

VABILO NA PREDAVANJE / INVITATION TO THE LECTURE

Dr. David M. Smith

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute,
Zagreb, Croatia

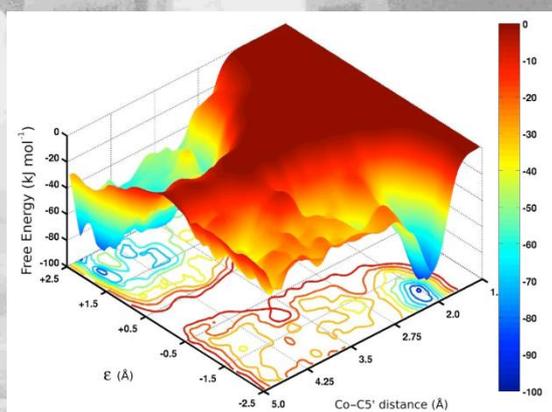
Sreda / Wednesday, 21. 12. 2011, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the
National Institute of Chemistry; Hajdrihova 19, Ljubljana

The Activation of Coenzyme B₁₂

Povzetek / Abstract

Enzymes that rely on coenzyme B₁₂ (5'-deoxyadenosylcobalamin) have generated a great deal of interest in the scientific community. One particular focus has been the activation of the Co-C bond of the coenzyme and its connection to the subsequent hydrogen-atom abstraction from the substrate. In this contribution, we address these issues with a state-of-the-art QM/MM first principles molecular dynamics study of the methylmalonyl-CoA mutase catalysed reaction. Using techniques such as constrained- and meta-dynamics, we evaluate the free energy profiles associated with the initial steps of this reaction.



By analysing the dynamics of the natural cofactor and two dideoxy analogues, we shed new light on the important catalytic effects as well as the way in which the enzyme controls the highly reactive 5'-deoxyadenosyl radical intermediate.

Vljudno vabljeni! / Kindly invited!

Info: Dr. Robert Vianello; robert.vianello@ki.si