



University of zabol  
Graduate school  
Faculty of science  
Department of Bioinformatics

The Thesis Submitted for the Degree of Master of Science  
(In the field of Bioinformatics)

Title:

**A study of the interaction space of lactate dehydrogenase  
isoforms and its some inhibitors using proteochemometric  
modeling**

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Summer ۲۰۲۱

**Abstrac:**

Lactate dehydrogenase (LDH) is a tetramer enzyme that reversibly catalyzes the conversion of pyruvate to lactate. This enzyme is important because LDH isoenzymes are associated with a variety of diseases, including cancers, heart disease, liver problems, and most importantly, corona disease. The aim of this study was to model LDHA and LDHB isoenzyme inhibitors using proteochemetric method. This method is system-based and does not require knowledge of the three-dimensional structure of the protein, but it depends on the sequence of amino acids and descriptors. To implement the proteochemetric method, the camb package in the R Studio Server programming environment as well as the data set of LDHA and LDHB isoenzyme inhibitors from the valid Binding DB database were used. The proteochemometric method uses three machine learning algorithms gradient amplification model, random forest and support vector machine as regression methods to find the best model. Finally, by examining the statistical parameters such as RMSE,  $R^2$  and  $Q^2$ , the most appropriate model for inhibitors of LDHA and LDHB isoenzymes was selected using the best random forest method.

**Keywords:** descriptor, proteochemetric, machine learning algorithm, inhibitor, isoenzyme, camb package.