MOLECULAR MODELING OF SHIKIMATE KINASE FROM *BACILLUS ANTHRACIS*

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Among potential targets on development of new drugs against B. Anthracis, enzymes from Shikimate pathway deserve attention. It is a seven step biosynthetic route that leads to the synthesis of aromatic amino acids, ubiquinone, and secondary metabolites, from phosphoenol pyruvate and erythrose-4-phosphate. This pathway is essential for algae, bacteria, fungi, parasite, whereas it's absent in mammals. Therefore, these enzymes are potential targets for the development of nontoxic antimicrobial agents, herbicides and anti-parasite drugs. Shikimate Kinase (SK), the fifth enzyme, catalyzes the specific phosphorilation of shikimic acid, using ATP as a co-substrate, resulting in shikimate-3-phosphate and ADP. The three-dimensional structure of SK from *Bacillus anthracis* (BaSK) was modeled. We used as template crystallographic structure of SK from *Mycobacterium tuberculosis*. The structural mechanism of the catalytic functioning of BaSK was investigated on the basis of a series of structures of SK from *Mycobacterium tuberculosis* corresponding to individual steps in the enzymatic reaction. Based on a comparison of the structural states before initiation of the reaction and immediately after the catalytic step, we derived a structural model of the transition state. This work discuss the structural features of the homology models, obtained for SK from *B. anthracis* and the potential of this structure on the studies of new inhibitors that may generate a new generation of drugs against *B. anthracis.*