



Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.elsevier.com/locate/saa

Novel pure component contribution, mean centering of ratio spectra and factor based algorithms for simultaneous resolution and quantification of overlapped spectral signals: An application to recently co-formulated tablets of chlorzoxazone, aceclofenac and paracetamol

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ARTICLE INFO

Article history:

Received 26 November 2015

Received in revised form 8 March 2016

Accepted 20 March 2016

Available online 24 March 2016

Keywords:

Chlorzoxazone

Aceclofenac

Paracetamol

PCCA

MCR

PLS

ABSTRACT

In this work, resolution and quantitation of spectral signals are achieved by several univariate and multivariate techniques. The novel pure component contribution algorithm (PCCA) along with mean centering of ratio spectra (MCR) and the factor based partial least squares (PLS) algorithms were developed for simultaneous determination of chlorzoxazone (CXZ), aceclofenac (ACF) and paracetamol (PAR) in their pure form and recently co-formulated tablets. The PCCA method allows the determination of each drug at its λ_{\max} . While, the mean centered values at 230, 302 and 253 nm, were used for quantification of CXZ, ACF and PAR, respectively, by MCR method. Partial least-squares (PLS) algorithm was applied as a multivariate calibration method. The three methods were successfully applied for determination of CXZ, ACF and PAR in pure form and tablets. Good linear relationships were obtained in the ranges of 2–50, 2–40 and 2–30 $\mu\text{g mL}^{-1}$ for CXZ, ACF and PAR, in order, by both PCCA and MCR, while the PLS model was built for the three compounds each in the range of 2–10 $\mu\text{g mL}^{-1}$. The results obtained from the proposed methods were statistically compared with a reported one. PCCA and MCR methods were validated according to ICH guidelines, while PLS method was validated by both cross validation and an independent data set. They are found suitable for the determination of the studied drugs in bulk powder and tablets.

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1. Introduction

Nowadays, multi-component formulations have been taking up a great importance in the market due to their synergistic effects, quick relief, multiple actions, tolerability, and patient acceptance. Many of such combinations are now available in market, the raised points in quality control laboratories is how to simultaneously determine these drugs in formulations with simple, sensitive and lower cost analytical methods. One of such formulations is the recently co-formulated tablets of chlorzoxazone (CXZ), aceclofenac (ACF) and paracetamol (PAR). CXZ, (5-chloro-2(3H)-benzoxazolone), inhibits histamine release and has skeletal muscle relaxant property. It is used to decrease muscle tone

and tension and thus to relieve spasm and pain associated with musculoskeletal disorders. ACF is 2-[(2,6-dichloro phenylamino) phenyl] acetoxy-acetic acid. It is an orally administered drug which affects a variety of inflammatory mediators. The mode of action of ACF is largely based on the inhibition of prostaglandin synthesis. PAR is chemically designated as (N-(4-hydroxyphenyl) acetamide, it is a centrally and peripherally acting analgesic agent. It has weak anti-inflammatory effects and antipyretic effect through direct activity on the center for the body temperature regulation in the hypothalamus [1]. The three drugs are official in United States Pharmacopeia (USP) [2]. The structures of the three drugs are presented in Fig. 1. Survey of literature revealed that many methods were reported for determination of these drugs either individually [3–5] or in their ternary mixtures by chromatographic methods [6–14], while only one spectrophotometric method was reported in their ternary mixture [15].

So, in this work, the efficiency of pure component contribution algorithm (PCCA) as a novel algorithm was compared with both univariate

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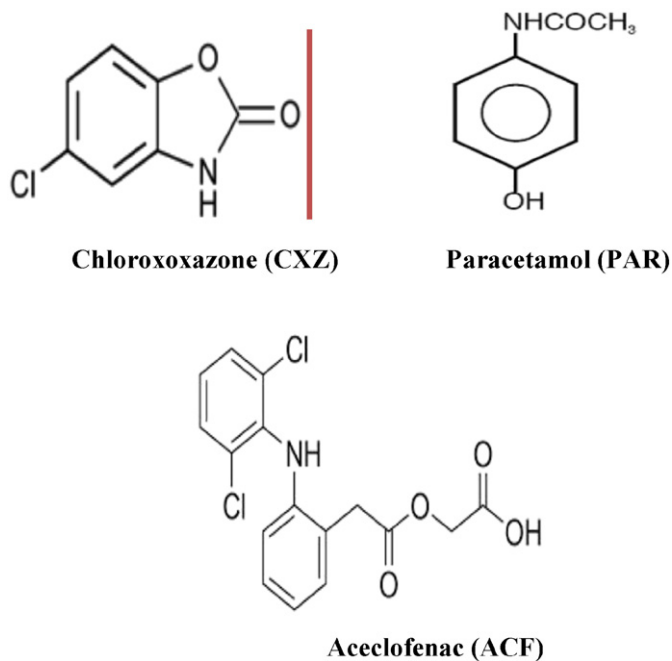


Fig. 1. Chemical structure of the studied drugs.

mean centering of ratio spectra (MCR) and multivariate partial least squares (PLS) for spectral resolution and quantitation of the studied drugs in their pure forms and in two different brands of tablet dosage forms.

1.1. Theoretical background

1.1.1. Pure component contribution algorithm (PCCA)

Hegazy [16] developed and validated this novel algorithm which is efficiently extracts the pure contribution of each component in binary and ternary mixtures. The algorithm involves coded function where the following equations were run automatically upon using the code. The following theory was reported for the developed algorithm [16].

$$A_m = \alpha_X C_X + \alpha_Y C_Y + \alpha_Z C_Z \quad (1)$$

$$B = A_m / \alpha_Z = \alpha_X C_X / \alpha_Z + \alpha_Y C_Y / \alpha_Z + C_Z \quad (2)$$

$$C = MC(B) = MC(\alpha_X C_X / \alpha_Z) + MC(\alpha_Y C_Y / \alpha_Z) \quad (3)$$

$$D = C / MC(\alpha_Y / \alpha_Z) = MC(\alpha_X C_X / \alpha_Z) / MC(\alpha_Y / \alpha_Z) + C_Y \quad (4)$$

$$E = MC(D) = MC[MC(\alpha_X C_X / \alpha_Z) / MC(\alpha_Y / \alpha_Z)] \quad (5)$$

$$F = MC[MC(\alpha_X C_X / \alpha_Z) / MC(\alpha_Y / \alpha_Z)] / MC[MC(\alpha_X / \alpha_Z) / MC(\alpha_Y / \alpha_Z)] = C_X \quad (6)$$

$$G = C_X * \alpha_X = \alpha_X C_X \quad (7)$$

where, A_m is the vector of the absorbance of the mixture, α_X , α_Y and α_Z are the molar absorptivity vectors of X, Y and Z and C_X , C_Y and C_Z are the concentrations of X, Y and Z, respectively and MC is the mean centering process, the detailed description of the equations were reported [16]. As eq. (7) shows, the obtained spectra permits the determination of component X by direct measurement of the estimated absorbance value at its λ_{max} using the corresponding regression equation obtained by plotting the absorbance of the pure spectra of X at its λ_{max} versus its corresponding concentration. Pure component contribution for Y and Z could also be obtained as described for X.

1.1.2. MCR method

This method was a well-established one [17,18] and the theoretical background was explained where it was successfully applied for resolving binary and ternary mixture.

1.1.3. PLS method

It is the conventional chemometric algorithm applied for separation and resolution of complex mixture, its theory was well established and based on factor analysis [19].

2. Experimental

2.1. Instruments and software

All absorbance measurements were carried out using Jasco (V-530) double beam UV–Visible spectrophotometer (Japan), with 1 cm matched quartz cell. Spectra were automatically obtained by Jasco UV-Probe (VWS-580 Spectra Manager software). The spectra were scanned from 200 to 400 nm using 0.1 nm interval. All computations were performed in Matlab® for Windows™ version 6.5. The PLS procedure was taken from PLS-Toolbox 2.0 for use with Matlab® 7.9.

2.2. Chemicals and solvents

2.2.1. Pure samples

Pure samples of CXZ and PAR were kindly supplied by EVA Pharma Pharmaceutical Company, Giza, Egypt. The purity of the samples was certified to be 100.6% and 100.4%, respectively. ACF was kindly supplied by Amriya, Pharmaceutical Company, Alexandria, Egypt. It has a certified purity of 100.8%.

2.2.2. Market samples

Two tablet dosage forms were purchased from the market, Hifenac-MR® tablet, Batch No. KP2481 (labeled to contain 500 mg CXZ, 100 mg ACF, and 500 mg PAR per tablet) is manufactured by INTAS, Pharmaceuticals, India. Dolokind-MR® tablet, Batch No. C1AGM016 (labeled to contain 250 mg CXZ, 100 mg ACF and 325 mg PAR) is manufactured by Mankind Pharma, Delhi, India.

2.2.3. Solvents

Methanol of spectroscopic grade (sd fine-chem limited, Industrial state, Mumbai) and highly purified double distilled water were used.

2.3. Solutions

2.3.1. Standard solutions

Standard solutions containing $100 \mu\text{g mL}^{-1}$ of each of CXZ, ACF and PAR were prepared by dissolving 10 mg of each drug in 100 mL methanol.

2.4. Procedure

2.4.1. Construction of calibration curves for univariate methods

Aliquots equivalent to 0.2–5.0 mL of CXZ, 0.2–4.0 mL of ACF and 0.2–3.0 mL of PAR were accurately and separately transferred from their corresponding standard solutions ($100 \mu\text{g mL}^{-1}$) using calibrated micro pipettes to a series of 10-mL volumetric flasks. Each flask was completed to volume with methanol to reach a final concentration range of 2.00–50.00 $\mu\text{g mL}^{-1}$ for CXZ, 2.00–50.00 $\mu\text{g mL}^{-1}$ for ACF and 2.00–30.00 $\mu\text{g mL}^{-1}$ for PAR. The spectra of the prepared standard solutions were scanned from 200 to 400 nm with 0.1 nm interval.

2.4.1.1. PCCA method. The values of absorbance of the previously scanned spectra at 278, 272 and 245 nm for CXZ, ACF and PAR, respectively, were recorded, plotted against the corresponding concentrations and the regression parameters were calculated.

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