



Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Velika predavalnica Kemijskega inštituta /
Great Lecture Hall
National Institute of Chemistry
Hajdrihova 19, Ljubljana, Slovenia

Computational Design of the Temperature Dependence of Enzyme Reactions

Cold-adapted enzymes from psychrophilic species are generally among most highly optimized enzymes found in nature. They thus invariably outperform their orthologous mesophilic counterparts, in terms of activity, below and around room temperature. It is therefore not so surprising that no successful attempts to enhance the activity of cold-adapted enzymes appear to have been reported yet. We will address this problem for two bacterial enzymes from arctic environments to illustrate our strategy. In the case of a small extracellular lipase, our results show that it is possible to construct variants, with just a few mutations, that both markedly increase the catalytic rates over the entire examined temperature range and also move the temperature optimum upwards. Of particular interest here is the fact that our most efficient cold-adapted enzyme variant only has mutations that are 15-20 Å away from the reaction center. This underscores the high degree of optimization of the native enzyme and thus suggests that mutation sites for further improvement may have to be sought at more distant amino acid positions.

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Vljudno vabljeni / Kindly invited