

Supplementary Materials

Solvents, Chemicals, and Standards

Maceration and extraction solvents (ethanol and glycerol), analytical HPLC grade solvents (acetonitrile, methanol, and formic acid), reagents for HPLC buffer (potassium dihydrogen phosphate and phosphoric acid) were purchased from Fluka Biochemika (Buchs, Switzerland) and Sigma–Aldrich (St Louis, MO, USA). Cetyltrimethylammonium bromide (cetrimide) was purchased from Extrasynthèse (Genay, France), while 1,2-phenylenediamine dihydrochloride (OPDA) was purchased from Sigma–Aldrich.

All polyphenolic standards (caffeic acid, chlorogenic acid, coumaric acid, ferulic acid, hyperoside, isoquercitrin, quercetin, quercitrin, rutin, ellagic acid, gallic acid, catechin, epicatechin, castalagin, vescalagin) were purchased from Sigma–Aldrich, while organic acids (citric acid, malic acid, oxalic acid, quinic acid, succinic acid, and tartaric acid) were purchased from Fluka Biochemika. Ascorbic acid and dehydroascorbic acid were purchased from Extrasynthèse. Milli-Q ultrapure water was produced by Sartorius Stedim Biotech mod. Arium (Sartorius, Göttingen, Germany).

Stock solutions of cinnamic acids and flavonols with a concentration of 1.0 mg mL^{-1} were prepared in methanol. From these solutions, four calibration standards (1000 ppm, 50 ppm, 250 ppm, 125 ppm) were prepared by dilution with methanol; stock solutions of benzoic acids, tannins, and catechins with a concentration of 1.0 mg mL^{-1} were prepared in a solution of 95% methanol and 5% water. From these solutions, four calibration standards were prepared by dilution with 50% methanol-water. Stock solutions of organic acids with a concentration of 1.0 mg mL^{-1} were prepared in ultrapure water. From these solutions, four calibration standards were prepared by dilution with water. Finally, stock solutions of ascorbic and dehydroascorbic acids with a concentration of 1.0 mg mL^{-1} were prepared in methanol. From these solutions, four calibration standards were prepared by dilution with methanol.

Table S1. Chromatographic conditions of the used methods.

Method	Compounds of Interest	Stationary Phase	Mobile Phase	Flow (mL min ⁻¹)	Wavelength (nm)
A	cinnamic acids, flavonols	KINETEX—C18 column (4.6 × 150 mm, 5 μm)	A: 10 mM KH ₂ PO ₄ /H ₃ PO ₄ , pH = 2.8 B: CH ₃ CN	1.5	330
B	benzoic acids, catechins, Tannins	KINETEX—C18 column (4.6 × 150 mm, 5 μm)	A: H ₂ O/CH ₃ OH/HCOOH (5:95:0.1 v/v/v), pH = 2.5 B: CH ₃ OH/HCOOH (100:0.1 v/v)	0.6	280
C	monoterpenes	KINETEX—C18 column (4.6 × 150 mm, 5 μm)	A: H ₂ O B: CH ₃ CN	1.0	250
D	organic acids	KINETEX—C18 column (4.6 × 150 mm, 5 μm)	A: 10 mM KH ₂ PO ₄ /H ₃ PO ₄ , pH = 2.8 B: CH ₃ CN	0.6	214
E	vitamins	KINETEX—C18 column (4.6 × 150 mm, 5 μm)	A: 5 mM C ₁₆ H ₃₃ N(CH ₃) ₃ Br/50 mM KH ₂ PO ₄ , pH = 2.5 B: CH ₃ OH	0.9	261, 348
F	sugars	SphereClone—NH ₂ column (4.6 × 250 mm, 5 μm)	A: H ₂ O B: CH ₃ CN	0.5	286

Method A—gradient analysis: 5% B to 21% B in 17 min + 21% B in 3 min (2 min conditioning time). Method B—gradient analysis: 3% B to 85% B in 22 min + 85% B in 1 min (2 min conditioning time). Method C—gradient analysis: 30% B to 56% B in 15 min + 56% B in 2 min (3 min conditioning). Method D—gradient analysis: 5% B to 14% B in 10 min + 14% B in 3 min (2 min conditioning time). Method E—*isocratic* analysis: ratio of phase A and B: 95:5 in 10 min (5 min conditioning time). Method F—*isocratic* analysis: ratio of phase A and B: 5:85 in 12 min (3 min conditioning time).