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The application of continuous wavelet transform and least squares support vector machine for the simultaneous quantitative spectrophotometric determination of Myricetin, Kaempferol and Quercetin as flavonoids in pharmaceutical plants

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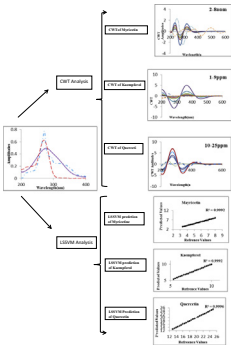
HIGHLIGHTS

- We examined simultaneous determination of Myricetin, Kaempferol and Quercetin of some pharmaceutical plants.
- We coupled UV spectroscopy with two signal processing methods of CWT and LS-SVM.
- CWT and LS-SVM methods are fast and low cost methods.
- We can determinate Myricetin, Kaempferol and Quercetin simultaneously without separating them.

GRAPHICAL ABSTRACT



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ABSTRACT

Flavonoids are γ-benzopyrone derivatives, which are highly regarded in these researchers for their antioxidant property. In this study, two new signals processing methods been coupled with UV spectroscopy for spectral resolution and simultaneous quantitative determination of Myricetin, Kaempferol and Quercetin as flavonoids in Laurel, St. John's Wort and Green Tea without the need for any previous separation procedure. The developed methods are continuous wavelet transform (CWT) and least squares support vector machine (LS-SVM) methods integrated with UV spectroscopy individually. Different wavelet families were tested by CWT method and finally the Daubechies wavelet family (Db4) for Myricetin and the Gaussian wavelet families for Kaempferol (Gaus3) and Quercetin (Gaus7) were selected and applied for simultaneous analysis under the optimal conditions. The LS-SVM was applied to build the flavonoids prediction model based on absorption spectra. The root mean square errors for prediction (RMSEP) of Myricetin, Kaempferol and Quercetin were 0.0552, 0.0275 and 0.0374, respectively. The developed methods were validated by the analysis of the various synthetic mixtures associated with a well- known flavonoid contents. Mean recovery values of Myricetin, Kaempferol and Quercetin, in CWT method were 100.123, 100.253, 100.439 and in LS-SVM method were 99.94, 99.81 and 99.682, respectively. The results achieved by analyzing the real samples from the CWT and LS-SVM methods were compared to the HPLC reference method and the results were very close to the reference method. Meanwhile, the obtained results of the one-way ANOVA (analysis of variance) test revealed that there was no significant difference between the suggested methods.

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1. Introduction

Flavonoids represent a group of naturally occurring polyphenoic compounds existed as pigment in various fruits, vegetables and pharmaceutical plants [1]. Their basic structure contains a phenol ring in the 2-phenyl-benzopyrone structure [2]. Based on the degree of oxidation of the central pyrene ring, flavonoids can be subdivided into six classes: flavones, flavanones, isoflavones, flavonols, flavanols and anthocynanins [3,4].

An increasing number of flavonoids have attracted much attention in relation to their biological activities, including anti-viral, anti-oxidant, anti-bacterial, anti-cancer and vasodilatory, anti-diabetic activities [1–6]. Nevertheless, the application of the flavonoids as drugs is yet in the investigation process [5].

The main role of these compounds as antioxidant is the ability to reduce active oxygen species and inhibit in vitro oxidation of low-density lipoproteins in turn reduces their thrombotic tendency. The total amount of flavonoids is an important index which reflects quality and medicinal value of traditional medicines [4,6]. In this study, Myricetin, Kaempferol and Quercetin are used as flavonoids, which possess anti-mutagenic and anti-oxidant effects in vitro and vivo. The chemical name of Myricetin is 3,5,7-trihy droxy-2-(3,4,5-trihydroxyphenyl)-4-chromenone. Similarly the chemical name of Kaempferol 3,5,7-trihydroxy-2-(4-hydroxyphen yl)-4*H*-chromen-4-one and the chemical name for Quercetin is 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4*H*-chromen-4-one. Chemical structures of the proposed flavonoids are shown in Fig. 1.

Analytical methods been reported for simultaneous quantitative determination of such flavonoids that included capillary electrophoresis method [7], gas chromatography analysis [8] and high-performance liquid chromatography (HPLC) [9]. However, all of these methods, particularly those involving chromatography, are generally time-consuming because they are usually include the extraction steps, need highly pure solvents that are commonly environmental contaminants and in some cases require rather expensive complicated analytical equipment. Hence, original, relatively naive and inexpensive analytical methods for the simultaneous determination of flavonoids such as Myricetin, Kaempferol and Quercetin would be effective[5–11]. The extension of such simpler methods is often facilitated by using Chemometric methods as an essential and powerful tool for data mining which can be used successfully for the discrimination between similar structural substances [12].

Recently, Chemometric methods are rapidly developed and widely applied in different fields of chemistry, especially analytical chemistry. De-noising, compression and variable reduction are major application areas of these methods in analytical chemistry.

A novel Chemometric technique known as wavelet transform (WT) has been coupled with the Fourier transform as a data-processing method in analytical chemistry [13,14].

Continuous wavelet transform is an application of wavelet analysis, which is an ideal method for the spectral resolution and prediction of multi-mixtures in the presence of original overlapping signals [15]. This approach provides an accurate, precise, rapid and low cost analysis which is used for the quality control and routine analysis of the commercial products in laboratories [16]. Lately, CWT and zero-crossing technique have been coupled with a mathematical model for increasing the spectra resolution of multi-component mixtures [15–22].

Another approach for Chemometrics is support vector machine, which introduced as a powerful tool to address classification and function regression problems [23]. Vapnik developed SVM for classification and nonlinear function estimation [24]. The SVM method is based on the statistical learning theory and structural risk minimization. Therefore, it has been shown to be superior to the traditional empirical risk minimization principle used by conventional neural networks [25,26].

Suykens and coworkers introduced a modified version of the SVM called least squares support vector machine [27]. A set of linear equations is required to be solved during the training of LS-SVM and the complexity of calculation is decreased much [28–30]. Due to the choice of quadratic function, LS-SVM loses more sparseness for empirical risk in comparison to SVM. Therefore, a trained LS-SVM can increase the computation load of decision function especially for large scales problems [31]. Recently, the LS-SVM method has been coupled with the spectral analysis as a rapid and non-destructive method for simultaneous quantitative analysis of multicomponent mixtures [27–32]

In order to existence strong overlapping among the absorption spectra of Myricetin, Kaempferol and Quercetin, the UV spectroscopy cannot be applied for simultaneous determination of them alone. Thus, Chemometric methods can be integrated with UV spectroscopy methods [11].

In this work, two Chemometrics methods CWT and LS-SVM techniques can be combined for the purpose of simultaneous spectrophotometric determination of Myricetin, Kaempferol and

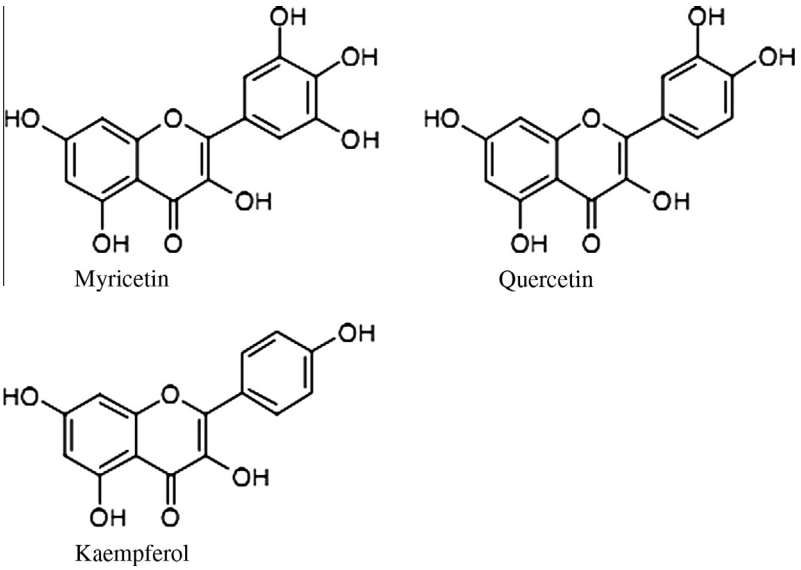

Fig. 1. Chemical structure of Myricetin, Kaempferol and Quercetin.

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