SCIENCESPRINGDAY

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Chemistry Department

Cellulosome: a molecular machine

Macromolecular Crystallography Group

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

requimte rede de química e tecnologia

Ana Luísa Carvalho

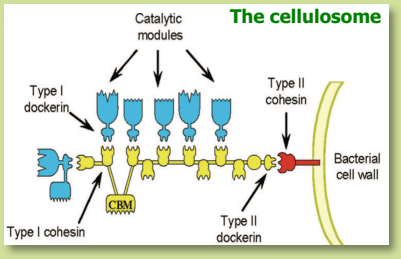
(Assistant Researcher, since 2003)

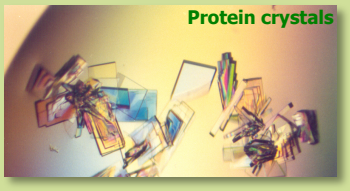
- Since 2012, Member of the Scientific Council of FCT-UNL
- 2002, PhD in Structural Biology
- 1998, Msc in Biophysics
- 1995, Graduation in App. Chemistry
- Citation metrics (WOK): Total articles in publication list: 25; Sum of the times cited: 543; Average citations per article: 24.68; h-index: 10

Objectives

The main focus of research is the functional and structural characterization of a megaDalton complex, the Cellulosome, present in some anaerobic bacteria and fungi. These organisms use the Cellulosome as a megadalton catalytic machine, to efficiently degrade cellulose and its derivatives, to ethanol.

The cellulosome comprises a molecular scaffold protein, whose cohesin domains interact with corresponding dockerin domains of glycoside hydrolases. These are also modular, comprising catalytic domains appended to one or more non-catalytic carbohydrate-binding modules (CBMs). Cellulosomes and CBMs play a central role in the enzymatic hydrolysis of plant cell wall polysaccharides.

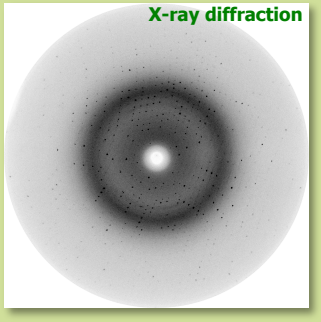


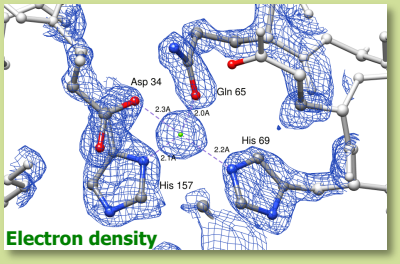


Methodology

To pursue my research interests, I have elected the X-ray Crystallography methodology, due to its power to provide detailed information at the atomic level. This allows me to specifically identify the structural determinants responsible for recognition of the different cellulosomal modules.

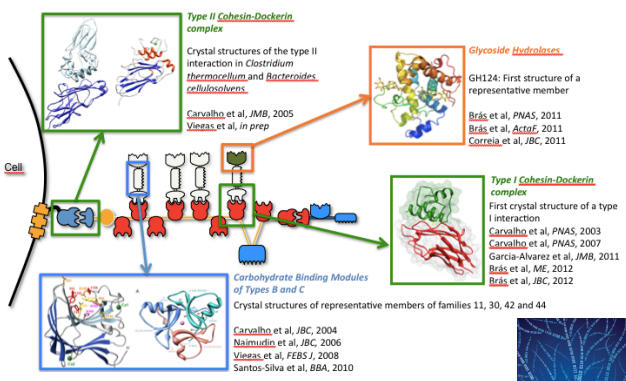
To achieve this, single crystals of each purified protein, isolated or in complex with other proteins or ligands, have to be produced. After X-ray diffraction experiments (either in the in-house X-ray equipment or in a synchrotron facility), the 3D structure solution is performed using the appropriate crystallographic methods. Once this is achieved, it is possible to visualize the resulting electron density map surrounding each atom in the structure.

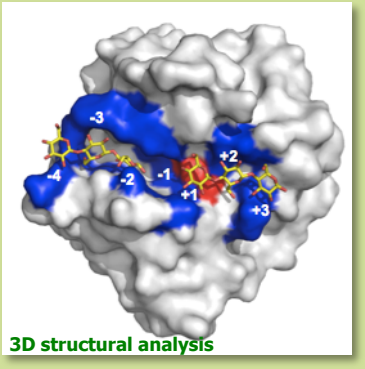




Expected Results

The observation of the electron density map allows us to unambiguously identify important residues in the binding interfaces, characterize atomic distances and surface contact areas.
The picture summarizes our progress in the structural characterization of the Cellulosome.





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