

Chemistry Department

Title

Macromolecular Crystallography Group



<http://xtal.dq.fct.unl.pt/>



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Post-doctoral Researcher
Publications:

https://www.researchgate.net/profile/Abhik_Mukhopadhyay/

Profile:
pt.linkedin.com/pub/abhik-mukhopadhyay/471555/149/

Objectives

Structural biology - Elucidation of Structure function relationship of proteins.

Characterization of protein ligand interaction – Structure guided drug design and development of novel metallodrugs .

Chemical crystallography – Organic and Inorganic molecules

Computational methods

Methodology

- Protein crystallography
- Protein expression and purification
- Small molecule crystallography
- X-ray diffraction methods
- Standard analytical and spectroscopic techniques
- Molecular dynamics and quantum mechanics calculations

Expected Results

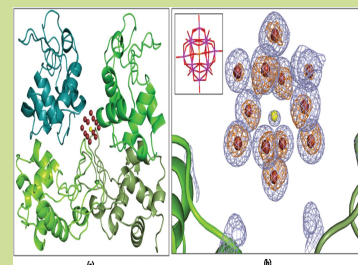
- High resolution crystal structures of proteins
- Crystal structures of target proteins with drug/ligand bound
- Crystal structures of small molecules (organic, inorganic and organometallic)
- Characterization of materials by x-ray diffraction methods
- Understanding thermodynamic properties of proteins by computational methods

Funding:

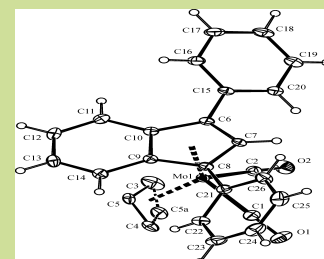
FCT postdoctoral grants SFRH/BPD/20142/2006 and SFRH/BPD/87725/2012



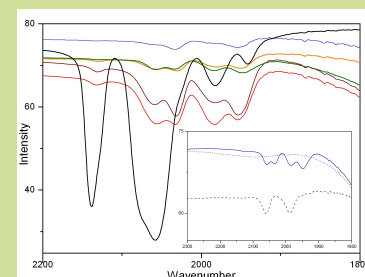
Bacterial Adenylate kinase



Keggin molecule inside lysozyme



Molybdenum complex



IR of protein-drug samples