Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 122 (2014) 744–750

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

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

Different approaches in Partial Least Squares and Artificial Neural Network models applied for the analysis of a ternary mixture of Amlodipine, Valsartan and Hydrochlorothiazide

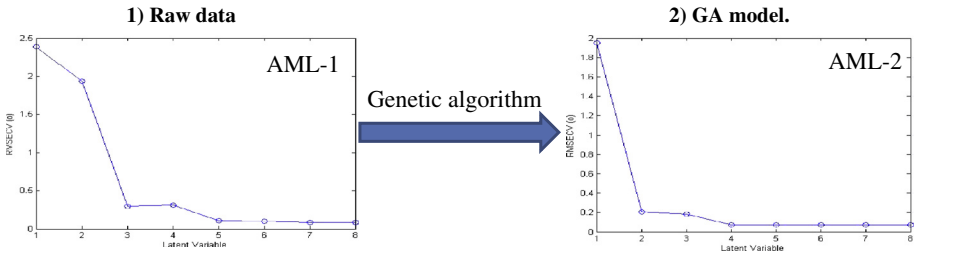
Hany W. Darwish [1], Said A. Hassan *, Maissa Y. Salem, Badr A. El-Zeany

Department of Analytical Chemistry, Faculty of Pharmacy, Cairo University, Kasr El-Aini Street, 11562 Cairo, Egypt

HIGHLIGHTS

- Advanced chemometric methods developed for this ternary mixture.
- Traditional (PLS) and advanced (ANN) chemometric models.
- Difference between GA and PCA as preceding step to chemometric models.
- GA can improve the prediction with less LVs or neurons.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 10 May 2013
Received in revised form 10 September 2013
Accepted 3 November 2013
Available online 20 November 2013

Keywords:
PLS
ANN
GA
Amlodipine
Valsartan
Hydrochlorothiazide

ABSTRACT

Different chemometric models were applied for the quantitative analysis of Amlodipine (AML), Valsartan (VAL) and Hydrochlorothiazide (HCT) in ternary mixture, namely, Partial Least Squares (PLS) as traditional chemometric model and Artificial Neural Networks (ANN) as advanced model. PLS and ANN were applied with and without variable selection procedure (Genetic Algorithm GA) and data compression procedure (Principal Component Analysis PCA). The chemometric methods applied are PLS-1, GA-PLS, ANN, GA-ANN and PCA-ANN. The methods were used for the quantitative analysis of the drugs in raw materials and pharmaceutical dosage form via handling the UV spectral data. A 3-factor 5-level experimental design was established resulting in 25 mixtures containing different ratios of the drugs. Fifteen mixtures were used as a calibration set and the other ten mixtures were used as validation set to validate the prediction ability of the suggested methods. The validity of the proposed methods was assessed using the standard addition technique.

Introduction

Amlodipine (AML), 2-[(2-aminoethoxy)methyl]-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-3,5-pyridine carboxylic acid 3-ethyl 5-methyl ester) [1] (Fig. 1a) is a dihydropyridine derivative acts as a calcium channel blocker. It is used in the management of hypertension, stable angina and variant angina [2].

Valsartan (VAL), N-[p-(o-1H-Tetrazol-5-ylphenyl)benzyl]-N-valeryl-L-valine [1] (Fig. 1b), is an antagonist of the angiotensin-II AT_1-receptor. It is used for treatment of hypertension, heart failure, and post-myocardial infarction [3].

Hydrochlorothiazide (HCT), 6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulphonamide-1,1-dioxide [1] (Fig. 1c), is a benzothiadiazines diuretic widely used in antihypertensive pharmaceutical formulations [4].

Literature survey revealed that AML and HCT are official in British Pharmacopoeia [5], while VAL, HCT and their mixture are official in United States Pharmacopoeia [6]. There are many reported methods for the determination of AML, VAL or HCT in different dosage forms [7–14], but only few chromatographic methods were reported for the simultaneous estimation of AML, VAL and HCT in their ternary mixture [15–19]. Also, spectrophotometric

* Corresponding author. Tel.: +20 1000994542.
E-mail address: saidmonem_84@yahoo.com (S.A. Hassan).
[1] Present address: Pharmaceutical Chemistry Department, College of Pharmacy, King Saud University, P.O. Box 2457, Riyadh 11451, Saudi Arabia.

1386-1425/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.saa.2013.11.045