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ELECTROCHEMICAL DETECTION OF ENANTIOMERIC TYROSINE BY MACHINE LEARNING

Tesfatsion W.T., Stekolshchikova A.A., Ivanov A.S., Nikolaev K.G.
teweldebrhan@scamt-itmo.ru
Scientific supervisor – Prof. Dr., Head of ISC of ITMO University Skorb E.V.
(Infochemistry Scientific Center, ITMO University)

Abstract. The work depicts an electrochemical hydrogel−eutectic gallium indium alloy interface for the recognition of enantiomeric chemicals. This interface allows for the recording of nonlinear current−voltage responses, depending on the composition of the hydrogel. The current–voltage data for the machine learning model are trained by a multilayer perceptron. This model accurately recognizes the enantiomeric tyrosine in mixture with interfering Phosphate-buffered saline with 79% accuracy. Thus, this interface can be used as a convenient method for expressed recognition of various chemicals and pathogens detection.

Biomedical research is a field of research that includes many areas of both life and physical sciences. The broad area of science looks for ways to prevent and treat diseases that cause illness and death in people and animals.

L-Tyrosine is a conditionally indispensable amino acid required to produce the neurotransmitter's dopamine, adrenaline, and noradrenaline, as well as for the skin pigment, melanin. Noradrenaline (norepinephrine) and adrenaline (epinephrine) are the main actors in the body's response to acute stress and, along with dopamine, help to support a positive mood and mental alertness. In addition, L-Tyrosine is especially critical for the normal function of the thyroid gland. On the other hand, D-tyrosine has been the precursor of many different anti-inflammatory. Thus, a simple and reliable method for determining D- and L-tyrosine in pharmaceutical formulations is highly desirable as such, chiral resolution of enantiomers plays an important role in the pharmaceutical industry.

There are different ways of determination of enantiomeric chemicals as D-tyrosine and L-tyrosine. We hypothesized that machine learning could be shown proof-of-concept in the following can be applied for miniaturized test-systems with potential application in the field. The machine learning method uses the database and does not need calibration each time. Also, the method is fast, versatile, cheap, robust, and sustainable.

For logical analysis, we propose use of a feedforward deep neural network model (multilayer perceptron). The backpropagation algorithm does the training of such a machine learning model. Different computer and machine learning methods are able to solve a lot of biological and chemical problems, in particular, establishing the structure of proteins and their interactions, as well as predicting the effect of mutations on their assembly. Multilayer perceptron supervised learning allows the detection of individual states on an eGaIn/hydrogel interface that depends on hydrogel composition. A database is necessary for model training. In the database columns consist of attributes by which responses are determined. Since the redox peaks are individual for hydrogel compositions, currents are attributes and compositions are responses. This approach can be used to recognize and determine their stages using I−V curves as a fingerprint for identifying L-tyrosine and D-tyrosine.

A multilayer perceptron is one of the most and simplest algorithms in machine learning can be able to supervise and unsupervised and also can analyze our sample composition from the obtained curves. Presently this is fast learning algorithm of perceptron training and that's algorithm for perceptron learning capability. The overall computation approach of this algorithm uses for exploring the perceptron training and learning capability in multilayer network. The used parametric conditions for a multilayer perceptron to train the machine learning model's (learning rate 0.3, momentum 0.2, training time 10000) and layers of 7, 14, 20 on big electrodes, tyrosine diffusion through the gel, and

combined data, respectively. In our work, we exampled two processes, which are gel on large electrodes and diffusion system. The mode identified the enantiomeric compounds as L-tyrosine and D-tyrosine with 79.0%, 99.5%, and 98.2% correctly on big gel electrodes, diffusion systems, and combined data. Thus, this interface can be used as a convenient method for expressed recognition and identification of chemicals.

A new simple and sensitive electrochemical method have been developed and validated to determine L-tyrosine and D-tyrosine in pharmaceutical formulations. This study describes determining the qualified and quantified enantiomeric chemical tyrosine based on the current-voltage data for the data processing using a machine learning model, which results more admirable and usable in different biomedical areas. Such a machine learning system demonstrates a new approach for identifying and determining tyrosine, which is useful in pharmaceuticals.