

Theoretical study of acceptance features of adenosine and its aza-, carba- and deoxyanalogues in active site of adenosine deaminase

© Yuriy P. Zarubin,¹⁺ Prokofiy V. Sklyuev,¹ and Pyotr P. Purygin¹

Chair of Organic, Bioorganic and Medicinal Chemistry. Samara State University. Akad. Pavlova St., 1. Samara, 443011. Samara Region. Russia. Phone: +7 (846) 334-54-59. E-mail: zarubin@ssu.samara.ru.

*Supervising author; ⁺Corresponding author

Keywords: adenosine deaminase, mechanism of the substrate specificity, adenosine, analogues, aza-, carba-, deoxy-, features of acceptance, theoretical study.

Abstract

Conformational models of enzyme-ligand complexes of adenosine deaminase with adenosine and its aza-, carba- and deoxyanalogues applying methods of docking and molecular mechanical optimization are constructed. Optimization conformational energy of enzyme-ligand complexes was made using molecular mechanics of MM3 force field. Features of adenosine deaminase acceptance of molecules of adenosine and its analogues in *N*- and *S*-areas of pseudorotation of furanose cycle are considered. Interrelations between structure of enzyme-ligand complexes and biochemical properties of ligands in the relation adenosine deaminase are established.