SCIENCESPRINGDAY

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Chemistry Department

Macromolecular Crystallography

xtal
Crystallography Group @ REQUIMTE
http://xtal.dq.fct.unl.pt/

requimte
rede de química e tecnologia

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- Aldino Viegas, *post-doc*
- Marino Santos, Ana Rita Cardoso, Hugo Correia, *PhD students*

Maria João Romão

Full Professor
Group leader

Since 2012, Full Professor

1998-2012, Associate Professor, FCT-UNL

2001, Habilitation, FCT-UNL

1989, PhD in Chemistry, IST

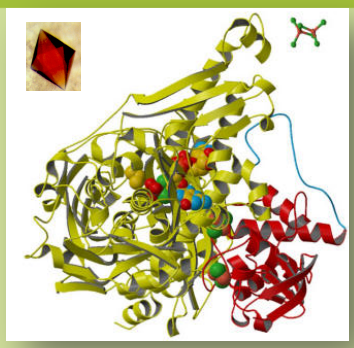
Objectives

A - Molybdenum enzymes – Molybdopterin-containing enzymes (Mo active site, associated to other electron transfer redox centers (Fe/S, hemes and flavins)).
Novel enzymes; reaction mechanisms; co-factor assembly and enzyme maturation.

B - The Cellulosome: a cellulose degradation machinery – Enzymatic and molecular recognition components of the Cellulosome assembly.

C - Interaction of CO releasing molecules (CORM) with plasma proteins.

D - New tools and methodologies for protein crystallization and optimization.



Molybdoenzymes

Methodology

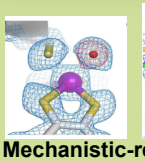
- Crystallographic methods using data collected at the ESRF, SLS, SOLEIL & DIAMOND SR sources.

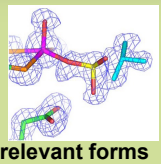
- SAXS data are being used as complementary information on complexes, protein-protein interactions and multiple enzyme conformations (ESRF & DESY).

- Structural data complemented by NMR data, in particular for defining a structural basis for substrate binding to CBMs (collab. NMR@REQUIMTE).

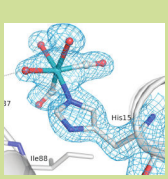
- Cryo-EM studies on mini-cellulosomes (collab.Madrid University).

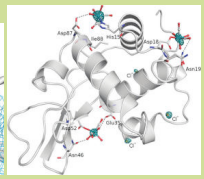
- Carbohydrate microarrays for ligand discovery; protein-protein microarrays.





Mechanistic-relevant forms





CORMs Reactivity toward Proteins

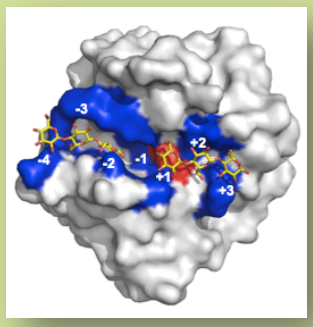
Expected Results

A- Novel crystal structures – first mammalian aldehyde oxidase crystal structures; Substrate and inhibitor-bound forms. Structures of complexes with broad impact for drug companies (e.g. Pfizer).
Structure-derived enzymatic mechanisms; Moco-binding and maturation mechanisms.

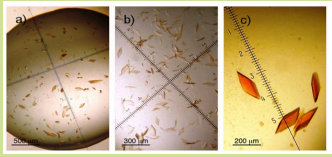
B- Novel enzymes and carbohydrate binding modes. Definition of molecular determinants for the function of the cellulosome machinery.

C- Mechanisms of drug binding to plasma proteins (model proteins; hemoglobin; transferrin; albumin) and in drug design strategies (collab. ITQB/Alfama (C.Romão).

D - The effect of ionic liquids in protein crystallization with model proteins as well as real cases; the use of nanoparticles as crystallization inducers (collab. ITQB (L.Rebelo)) and REQUIMTE (R. Franco)).



Cellulosomal Proteins & Enzymes



Crystallization with IL

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MINISTÉRIO DA EDUCAÇÃO E CIÊNCIA

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Univ. Potsdam; Magrio Negri Institute Milan