Introduction

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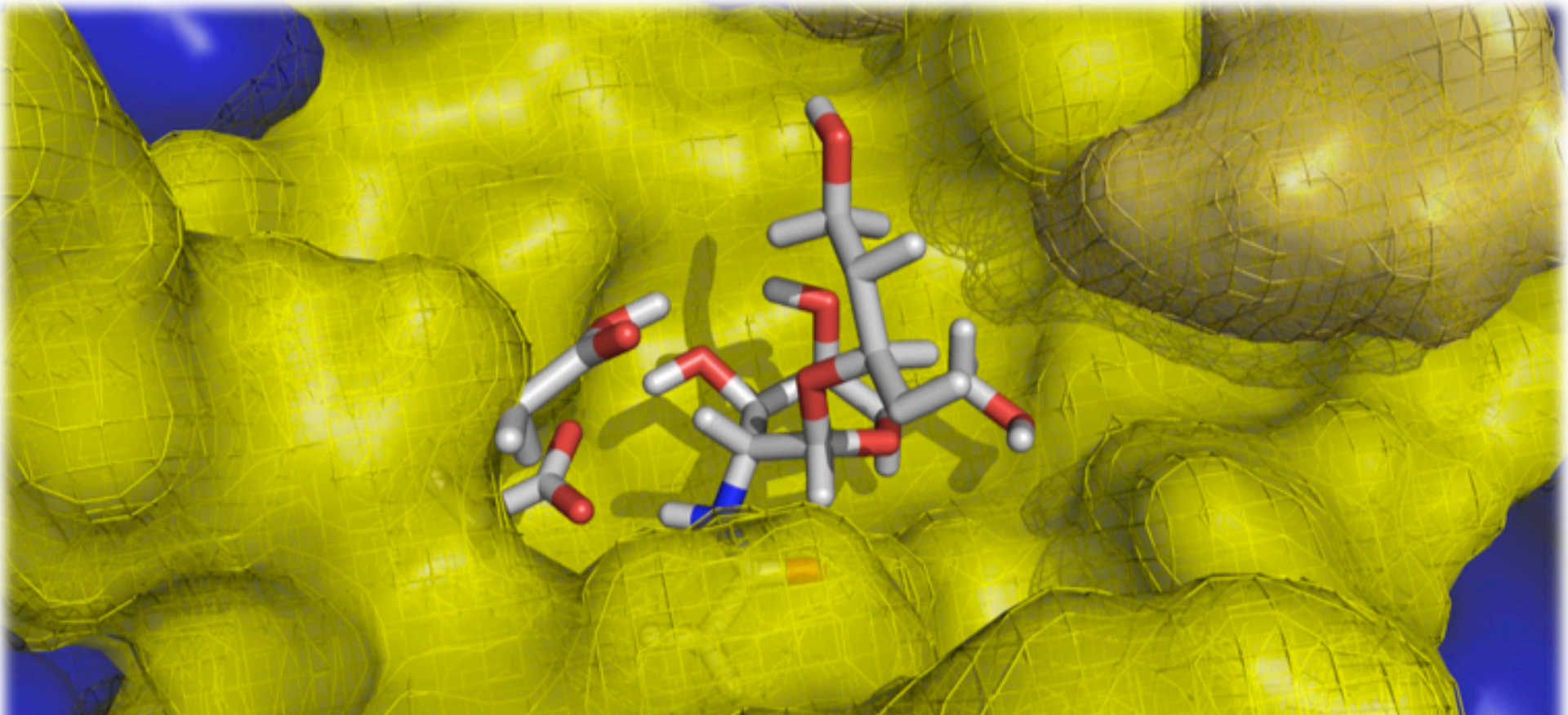

Chile & Portugal

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Porto – World Heritage City

Department of Chemistry & Biochemistry

Theoretical Chemistry & Computational Biochemistry

Research Fields

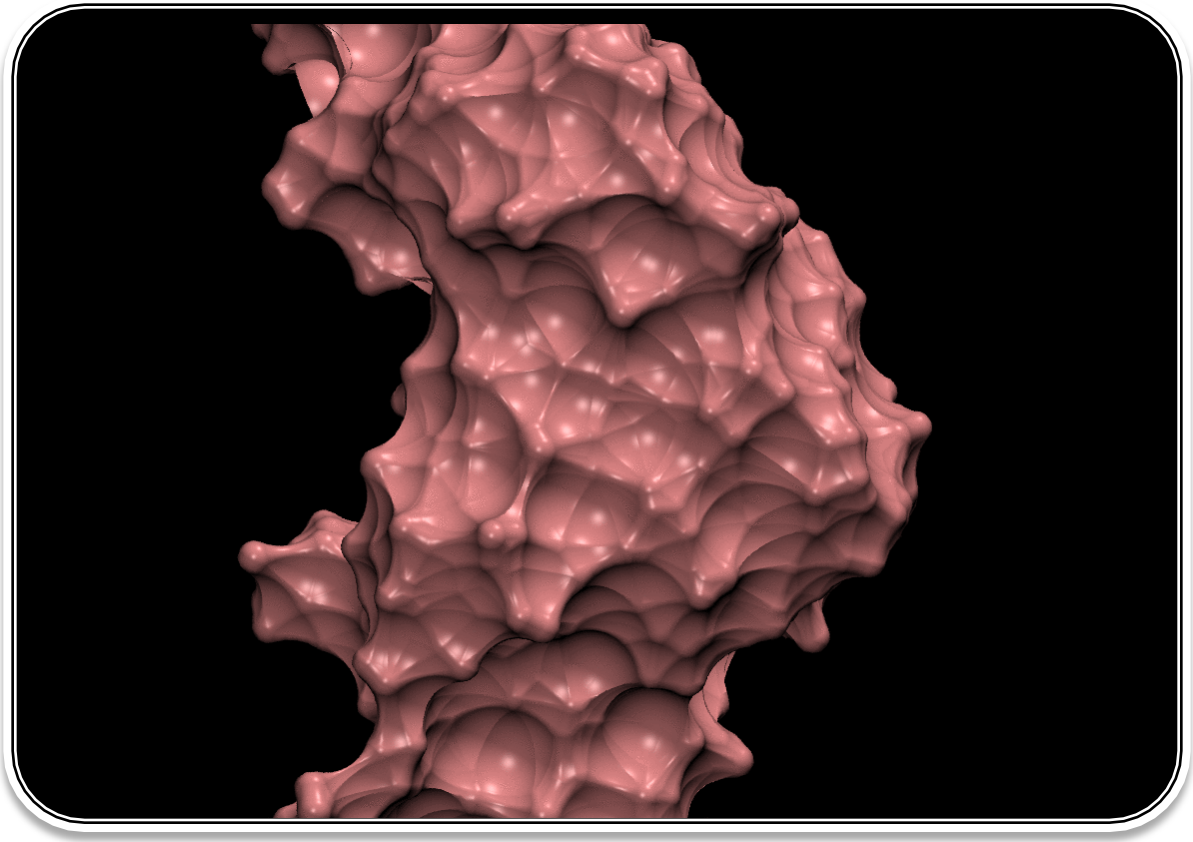
Enzymatic Mechanisms & Inhibition.

Structure & Dynamics of Proteins.

Comp. Mutagenesis & P:P Docking.

Software & Algorithms

Drug Discovery.



- Catalytic mechanism with atomic detail
- DG of each elementary reaction step
- Transition state structure
- Inhibition mechanism with atomic detail

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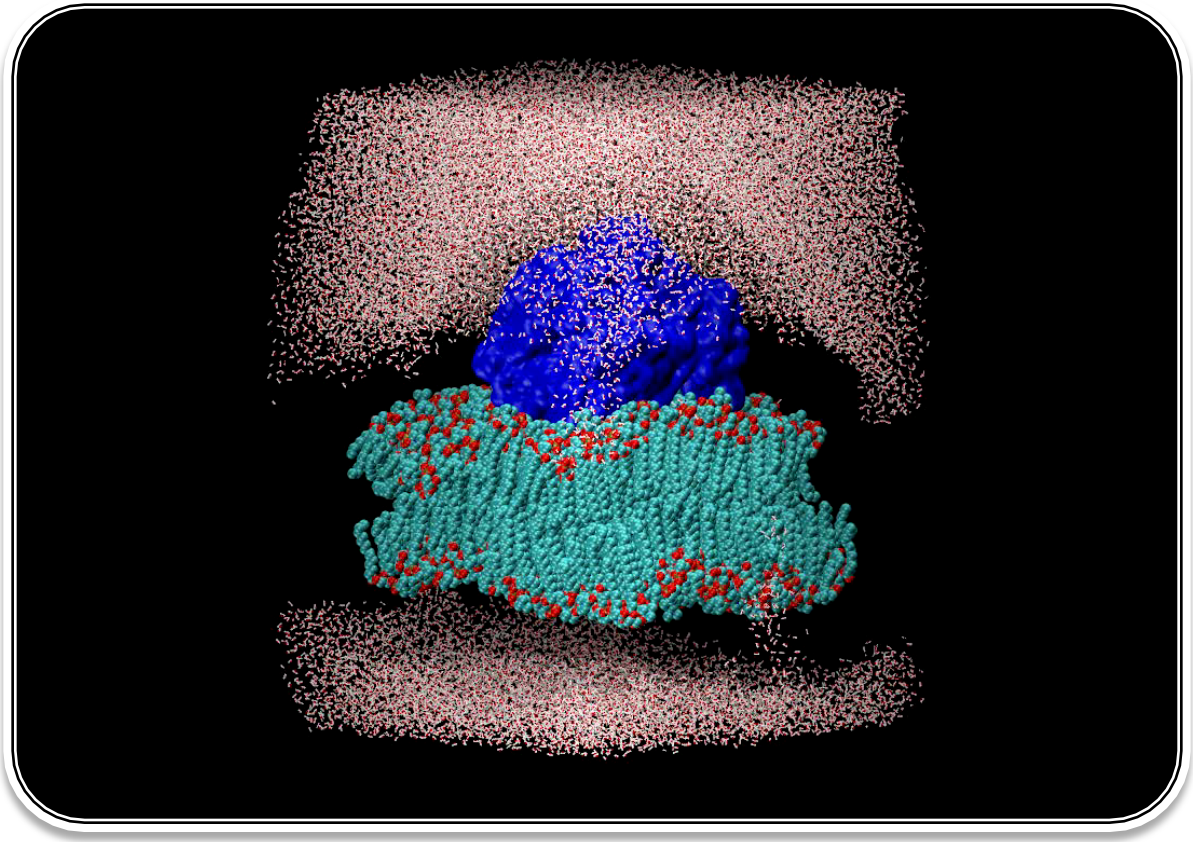

- Protein modelling
- Conformational rearrangements
- Molecular Recognition
- Free energy for ligand binding

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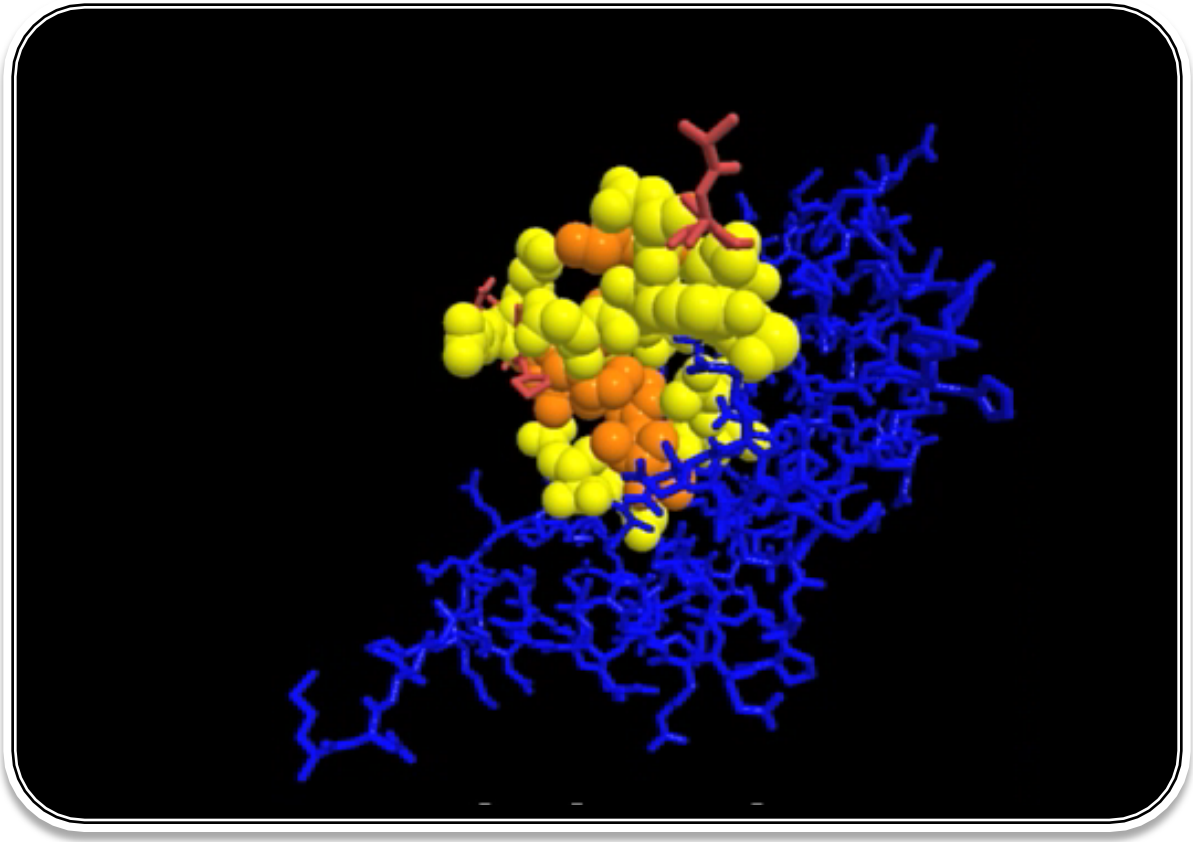

- Effect of Ala mutations in binding free energy
- Mapping of protein:protein interfaces
- Hot-spot detection
- Based in MM-PBSA but as accurate as TI

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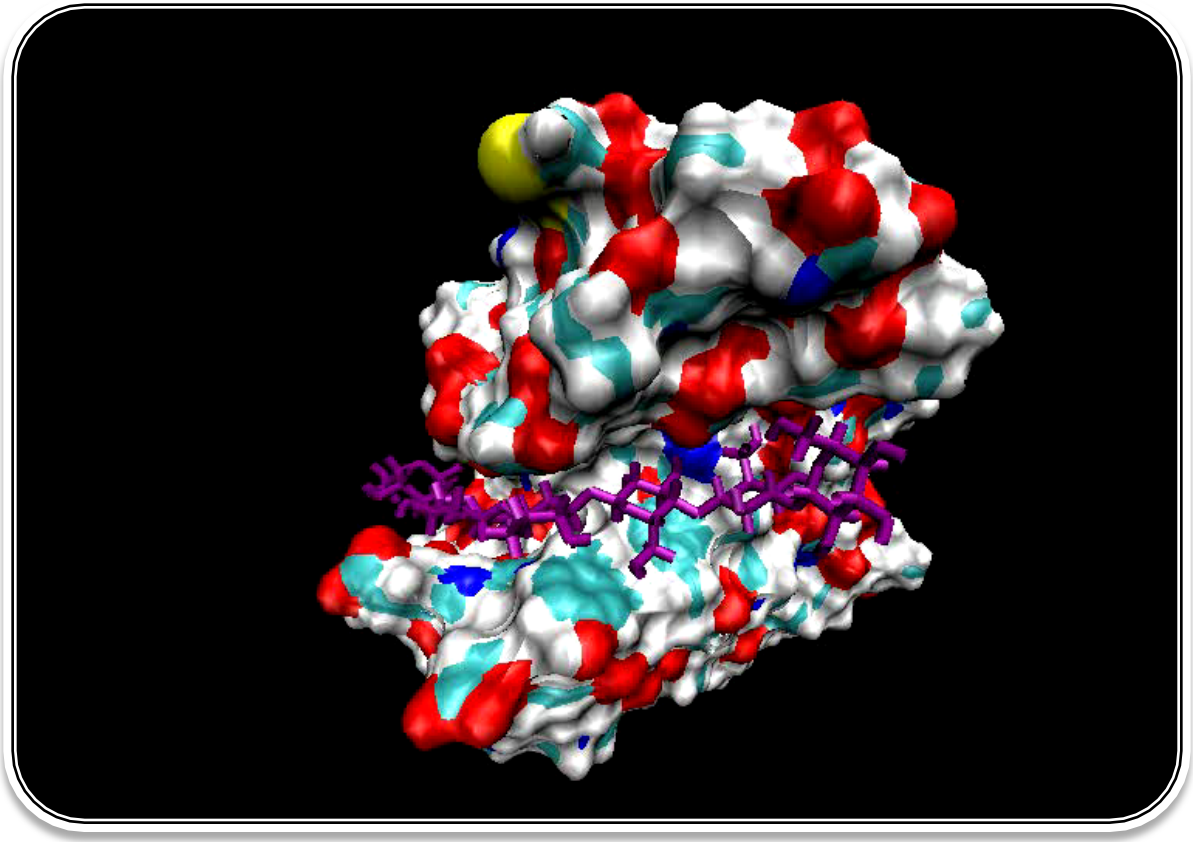

- MADAMM – flexible receptor docking
- CompASM –Alanine Scanning Mutagenesis
- VSLab- Virtual Screening Laboratory
- VolArea – Molecular area and volume

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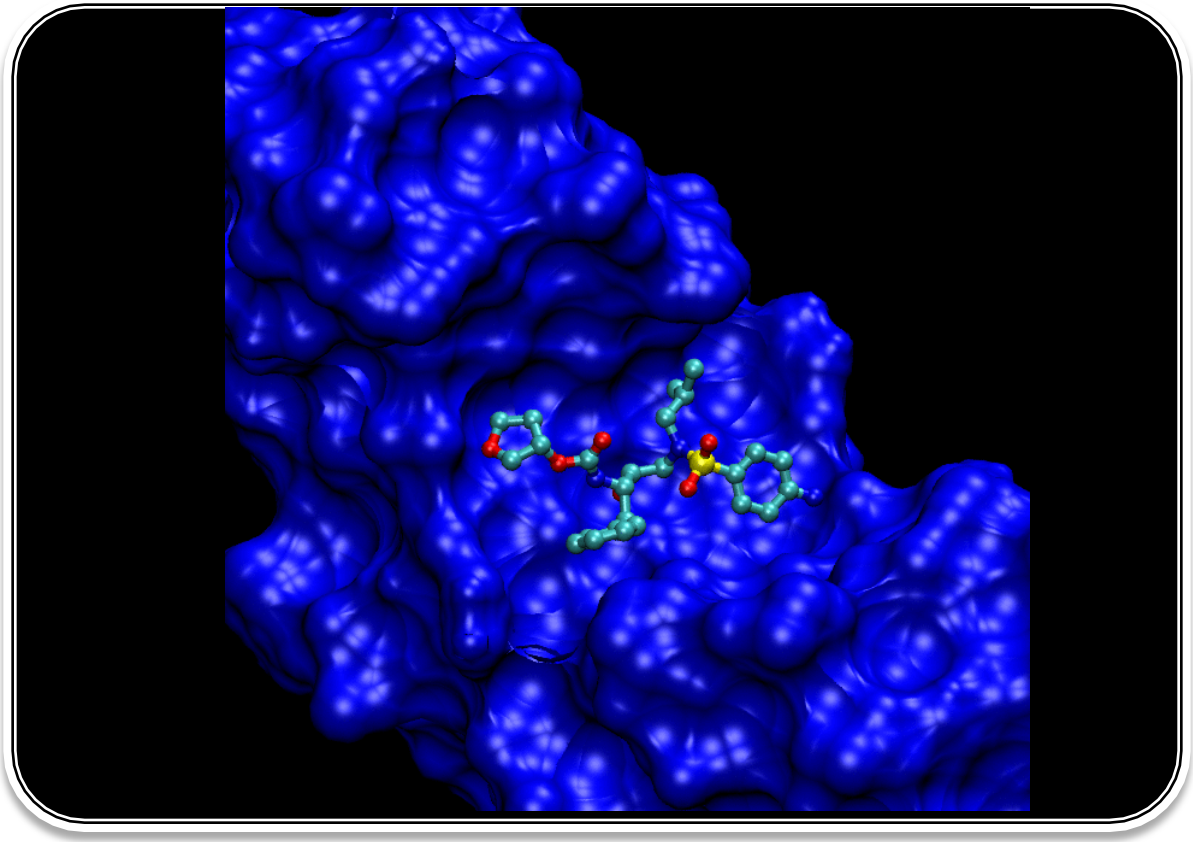

- Virtual Screening
- Scoring functions
- Hit to Lead Optimization

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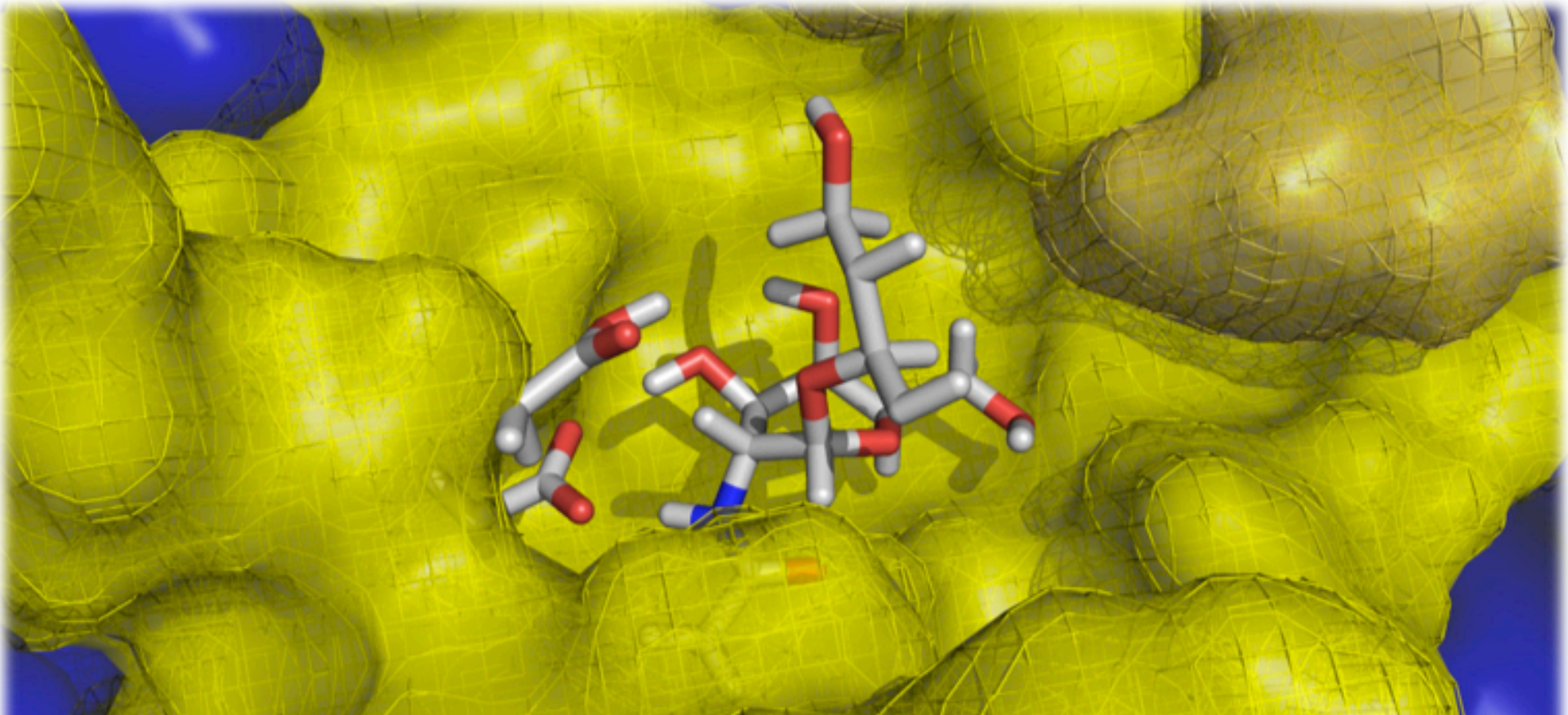

Course Outline

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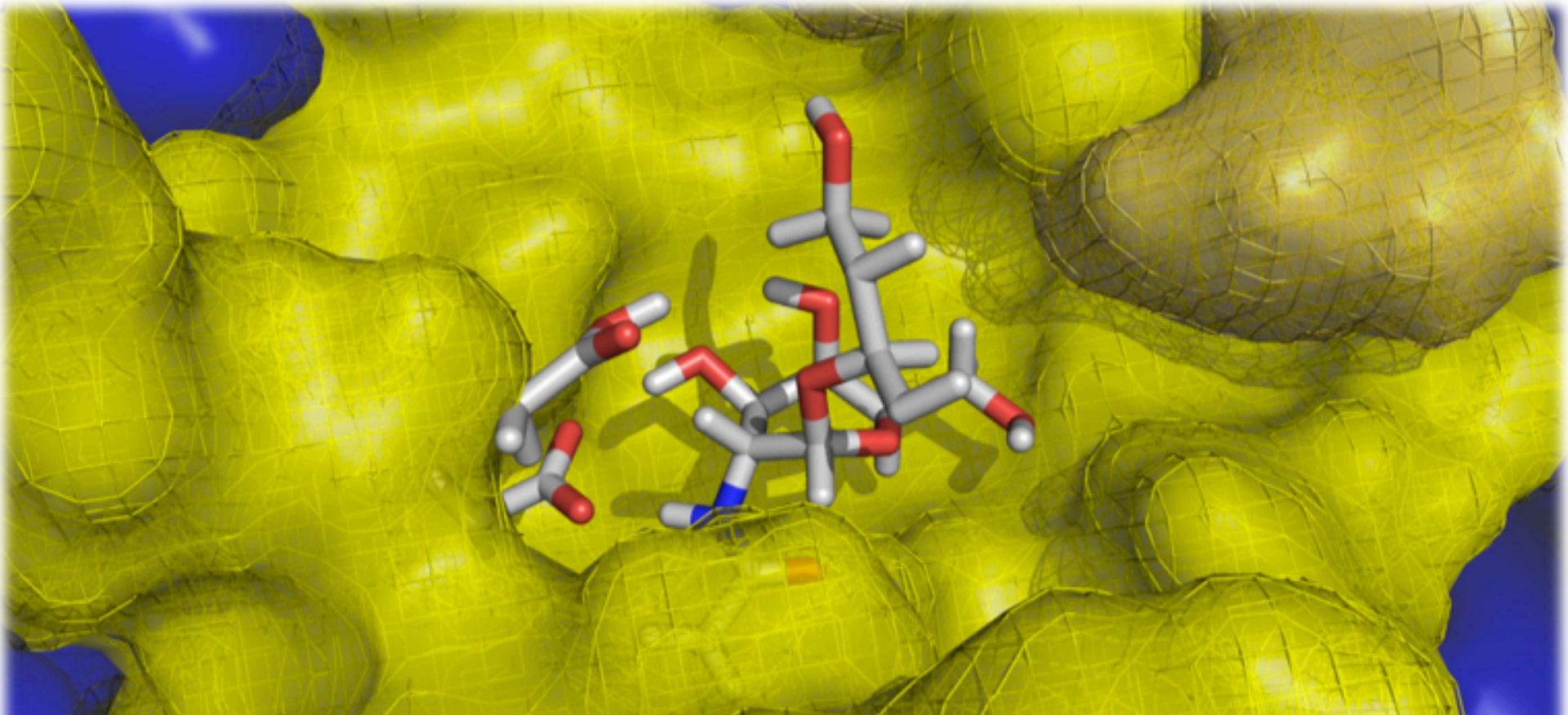

Course Outline

1. Challenges Facing the Simulation of Biomolecular systems

2. Enzymatic Catalysis.
2.1. Basics about enzyme catalysis.
2.2. Why are enzymes so difficult to simulate?
2.3. Determination the chemical mechanism of an enzymatic reaction.
2.4. Examples.

3. Molecular Dynamics/Free Energy Calculations.
3.1. Principles of molecular dynamics simulations.
3.2. Challenges for the simulation of biomolecules.
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4. Computational Mutagenesis.
4.1. The anatomy of protein interfaces.
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5. Molecular docking and Virtual Screening
5.1. Challenges for computational drug discovery.
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Computational Biochemistry, University of Porto

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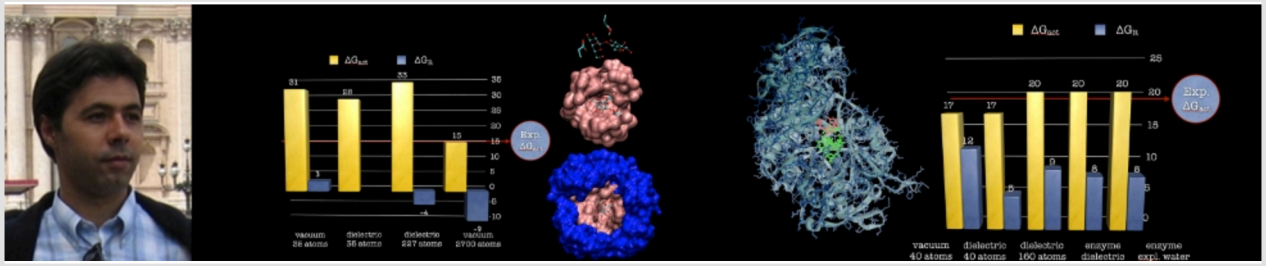

Academic

I have got a degree in chemistry at the University of Porto, Portugal, in 1993. After teaching chemistry in the high school for three years, I have started my PhD studies (1997), under the supervision of Prof. José Gomes. The subject of my work has been aimulations of liquid|liquid Interfaces and ion transfer across them. Upon finishing the PhD (2000) I become an Assistant Professor at the Chemistry Department of the Faculty of Sciences of Porto, Portugal, and later (2009) an associate Professor of the same Faculty. I teach courses for the degrees and MSc of Chemistry and of Biochemistry, mostly in the field of quantum chemistry, computational biochemistry and drug discovery.

Research

My research began with a brief passage through path integral Monte Carlo simulations. Afterwards I have spent a few (PhD) years dedicated to classical molecular dynamics simulations of liquid phase. My interests shifted towards biological systems after finishing my PhD, and I begun studying the catalytic mechanism of enzymes, first using Density Functional Theory and afterwards QM/MM methods. From then on, my research areas have broadened to encompass the energetics and dynamics of proteinsand membranes, molecular dynamics free energy calculations, computational mutagenesis (mostly alanne scanning mutagenesis), docking algorithms and software, and drug discovery.

Curso de PostGrado - Bioquímica Computacional

Universidad de Concepción, 18-19 Mayo 2015 - Diapositivas de las Charlas

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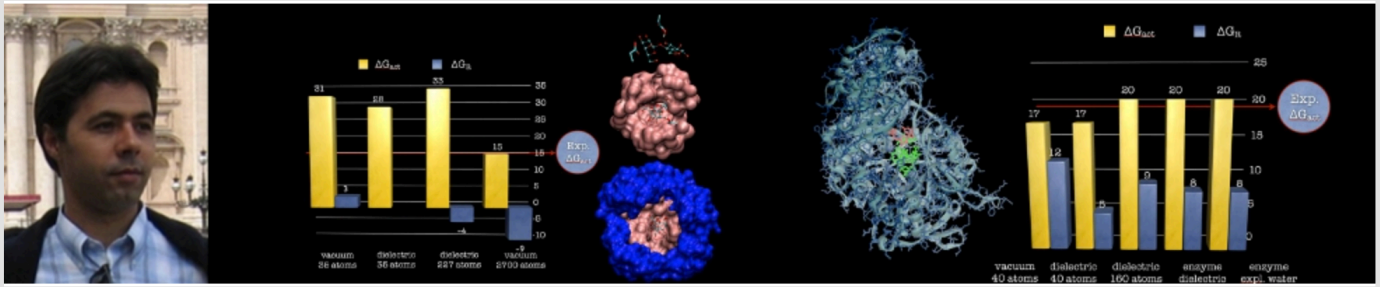

Curso de Bioquímica Computacional

Universidad de Concepción, 18-19 de Mayo de 2015 - Diapositivas de las Charlas

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