

Chemical analysis of *C. intybus* leaf extract using UPLC-TOF-MS positive mode (ESI+)

Description	Adducts	Formula	m/z	Mass Error (ppm)
Alanine	M+H	C ₃ H ₇ NO ₂	90.0554	4.4417
Asparagine	M+H	C ₄ H ₈ N ₂ O ₃	133.0610	1.5030
Glutamine	M+H	C ₅ H ₁₀ N ₂ O ₃	147.0771	4.7594
Tartaric acid	M+H	C ₄ H ₆ O ₆	151.0231	-3.9729
caffeic acid	M+H, M+Na	C ₉ H ₈ O ₄	181.0489	-3.3140
Fructose	M+H	C ₆ H ₁₂ O ₆	181.0701	-3.3136
Glucose	M+H	C ₆ H ₁₂ O ₆	181.0714	3.8659
Tyrosine	M+H	C ₉ H ₁₁ NO ₃	182.0754	-0.5492
Favan-3-ol	M+H	C ₁₅ H ₁₄ O ₂	227.1070	1.3210
Flavan-4-ol	M+H	C ₁₅ H ₁₄ O ₂	227.1070	1.3210
7-Hydroxyflavan	M+H	C ₁₅ H ₁₄ O ₂	227.1070	1.3210
Caftaric acid	M+H	C ₁₃ H ₁₂ O ₉	313.0558	1.2778
Sucrose	M+H	C ₁₂ H ₂₂ O ₁₁	343.1219	-4.6630
p-Coumaric acid glucoside	M+H, M+Na	C ₁₅ H ₁₈ O ₈	327.1069	-1.5286
Chlorogenic acid isomers	M+H	C ₁₆ H ₁₈ O ₉	355.1017	-0.7836
Cyanidine-3-O-glucoside	M+	C ₂₁ H ₂₁ O ₁₁	449.1078	-0.6679
Kaempferol-3-O-glucoside	M+H	C ₂₁ H ₂₀ O ₁₁	449.1085	1.4681
Quercitin-3-glucuronide	M+H	C ₂₁ H ₁₈ O ₁₃	478.0733	-2.9284
Chicoric acid	M+H, M+Na	C ₂₂ H ₁₈ O ₁₂	497.0693	0.5519
Dicaffeoyl quinic acid isomers	M+H	C ₂₅ H ₂₄ O ₁₂	517.1339	-0.3867
Rutin	M+H	C ₂₇ H ₃₀ O ₁₆	611.1634	-2.4491