₂ O ₆	299.0548	-4.4455
4-Hydroxybenzoyl glucose	M-H	C ₁₃ H ₁₆ O ₈	299.0761	-3.8020
4-Hydroxybenzoic acid 4-O-glucoside	M-H	C ₁₃ H ₁₆ O ₈	299.0761	-3.8020
glucosyl salicylate	M-H	C ₁₃ H ₁₆ O ₈	299.0761	-3.8020
Caftaric acid	M-H	C ₁₃ H ₁₂ O ₉	311.0409	0.2301
gentisic acid 5-beta-glucoside	M-H	C ₁₃ H ₁₆ O ₉	315.0713	-2.6976
Fertaric acid	M-H ₂ O-H, M-H	C ₁₄ H ₁₄ O ₉	325.0559	-2.3264
sinapoyltartronic acid	M-H ₂ O-H, M-H	C ₁₄ H ₁₄ O ₉	325.0559	-2.3264
6-O-Galloylglucose	M-H	C ₁₃ H ₁₆ O ₁₀	331.0656	-4.4879
Glucogallin	M-H	C ₁₃ H ₁₆ O ₁₀	331.0656	-4.4879
Ascorbyl glucoside	M-H	C ₁₂ H ₁₈ O ₁₁	337.0779	0.8319
dalpatein	M-H	C ₁₈ H ₁₄ O ₇	341.0668	0.3146
Rosmarinic acid	M-H ₂ O-H	C ₁₈ H ₁₆ O ₈	341.0668	0.3147
Chlorogenic acid isomers	M-H	C ₁₆ H ₁₈ O ₉	353.0872	-1.7756
Syringin	M-H	C ₁₇ H ₂₄ O ₉	371.1346	-0.4712
abscisic acid glucoside	M-H	C ₂₁ H ₃₀ O ₉	425.1810	-1.7007
6-Hydroxyluteolin 7-glucoside	M-H ₂ O-H	C ₂₁ H ₂₀ O ₁₂	445.0776	-0.1085
Hypolaetin-8-glucoside	M-H ₂ O-H	C ₂₁ H ₂₀ O ₁₂	445.0776	-0.1085
Gossypetin 8-rhamnoside	M-H ₂ O-H	C ₂₁ H ₂₀ O ₁₂	445.0776	-0.1085
Genistein-7-O-glucuronide	M-H	C ₂₁ H ₁₈ O ₁₁	445.0779	0.6321
7-Hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-5-yl beta-D-glucopyranosiduronic acid	M-H	C ₂₁ H ₁₈ O ₁₁	445.0779	0.6321
apigenin 7-glucuronide	M-H	C ₂₁ H ₁₈ O ₁₁	445.0779	0.6321
apigenin 7-glucuronide	M-H	C ₂₁ H ₁₈ O ₁₁	445.0788	2.6623
Genistein-7-O-glucuronide	M-H	C ₂₁ H ₁₈ O ₁₁	445.0788	2.6623
Luteolin-5-O-glucopyranoside	M-H	C ₂₁ H ₂₀ O ₁₁	447.0935	0.5352
Kaempferol-7-O-glucoside	M-H	C ₂₁ H ₂₀ O ₁₁	447.0935	0.5352
Luteolin-7-O-glucopyranoside	M-H	C ₂₁ H ₂₀ O ₁₁	447.0935	0.5352
Carthamone	M-H, 2M-H	C ₂₁ H ₂₀ O ₁₁	447.0947	3.1519
Plantagin	M-H, 2M-H	C ₂₁ H ₂₀ O ₁₁	447.0947	3.1519
Kaempferol-7-O-glucoside	M-H, 2M-H	C ₂₁ H ₂₀ O ₁₁	447.0947	3.1519
Isorhamnetin 4'-O-glucuronide	M-H ₂ O-H	C ₂₂ H ₂₀ O ₁₃	473.0736	2.0915
Chicoric acid	M-H	C ₂₂ H ₁₈ O ₁₂	473.0738	2.6795
Carmine	M-H	C ₂₂ H ₂₀ O ₁₃	491.0836	0.9801
Isorhamnetin 4'-O-glucuronide	M-H	C ₂₂ H ₂₀ O ₁₃	491.0836	0.9801
Raffinose	M-H	C ₁₈ H ₃₂ O ₁₆	503.1626	1.5941
Maltotriose	M-H	C ₁₈ H ₃₂ O ₁₆	503.1626	1.5941
D-Cellotriose	M-H	C ₁₈ H ₃₂ O ₁₆	503.1626	1.5941
Isomaltotriose	M-H	C ₁₈ H ₃₂ O ₁₆	503.1626	1.5941
Dicaffeoylquinic acid isomers	M-H	C ₂₅ H ₂₄ O ₁₂	515.1199	0.7406
5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 5-O-beta-D-glucopyranosyl-beta-D-xylofuranoside	M-H	C ₂₆ H ₂₈ O ₁₅	579.1370	2.5476
5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 6-O-beta-D-xylofuranosyl-beta-D-glucopyranoside	M-H	C ₂₆ H ₂₈ O ₁₅	579.1370	2.5476
Luteolin 7-O-rutinoside	M-H	C ₂₇ H ₃₀ O ₁₅	593.1518	0.9918
Luteolin-7-O-neohesperidoside	M-H	C ₂₇ H ₃₀ O ₁₅	593.1518	0.9918
Kaempferol 3-O-neohesperidoside	M-H	C ₂₇ H ₃₀ O ₁₅	593.1518	0.9918
Multinose A	M-H	C ₂₇ H ₃₀ O ₁₆	609.1470	1.4808
luteolin-7-O-gentiobioside	M-H	C ₂₇ H ₃₀ O ₁₆	609.1470	1.4808
Quercetin 3-O-rhamnoside 7-O-glucoside	M-H	C ₂₇ H ₃₀ O ₁₆	609.1470	1.4808
Rutin	M-H	C ₂₇ H ₃₀ O ₁₆	609.1470	1.4808