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REGULAR ARTICLE

Estimation of antioxidant activity of different mixed herbal infusions using attenuated total reflectance Fourier transform infrared spectroscopy and chemometrics

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ABSTRACT

Antioxidant activity of 19 different mixed herbal infusion as it was calculated by 2,2-diphenyl-1-picrylhydrazyl (DPPH) and 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) assays was correlated using attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) and chemometrics. The spectral region 1538- 843 cm^{-1} in 2^{nd} derivative mode and the partial least squares (PLS) regression were used. The correlation coefficient, the root-mean-square error of calibration (RMSEC) and the root-mean-square error of prediction (RMSEP) for the DPPH assay were 0.97, 130 and 118 respectively. The corresponding values for the ABTS assay were 0.99, 148 and 121. The above results show that it is possible to estimate the antioxidant activity according to DPPH and ABTS assays of different mixed herbal infusions using ATR-FTIR spectroscopy. Furthermore the proposed methods are simple, rapid and economical.

Keywords: Antioxidant activity; ATR-FTIR; Chemometrics; Herbal infusions; PLS

INTRODUCTION

Free radicals are products of oxygen and nitrogen that come from the metabolic paths. The excessive amount of these free radicals is the cause of chronic diseases in human (Dhar et al., 2012; Aktumsek et al., 2013). Antioxidants in food play an important role for human's health since the scientific community has proven that they can reduce the risk of chronic diseases such as cancer, heart disease and Alzhemier's disease (Aktumsek et al., 2013; Rautiainen et al., 2013; Saeidnia and Abdollahi, 2013). Phenolic compounds are responsible for the antioxidant activity and the main sources of them are fruit, vegetables, legumes, fats/oils and herbal infusion (Dhar et al., 2012; Reutenbach and Venter, 2013; Lou et al., 2014). The last years it has been found that the consumption of herbal infusions made of a great variety of herbs such as oregano, sage, rosemary etc., can be very helpful for someone's health as far as the antioxidant intake is concerned (Atoui et al., 2005; Boskou 2006; Pincemail et al., 2012).

There are many assays for the determination of antioxidant activity. The 2,2-diphenyl-1-picrylhydrazyl (DPPH) (Brand-Williams and others 1995) and 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) methods (Re et al.,1999) were used widely.

Fourier transform infrared spectroscopy (FTIRS) is recognized as a very good analytical tool when it combined with various statistical methods (Fagan et al., 2007; Karoui et al., 2010; Khanmohammadi and Garmarudi, 2011; Ferreira et al., 2014). In recent years more publications are referenced in the statistical analysis of infrared Fourier transform (FT-IR) spectroscopic data for the study of herbs (Fu et al., 2013; Lee et al., 2014; Mncwangi et al., 2014). In recent years the near infrared spectroscopy (NIRS) was employed with linear

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and nonlinear regressions tools for the determination of antioxidant activity in green tea (Chen Q et al., 2012), in bamboo leaf extract (Wu et al., 2012), and in *Salvia miltiorrhiza* (Duan et al., 2014). Mid infrared spectroscopy (MIRS) in combination with multivariate analysis tools has recently been used for the study of antioxidant activity in propolis (Mot et al., 2011), in phosphorylated chitosan (Subhapradha et al., 2013), in sulphated polysaccharides (Li and Shah, 2014), in tea polysaccharides (Zhao et al., 2014), and in extracts from edible mushrooms (Ren et al., 2014).

The attenuated total reflectance (ATR)-FTIR spectroscopy is an interesting technique that is increasingly used in recent years (Karoui et al., 2010; Wang and Rodriguez-Saona, 2012; Helmdach et al., 2013; Cozzolino et al., 2014). The above spectroscopic technique combined with multivariate analysis was used for the determination of the total antioxidant capacity of red wine samples (Versari et al., 2009).

The aim of this work is to develop an alternative methodology for the antioxidant activity estimation, according to DPPH and ABTS assays, of various herbal infusions for routine analysis. The proposed methods combine the ATR-FTIR and the partial least squares (PLS) regression. The proposed methods are simple, fast and economical.

MATERIALS AND METHODS

Materials

For mixed herbal infusions we used the following: Seven commercial products of mixed herbals such as rosemary-thyme (of biological and conventional cultivation), sage-lemon verbena, cinnamon-clove, honey-orange, green tea-ginger-licorice, black tea-lemon-spearmint and seven non-mixed commercial products of spearmint, sage, lemon verbena and plant material of black tea from Trapezounta (Turkey, 2013 yield), oregano from Kalamata (Greece, 2013 yield), rosemary from Olympic village-Athens (Greece, 2013 yield) and thyme from Agrinio (Greece, 2013 yield). Furthermore a set of five samples which were prepared by mixing the above samples. A total of 19 samples were studied.

For DPPH assay: DPPH Sigma Aldrich, ethanol 99.8 % Merck.

For the ABTS assay: ABTS Sigma Aldrich, $K_2S_2O_8$ Sigma Aldrich.

Trolox Sigma Aldrich.

Determination of the antioxidant activity using the DPPH and ABTS assays

Mixed herbal infusions were prepared by adding 2 g of each mixed herbal samples in 200 mL (about 1 cup) deionized hot water (85°C) and steeped for five minutes. The herbal infusions were then filtered through a Whatman filter No. 1. Prior to analysis, an aliquot was further filtrated with a polytetrafluoroethylene filter with 0.45 μm pore size. Then, the infusions were examined for their antioxidant activity with the methods of DPPH (Brand-Williams et al., 1995) and ABTS (Re et al., 1999). The antioxidant activity of each sample was expressed in μmol/mL of Trolox. The measured Trolox values will be called actual values.

FT-IR spectroscopy

FT-IR spectra of the 19 samples were obtained in ATR mode using a standard ZnSe 45^0 flat plate against a ZnSe background on a Nicolet 6700 FT-IR (Thermo Electron Corporation) spectrometer (Deuterated TriGlycine Sulfate detector; Nichrome source; KBr beamsplitter), with a total of 100 scans (resolution, 4 cm^{-1}). A sample of 750 μL was added from every herbal infusion in ZnSe plates. The samples were left to dry for approximately an hour and a half in the oven in 40°C. Every spectrum was smoothed using the Savitsky–Golay algorithm (5-point moving, second-degree polynomial). Then the baseline was corrected (second-degree polynomial, 20 iterations). The OMNIC 7.3 (Thermo Fisher Scientific Inc.) software, that accompanies the spectrophotometer, was used for the previous functions.

Chemometrics

Two PLS models were developed using the TQ analyst software (version 8.0.0.245; Thermo Fisher Scientific Inc.) The first PLS model relating the estimation of antioxidant activity in accordance with DPPH assay and the second to ABTS assay. For this purpose the spectral region 1538-843 cm^{-1} in 2^{nd} derivative mode and the actual Trolox values, according to DPPH and ABTS assays, were used. The actual Trolox values and the corresponding spectra were entered in TQ analyst software to develop the PLS models. The 19 samples were split into two sets randomly by the software (Chen Y et al., 2012). The first set of 14 samples was used for the calibration of the PLS model and the second of five samples for the validation of the model. Two linear calibrations model were built as follows. The PLS model correlated the actual Trolox values with the corresponding spectral data and it calculated the new Trolox values (calculated values). The first PLS model concerns the Trolox values according to the DPPH assay, and the second to the ABTS assay. The optimum number of PLS factors was determined by the leave-one-out cross-validation procedure. Three factors were used for DPPH-PLS model and six for ABTS. The existence of outliers

was examined in calibrations data according to Chauvenet test and Leverage diagnostic on basis of spectral or Trolox actual values difference. The correlation coefficient (R^2), root-mean-square error of validation (RMSECV), and root-mean-square error of prediction (RMSEP) for each PLS model were calculated.

RESULTS AND DISCUSSION

Antioxidant activity according to DPPH and ABTS assays

The antioxidant activity of the 19 herbal infusions was determined using the DPPH and ABTS assays (Tables 1 and 2). The values, called actual, were ranged between 2470 (oregano) – 580 (cinnamon-clove) μmol/mL of Trolox for the DPPH assay and 4680 (oregano) – 200 (thyme) μmol/mL of Trolox for the ABTS assay.

Spectroscopic analysis

Typical ATR-FTIR spectra of some herbal infusions are shown in Fig. 1. The peaks at 3400-3100 cm^{-1} correspond to –OH bond (Boeriu et al., 2004), 2970-2900 cm^{-1} to the C-H stretching (Boeriu et al., 2004), 1740-1720 cm^{-1} to C=O stretching (Boeriu et al., 2004), 1620-1590 cm^{-1} to the aromatic C=C stretching (Lu et al., 2011), 1410-1390 cm^{-1} mainly to $–CH_3$ asymmetric deformation (Lu et al., 2011), 1270-1220 cm^{-1} to the C-O stretching of glycosides (Liu et al., 2012). Finally the peak at 1000-1300 cm^{-1} correspond to the combination of C-OH hydrogen bond with C-OH oligosaccharides and C-O stretching coupled with C-O bending of C-OH of carbohydrates (Lu et al., 2011).

The antioxidant activity has been correlated with the presence of various phenolic compounds linked, or not, with sugars (Boskou, 2006; Kamiloglu et al., 2014; Vallverdu-Quevalt et al., 2014). The above compounds mainly absorb in the 1600-800 cm^{-1} spectral region. The spectra in this spectral region are very similar. So the 1538-843 cm^{-1} spectral region in 2nd derivative mode has been selected (Ritthiruandej et al., 2011).

Chemometrics

TQ analyst software is a commercial package for multivariate analysis particularly user friendly. In the last years many works have been published describing PLS models using the TQ analyst software and the ATR spectroscopy (Kandhro et al., 2013; Jawaid et al., 2013; Kaya-Celiker et al., 2014; Silva et al., 2014; Talpur et al., 2014).

For the developing of the PLS models the actual values of Trolox and the corresponding ATR-FTIR spectra were combined using the TQ analyst software. Then the 1538-843 cm^{-1} spectral region in 2nd derivative mode was chosen.

The software divided the samples in two sets automatically (Shen et al., 2011; Chen Y et al., 2012). A set of 14 samples was used for the calibration and another of five samples for the validation.

The statistical approach followed in this work is based on the linear combination of spectroscopic variables, so-called factors. A factor is a set of components that contains

Table 1: Antioxidant activity and the recovery of the different mixed herbal infusions with the DPPH assay (actual values) and with the proposed PLS – ATR-FTIR method (calculated values)

Mixed herbal infusions	Actual value (μmol Trolox/mL)	Calculated value (μmol Trolox/mL)	Recovery (%)
Bio rosemary-thyme	1490	1351	90.7
Rosemary-thyme	1280	1361	106.3
Cinnamon-clove	580	586	101.0
Sage-lemon verbena	1670	1738	104.1
Honey-orange	790	769	97.3
Green tea-ginger-licorice	2170	2470	113.8
Black tea-lemon-spearmint	2040	1868	91.6
Spearmint	1100	1156	105.1
Thyme	2180	2119	97.2
Sage	1680	1667	99.2
Rosemary	630	644	102.2
Lemon verbena	1590	1547	97.3
Black tea	820	818	99.8
Oregano	2470	2395	97.0
Oregano – black tea	1871	1996	106.7
Rosemary – lemon verbena	1391	1261	90.7
Thyme - sage	2123	2102	99.0
Sage – lemon verbena – honey - orange	1432	1334	93.2
Rosemary – thyme – cinnamon - clove	818	720	88.0

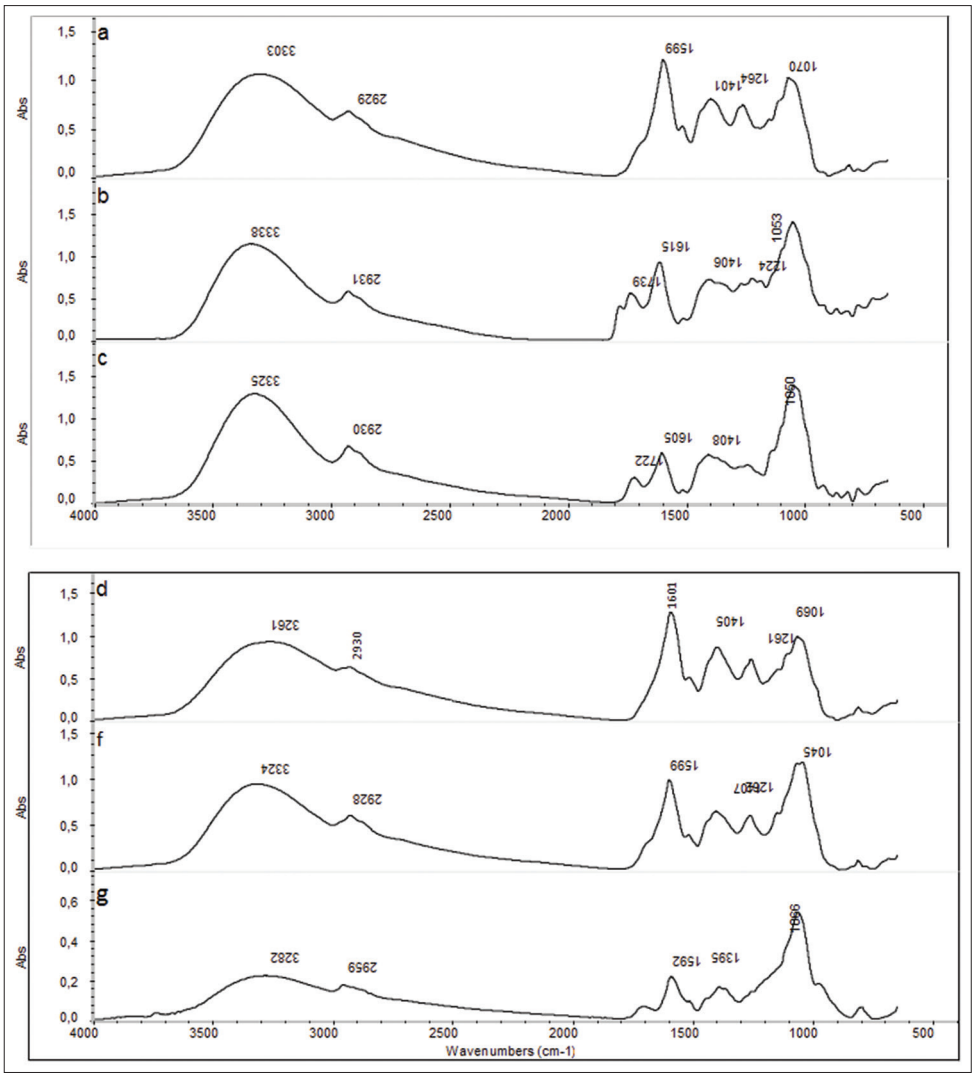

Fig 1. FT-IR spectra of the mixed herbal infusions: a) Sage - lemon verbena, b) cinnamon – clove, c) honey – orange, d) spearmint, f) lemon verbena g) rosemary.

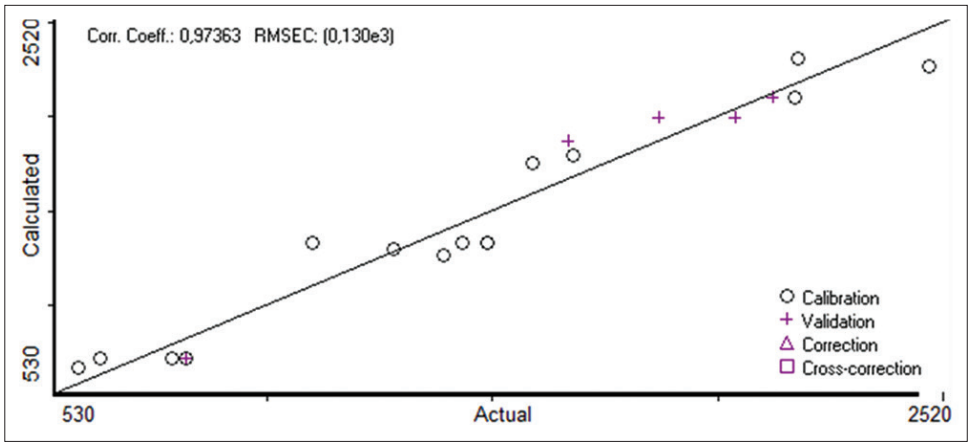

Fig 2. The linear correlation between the antioxidant activity according to the DPPH assay and proposed ATR-FTIR-PLS method. Correlation coefficient and RMSEC are also given.

spectral and actual values of Trolox information and it is used to describe the variation in a PLS method model. The optimum number of the factors was determined using of leave-one-out cross validation by plotting the

number of factors against the root mean square error cross validation (RMSECV) and determining the minimum factors. So for the DPPH determination were used three factors (RMSECV=241.7) (Fig. 2, Table 3) and for ABTS six (RMSECV=753.3) (Fig. 3, Table 3).

Outliers were detected on the basis of spectral or Trolox concentration difference with two widely used methods, Chauvenet test and Leverage diagnostic (Chen Y et al., 2012). Outliers not found.

Calibration evaluation was done using the RMSEC and determination coefficients. The RMSEC correlated with the differences between the actual Trolox values and the corresponding calculated, based on the FTIR spectra, values for the calibration set. The correlation coefficients (R^2) show how close the calculated with the actual values are. So for the DPPH evaluation R^2=0.97 and RMSEC=130 (Fig. 2, Table 3). For the ABTS evaluation the corresponding values were found 0.99 and 148 respectively (Fig. 3, Table 3). These values show a very good linear correlation between the actual and calculated Trolox values for both evaluations. Furthermore the low RMSEC values, compared with the corresponding actual Trolox values, show that the calibration models are very satisfactory.

The RMSEP is associated with the differences between the actual and the predicted values by the model. The RMSEP values were found 118 for the DPPH-PLS model and 121 the corresponding ABTS-PLS (Table 3). The above values are low compared with the corresponding actual Trolox values.

The RMSEC and RMSEP values are closed together on each proposed PLS model. This observation coupled with the low values of RMSEC, RMSEP and the high R^2 show the robustness of the proposed models (Chen Y et al., 2012; Kandhro et al., 2013).

Table 2: Antioxidant activity and the recovery of the different mixed herbal infusions with the ABTS assay (actual values) and with the proposed ATR-FTIR-PLS method (calculated values)

Mixed herbal infusions	Actual value (μmol Trolox/mL)	Calculated value (μmol Trolox/mL)	Recovery (%)
Bio rosemary-thyme	1790	1820	101.7
Rosemary-thyme	1630	1413	86.7
Cinnamon-clove	1110	1161	104.6
Sage-lemon verbena	1880	2038	108.4
Honey-orange	1340	1273	95.0
Green tea-ginger-licorice	1730	1718	99.3
Black tea-lemon-spearmint	3260	2850	87.4
Spearmint	2130	2043	95.9
Thyme	200	231	115.5
Sage	2510	2052	81.8
Rosemary	820	1107	135.0
Lemon verbena	1800	1764	98.0
Black tea	1260	1233	97.9
Oregano	4680	4710	100.6
Oregano – black tea	3181	2850	89.6
Rosemary – lemon verbena	1794	1358	75.7
Thyme - sage	1317	1519	115.3
Sage – lemon verbena – honey - orange	2112	2052	97.2
Rosemary – thyme - cinnamon - clove	1235	1251	101.3

Table 3: The PLS regression results of the proposed FTIR models for the estimation of the antioxidant activity according to DPPH, ABTS assays using the 1538-843 cm^{-1} spectral region in 2nd derivative mode

Proposed method	R^2	RMSECV	Factors	RMSEC	RMSEP
DPPH estimation	0.97	241.7	3	130	118
ABTS estimation	0.99	753.3	6	148	121

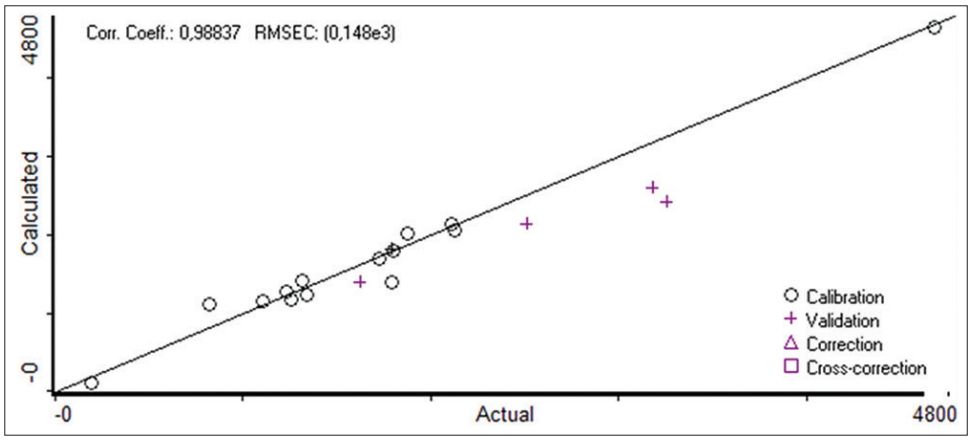

Fig 3. The linear correlation between the antioxidant activity according to the ABTS assay and proposed ATR-FTIR-PLS method. Correlation coefficient and RMSEC are also given.

The Trolox values for the DPPH assay as they were calculated by the proposed ATR-FTIR-PLS method fluctuated from 2470 (green tea-ginger-licorice) to 586 (cinnamon-clove) μmol/mL (Table 1). For the ABTS assay the calculated Trolox values were ranged between 4710 (oregano) and 231 (thyme) μmol/mL (Table 2).

The recovery was calculated and its value was oscillated between 88.0 and 113.8 % for the DPPH assay (Table 1). Each recovery value is between 80 and 120%, which are the generally accepted limits. In case of ABTS assay (Table 2), only two values are outside the generally accepted limits. Hence the variability of the recovery value is considered satisfactory.

CONCLUSION

In this work two ATR-FTIR-PLS methods are proposed for the estimation of the antioxidant activity in different herbal infusions according to DPPH and ABTS. The proposed models are based on the ATR-FTIR spectroscopy. The spectral region 1538-843 cm^{-1} in 2^{nd} derivative mode and the PLS regression were used. The R^2, RMSEC RMSEP and recovery values show that the proposed methods can be applied in routine analysis for the estimation of the antioxidant activity. In addition the proposed methods are simple, non time-consuming and economical.

Author's contributions

All authors contributed equally in this article.

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