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Avviso di Seminario

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Computational Design of Enzymes – Are We There Yet?

Lunedì 29 Maggio 2017, ore 11:00

Aula A, Plesso Polifunzionale

Summary

Enzymes catalyze chemical reactions with great speed and high specificity, using water as the medium. Thus, they could provide great advantage in processes such as bioremediation, by converting toxic pollutants harmless compounds, and chemical synthesis, by converting multistep process that use organic solvents into one-step syntheses in water. One emerging technique for the development of new enzymes is based on computation: entire enzymes are designed in-silico by optimizing the environment around the known transition state of the reaction of interest.

The most successful example of computational design is represented by the Kemp eliminases. These designed enzymes catalyze a reaction not found in any metabolic pathway (the "Kemp elimination") with rate accelerations of up-to 7 orders of magnitude. Using the Kemp elimination as a benchmark, these remarkable accelerations have often been used to underscore the success of design.

But is the Kemp elimination a good benchmark for the design of enzymes? Does this reaction represent a significant challenge for macromolecules? How easy is it to find proteins that promiscuously catalyze the Kemp elimination with rate accelerations similar to those of the designed enzymes? In this talk, I am going to use examples from the literature and recent advances in our lab to answer these questions.

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