PROJECTION TO LATENT STRUCTURES FOR RECOGNITION OF ATENOLOL BY MANUFACTURERS

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Atenolol is a selective β1-adrenoblocker. It is used in the treatment of cardiovascular diseases, such as arterial hypertension, angina pectoris, acute myocardial infarction, tachycardia, etc. One of the enantiomers of the medicinal product has pronounced pharmacological properties, unlike the other. This stimulates the development of studies on the recognition and determination of atenolol enantiomers in pharmaceuticals. In this work, pharmaceuticals from various manufacturers (Belupo, Pranapharm etc.) were chosen as real samples. The voltammograms were obtained by oxidation of atenolol on glassy carbon electrodes (GCE) modified by composites of polyelectrolyte complexes of chitosan (CS) and chitosan succinamide (SCS) with cyclodextrins (CD).

Projection to Latent Structures (PLS) was used for atenolol recognition by manufacturers. PLS regression is a recent technique that generalizes and combines features from the principal component analysis and multiple regression. It is particularly useful when we need to predict a set of independent variables. PLS regression is a statistical method that finds a linear regression model by projecting the predicted variables and the observable variables to a new space. A PLS model will try to find the multidimensional direction in the X space that explains the maximum multidimensional variance direction in the Y space. Results were considered positive if reference sample was correctly assigned to the test sample. The reference set and the test set were prepared independently. Values of discriminant responses of PLS model for real samples using sensory system based on three GCEs modified by composites of CS-SCS with α-, β- and γ-CD were calculated and it is shown in table. It can be seen that all samples were correctly recognized.

Table. Discriminant responses (RS/TS) of PLS model in percentage (%) for real samples using sensory system based on three GCEs modified by composites of CS-SCS with α-, β- and γ-CD

RS* / TS**	Sample 1	Sample 2	Sample 3
Sample 1	98.80	0.83	0.38
Sample 2	0.83	98.96	0.21
Sample 3	0.37	0.21	99.42

* RS − reference sample, TS − test sample

Thus, the partial least squares regression method was successfully applied to the recognition of atenolol by the manufacturers, which will allow expressly evaluating the quality of the medicament on its basis.