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A new optical technique for the quantitative and functional analysis of botanical extracts for oenological use☆

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ABSTRACT

Eighty-six oenological tannins including condensed (TanCondx) and ellagitannins (TanElx) were analyzed for their total polyphenols content (TPC), polymeric tannins content (TAC) and antiradical activity (AA). Results from the reference spectrophotometric methods (Adams-Harbertson AH assay and DPPH• radical scavenging) were compared with the optical measurements obtained using a technique related to the Spectral Sensitive Pulsed Photometry (SSPP) - a new method suggested in a patented industrial invention for the quantification of tannins, and based on the reactivity of the polyphenolic compounds against targeted reagents: (i) a buffered bovine serum albumin (BSA) solution to measure TAC, and (ii) a soluble polyvinylpyrrolidone (PVP) resin for the TPC and AA measurements. Reactions of polyphenols with BSA and PVP enabled a dose-dependent turbidity development which was monitored under irradiation detected by the 875 nm sensitivity peak photodiode. The SSPP-BSA estimated the TAC in the extracts with appreciable precision (adj. $R^2 = 0.966$ against AH, Root Mean Square Error RMSE 22.18 mg CE /g dw); The TPC and AA estimates were good (TPC: adj. $R^2 = 0.917$ against AH, RMSE 75.13 mg CE /g dw; AA: adj. $R^2 = 0.913$ against DPPH•, RMSE 6.41 % scavenging), although affected by some scatter phenomena. TAC, TPC and AA are key parameters for the classification of oenological extracts and the extraction process from by-products can be improved by the rapid quality control through the proposed assay.

1. Introduction

Sustainability and quality control are the most relevant topics to emerge in recent years, particularly with reference to agri-food supply chains; a combination of lean production and high-level quality management are now core to the strategy of the food industry at the global level (Hassoun et al., 2022; Hassoun et al., 2024). In particular, the European Community encourages its Member States to adopt new and virtuous direction towards the global economy and production, by ensuring that policy actions are firmly anchored in latest science and knowledge (*European Commission: Directorate-General for Research and Innovation, horizon Europe, pillar II - global challenges and European industrial competitiveness*, 2021). In the context of the food system, each unit operation and/or process has the potential to be monitored using emerging and low-impact technologies to reduce quality uncertainty. On this view, the development of innovative, portable measuring devices coupled with smart data management systems is gaining increasing interest for the industry, as they allow to adopt decision-making strategies supported by knowledge (Grassi & Casiraghi, 2022; Levy, Hashiguchi, & Cecchini, 2022; Marvin et al., 2022).

The wine sector is a special case that effectively summarizes the requirements and challenges of an innovative and high-quality food chain, since its management implies a high level of control over the different transformations taking place from the initial processing of raw materials (grapes) to the customers' delivery of bottled wines (Costa, Catarino, Escalona, & Comuzzo, 2022; Ma et al., 2022; Vieira, Figueira, & Fragoso, 2023).

The variety of materials, machinery, and products used in oenology

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contribute to the supply chain and request specific quality assurance protocols.

At this proposal, the wine industry makes extensive use of processing aids, i.e., 'substances which are added during food processing to confer particular characteristics' (EFSA https://www.efsa.europa.eu/en/glossary/processing-aid); these include oenological tannins, natural botanical extracts which are approved for use in grapes, must, and wines at the different levels of the production process, and can be added as lyophilized powders/ stabilized solutions in pure or blended formulations (OIV, 2022, 2024). Extensive research on oenological tannins performed over the last two decades has demonstrated their technological relevance, along with their role as alternative to more impactful oenological practices, encouraging their exploitation thorough the wine chain (Fracassetti, Messina, Saligari, & Tirelli, 2023; Motta et al., 2025; Paissoni et al., 2022a; Ricci et al., 2016; Vignault et al., 2018). Following this trend, the commercially-available formulations have increased significantly; nevertheless, it is still somewhat challenging to achieve a full characterization of commercial oenological formulations in terms of composition and functional characteristics. For instance, the content of polyphenolic compounds must meet minimum content set by regulatory authorities, and producers must adhere to strict safety, authentication and functional protocols; these require intense sample preparations coupled with costly and time-consuming analytical methods, and highly qualified personnel for processing complex datasets (Paissoni et al., 2022a). Whether traditional methods offer a broad and detailed perspective on the composition of the oenological extracts, the use of smart and portable devices may provide relevant analytical information to optimize the extraction processes, to rank the quality of the extracts, or for timely identification of defective batches, with a clear advantage in terms of cost and quality of the commercial formulations.

Recent studies introduced innovative approaches to the analytical characterization of polyphenols and tannins (Alfieri, Modesti, Bellincontro, Renzi, & Aleixandre-Tudo, 2024; Dos Santos, Bosman, du Toit, & Aleixandre-Tudo, 2023; Johnson, Walsh, Naiker, & Ameer, 2023; Motta et al., 2025; Nghia et al., 2023), acting as benchmarks for the innovation in quality control systems. In our previous work (Ricci et al., 2020) we suggested the Spectral Sensitive Pulsed Photometry, (SSPP) (Patent nr.102019000002585) as rapid optical method for the quantification of tannins in wine. In the present work, some functions of SSPP were used to characterize a selection of tannin extracts in relation to the following parameters: (i) total polyphenols content TPC; (ii) tannic (polymeric) fraction TAC; (iii) anti-radical activity AA determined against the synthetic radical 2,2-diphenyl-1-picrylhydrazyl (DPPH•) - a common method for measuring the antioxidant activity of oenological extracts (Magalhães, Ramos, Reis, & Segundo, 2014; Paissoni et al., 2022b; Ricci, Parpinello, Teslić, Kilmartin, & Versari, 2019). The potential of the method is discussed with a view to its possible implementation as part of large-scale quality control strategies.

2. Materials and methods

2.1. Chemicals

Chemicals included sodium chloride, sodium acetate, sodium dodecyl sulfate, triethanolamine, iron(III) chloride, bovine serum albumin (BSA, ≥ 98 %) to prepare buffers and working solutions; the (+)-catechin monohydrate standard (≥ 98 %) used to calibrate the spectrophotometric methods; the 2,2-diphenyl-1-picrylhydrazyl synthetic radical for the colorimetric DPPH• assay; the polyvinylpyrrolidone (PVP) with average molecular weight 10,000 for the optical determination of polyphenols. All reagents were from Sigma (Sigma-Aldrich, St. Louis, MO, US). The working solutions were prepared with ultrapure water from a MilliQ gradient system (Millipore Corporation, Billerica, MA, USA), except the methanol used for the DPPH• assay (HPLC grade, ≥ 99.9 %) which was from Merck (Merck Millipore, Darmstadt, Germany).

2.2. Tannins

A selection of 86 experimental extracts from different botanical sources, 44 of which ellagic (TanEl*x*, **Supplementary Material SM1**) and 42 condensed (TanCond*x*, **Supplementary Material SM1**) was supplied by Italiana Biotecnologie Srl (San Martino di Trecate, NO, IT); the samples were extracted by different production companies, gathered from various process conditions and designed to develop commercial formulations for precision oenological purposes. Tannins were dissolved in MilliQ water at the concentration of 1 g/L, and the compositional data were reported with reference to the g of dry weight (g dw); the same solutions were used for all analytical determinations.

2.3. Spectrophotometric determinations

All the spectrophotometric/colorimetric determinations were made in 1 cm-optical path disposable plastic cuvettes using a Cary 60 UV–Vis spectrophotometer (Agilent Technologies, Santa Clara, CA, US); each experiment was run in duplicate, and results were provided as averaged values. Blank measurements were obtained mixing the reagent solutions with appropriate volumes of distilled water. The tannins solutions were analyzed for their total polyphenols (TPC) and tannins (TAC) content using the Adams-Harbertson gravimetric-colorimetric assay (AH) previously reported in the literature (Harbertson, Kennedy, & Adams, 2002) as the reference method. Calibration was performed using (+)-catechin as the reference standard and results were expressed as mg (+)-catechin equivalents per gram of dry weight (mg CE / g dw).

The antiradical activity (AA) was determined using the DPPH• assay, previously adapted for the analysis of oenological botanical extracts (Ricci et al., 2019); briefly, the tannin solutions were diluted 20 times in ultrapure water and 100 μL were mixed to 2.9 mL of 200 μM DPPH• (molar mass: 394.32 g/mol) in methanol; the resulting mixture was incubated up to 24 h until reaching the steady-state (Ricci et al., 2019). Results were expressed as percentage of DPPH• radical scavenged at the wavelength of 517 nm according to the following:

$$\%\text{inhibition} = [(\text{Ab} - \text{As})/\text{Ab}] \times 100$$

where: *Ab* = absorbance of the reagent blank ($\text{Ab}_{517\text{nm}}$ = 0.810 a.u.), and *As* = absorbance of the sample.

2.4. Optical determinations from SSPP

The optical determinations were performed using the Spectral Sensitive Pulsed Photometry (SSPP) prototype detailed in the literature (Ragni, Iaccheri, Cevoli, & Berardinelli, 2016) and previously applied in case study to determine the tannins content in liquids (Patent nr.102019000002585; Ricci et al., 2020). The optical prototype was equipped with a photodiode with a peak intensity around 875 nm, which enable to monitor the relevant optical phenomena (i.e., development of turbidity) involved in the attenuation of the source intensity, also removing interference due to the color of the extracts (Ricci et al., 2020). For the purpose of the present experiment, the peak value of the light intensity (LI) was used to build univariate statistical models to estimate TPC, TAC, AA (subsequently, for brevity, the peak is indicated as SSPP and expressed as light intensity (LI)). Different reaction mixtures were evaluated (see **2.4.1** and **2.4.2**) to interpolate the LI with the TPC, TAC and AA obtained from the spectrophotometric determinations.

The tannin solutions were directly mixed with the PVP and BSA reagents at different volumetric ratios (see **2.4.1** and **2.4.2**) to enable the formation of the colloidal suspensions; blank measurements were obtained by mixing the reagent solutions with appropriate volumes of distilled water. Disposable plastic cuvettes with 1 cm optical path were used to prepare the reaction mixture for the SSPP determinations.

Each sample was prepared in duplicate; for each determination, the instrument takes and averages 3 subsequent optical measurements. The

average of the three is directly displayed in the screen of the prototype via an Arduino board system (Ricci et al., 2020).

2.4.1. SSPP-PVP / TPC and SSPP-PVP / AA

The PVP was dissolved in a acetate buffer (pH 4.9) at the fixed concentration of 1 g/L. For the optical determination of tannins, the aqueous solutions of the extracts (section 2.2) were mixed with the PVP solution in a 0.5: 3.50 volumes ratio, enabling a linear response against TPC. The SSPP measurement was performed every minute for 10 min after mixing; nevertheless, a reproducible measurement was achieved only after 1 min incubation. The results expressed as LI were compared to the TPC (mg CE/ g dw) obtained by the reference method (Harbertson et al., 2002).

In addition, the SSPP-PVP signals were correlated to the % DPPH• scavenging results for the AA determination.

2.4.2. SSPP-BSA / TAC and SSPP-BSA / TAC st

For the optical determination of TAC, the aqueous solutions of the extracts were mixed with a solution of reagent-grade BSA dissolved at the fixed concentration of 500 mg/L in a acetate buffer (pH 4.9). The tannin-to-protein ratio was 0.25: 3.75 *v*/v; this volumetric ratio ensured an excess of protein improving stability, reproducibility and linearity of the optical response. After mixing, the SSPP measure was performed every minute for 10 min, and an optimum incubation time of 5 min was determined.

Under our experimental conditions the working solutions contained a maximum 426 mg/L CE of tannins (see **3.1** and Table 2); in order to assess the linearity of the method under an extended concentration range, standard aqueous solutions were prepared using a commercial grape pomace extract (Laffort Italia, Tortona, IT) with known composition (i.e., TPC 667 ± 15 mg CE / g dw; TAC 259 ± 6 mg CE / g dw), to obtain standard TAC values ranging 55–1400 mg CE/L (TAC st). The solutions obtained were measured with the AH assay and with SSPP-BSA up to 10 min incubation time to verify the stability of the LI values.

2.5. Statistical analysis

The data and model performances were evaluated using the XLSTAT version 2023.1.1 (Addinsoft, Anglesey, UK). Linear functions were exploited to predict the TPC and TAC contents, along with the AA of the extracts, with the arbitrary unit LI from SSPP-BSA and SSPP-PVP as x and the spectrophotometrically determined TPC, TAC, AA as $f(x)$. The 86 samples were randomly divided into a calibration set for model building (58 samples) and validation set for model validation (28 samples). The accuracy and precision of the calibration model were evaluated using the determination coefficient of calibration (R^2cal) and the root mean standard error of calibration (RMSEcal) as the main indicators, while the reliability and stability of the model were evaluated through the determination coefficient of validation (R^2val) and the root mean standard error of validation (RMSEval). In particular, the RMSEcal informs on the potential error of future predictions, whereas the RMSEval detects the real error when adding further samples (Aleixandre-Tudo, Nieuwoudt, Olivieri, Aleixandre, & du Toit, 2018; Liu et al., 2024). Both the residual predictive deviation of calibration (RPDcal) and validation (RPDval) were used as further indicators to evaluate the predictive ability, assuming that a model with RPD value >2.5 can be effectively used for prediction purposes due to larger standard deviation coupled to smaller prediction error, while a model with 1.5 < RPD > 2.5 performs well for screening (Liu et al., 2024; Versari, Parpinello, & Laghi, 2012).

The Bland-Altman method was used to assess the agreement between the proposed and reference methods. Consistency plots were drawn using XLSTAT version 2023.1.1 (Addinsoft, Anglesey, UK). Data were presented as the mean ± standard deviation (n = 3). The Limit Of Agreement (LOA) was determined at the $p < 0.05$ statistical significance.

3. Results and discussion

3.1. Spectrophotometric determination of TPC, TAC and AA

Table 1 reports the averaged values and standard deviation of the TPC and TAC determined by spectrophotometry (AH). TPC of the extracts varied over three orders of magnitude (CV 133.2 %) with min-max 33–1101 mg CE / g dw and average 567 mg CE / g dw. The measured values occasionally exceeded the dry weight, possibly due to the standard used for the calibration of the colorimetric method, as previously reported by Haslam (1989), or to random weighing error. The TCA, corresponding to the protein-reactive polyphenolic polymers/macromolecules, varied with min-max 0–426 mg CE / g dw and averaged 213 mg CE / g dw (CV 141.4 %). Few samples showed limited or missing polymeric fraction, possibly related to the botanical source and extraction method used or to a limited reactivity against the BSA used in the spectrophotometric assay.

The extracts displayed variable reactivity against the DPPH• radical, and the TPC was a factor in this trend. The R^2 value obtained with a linear regression of the TPC and AA parameters was 0.986 (adj.), with RMSE of 2.6 % AA (detailed model parameters in the **Supplementary Material SM2**); on the reverse, the interpolation of the DPPH• results with the measured TAC failed to provide an appropriate regression model for the prediction of AA (adj. $R^2 = 0.515$), despite the coefficient of x and the intercept being significant (*data not reported*). The poor correlation between TAC and AA can be related to the fact that the botanical extracts usually contain a consistent fraction of active polyphenolic monomers, making relevant contributions as antioxidants (Fracassetti, Messina, et al., 2023; Ricci et al., 2016; Vignault et al., 2018); indeed, the experimental results are consistent with the previous literature, reporting that the AA exhibits a positive linear correlation with the TPC of the extracts (Motta, Guaita, Cassino, & Bosso, 2020, 25). The occurrence of an extensive TAC may rather influence the incubation times required to obtain a steady state for the radical neutralization reaction, as observed in a previous work (Ricci et al., 2019).

3.2. Prediction of TPC, AA, and TAC of the extracts using the SSPP method

Table 1 reports the optical and reference measurements, and Table 2 summarizes the model performances according to the calibration and validation sets; overall, a few outliers (samples≤4) were identified and removed during models calibration.

The polyvinylpyrrolidone (PVP) was selected to determine the TPC of the extracts as this synthetic resin exhibits lower selectivity compared to the proteins, being able to aggregate the polyphenols - regardless their molecular weight - by hydrogen bonding, with development of turbidity; this property has been previously exploited to determine the TPC of botanical extracts (Makkar, Blümmel, & Becker, 1995). The same study also showed an optimal pH range (5–7) to elicit the PVP-polyphenols intermolecular association (Makkar et al., 1995). With reference to the TPC values, an adj. R^2cal = 0.917 was obtained wit RMSEcal of 75.16 mg CE / g dw, suggesting that the TPC of the extracts can be predicted by linear regression with the SSPP-PVP optical measurement, with significant model parameters and good agreement between predicted and experimental values (Fig. 1a; Table 2,); on the other hand, SSPP measurements performed over time after reagent mixing showed low reproducibility when one minute incubation was exceeded (*data not reported*), suggesting that further experiments are mandatory to achieve a robust measurement. The SSPP-PVP values obtained under 1 min incubation have proven to be also suitable for the prediction of AA of oenological tannins: the linear regression had an adj. R^2 of 0.913, with RMSEcal of 6.41 % scavenging and significant model parameters (Fig. 1b; Table 2).

When SSPP-BSA measurements (Table 1) were considered for the prediction of TAC, the standardization of the reaction mixture with large

Table 1
Set of experimental data including spectrophotometric and optical determinations.

Sample code	TAC (mg CE / g dw)	TPC (mg CE / g dw)	AA (% scavenging)	SSPP-BSA (LI)	SSPP-PVP (LI)
TanCond1	144 ± 18	300 ± 13	39.1 ± 2.3	19,382 ± 1	19,986 ± 37
TanCond2	148 ± 1	302 ± 25	36.0 ± 1.6	19,662 ± 4	20,654 ± 35
TanCond3	320 ± 16	518 ± 7	59.6 ± 0.8	17,232 ± 9	16,631 ± 134
TanCond4	271 ± 7	564 ± 31	58.6 ± 1.0	18,107 ± 11	17,207 ± 45
TanCond5	170 ± 9	368 ± 1	47.1 ± 1.5	18,938 ± 56	20,038 ± 52
TanCond6	349 ± 8	802 ± 28	86.0 ± 1.7	16,715 ± 11	14,474 ± 83
TanCond7	352 ± 4	1101 ± 16	98.7 ± 0.3	16,453 ± 9	13,077 ± 110
TanCond8	254 ± 4	613 ± 18	63.9 ± 2.7	17,955 ± 10	15,629 ± 156
TanCond9	285 ± 0	664 ± 18	74.1 ± 2.0	17,794 ± 7	16,473 ± 27
TanCond10	212 ± 36	555 ± 14	63.0 ± 0.4	19,180 ± 25	17,282 ± 159
TanCond11	315 ± 1	650 ± 29	70.4 ± 1.5	17,202 ± 4	16,113 ± 11
TanCond12	280 ± 16	659 ± 39	72.6 ± 0.5	17,274 ± 4	17,344 ± 13
TanCond13	360 ± 2	985 ± 12	96.4 ± 1.2	16,829 ± 10	14,269 ± 207
TanCond14	323 ± 7	886 ± 12	94.6 ± 0.7	17,003 ± 11	15,196 ± 146
TanCond15	201 ± 2	1000 ± 8	97.5 ± 1.2	18,787 ± 39	15,161 ± 279
TanCond16	396 ± 30	803 ± 1	85.0 ± 0.4	15,938 ± 54	15,967 ± 20
TanCond17	287 ± 21	582 ± 3	65.1 ± 0.6	17,573 ± 16	17,035 ± 47
TanCond18	216 ± 11	327 ± 18	44.1 ± 0.8	19,143 ± 10	20,419 ± 132
TanCond19	124 ± 32	295 ± 5	41.5 ± 1.0	20,164 ± 17	20,720 ± 43
TanCond20	148 ± 3	957 ± 26	96.9 ± 1.5	19,753 ± 351	14,329 ± 28
TanCond21	153 ± 7	975 ± 1	94.3 ± 7.4	19,179 ± 37	13,965 ± 51
TanCond22	18 ± 0	640 ± 28	70.2 ± 0.5	20,974 ± 33	16,996 ± 80
TanCond23	334 ± 35	862 ± 5	90.3 ± 0.7	16,681 ± 21	14,412 ± 210
TanCond24	278 ± 9	574 ± 4	64.4 ± 0.7	17,826 ± 29	17,514 ± 148
TanCond25	371 ± 19	621 ± 11	69.1 ± 0.1	16,039 ± 10	17,677 ± 98
TanCond26	98 ± 7	453 ± 12	56.2 ± 2.5	20,815 ± 263	18,258 ± 59
TanCond27	28 ± 1	486 ± 8	57.7 ± 0.5	21,007 ± 10	16,855 ± 195
TanCond28	387 ± 12	885 ± 43	92.3 ± 0.8	16,009 ± 13	15,213 ± 6
TanCond29	165 ± 9	1078 ± 2	98.2 ± 0.8	19,234 ± 17	14,125 ± 129
TanCond30	11 ± 0	286 ± 8	40.0 ± 0	21,026 ± 6	19,811 ± 17
TanCond31	124 ± 5	257 ± 5	38.0 ± 0.7	19,816 ± 85	19,964 ± 22
TanCond32	9 ± 2	179 ± 3	30.0 ± 1.1	20,996 ± 5	21,010 ± 18
TanCond33	2 ± 0	65 ± 5	19.4 ± 2.1	21,182 ± 12	20,855 ± 168
TanCond34	241 ± 31	500 ± 7	58.9 ± 0.5	17,946 ± 9	16,814 ± 158
TanCond35	9 ± 0	234 ± 34	35.2 ± 0.4	20,974 ± 25	20,287 ± 46
TanCond36	0	33 ± 2	18.0 ± 0.3	21,154 ± 7	21,167 ± 54
TanCond37	312 ± 17	681 ± 13	74.3 ± 0.2	16,895 ± 5	18,107 ± 6
TanCond38	380 ± 2	791 ± 5	83.9 ± 0.4	16,057 ± 3	16,480 ± 53
TanCond39	338 ± 6	668 ± 2	74.4 ± 1.9	16,927 ± 15	15,923 ± 20
TanCond40	323 ± 43	733 ± 14	79.3 ± 0.9	16,392 ± 10	17,626 ± 21
TanCond41	254 ± 1	884 ± 20	93.0 ± 1.8	18,524 ± 31	16,213 ± 170
TanCond42	348 ± 1	815 ± 17	85.1 ± 0.8	16,875 ± 7	14,857 ± 91
TanEl1	282 ± 4	516 ± 10	60.2 ± 0.4	16,306 ± 8	17,764 ± 118
TanEl2	323 ± 2	690 ± 17	76.2 ± 1.8	17,462 ± 20	17,129 ± 18
TanEl3	157 ± 3	287 ± 13	42.3 ± 3.0	19,543 ± 11	19,789 ± 16
TanEl4	185 ± 1	309 ± 3	40.7 ± 1.8	18,507 ± 10	18,756 ± 192
TanEl5	0	70 ± 3	21.8 ± 0.6	21,421 ± 16	20,826 ± 43
TanEl6	278 ± 3	506 ± 3	60.3 ± 1.7	17,044 ± 17	19,041 ± 8
TanEl7	68 ± 1	97 ± 7	24.9 ± 1.8	20,143 ± 37	21,558 ± 83
TanEl8	66 ± 3	128 ± 10	26.8 ± 0.6	20,479 ± 19	20,286 ± 105
TanEl9	130 ± 1	291 ± 5	41.3 ± 1.2	19,114 ± 5	19,759 ± 25
TanEl10	201 ± 0	397 ± 3	48.4 ± 1.6	18,164 ± 2	18,777 ± 34
TanEl11	258 ± 1	420 ± 5	51.2 ± 0.6	17,492 ± 10	17,553 ± 69
TanEl12	149 ± 1	279 ± 5	38.1 ± 1.9	19,185 ± 1	20,865 ± 6
TanEl13	330 ± 4	577 ± 2	66.3 ± 1.7	16,559 ± 11	16,052 ± 89
TanEl14	322 ± 3	748 ± 12	85.2 ± 0.4	16,768 ± 16	15,991 ± 18
TanEl15	195 ± 0	400 ± 5	48.0 ± 2.7	18,929 ± 10	18,758 ± 83
TanEl16	230 ± 1	339 ± 2	46.9 ± 3.2	18,036 ± 6	18,314 ± 13
TanEl17	143 ± 0	209 ± 10	34.1 ± 1.1	20,242 ± 16	19,530 ± 100
TanEl18	83 ± 1	158 ± 2	30.5 ± 2.2	20,291 ± 11	21,008 ± 14
TanEl19	61 ± 1	137 ± 17	26.1 ± 1.5	20,567 ± 3	21,210 ± 16
TanEl20	78 ± 2	139 ± 5	31.9 ± 2.3	20,442 ± 20	21,183 ± 9
TanEl21	135 ± 0	209 ± 13	31.6 ± 2.5	19,801 ± 2	20,528 ± 127
TanEl22	338 ± 5	443 ± 12	53.4 ± 0.4	16,989 ± 18	18,333 ± 37
TanEl23	157 ± 2	234 ± 2	35.8 ± 0.5	19,543 ± 14	19,981 ± 51
TanEl24	327 ± 1	486 ± 2	57.8 ± 0.7	17,460 ± 17	18,935 ± 60
TanEl25	279 ± 0	429 ± 8	50.6 ± 0.9	17,231 ± 1	18,974 ± 42
TanEl26	150 ± 0	291 ± 2	40.6 ± 0.2	19,088 ± 54	19,753 ± 53
TanEl27	50 ± 2	137 ± 13	29.3 ± 3.0	20,725 ± 14	21,189 ± 16
TanEl28	85 ± 1	309 ± 10	46.3 ± 6.1	20,242 ± 29	19,184 ± 45
TanEl29	0	59 ± 7	16.9 ± 4.9	20,411 ± 204	20,932 ± 38
TanEl30	168 ± 3	347 ± 0	43.9 ± 0.5	19,078 ± 41	19,237 ± 19

(*continued on next page*)

Table 1 (*continued*)

Sample code	TAC (mg CE / g dw)	TPC (mg CE / g dw)	AA (% scavenging)	SSPP-BSA (LI)	SSPP-PVP (LI)
TanEl31	278 ± 1	415 ± 8	54.0 ± 1.2	17,734 ± 52	17,900 ± 8
TanEl32	281 ± 2	568 ± 3	63.0 ± 2.1	17,460 ± 69	18,156 ± 18
TanEl33	234 ± 0	372 ± 2	47.8 ± 0.5	18,373 ± 1	18,997 ± 8
TanEl34	20 ± 2	208 ± 8	32.6 ± 0.9	21,093 ± 9	20,535 ± 8
TanEl35	300 ± 2	423 ± 3	51.4 ± 0.7	17,017 ± 9	19,522 ± 14
TanEl36	201 ± 7	337 ± 10	41.6 ± 4.1	18,883 ± 13	20,323 ± 8
TanEl37	288 ± 2	516 ± 7	62.8 ± 1.1	17,584 ± 20	16,655 ± 18
TanEl38	313 ± 1	581 ± 8	67.0 ± 2.0	17,121 ± 18	17,041 ± 27
TanEl39	386 ± 2	591 ± 8	67.1 ± 2.4	16,075 ± 16	16,956 ± 64
TanEl40	426 ± 0	627 ± 5	68.6 ± 1.2	15,339 ± 15	15,918 ± 23
TanEl41	379 ± 1	639 ± 12	77.3 ± 1.0	16,538 ± 27	16,895 ± 9
TanEl42	382 ± 1	710 ± 5	69.1 ± 0.3	16,036 ± 37	15,837 ± 18
TanEl43	383 ± 3	608 ± 5	66.0 ± 2.6	16,150 ± 9	15,996 ± 16
TanEl44	362 ± 4	545 ± 7	61.7 ± 0.9	16,590 ± 7	18,085 ± 5

excess of protein enabled to achieve a significant linear correlation, with adj. R^2 0.966 and RMSEcal 22.18 mg CE / g dw (Fig. 1c; Table 2). Furthermore, the SSPP measurements performed on standard solutions with TAC concentrations up to 1400 mg/L CE (SSPP-BSA / TAC st) confirmed an extended linearity of the optical response, with improvement of the model's performances (Table 3). In addition, stepwise determinations were performed up to 10 min after mixing, showing that the signal was stable up to 5 min before experiencing a decline in the linearity of the spectral response (Table 3); alternative functions failed to interpolated the 10-min SSPP-BSA data, showing rather random distribution. In previous work where different tannin-to-protein ratio was applied along with a different protein source (Ricci et al., 2020), the higher coefficient of determination (R^2 up to 0.9657) was associated with a quadratic regression between the SSPP optical signal and TAC, and the nonlinear correlation between higher TAC and light signal was tentatively attributed to a saturation effect (Ricci et al., 2020). On the other hand, Le Bourvellec and Renard (2012) demonstrated that the morphology of aggregates can be modulated according to the tannin-to-protein content: in more detail, a low tannin-to-protein ratio encouraged the interlinking between small complexes, delaying clusters growing and precipitation, whereas a higher ratio resulted in coarse and unstable aggregates. After 10 min incubation the effect observed by Le Bourvellec and Renard (2012) was relevant for standard solutions with higher TAC values (> 400 mg/L CE), with the tannin-to-protein complexes evolving into unstable colloids which were readily apparent to the naked eye; nonetheless, the effect was delayed through the use of an appropriate volumetric ratio between the reagents, with positive impact on the predictivity of TAC.

The TPC, TCA and AA prediction models constructed based on SSPP-PVP and SSPP-BSA achieved the purpose of prediction due to the RPDcal and RPDval values sistematically higher than 2.5 (Table 2), which was considered a suited arbitrary threshold in agreement with previous reports (Aleixandre-Tudo et al., 2018; Liu et al., 2024; Versari et al., 2012).

With reference to the original dataset reported in Table 1, the Bland-Altman plots (Fig. 2) were used to evaluate consistency between the proposed optical method and the reference methods, with the x-axes as the respective methods' mean values, and the y-axes as the difference between the same values. The differences between the averages of the two variables are reported as bias, i.e., systematic pattern of deviation between the methods. According to the mean differences observed between the observations, a systematic bias in the measurement techniques was not observed. For the TPC determination (Fig. 2a) all the data points fell within the 95 % LOA of the difference between predicted values and observed values, reporting a ± 76.06 mg CE / g dw SD and corroborating the potential for implementation of the optical method through the stabilization of reagents. For TAC, an effective comparability between the methods was achieved; most of the data points fell within the LOA (±21.29 mg CE / g dw SD), with a few exceptions which is associated to extracts retaining a lower tannin fraction (Fig. 2b); it follows that a random error in the data is likely to occur in samples with lower TAC (< 200 mg CE / g dw). The optical method performed well in predicting the AA compared to the DPPH• assay: the mean line fell well within the confidence interval with mean - 0.114 and outliers were not observed (Fig. 2c). For all models, the differences between the experimental values were evenly dispersed on two sides of the zero-bias line, indicating the suitability of the optical method in prediction of the TPC, TAC and AA parameters.

Several studies have been conducted on the determination of polyphenolic compounds in plant matrices and plant-derived food and numerous methods have been proposed for their quantification, gaining

Table 2
Regression model indicators and standardized coefficients based on characteristic LI (peak intensity) of the SSPP. Notes: RMSEcal, root mean square error of calibration; R^2cal, coefficient of determination of calibration; RPDcal, residual predictive deviation of calibration; RMSEval, root mean square error of validation; R^2val, coefficient of determination of validation; RPDval, residual predictive deviation of validation.

Dependent variable	Method	Calibration					Standardized calibration coefficients				
		Nr samples	*Range*	*R^2cal*	*RSMEcal*	*RPDcal*	*Slope*	*Standard error*	*p-values*	*Lower bound (95 %)*	*Upper bound (95 %)*
TPC (mg CE / g dw)	SSPP-PVP	55	0–1101	0.917	75.16	3.12	−0.96	0.039	<0.0001	−1.037	−0.879
TAC (mg CE / g dw)	SSPP-TAC	57	0–396	0.966	22.18	3.60	−0.98	0.025	<0.0001	−1.033	−0.934
AA (% scavenging)	SSPP-AA	55	24.9–98.7	0.913	6.41	3.09	−0.96	0.040	<0.0001	−1.037	−0.876
Dependent variable		**Validation**									
		Nr samples	*Range*	*R^2val*	*RSMEval*	*RPDval*					
TPC (mg CE / g dw)	SSPP-PVP	28	71–886	0.890	82.16	2.90					
TAC (mg CE / g dw)	SSPP-TAC	28	2–426	0.974	20.59	3.72					
AA (% scavenging)	SSPP-AA	28	11.7–97.6	0.877	8.06	3.11					

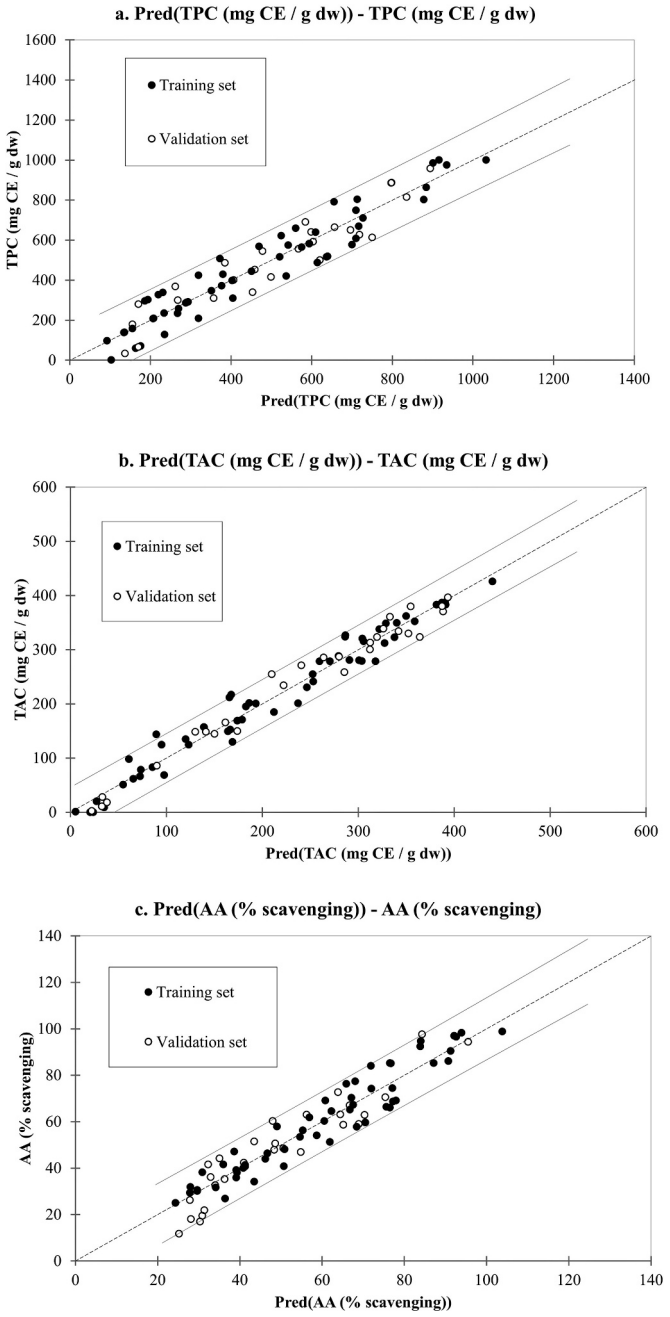

Fig. 1. Linear regression plots between predicted and observed values of TPC (a), TAC (b) and AA (c).

a high predictive capacity compared to traditional applications (Cozzolino, 2022; Cozzolino, Cynkar, Shah, & Smith, 2011; Dos Santos et al., 2023; Liu et al., 2024). The optical solution proposed in this work has advantages in (i) being extremely cost-effective and easily transferable on an industrial scale; (ii) being suited for the supply chain monitoring with minimum sample preparation required and easy, multiparametric processing of instrument data. The optical method showed potential to provide key quality control parameters within acceptable tolerances for industrial applications (with SD < 10 %); on the other hand, the implementation of the dataset can definitely improve the performance of predictive models.

As a further potentiality for implementation, in this work the AA of the extracts was evaluated according to the radical scavenging capacity: nevertheless, the polyphenolic compounds exert their antioxidant capacity through different mechanisms, which were extensively reported

Table 3
Stability of the SSPP-BSA / TAC st experiments over 5 and 10 min incubation times.

Measured TAC - mg/L CE	SSPP-BSA 5 min - LI	SSPP-BSA 10 min - LI
55	20,430 ± 160	20,416 ± 29
327	16,933 ± 86	16,925 ± 17
456	15,363 ± 54	16,001 ± 88
542	14,094 ± 94	14,979 ± 263
560	13,763 ± 38	14,286 ± 301
578	13,613 ± 98	14,302 ± 247
614	13,001 ± 11	13,823 ± 125
685	12,254 ± 18	13,027 ± 352
828	10,398 ± 49	12,987 ± 360
972	8065 ± 68	10,197 ± 262
1115	6390 ± 288	8182 ± 327
1186	5996 ± 19	11,942 ± 168
1330	3399 ± 156	12,897 ± 431
1400	2582 ± 6	9223 ± 109
Linear R^2 adj.	**0.987**	**0.692**

(Fracassetti et al., 2023; Fracassetti, Messina, et al., 2023; Paissoni et al., 2022a). In this regard, future comprehensive studies on the suitability of SSPP in the AA prediction are envisaged.

4. Conclusion

In this work, the potentialities of the SSPP method were explored for the quantitative and functional characterization of botanical extracts for enological use, including a large selection of ellagic and condensed industrial extracts to improve representativity of the dataset. The optical method based on SSPP showed valuable performances for the prediction of selected parameters through simple linear régressions. The highest R^2 value (0.966, RMSE of 22.18 mg CE / g dw of the extract), along with stability of the optical response over 5 min incubation, was observed in the prediction of TAC using the BSA as targeted reagent for the complexation of tannins and turbidity development. The SSPP-PVP failed to provide robust optical measurements over time, but showed potentialities to predict both the TPC and AA of the extracts when the optical measurements were performed immediately after preparing the reaction mixture; further experiments will be mandatory to improve stability of the PVP-polyphenol complexes, and therefore the SSPP signal associated with turbidity development. This work complements previous studies by the Authors and supports the technological advancement of the patented method (Patent nr.102019000002585); the SSPP-related optical method was confirmed as a valid tool for quality control related to the oenological tannins production.

5. Metadata

Metadata will be made available and searchable on AMS Acta repository (https://amsacta.unibo.it/) by recording the DOI of the article soon after publishing.

CRediT authorship contribution statement

Arianna Ricci: Writing – original draft, Validation, Project administration, Methodology, Formal analysis, Conceptualization. **Eleonora Iaccheri:** Writing – review & editing, Validation, Data curation, Conceptualization. **Giuseppina Paola Parpinello:** Writing – review & editing, Methodology, Data curation, Conceptualization. **Luigi Ragni:** Writing – review & editing, Validation, Supervision, Project administration, Methodology. **Matteo Bosaro:** Writing – review & editing, Visualization, Investigation. **Andrea Versari:** Writing – review & editing, Supervision, Methodology, Conceptualization.

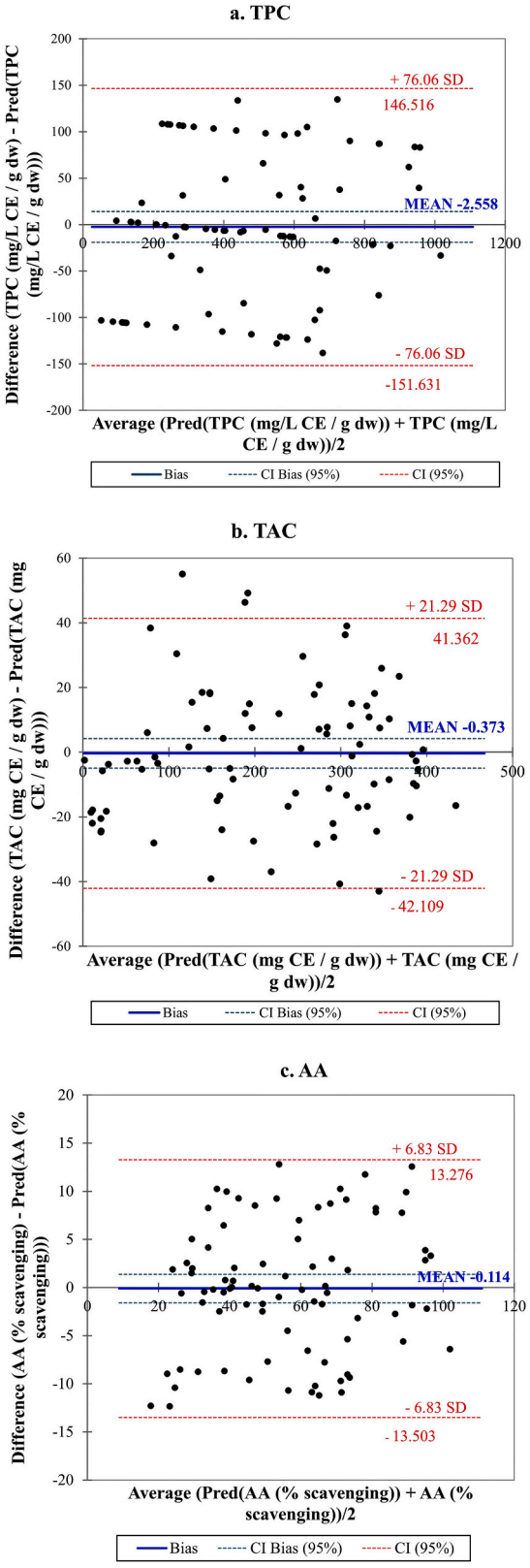

Fig. 2. Bland-Altman validation between the PLS predicted values and the observed values of TPC (a), TAC (b) and AA (c). X-axes report the mean of predicted and observed values; Y-axes denote the difference between predicted and observed values; dotted blue lines: zero bias; solid blue lines: overall bias; dotted red lines: LOA. The middle areas indicate their 95 % confidence intervals. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Declaration of competing interest

The authors declare the following which may be considered as potential competing interests: authors AR, GPP, LR, EI and AV are listed as inventors in the Patent n. 1020190000002585 holded by the University of Bologna (IT). Author MB has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodres.2025.116562.

Data availability

Metadata will be made available and searchable on AMS Acta repository (https://amsacta.unibo.it/) by recording the DOI of the article soon after publishing.

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Supplementary Material 1

Samples list and description: botanical extract used in the experiment.

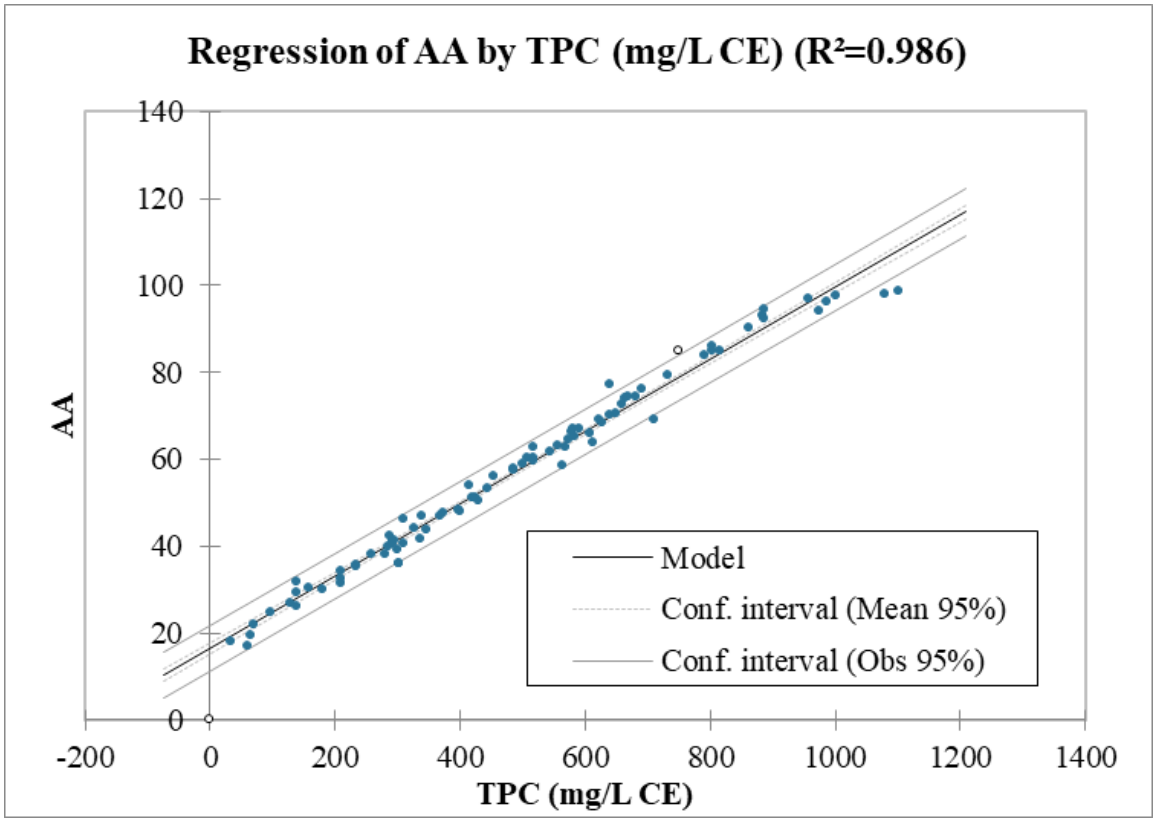
E = ellagitannin; Proc/prod = procyanidin/prodelphinidin; Prof/pror = profisetinidin/ prorobinetidin, according to OIV classification (OIV, 2024).

Sample code	**Botanical source**	**Classification**
TanCond1	Mimosa	Prof/pror
TanCond2	Mimosa	Prof/pror
TanCond3	Grape seed	Proc/prod
TanCond4	Grape pomace	Proc/prod
TanCond5	Mimosa	Prof/pror
TanCond6	Grape seed	Proc/prod
TanCond7	Green tea	Proc/prod
TanCond8	Grape pomace	Proc/prod
TanCond9	Quebracho	Prof/pror
TanCond10	Grape pomace	Proc/prod
TanCond11	Grape seed	Proc/prod
TanCond12	Grape pomace	Proc/prod
TanCond13	Quebracho	Prof/pror
TanCond14	Quebracho	Prof/pror
TanCond15	Green tea	Proc/prod
TanCond16	Grape seed	Proc/prod
TanCond17	Grape pomace	Proc/prod
TanCond18	Mimosa	Prof/pror
TanCond19	Mimosa	Prof/pror
TanCond20	Green tea	Proc/prod
TanCond21	Green tea	Proc/prod
TanCond22	Green coffee	Proc/prod
TanCond23	Grape seed	Proc/prod
TanCond24	Grape pomace	Proc/prod
TanCond25	Grape seed	Proc/prod
TanCond26	Cherry wood	Proc/prod
TanCond27	Acacia	Prof/pror
TanCond28	Grape seed	Proc/prod
TanCond29	Green tea	Proc/prod
TanCond30	Green tea	Proc/prod
TanCond31	Grape pomace	Proc/prod
TanCond32	Grape seed	Proc/prod
TanCond33	Grape pomace	Proc/prod
TanCond34	Quebracho	Prof/pror
TanCond35	Cherry wood	Proc/prod
TanCond36	Bamboo	Proc/prod
TanCond37	Grape pomace	Proc/prod
TanCond38	Grape seed	Proc/prod
TanCond39	Grape seed	Proc/prod
TanCond40	Grape seed	Proc/prod
TanCond41	Grape seed	Proc/prod

TanCond42	Grape seed	Proc/prod
TanEl1	Chestnut	Ell
TanEl2	Lemon wood	Ell
TanEl3	Oak	Ell
TanEl4	Pine bark	Ell
TanEl5	American oak	Ell
TanEl6	Chestnut	Ell
TanEl7	French oak petraea	Ell
TanEl8	Oak	Ell
TanEl9	American oak	Ell
TanEl10	Oak	Ell
TanEl11	French oak robur	Ell
TanEl12	Oak	Ell
TanEl13	Chestnut	Ell
TanEl14	Oak	Ell
TanEl15	French oak robur	Ell
TanEl16	French oak robur	Ell
TanEl17	French oak robur	Ell
TanEl18	French oak robur	Ell
TanEl19	French oak robur	Ell
TanEl20	French oak robur	Ell
TanEl21	American oak	Ell
TanEl22	French oak robur	Ell
TanEl23	French oak petraea	Ell
TanEl24	French oak robur	Ell
TanEl25	French oak robur	Ell
TanEl26	French oak petraea	Ell
TanEl27	French oak robur	Ell
TanEl28	American oak	Ell
TanEl29	American oak	Ell
TanEl30	French oak robur	Ell
TanEl31	French oak robur	Ell
TanEl32	Mixed oaks (*robur*, *petraea alba*)	Ell
TanEl33	Oak	Ell
TanEl34	Oak	Ell
TanEl35	Unstoasted oak	Ell
TanEl36	Unstoasted oak	Ell
TanEl37	Chestnut	Ell
TanEl38	Chestnut	Ell
TanEl39	Chestnut	Ell
TanEl40	Chestnut	Ell
TanEl41	Chestnut	Ell
TanEl42	Chestnut	Ell
TanEl43	French oak	Ell
TanEl44	French oak	Ell

Supplementary Material SM2.

Regression and model parameters for the prediction of AA by the measured TPC of the extracts



Equation coefficients	Estimate	St. error	p-value	95% lower limit	95% upper limit
x (TPC)	0.083	0.001	< 0.0001	0.081	0.085
intercept	16.483	0.607	< 0.0001	15.276	17689