STUDYING ENZYMATIC REACTIONS WHICH CHANGE DNA TOPOLOGY

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Two classes of enzymes, DNA topoisomerases and site-specific recombinases, catalyze reactions which change topology of circular DNA molecules. One approach to study the mechanisms of such reactions is to compare the distribution of DNA topological states obtained in a particular reaction experimentally with the distributions calculated for different models of the reaction mechanism. The major attention in the talk will be paid to the theoretical part of the approach. The theoretical analysis assumes that the substrate DNA has equilibrium distribution of conformation. A set of DNA conformations, which correspond to the distribution, can be simulated with a good accuracy. Then, we select from the constructed set the conformations which have two properly juxtaposed segments, so they can form the reaction substrate. For each of the selected conformations we can calculate the topology of the reaction products. Thus, we directly simulate the distribution of topological states of the reaction products. Two applications of the approach are considered, to type II DNA topoisomerases and to Cre and Flp recombinases.

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