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Comparative study of the continuous wavelet transform, derivative and partial least squares methods applied to the overlapping spectra for the simultaneous quantitative resolution of ascorbic acid and acetylsalicylic acid in effervescent tablets

Erdal Dinç[a,*], Abdil Ozdemir[b], Dumitru Baleanu[c,d]

[a] *Department of Analytical Chemistry, Faculty of Pharmacy, Ankara University, 06100 Tandoğan, Ankara, Turkey*
[b] *Department of Chemistry, Faculty of Arts and Sciences, Sakarya University, 54100 Serdivan, Sakarya, Turkey*
[c] *Department of Mathematics and Computer Sciences, Faculty of Arts and Sciences, Çankaya University, 06530 Ankara, Turkey*
[d] *National Institute for Laser, Plasma and Radiation Physics, Institute of Space Sciences, Magurele-Bucharest, P.O. Box MG-23, R 76911, Romania*

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Abstract

The simultaneous spectrophotometric determination of ascorbic acid (AA) and acetylsalicylic acid (ASA) in effervescent tablets in the presence of the overlapping spectra was accomplished by the continuous wavelet transform (CWT), derivative spectrophotometry (DS) and partial least squares (PLS) approaches without using any chemical pre-treatment. CWT and DS calibration equations for AA and ASA were obtained by measuring the CWT and DS amplitudes corresponding to zero-crossing points of spectra obtained by plotting continuous wavelet coefficients and first-derivative absorbance values versus the wavelengths, respectively. The PLS calibration was constructed by using the concentration set and its full absorbance data consisting of 850 points from 220 to 305 nm in the range of 210–310 nm. These three methods were tested by analyzing the synthetic mixtures of the above drugs and they were applied to the real samples containing two commercial pharmaceutical preparations of subjected drugs. A comparative study was carried out by using the experimental results obtained from three analytical methodologies and precise and accurate results were obtained.

Keywords: Continuous wavelet transform; Derivative spectrophotometry; Partial least squares; Ascorbic acid; Acetylsalicylic acid; Effervescent tablets

1. Introduction

A mixture of ascorbic acid (AA) and acetylsalicylic acid (ASA) has worldwide use for pain and fever relief in the pharmaceutical preparations. The content of AA and ASA drugs have been analyzed simultaneously by LC [1,2]. The above drugs in combination with other active compounds were determined by differential spectrophotometry [3], spectrofluorimetry [4], HPLC [5,6], potentiometry [7], derivative spectrophotometry [8,9], voltametry [10], ratio-spectra derivative methods [11].

Although HPLC and other conventional spectrophotometric methods have been extensively applied to the simultaneous analysis of mixtures concerning biological, environmental and pharmaceutical problems, they have some well-known disadvantages in the analytical applications. However, the advent of the new mathematical methods, namely the wavelet transforms [12–18] and the chemometric methods [19–22] have fostered the development of the curve resolution of the overlapping peaks in the spectra of multi-mixtures. In analytical chemistry, the wavelet method has been used in combination of other calibration techniques such as partial least squares (PLS) [23–25] and zero-crossing techniques [26–28] for the quantitative determination of active compounds in samples.

* Corresponding author. Tel.: +90 312 215 4886; fax: +90 312 213 1081.
E-mail address: dinc@pharmacy.ankara.edu.tr (E. Dinç).

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In analytical chemistry, for a long period of time, derivative spectrophotometry (DS) has been considered as a comparative method for the quantitation of active compounds in pharmaceutical samples. On the other hand this method contains various disadvantages including fair resolution of mixture spectra due to the diminished peak amplitude with higher order derivation procedure.

PLS and other chemometric methods can be applied with great success to complex pharmaceutical mixtures. These chemometric methods need to use an abstract mathematical content and it is not easy to apply and understand the theory of these chemometric techniques particularly PCR and PLS calibration theory. Although they have abstract theories and other shortcomings, they have been already applied to many fields of applied science as well as analytical chemistry.

For these reasons, we strongly believe that new methods should be presented for the quality control, quantitative analysis and routine analysis of the drugs in their samples.

Continuous wavelet transform (CWT) method is a quite new and promising method in the area of pharmaceutical [21–23] and other signal processing area. The importance of CWT comes from the signal transformation of the original one to the other form of signal giving opportunity of many families including Haar, Daubechies and Mexican hat function to obtain the best calibration signals. The selection of wavelet family is the most important step to get the best signal transformation for a given mixture. It may happen that two or more families give satisfactory results, so there is possibility to choose one of them for the problem solution.

The main purpose of this study is to show the applicability of CWT to quantitate the amount of active ingredients in pharmaceutical samples. CWT as a graphical method was applied to a rapid simultaneous determination of AA and ASA in the synthetic mixtures and two commercial pharmaceutical effervescent tablet formulations. A detailed comparison was carried out by derivative spectrophotometry and PLS techniques and good agreements were found between the obtained results.

2. Experimental

2.1. Apparatus and software

A Shimadzu UV-160 double beam UV–Vis spectrophotometer possessing a fixed slit width (2 nm) connected to a computer loaded with Shimadzu UVPC software and a HP DeskJet 600 printer were used to record the absorption spectra. All the measurements were realized at ambient temperature. The absorption spectra were recorded over the wavelength range of 210–310 nm against a blank (0.1 M HCl).

The data treatment was done in a Pentium 4 2.8 GHz (512 Mb RAM) computer using MATLAB 7.0 software (The MathWorks, Natick, MA, USA). CWT calculations were performed by means of Wavelet toolbox in MATLAB 7.0 and PLS calculations were done in PLS-Toolbox 3.0. The DS calculations and calibrations were performed by using Microsoft Excel.

2.2. Pharmaceutical preparation

Two commercial effervescent tablet formulations were considered in this study, namely, SEDERGINE® effervescent tablets (produced by Laboratories UPSA, France, Batch no. G 0611) consisting of 200 mg AA and 330 mg ASA per tablet and ASPIRIN® Plus C effervescent tablets (produced by Bayer Drug Industry, Istanbul-Turkey, Batch no. 3 E 173) containing 240 mg AA and 400 mg ASA per tablet were studied by using CWT, DS and PLS methods.

2.3. Standard solution

Stock solutions of 50 mg/100 mL AA and ASA for each compound were prepared in 0.1 M HCl. A standard series of the solutions containing 4–20 μg/mL were obtained from the stock solutions for CWT and DS. A concentration set of 16 mixture solutions containing in the concentration range of 0–20 μg/mL AA and ASA was freshly prepared from the stock solutions. A validation set of 10 mixture solutions containing two compounds was also prepared by using the same stock solutions.

2.4. Effervescent tablet analysis

Twenty effervescent tablets were weighted and powdered in a mortar. A tablet amount was transferred to a 100 mL calibrated flask and dissolved in 100 mL 0.1 M HCl and stirred until effervescence tablet particles dissolved completely. After dissolution process prepared solutions were filtered with 0.2 μm disposable membrane filter (Sartorious, minisart, $\phi = 0.20$ μm) by using an injector. The final solution was diluted to the working range for application of the three methods. An analogous procedure was applied to both SEDERGINE® (I) and ASPIRIN® Plus C (II) tablets. (I) and (II) solutions were diluted in the working concentration range with the 0.1 M HCl. All the solutions prepared freshly and protected from light.

3. Results and discussion

The absorption spectra of AA and ASA in the same mixture are strongly overlapping in the wavelength range of 210–310 nm as it can be seen in Fig. 1. The direct determination of subjected compound in the pharmaceutical formulation is not possible due to their overlapping spectra. Therefore, a new approach, CWT was developed for the simultaneous determination of the above-mentioned compounds. The confirmation of CWT was carried out by applying DS and PLS to the same binary mixtures and pharmaceutical samples. The different concentration ranges were tested for the preparation of calibrations for both drugs and

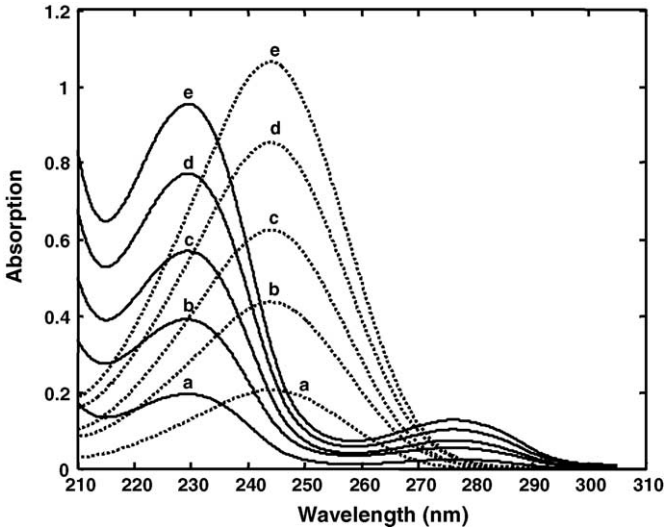

Fig. 1. Absorption spectra of AA (···) and ASA (—) in the concentration of (a) 4 μg/mL, (b) 8 μg/mL, (c) 12 μg/mL, (d) 16 μg/mL and (e) 20 μg/mL.

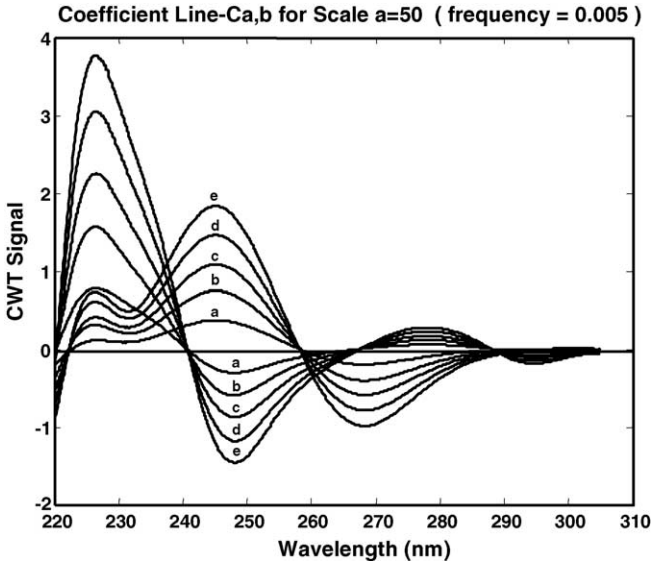

Fig. 2. CWT spectra of AA and ASA in the concentration range of (a) 4 μg/mL, (b) 8 μg/mL, (c) 12 μg/mL, (d) 16 μg/mL and (e) 20 μg/mL in 0.1 M HCl.

the working range between 4 and 20 μg/mL was selected as an appropriate spectral window.

CWT method was utilized and applied for the simultaneous determination of AA and ASA in the mixtures and two commercial pharmaceutical effervescent tablet formulations without any separation or any other chemical process. CWT based on an integration procedure was compared with DS and PLS methods regarding the performance of these three methods. In the last section, first DS and PLS as well known and favored methods of analysis were applied to the mixtures of AA and ASA with the aim of comparison of the developed CWT method. We observed that these three methods give us the successful results for the determination of two drugs. The procedures of these methods were given in the following sections.

3.1. CWT method

A wavelet transform involves the decomposition of a signal function or vector into simpler, fixed building blocks at different scales and positions:

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

Here a denotes the scale parameter which is a variable used to control the scaling, b represents the translation parameter controlling the translation and R is the domain of real numbers. A mother wavelet $\Psi(\lambda)$ generates the set of functions $\Psi_{a,b}(\lambda)$ by scaling (or dilatation) and shifting (or translation).

In our case, the absorbance values of standard series of AA and ASA in the concentration range of 4–20 μg/mL were transferred as absorbance data vectors from EXCEL to wavelet domain. The transferred absorbance data vectors were processed by Mexican CWT at the scaling factor $a = 50$ and CWT spectra were obtained by plotting $C_{a,b}$ coefficients versus wavelengths as could be seen in Fig. 2. By using zero-crossing technique, CWT calibration equations were obtained by measuring the CWT signals at 258.1 nm for ASA and at 267.5 nm for AA and their statistical results were summarized in Table 1. The correlation coefficients of equations' straight-lines were calculated as higher than 0.999 and also other statistical parameters are in acceptable range for the utilization of calibration lines for the determination of both drugs. In the recovery studies, the obtained CWT calibration equations for both drugs were tested by analyzing an independent validation set of 10 mixture solutions of AA and ASA in the working concentration region of 4–20 μg/mL. Their results as mean and relative standard deviation were given in Table 4. The analytical values indicate the preci-

Table 1
Linear regression analysis and its statistical results by CWT and DS

λ	Regression equation	r	S.E. (m)	S.E. (n)	S.E. (r)
CWT					
258.1	$A = -0.02611C_{ASA} - 0.00411$	0.9996	0.0004	0.0056	0.0053
267.5	$A = -0.04884C_{AA} - 0.00468$	0.9998	0.0005	0.0071	0.0068
DS					
244.0	$A = -0.02624C_{ASA} - 0.00045$	0.9999	0.0002	0.0029	0.0027
258.6	$A = -0.02514C_{AA} - 0.00071$	0.9997	0.0004	0.0047	0.0044

sion and accuracy of the application of CWT method to the samples.

CWT calibration graphs were also applied to real samples containing two commercial effervescent tablet formulations. The experimental results of this CWT application showed good agreement with the label claim of both commercial dosage forms.

3.2. Derivative spectrophotometry

In this method, the calibration graphs of AA and ASA in the concentration range of 4–20 μg/mL were obtained by measuring the dA/dλ values at 244.0 and 258.6 nm corresponding to zero-crossing points, respectively. The zero-crossing points give the opportunity of determining AA and ASA amount in their mixture without any priori separation step. Table 1 shows the statistical parameters corresponding to the calibration graphs for both drugs in the chosen wavelengths.

In the optimization of the experimental conditions of DS, the effect of Δλ and scaling factor was tested to find the best derivative spectra. The values of Δλ = 4 nm and scaling factor 10 in the first derivative of the absorption spectra were found as considerable values for both drugs determination. Fig. 3 shows the first derivative spectra obtained with Δλ = 4 nm interval and scaling factor 10 from the absorption spectra shown in Fig. 1.

The validation of DS was checked by using various mixtures consisting of AA and ASA in the working range of two drugs. The means and their relative standard deviations were found to be 99.5 and 1.67% and 101.6 and 2.11% for AA and ASA, respectively, in the synthetic mixtures prepared by adding known amounts of AA and ASA. As seen in Table 4 the recovery results were found reliable for the ability of this method.

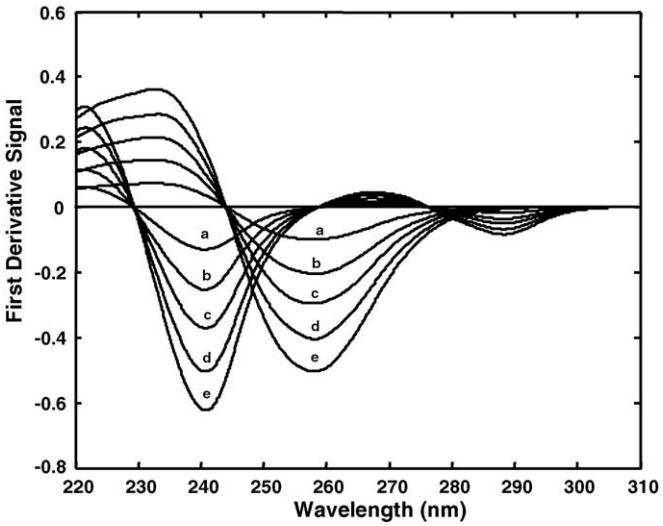

Fig. 3. First derivative spectra of AA and ASA in the concentration range of (a) 4 μg/mL, (b) 8 μg/mL, (c) 12 μg/mL, (d) 16 μg/mL and (e) 20 μg/mL in 0.1 M HCl.

Table 2
The matrix of concentration set consisting of two drugs

No	AA (μg/mL)	ASA (μg/mL)
1	4.0	16.5
2	8.0	16.5
3	12.0	16.5
4	16.0	16.5
5	20.0	16.5
6	0.0	12.0
7	10.0	4.0
8	10.0	8.0
9	10.0	12.0
10	10.0	16.0
11	10.0	20.0
12	12.0	0.0
13	10.0	17.0
14	18.0	12.0
15	20.0	20.0
16	4.0	4.0

3.3. PLS method

In our case, the simultaneous prediction of AA and ASA in samples was accomplished by PLS calibration. The PLS calibration is done by the composition of both concentration and absorbance matrix into latent variables, $A = TP^T + E$ and $C = UQ^T + F$. The vector b is given as $b = W(P^TW)^{-1}Q$, where W is a weight matrix. By using the linear regression $C = a + bA$, the constant a is given by $a = C_{mean} - A^T_{mean}b$.

A concentration set design of the concentration data corresponding to the 16 samples containing the AA–ASA mixtures in the range of 0–20 μg/mL was randomly organized in the PLS calibration as shown in Table 2. The selection of optimal factor was done by cross-validation procedure by using 16 absorption spectra of samples. This procedure was carried out by PLS Toolbox 3.0. According to the cross-validation process, the different factor numbers were tested and the RMSECV values versus factor numbers were plotted and indicated in Fig. 4. In our case, the first four factors having minimum values of PRESS (prediction residual error sum of squares) were found appropriate for PLS calibration. On the other hand PRESS, SEC, correlation coefficient, intercept and slope of PLS calibration using the first four factors were calculated and shown in Table 3.

In the prediction step, the constructed PLS calibration was applied to the synthetic mixtures (Table 4) and the ability of this calibration was checked by using the statistical parameters namely SEP, correlation coefficient, intercept and slope according to the relation between added and found

Table 3
Statistical parameters of the concentration matrix in the PLS calibration steps

Parameter	AA	ASA
PRESS	0.1296	0.0745
SEC	0.0900	0.0682
R	0.9999	0.9999
N	0.0030	0.0018
M	0.9997	0.9999

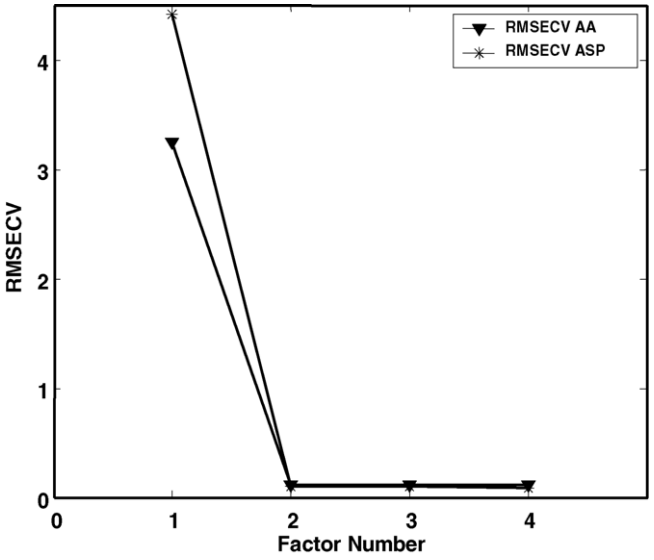

Fig. 4. RMSECV graph of the calibration set in PLS calibration step.

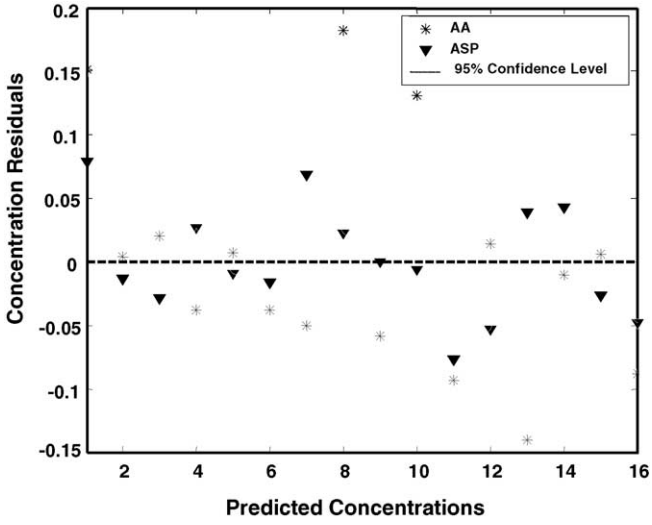

Fig. 5. Concentration residuals for the predicted concentration of AA and ASA by using PLS.

concentration were studied for the constructed PLS calibration. The SEP values were found as 0.130 for AA and 0.085 for ASA. The correlation coefficients are 0.9987 for AA and 0.9997 for ASA and these values indicate good predictive ability of PLS calibration in the prediction of the AA and ASA amounts in the mixture solutions. In another analytical test was done by plotting the concentration residuals against the predicted concentrations. We observed that the residuals randomly scattered around zero as shown in Fig. 5

The PLS calibration is used for the estimation of two drugs in the samples. The applicability of PLS method was confirmed by determining AA and ASA in the synthetic binary mixtures. The various mixtures consisting of AA and ASA in the working range of two drugs were used for the validation of PLS. As it can be seen in Table 4, mean and their relative standard deviations were found to be 99.9 and 1.70% and 101.1 and 1.80 % for AA and ASA, respectively. The synthetic mixtures were prepared by adding known quantities of AA and ASA.

The matrix effect of excipients in the effervescent tablets was tested for CWT, DS and PLS methods. For this reason, standard edition method was applied to commercial effervescent tablets. In application of standard addition method to effervescent tablets, the mean percentage recoveries and their standard deviation for the CWT, DS and PLS were calculated as $99.0 \pm 1.11\%$ (I), $100.05 \pm 1.30\%$ (II); $98.9 \pm 1.45\%$ (I), $101.10 \pm 1.81\%$ (II); $99.5 \pm 1.62\%$ (I), $98.05 \pm 1.95\%$ (II) for AA and $100.8 \pm 0.98\%$ (I), $98.50 \pm 2.05\%$ (II); $102.10 \pm 1.75\%$ (I), $97.50 \pm 2.52\%$ (II); $98.80 \pm 1.52\%$ (I), $100.95 \pm 1.09\%$ (II) for ASA, respectively for five replicates. According to the obtained results a good precision and accuracy was observed for three methods. Consequently, the matrix effect of the excipients in tablet analysis was not observed.

Table 4
Recoveries of AA and ASA in various synthetic mixtures by CWT, DS and PLS

No.	CWT						DS				PLS			
	Added (μg/mL)		Found (μg/mL)		Recovery (%)		Found (μg/mL)		Recovery (%)		Found (μg/mL)		Recovery (%)	
	AA	ASA	AA	ASA	AA	ASA	AA	ASA	AA	ASA	AA	ASA	AA	ASA
1	4.0	16.5	3.89	16.49	97.3	100.0	3.94	16.49	98.5	99.9	3.93	16.47	98.2	99.8
2	8.0	16.5	7.99	16.58	99.9	100.5	7.96	16.52	99.5	100.1	8.02	16.47	100.2	99.8
3	12.0	16.5	11.81	16.63	98.5	100.8	11.93	16.47	99.4	99.8	11.89	16.45	99.1	99.7
4	16.0	16.5	16.03	16.79	100.2	101.7	16.15	16.67	100.9	101.0	16.10	16.58	100.6	100.5
5	20.0	16.5	20.12	16.94	100.6	102.7	20.17	16.84	100.9	102.1	20.11	16.67	100.6	101.1
6	10.0	4.0	9.81	4.03	98.1	100.8	9.81	4.10	98.1	102.6	9.97	4.08	99.7	102.1
7	10.0	8.0	10.12	8.37	101.2	104.6	10.14	8.18	101.4	102.2	10.26	8.09	102.6	101.1
8	10.0	12.0	9.97	12.36	99.7	103.0	9.71	12.24	97.1	102.0	9.77	12.09	97.7	100.7
9	10.0	16.0	10.11	16.39	101.1	102.4	10.16	16.23	101.6	101.4	10.21	16.12	102.1	100.7
10	10.0	20.0	9.94	20.00	99.4	100.0	9.75	21.45	97.5	107.3	9.79	21.18	97.9	105.9
Mean					99.6	101.7			99.5	101.8			99.9	101.1
R.S.D.					1.30	1.49			1.67	2.11			1.70	1.80

R.S.D.: relative standard deviation.

Table 5
Results of the commercial effervescent tablet preparations by investigated methods

Method	CWT				DS				PLS			
Parameter	AA		ASA		AA		ASA		AA		ASA	
	I	II	I	II	I	II	I	II	I	II	I	(II)
Mean	197.7	236.7	344.8	395.9	199.4	238.5	340.5	395.1	197.5	239.4	342.0	389.4
S.D.	1.52	2.22	4.88	3.87	1.88	0.88	8.44	14.95	1.42	1.64	2.40	3.25
R.S.D.	0.77	0.94	1.41	0.98	0.94	0.37	2.48	3.78	0.72	0.69	0.70	0.84
S.E.	0.88	1.28	2.81	2.24	1.09	0.51	4.87	8.63	0.82	0.95	1.39	1.88
CL ($P = 0.05$)	1.77	2.58	5.67	4.51	2.19	1.02	9.82	17.40	1.65	1.91	2.79	3.79

SEDERGINE® VITAMINÉE C effervescent tablet: 200 mg AA and 330 mg ASA per tablet (I). ASPIRIN® Plus C effervescent tablet: 230 mg AA and 400 mg ASA per tablet (II).

3.4. Analysis of effervescent tablets

The obtained results by applying CWT, DS and PLS methods to two commercial effervescent tablet preparations were shown in Table 5. A good coincidence was observed between the experimental results and label claim of the commercial effervescent preparation in this study. The numerical values of all statistical parameters calculated in Table 5 are acceptable determination limits in application of two methods to the effervescent tablets.

To compare CWT, DS and PLS, one-way ANOVA test was applied to the obtained results for two commercial effervescent tablet formulations. The calculated F-values ($P = 0.05$, $n_1 = 4$ and $n_2 = 12$) were found lower than the tabulated F-value and the ANOVA test results were not significant; the variances differ only randomly. The results of one-way ANOVA test were shown in Table 6. We can accept by these three methods that there is no difference between the three sets of sub-samples.

Table 6
The ANOVA results by applying three methods to two commercial pharmaceutical effervescent preparations

	Drug	Sample	Source of variations		
			Between groups	Within groups	Total
Sum of squares	AA	I	11.17	31.50	42.67
		II	17.64	33.59	51.23
	ASA	I	47.48	403.04	450.52
		II	127.69	996.79	1124.48
Degree of freedom	AA	I	2	12	14
		II			
	ASA	I			
		II			
Mean squares	AA	I	5.59	2.62	
		II	8.82	2.80	
	ASA	I	23.74	33.59	
		II	63.84	83.07	
Calculated F-value	AA	I	2.13		
		II	3.15		
	ASA	I	0.71		
		II	0.77		
Tabulated F-value	AA	I	3.89		
		II			
	ASA	I			
		II			

4. Conclusion

The main purpose of this study was to apply CWT method to the simultaneous determination of AA and ASA drugs in their mixtures and effervescent tablets without using any prior chemical pre-treatment in the presence of the strongly overlapping spectra.

Good results were obtained by utilizing CWT, DS and PLS methods as a comparative study for the quantitation of AA and ASA and a good agreement with the literature results was found [25].

Although CWT and DS are based on the use of signal analysis, their theoretical aspects are different from each other. Comparing to DS method, CWT gives us many advantages as big peak intensity and more zero-crossing points. The increased peak intensity provides a higher sensitivity for CWT approach.

We believe that the ability of CWT based on zero-crossing technique to drug analysis will gain importance in the field of analytical chemistry as an alternative to the derivative method. This approach gives us repeatable, rapid and reliable results for the quantitation of active compounds in samples, as could be seen in this study.

These three methods were found suitable for simple and precise routine quality control analysis of the selected pharmaceutical samples.

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