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ORIGINAL ARTICLE

Simultaneous spectrophotometric determination of overlapping spectra of paracetamol and caffeine in laboratory prepared mixtures and pharmaceutical preparations using continuous wavelet and derivative transform

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Abstract In the present paper, two spectrophotometric methods were used for the simultaneous analysis of paracetamol (PCT) and caffeine (CAF) in their laboratory prepared mixtures and pharmaceutical preparations. Simple spectrophotometric analysis of PCT and CAF is not possible due to their complete spectral overlap. The proposed methods are based on the application of continuous wavelet transform (CWT) and derivative transform (using Savitsky–Golay filters) on the ratio spectra to predict each of CAF and PCT. Several wavelet families were tested. Coif1 and Sym2 were found to give best results under optimum conditions. The transformed signals of ratio spectra were used to plot the calibration curves for both components. The predictability of the built calibrations was validated through their application on several synthetic mixtures of both drugs. The proposed methods were used for the prediction of CAF and PCT in pharmaceutical preparation. The obtained results were statistically compared to a reference HPLC method. No significant differences

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were found between the obtained results and those from the reference method. Being simple, rapid, cheap and sensitive, the proposed methods are recommended for the routine daily analysis of these two drugs in their mixtures in quality control laboratories.

1. Introduction

PCT (*N*-(4-hydroxyphenyl)acetamide) usually used in combination with CAF (3,7-dihydro-1,3,7-trimethyl-1*H*-purine-2,6-dione) for the temporary relief of pain and discomfort associated with a number of conditions.

The pharmaceutical mixture of [PCT-CAF] had been analyzed with several techniques including: HPLC (Zhang et al., 2010; Lotfy et al., 2010; Hashem, 2010; Li et al., 2009; Mo et al., 2008; Crevar et al., 2008), gas chromatography (GC) Guo et al., 2010, liquid chromatography- mass spectrometry (LC/MS) (Feng et al., 2009; Di et al., 2008), thin layer chromatography (TLC) Soponar et al., 2009 and voltametric (Sanghavi and Srivastava, 2010; Lourencao et al., 2009). The mixture was also analyzed spectrophotometrically using second derivative zero crossing point (Tavallali and Salami, 2009) and chemometrically by genetic algorithm optimized methods (GCLS and GILS) (Ozdemir et al., 2010), PLS (Mot et al., 2010) and PCR (Mot et al., 2010).

In this paper, two signal processing techniques called derivative spectrophotometry using Savitsky–Golay filters and continuous wavelet transform are proposed for the simultaneous analysis of this drug mixture without need for any preceding extraction procedures or use of a time consuming, expensive instrumental technique like HPLC.

2. Theory

2.1. Savitsky–Golay method

In higher order derivatives, polynomials can be used to approximate spectra. This aims to improve SNR. The polynomial is moved point by point along spectra. Computation is repeated each time, which is time consuming.

Savitsky and Golay (1964) presented an alternative and simplified method of determining the new value of each data point. Where, instead of calculating each time, Savitsky and Golay tabulated polynomial coefficients. The values of the coefficients depend on the number of data points to be approximated, and the order of polynomial function.

To calculate the approximated spectral values, the absorbance data in certain window widths are multiplied by the corresponding coefficients and the sum of multiplications is divided by the normalization constant. According to the polynomial order used, the level of noise removed is determined.

2.2. Wavelet transform

Wavelet transform is a very powerful recent tool in signal processing. It is similar to Fourier transform with the advantage of having many basic functions called wavelets while the basic functions in Fourier transform are the trigonometric functions (sine and cosine). A wavelet transform is the representation of a function by wavelets. A wavelet is defined as a number of scaled and dilated functions $\Psi_{a,b}(\lambda)$ derived from a basic function $\Psi(\lambda)$. Therefore the basic function is often called a mother wavelet since it gives birth to a family of wavelets.

$$\psi_{a,b} = \frac{1}{\sqrt{|a|}}\psi\left(\frac{\lambda - b}{a}\right), \quad a \neq 0 \quad a, b, \in R \tag{1}$$

Where a is the scale parameter and b is called translation parameter.

Both CWT and DWT can be used for derivative calculation. However, CWT is preferred to be used for approximate derivative calculation. This is because of two major limitations of DWT in derivative calculations. DWT cannot be used for signals with low SNR as some noise may be retained at lower decomposition levels. Also it requires the number of data points not to be small because of the 50% reduction in data points for each derivative order computation (Nie et al., 2002).

Due to the presence of large number of basic wavelets, wavelet transform provides a solution for almost all chemistry problems with one or more of its wavelets by choosing the suitable scaling parameter.

Wavelet transform had been used over the past decade in many areas like de-noising, data compression and quantitative analysis of multicomponent systems. It had been used associated with zero crossing point in some papers in pharmaceutical

Table 1 Concentrations of caffeine and paracetamol in the 25 laboratory prepared mixtures.

Sample no.	Caffeine (μg/mL)	Paracetamol (μg/mL)
1	3.2	25.6
2	3.2	20.48
3	2.56	20.48
4	2.56	30.72
5	3.84	23.04
6	2.88	30.72
7	3.84	25.6
8	3.2	23.04
9	2.88	23.04
10	2.88	28.16
11	3.52	30.72
12	3.84	28.16
13	3.52	25.6
14	3.2	30.72
15	3.84	30.72
16	3.84	20.48
17	2.56	28.16
18	3.52	20.48
19	2.56	25.6
20	3.2	28.16
21	3.52	28.16
22	3.52	23.04
23	2.88	20.48
24	2.56	23.04
25	2.88	25.6