PIRAMID

PROTEIN INTERACTIONS
IN RATIONAL APPROACHES
FOR MEDICINAL
INNOVATIVE DRUGS

Conférence Pedro Alexandrino FERNANDES

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Salle Marie Curie, Laboratoire CEISAM
Faculté des Sciences et Techniques de Nantes

Challenges in Computational Enzymology

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This talk will focus in the study of enzyme reaction mechanisms with computational QM/MM methods. The relationship between enzyme rate and enzyme dynamics/flexibility will be analysed in detail. The consequences of enzyme flexibility on the specific chemical pathway that is followed will be addressed as well. An example of "chemical disorder"- multiple reaction mechanisms for the same enzyme with the same substrate- will be discussed. Overall, the talk tries to shed some light into the relationship between enzymatic conformational diversity, reaction rate and chemical mechanism.