Supplementary material

Statistical analysis. PLS regression predicts a set of dependent variables from a set of independent variables (predictors) by combining features from principal component analysis and multiple linear regression. The prediction is achieved by extracting a set of orthogonal factors from the predictors, called latent variables, and the goal of PLS is to find a series of uncorrelated latent variables such that the covariance between them and the set of dependent variables is maximal. PLS is particularly useful in situations where there are many possibly correlated predictor variables and relatively few samples, and, similarly to principal components analysis, it also allows to explore the data in search of hidden correlations and patterns.

The predictors were stored in a data matrix X and the independent variables in a data matrix Y of mean-centered and normalized column vectors. To identify the number of latent variables that allows the PLS regression model to provide an optimal prediction of new observations we used the leave-one-out cross-validation technique. This is a resampling method that separates the data into a training set and a test set, and it thus allows to test the prediction capabilities of the PLS model.

Table S1. List of the chemical reagent used.

Reagent	CAS number	Purity	Company
Methanol	67-56-1	suitable for HPLC, gradient grade, ≥99.9%	Sigma-Aldrich
Water	7732-18-5	suitable for HPLC, high purity	Sigma-Aldrich
Trifluoroacetic acid	76-05-1	suitable for HPLC, ≥99.0%	Sigma-Aldrich
Chlorogenic acid	327-97-9	primary reference standard	Sigma-Aldrich
Folin & Ciocalteu's phenol reagent	not present	undeclared	Sigma-Aldrich
Sodium carbonate	497-19-8	ACS reagent, anhydrous, ≥99.5%	Sigma-Aldrich
2,2'-diphenyl-1-picrylhydrazyl (DPPH)	1898-66-4	undeclared	Sigma-Aldrich
6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (TROLOX)	53101-49-8	≥98%	Sigma-Aldrich
Sodium acetate	127-09-3	anhydrous, ReagentPlus®, ≥99.0%	Sigma-Aldrich
2,4,6-Tri(2-pyridyl)-s-triazine (TPTZ)	3682-35-7	for spectrophotometric det. (of Fe), ⩾98%	Sigma-Aldrich
Iron(III) chloride hexahydrate	10025-77-1	puriss. p.a., reag. Ph. Eur., ⩾99%	Sigma-Aldrich
2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid (ABTS)	30931-67-0	≥98% (HPLC)	Sigma-Aldrich
Potassium persulfate	7727-21-1	ACS reagent, ≥99.0%	Sigma-Aldrich
Tyrosol	501-94-0	analytical standard, ≥ 99.5 %	Sigma-Aldrich
(−)-Epicatechin	490-46-0	analytical standard, ≥ 97.0% (HPLC)	Sigma-Aldrich
(+)-Catechin	154-23-4	analytical standard, ≥ 99.0 %	Sigma-Aldrich
Procyanidin B1	20315-25-7	analytical standard, ≥ 90% (HPLC)	Sigma-Aldrich
Procyanidin B2	29106-49-8	analytical standard, ≥ 90% (HPLC)	Sigma-Aldrich
Phloridzin dihydrate	7061-54-3	analytical standard, ≥ 98.5% (HPLC)	Sigma-Aldrich
Quercetin-3-glucoside	482-35-9	analytical standard, ≥ 98% (HPLC)	Sigma-Aldrich

Table S2. Gradient conditions for polyphenols separation by HPLC.

Minutes	% Solvent A [a]	% Solvent B [a]
0-2	95%	5%
2-7	88%	12%
7-38	45%	55%
38-39	0%	100%
39-40	0%	100%
40-41	95%	5%
41-45	95%	5%

[a] Solvent A: water; Solvent B: methanol.