

Table S3. The characteristic fragment ions of flavonoids used in chemical identification of present work .

Compound	characteristic fragment ions in negative model [<i>m/z</i>]	Ref
Isorhamnetin derivatives	316.06 [<i>Y</i> ₀] ⁻ , 315.05 [<i>Y</i> ₀ -H] ⁻ , 271.02 [<i>M</i> -H-CO ₂] ⁻ , 300.03 [<i>M</i> -H-CH ₃] ⁻ , 255.03 [<i>M</i> -H-CH ₃ -H ₂ O-CO] ⁻ , 151.00 [^{1,3} A ⁻],	[1]
Quercetin derivatives	301.03 [<i>Y</i> ₀] ⁻ , 300.03 [<i>Y</i> ₀ -H] ⁻ , 271.02 [<i>M</i> -H-CH ₂ O] ⁻ , 255.03 [<i>M</i> -H-H ₂ O-CO] ⁻ , 151.00 [^{1,3} A ⁻]	[2]
Kaempferol	286.05 [<i>Y</i> ₀] ⁻ , 285.04 [<i>Y</i> ₀ -H] ⁻ , 255.03 [<i>M</i> -H-CH ₂ O] ⁻ , 227.03. [<i>M</i> -H-CH ₂ O-CO] ⁻ , 151.00 [^{1,3} A ⁻]	[2]
Luteolin	286.05 [<i>Y</i> ₀] ⁻ , 285.04 [<i>Y</i> ₀ -H] ⁻ , 241.05 [<i>M</i> -H-CO ₂] ⁻ , 217.05 [<i>M</i> -H-C ₃ O ₂] ⁻ , 175.04 [<i>M</i> -H-C ₃ O ₂ -C ₂ H ₂ O]	[3, 4]
Taxifolin	303.05 [<i>Y</i> ₀ -H] ⁻ , 285.04 [<i>M</i> -H-CO ₂] ⁻ , 125.02 [<i>M</i> -H-C ₂ H ₂ O] ⁻ , 151.00 [^{1,3} A ⁻]	[5]

1. Du, L.-y.; Zhao, M.-T.; Qian, J.-H.; Jiang, D.-W.; et al.. The Metabolic Profiling of Isorhamnetin-3-O-Neohesperidoside Produced by Human Intestinal Flora Employing UPLC-Q-TOF/MS. *Journal of Chromatographic Science*. 2016, **55**(3), 243-250.
2. Schieber, A.; Berardini, N.; Carle, R. Identification of Flavonol and Xanthone Glycosides from Mango (*Mangifera indica* L. Cv. "Tommy Atkins") Peels by High-Performance Liquid Chromatography-Electrospray Ionization Mass Spectrometry. *Journal of Agricultural and Food Chemistry*. 2003, **51**(17), 5006-5011.
3. Śliwka-Kaszyńska, M.; Anusiewicz, I.; Skurski, P. The Mechanism of a Retro-Diels–Alder Fragmentation of Luteolin: Theoretical Studies Supported by Electrospray Ionization Tandem Mass Spectrometry Results. *Molecules*, 2022. **27**(3).
4. Brito, A.; Ramirez, J.-E.; Areche, C.; Sepulveda, B.; Simirgiotis, M.-J. HPLC-UV-MS Profiles of Phenolic Compounds and Antioxidant Activity of Fruits from Three Citrus Species Consumed in Northern Chile. *Molecules*. 2014, **19**(11), 17400-17421.
5. Hvattum, E., Determination of phenolic compounds in rose hip (*Rosa canina*) using liquid

chromatography coupled to electrospray ionisation tandem mass spectrometry and diode-array detection. *Rapid Communications in Mass Spectrometry*. 2002, **16**(7), 655-662.