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Use of continuous wavelet transform approach for simultaneous quantitative determination of multicomponent mixture by UV–Vis spectrophotometry

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ABSTRACT

In the present paper, a multicomponent analysis approach based on spectrophotometry method was developed for simultaneous determination of Guaifenesin (GU), Chlorpheniramine (CHL) and Pseudoephedrine (PSE) without any separation steps. The method under study is signal processing method based on Continuous Wavelet Transform (CWT) coupled with zero cross point technique. In this paper, CWT method was tested by synthetic ternary mixtures and was applied to the commercial cough syrup as a real sample and assessed by applying the standard addition technique. For demonstrate the accuracy of the results, other applications of signal processing, such as Derivative Transform (DT), Partial Least Squares (PLS) regression and Principal Components Regression (PCR) were used as comparative methods. Afterwards, the obtained results from analyzing the cough syrup by all methods were compared to the High-Performance Liquid Chromatography (HPLC) as a reference method. One-way analysis of variance test at 95% confidence level showed no significant differences between CWT and other applications.

1. Introduction

Cough can be caused by air pollution, smoking, allergic and etc. Cough medicines are used for relieve of cough. They are made up of one or more pharmaceutical active drugs. Cough preparations consist of antihistamines, antitussives, decongestants, expectorants and sleep aids. In the recent years, combination dosage forms of Guaifenesin (GU), Chlorpheniramine maleate (CHL) and Pseudoephedrine hydrochloride (PSE) as an agent to cure of cough is introduced. Guaifenesin or [R, S-3-(2-methoxyphenoxy) propane-1, 2-diol] used as an expectorant for treatment of cough. It is reported to increasing the volume and reducing the viscosity of phlegm [1]. Chlorpheniramine maleate or [3-(4-chlorophenyl)-*N*, *N*-dimethyl-3-pyridin-2-yl-propan-1-amine maleate] is an alkylamine antihistamine that used for the treatment of allergic or common cold [2,3]. Pseudoephedrine hydrochloride or [S, S-2-methylamino-1-phenylpropan-1-ol hydrochloride] may show effectiveness as an antitussive drug [4] and is used for the symptomatic sedation of nasal decongestant [5]. Chemical structures of guaifenesin, chlorpheniramine maleate and pseudoephedrine hydrochloride have shown in Fig.1.

Many methods have been reported in the literature for the measurement of GU, CHL and PSE with or without other compounds used in cough and cold medicines. These methods include High-Performance Liquid Chromatography (HPLC) [6–8], high-performance thin layer chromatography [9], micellar liquid chromatography [10], liquid chromatography-tandem mass spectrometry [11,12], non-aqueous capillary electrophoresis [13] and liquid chromatography-mass-mass spectrometry [14]. Since these methods need a separation step before analysis thus, these methods are time-consuming, destructive and expensive. In addition, these methods used very pure solvents which are environmental pollutants.

On the other hand, Ultra Violet (UV) spectrophotometry method is simple, rapid, nondestructive and inexpensive, but the spectral overlapping in multicomponent chemical mixtures is a limiting factor for it. In the past years, simultaneous quantitative determination of multicomponent chemical mixtures by UV spectrophotometry method has been significantly improved by the use of variety of methods. One of these is signal processing methods. These methods have advantages, such as rapidity, simplicity, accessibility to most laboratories, no preliminary sample preparation, enhanced specificity and sensitivity in mixture analysis. They can also be used for increasing spectra resolution and improvement of Signal to Noise (S/N) ratio.

Various signal processing methods have been used for the measurement of each above component with other drugs. These methods include net analyte signal [15], ratio derivative spectrophotometry [16], discrete wavelet transform-partial least squares [17], principal

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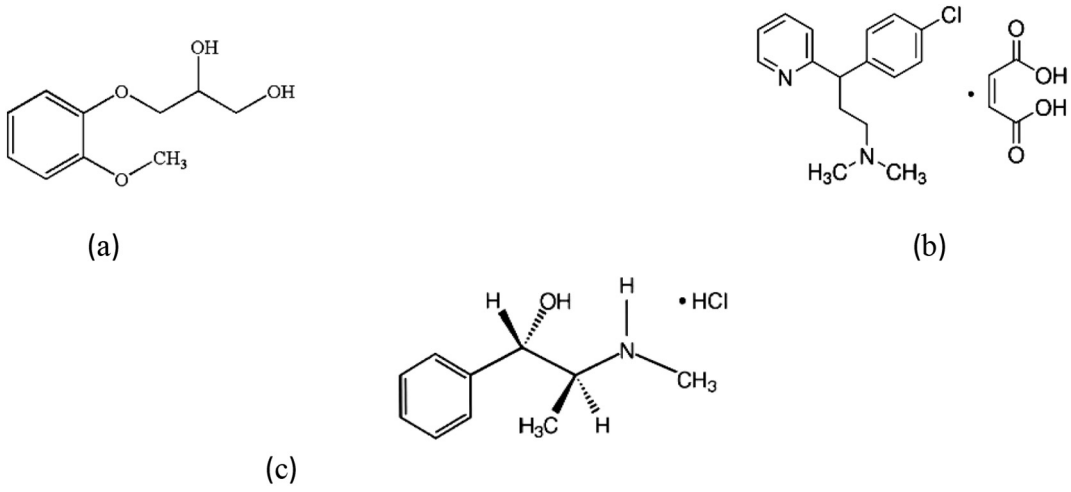

Fig. 1. Chemical structures of (a) guaifenesin, (b) chlorpheniramine maleate and (c) pseudoephedrine hydrochloride.

component analysis-artificial neural networks [18] and least squares support vector machine [19].

In this paper, signal processing method based on Continuous Wavelet Transform (CWT) coupled with zero cross point technique was used for simultaneous quantitative determination of GU, CHL and PSE by spectrophotometry method for the first time. Afterwards, other signal processing methods, such as Derivative Transform (DT), Partial Least Squares (PLS) regression and Principal Components Regression (PCR) were used as comparative methods. The all signal processing methods were validated by synthetic ternary mixtures and assessed by commercial cough syrup as a real sample.

Comparison of the results by one-way Analysis of variance (ANOVA) test between all signal processing methods and HPLC as a reference method shows good agreement between HPLC and signal processing methods especially the application of CWT. Consequently, this method (CWT) is suitable for quality control laboratories.

2. Continuous Wavelet Transform

Wavelet Transform (WT) is a theory based on signal processing and developed from the Fourier transform. The WT is a powerful tool that used in analytical chemistry to resolve spectra, signal de-noising [20], higher separation efficiency in sharpened peaks, signal compression and processing, elimination of background or matrix interference, enhancement of sensitivity and specificity in mixtures analysis [21], time and labor saving and carry out the simultaneous quantitative determination [22]. WT's inclusive of calculation coefficients, which are internal products of the signal and a wavelet family. The WT function is known as mother wavelet and is used to produce all basis functions [23,24]. Eq. (1) describes this function as:

$$\psi b,a\,(t) = \frac{1}{\sqrt{a}}\,\psi\left(\frac{t-b}{a}\right)\begin{cases} a, b\in R \\ a\neq 0 \end{cases} \tag{1}$$

where "a" and "b" are the dilation (scale) and translation parameters, respectively. And "R" is the domain of real numbers. WT have many different methods. One of these is continuous wavelet transform. Eq. (2) describes the continuous wavelet transform function as:

$$\mathrm{CWT}\,(b,a) = C\,(b,a) = \int_{-\infty}^{\infty} f\,(t)\psi^{*}_{b,a}(t)\;\mathrm{dt} \tag{2}$$

Superscript * display that the complex conjugate is used in case of a complex wavelet. At every scale, the signal energy is normalized by dividing the wavelet coefficients by $1/\sqrt{a}$ [25].

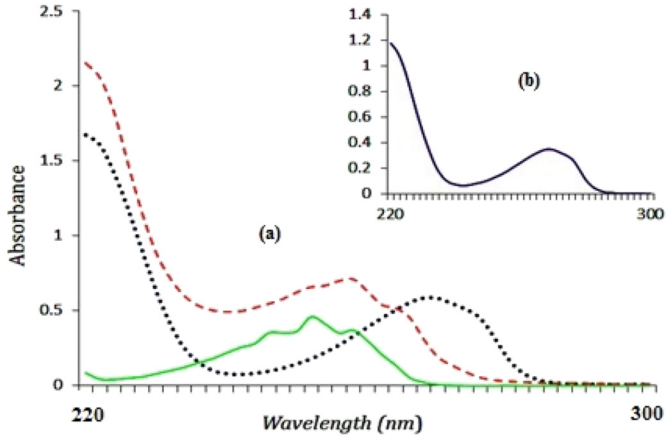

Fig. 2. (a) UV absorption spectra of guaifenesin 50 μg mL^{-1} (....), chlorpheniramine 50 μg mL^{-1} (- - -) and pseudoephedrine 500 μg mL^{-1} (__), and (b) UV absorption spectra of commercial cough syrup as real sample.

3. Experimental

3.1. Apparatus and Software

3.1.1. Spectrophotometry

For spectrophotometry determination, $T90^{+}$ double beam UV–Vis spectrophotometer (PG Instruments), equipped with 1 cm quartz cells was used. The scan range was 220–300 nm with 2 nm intervals and distilled water was used as the blank sample. The spectrophotometry determinations were carried out at room temperature (mean of about 20 °C). Calculations and the signal transforms were accomplished in Excel software and MATLAB 8.6.0 (R2015b) environment.

3.1.2. High-performance Liquid Chromatography

For HPLC method, Agilent (model 1200), equipped with a UV-detector set to 220 nm was used. By using Kromasil C18 column (150 mm × 4.6 mm, 5 μm particle size) and the mobile phase containing 45:55 (*v*/v) methanol/0.1 mol L^{-1} KH_2PO_4 buffer pH = 3 (with