Understanding enzymatic reactions

Maria João Ramos

UCIBIO@REQUIMTE, Department of Chemistry and Biochemistry Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n 4169-007 Porto, PORTUGAL

mjramos@fc.up.pt

We know that we can establish catalytic mechanisms of enzymatic reactions and, in doing so, explain the findings of experimentalists, but can we actually predict them? This talk is concerned with the computational needs that we come across to figure out results within computational enzymology. Calculations devised to study protein interactions and circumvent problems in some relevant systems will be reported as well as recent developments in the establishment of some catalytic mechanisms. We have resorted to QM/MM [1,2] as well as other calculations [3,4], in order to analyse the energetics of processes related to the systems under study and evaluate their feasibility according to the available experimental data.

References

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