PRINCIPAL COMPONENT ANALYSIS FOR SELECTIVE VOLTAMMETRIC RECOGNITION OF ATENOLOL ENANTIOMERS

Zilberg R. A., *Provorova Yu. R.*, Kabirova L. R., Habletdinova A. I.
Bashkir State University
32, Zaki Validi Street, 450074 Ufa, Republic of Bashkortostan, Russia
provorova-96@mail.ru

Atenolol (ATN) is a drug that helps to fight the diseases of the cardiovascular system. It has antiarrhythmic, antianginal, hypotensive biological actions. Biological activity of drugs is associated with one of the enantiomers. For atenolol, the S-enantiomer is usually 50–500 times more effective than the R-enantiomer.

In this study, voltammetric sensors based on glassy carbon electrodes (GCE) modified by composites of polyelectrolyte complexes of chitosan and chitosan succinamide (CS-SCS) with cyclodextrins (CD) for the recognition of ATN enantiomers have been developed. For more reliable recognition of enantiomers and their racemic mixtures, the obtained voltammograms were chemometrically processed using the principal component analysis (PCA). Chemometric processing of experimental data arrays by PCA allows to represent the ATN voltammograms in the form of points, grouping into ellipsoids or spheres in the new coordinate system X, Y, Z, etc., where the coordinate axes are the vectors of the main components. In this case, the main components should be considered as the directions of the greatest change in the space of the variables X, Y or Z. The graph on which the projections on the plane of the main components and parts of the explained data variance for each principal component are expressed as a percentage is usually called the chart of accounts. It describes the relative position of the voltammograms of the samples under study in the space of new coordinates and makes it possible to estimate the efficiency of the "compression" of the experimental data. Each point in the chart of accounts corresponds to a specific voltammogram, and the totality of nearby points and the space they occupy will correspond to the ATN enantiomers.

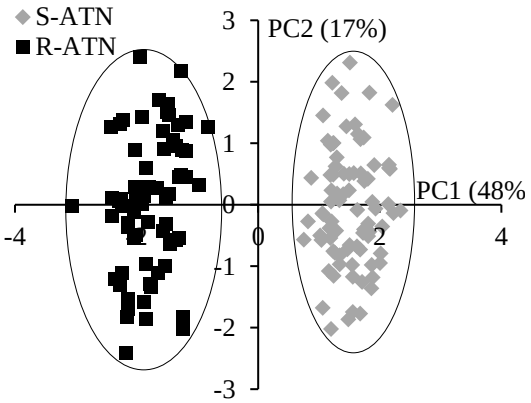

Fig. Score plot of PCA modelling of voltammograms obtained by differential pulse voltammetry for 0.5 mM solutions of ATN enantiomers using of sensory system with three GCEs electrodes modified by CS-SCS composites of CDs

Thus, the results of PCA modeling show the better specificity of voltammetric sensors based on glassy carbon electrodes modified with composites of polyelectrolyte complexes of chitosan and chitosan succinamide with cyclodextrins for recognition of ATN enantiomers.

This work was supported by the Russian Science Foundation (Grant No. 16-13-10257).