Mathematical Modeling of Bi-Substrate Enzymatic Reactions in the Presence of Different Types of Inhibitors

Authors : Rafayel Azizyan, Valeri Arakelyan, Aram Gevorgyan, Varduhi Balayan, Emil Gevorgyan

Abstract : Currently, mathematical and computer modeling are widely used in different biological studies to predict or assess behavior of such complex systems as biological ones. This study deals with mathematical and computer modeling of bi-substrate enzymatic reactions, which play an important role in different biochemical pathways. The main objective of this study is to represent the results from in silico investigation of bi-substrate enzymatic reactions in the presence of uncompetitive inhibitors, as well as to describe in details the inhibition effects. Four models of uncompetitive inhibition were designed using different software packages. Particularly, uncompetitive inhibitor to the first [ES1] and the second ([ES1S2]; [FS2]) enzyme-substrate complexes have been studied. The simulation, using the same kinetic parameters for all models allowed investigating the behavior of reactions as well as determined some interesting aspects concerning influence of different cases of uncompetitive inhibition. Besides that shown, that uncompetitive inhibitors exhibit specific selectivity depending on mechanism of bi-substrate enzymatic reaction.

Keywords : mathematical modeling, bi-substrate enzymatic reactions, reversible inhibition

Conference Title : ICBCBBE 2014 : International Conference on Bioinformatics, Computational Biology and Biomedical Engineering

Conference Location : Barcelona, Spain

Conference Dates : August 18-19, 2014