

# FÒRUM VIVES

Obrint **marcs**  
d'**intercanvi i reflexió**  
des de la **universitat**

## TÍTOL DE LA **PONÈNCIA** EN **UNA O DUES LÍNIES**

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Nom i cognoms  
Càrrec i Universitat

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**Xarxa Vives**   
d'universitats

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Universitat Abat Oliba CEU. Universitat d'Alacant. Universitat d'Andorra. Universitat Autònoma de Barcelona. Universitat de Barcelona. Universitat de Girona. Universitat de les Illes Balears. Universitat Internacional de Catalunya. Universitat Jaume I. Universitat de Lleida. Universitat Miguel Hernández d'Elx. Universitat Oberta de Catalunya. Universitat de Perpinyà Via Domitia. Universitat Politècnica de Catalunya. Universitat Politècnica de València. Universitat Pompeu Fabra. Universitat Ramon Llull. Universitat Rovira i Virgili. Universitat de Sàsser. Universitat de València. Universitat de Vic · Universitat Central de Catalunya.

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◆ 01 Text

◆ 02 Text

◆ 03 Text

# SUMARI

◆ 01 Text

◆ 02 Text

◆ 03 Text

◆ 04 Text

◆ 05 Text

# **Teaching Structural Bioinformatics at undergraduate level**

# BACKGROUND HISTORY

## ◆ Objectives of Structural Biology

1. Introduction to the basic molecular principles of biophysics
2. Structural principles of biopolymers: proteins and DNA
3. Methods for determining the 3D structure of biomolecules.
4. Relationship between structure, function and sequence of proteins.
5. Molecular simulation of proteins and DNA

## ◆ Competences of Structural Biology

1. Recognizing structural patterns of biomolecules and drugs
2. Relationship between 3D structure and function of biomolecules
3. Handling basic software and datasets of sequences and structures of biomolecules
4. Knowledge on experimental methods to analyze structures and biological systems.

# BACKGROUND HISTORY

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Printed in U.S.A.

BIOCHEMISTRY AND MOLECULAR BIOLOGY EDUCATION  
Vol. 31, No. 6, pp. 386-391, 2003

## Articles

### Teaching Structural Bioinformatics at the Undergraduate Level

Received for publication, July 19, 2002

**Nuria B. Centeno, Jordi Villà-Freixa, and Baldomero Oliva†**

*From the Laboratori de Bioinformàtica Estructural (GRIB-IMIM), Departament de Ciències Experimentals i de la Salut, Universitat Pompeu Fabra, 08003 Barcelona, Spain*

**Understanding the basic principles of structural biology is becoming a major subject of study in most undergraduate level programs in biology. In the genomic and proteomic age, it is becoming indispensable for biology students to master concepts related to the sequence and structure of proteins in order to develop skills that may be useful in a wide range of applications. Within this context, this article shows a scheme for teaching structural biology based on hands-on computer approaches, including computational genomics, and structural bioinformatics tools. The students learn to use most of the leading computer programs available for the complete path that goes from sequence to structure and eventually function. During the course, they are taught to build models of proteins based on sequence and structure information. The students are also provided with a critical point of view on automatic procedures and learn to discern between likely and unlikely structures of their final models.**

**Keywords:** Structural biology; homology modeling; computer simulations.

# BACKGROUND HISTORY

- ◆ Evaluation

Theory: Multiple Choice + Assay (40%)

Practical (30%)

Presentation (30%)

- ◆ Competences acquired by presentation

Group management

Technical (IT)

Oral communication

Write and summarize

All members of a team have to present

# BACKGROUND HISTORY

- ◆ Already in 2002-2003 many presentations were in English

## **Undergraduated students projects (2003-2004)**

Transcription factors - Marta Arcabell, Dora Cano, Blanca Puchau and Verónica Rodilla [PPT file].

Chaperones - Anaís Estrada, Edurne Gallastegui, Mercè Garí, Marta Guerra and Jordi Milà [PPT file].

Rhodopsin - Laia Font, Mireia Gimeno, Maria Larroy, Paola Paoletti and Laura Vicente [PDF file][PPT file].

Cyclin-dependent kinases - Yolanda Acosta, Naiara Aquizu, Elisabeth Castellanos, Ana Corrionero and María Ruiz [PPT file].

Nuclear magnetic resonance - Míriam Onrubia, Laura Plaza and Patricia Resa [PPT file].

High resolution electronic microscopy - Esther Melo, Susagna Sastre, Ingrid Sebastià, Roser Soler and Lidia Tubert [PPT file].

Circular dichroism and infra-red - Elena Echarte and Marta Mancebo [PPT file].

X-ray crystallography - Marta Costa, Guillem Galofré and Meritxell Pellicer [PPT file].

Ribosome - Jaume Bonet, Melquíades Calzado, Ana Campillo and Laura Ortet [PPT file].

Spliceosome - Manuel Beltran, Javier Garcia, Gerard Ill and Xavi Jalencas [PPT file].

Nucleosome - Anna Garcia-Elias, Marta Gimenez, Alba Llop and Mireya Plass [PPT file].

RNA polymerase - Ana Cuadrado, Montserrat Roura, Noemí de los Santos and Marta Valiente [PPT file].

RNA fold - Neus Romo, Jesús Sánchez, Anna Serra and Núria Torras [PDF file][PPT file].

## **Undergraduated students projects (2002-2003)**

DNA Structure - Laura Aguilera, Cristina Carreño, Irene Oliver and Blanca Reyes.

Helix-turn-helix and transcription factors - Alexandra Ballester, Patricia Gordillo and M. del Carmen Molina.

DNA polymerases - Mathieu Lichtenstein, Martin Nolla, Neus Rafel and Vidalba Rocher.

Aminoacyl-t-RNA synthase - Montserrat Ferrer, Sara Fernandez, Cristina Fuentes, Eva Lambea and David Dominguez.

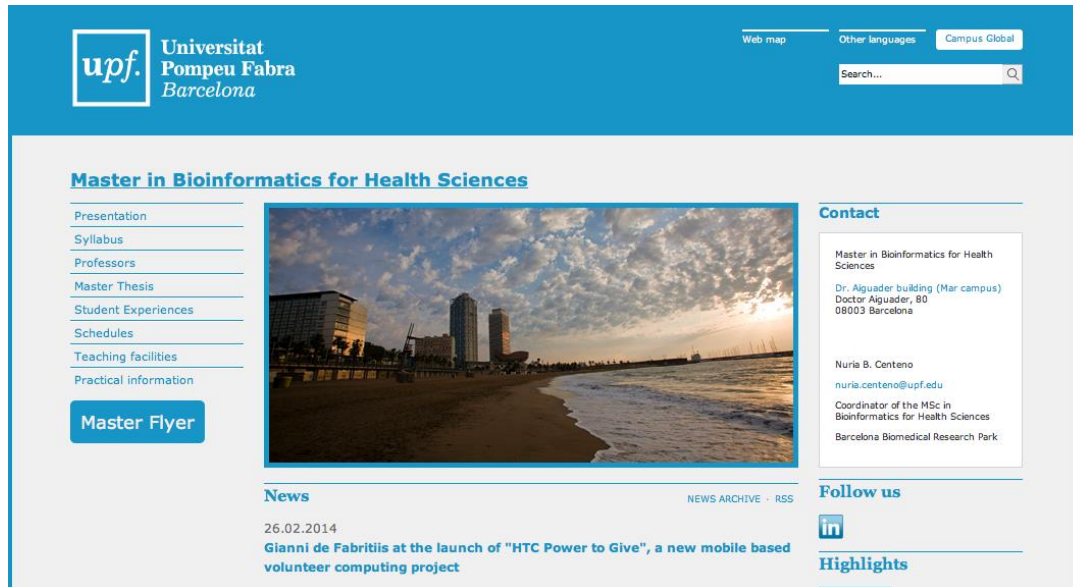
Ribosome - Silvia Bea, Marta Beltran, Ana Igea, Montserrat Sole and Iris Uribesalgo.

Enzymes with NAD motifs - Anna Boix, Aitzol Illarramendi, Ricard Perez, Ferran Pons and Roser Zaurin.



# BACKGROUND HISTORY

- ◆ 2004-2005 starts the Master of Bioinformatics for Health Sciences  
ALL COURSES WERE IN ENGLISH



The screenshot shows the website for the Master in Bioinformatics for Health Sciences at Universitat Pompeu Fabra. The header includes the UPF logo and navigation links for 'Web map', 'Other languages', and 'Campus Global'. A search bar is also present. The main content area features a navigation menu on the left with options like 'Presentation', 'Syllabus', 'Professors', 'Master Thesis', 'Student Experiences', 'Schedules', 'Teaching facilities', and 'Practical information'. A prominent blue button labeled 'Master Flyer' is located below the menu. The central part of the page displays a large image of a beach at sunset. To the right of the image is a 'Contact' section with the following text: 'Master in Bioinformatics for Health Sciences', 'Dr. Alguader building (Mar campus)', 'Doctor Alguader, 80', '08003 Barcelona', 'Nuria B. Centeno', 'nuria.centeno@upf.edu', 'Coordinator of the MSc in Bioinformatics for Health Sciences', and 'Barcelona Biomedical Research Park'. Below the image is a 'News' section with a date of '26.02.2014' and a headline: 'Gianni de Fabritiis at the launch of "HTC Power to Give", a new mobile based volunteer computing project'. The page also includes 'Follow us' and 'Highlights' sections.

# BACKGROUND HISTORY

- ◆ 2004-2005 starts the Master of Bioinformatics for Health Sciences  
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## Syllabus

The master provides different areas of specialization depending on the election of optional subjects:

- **Genome Bioinformatics**  
Automatic analysis, alignment, comparison and annotation of biological sequences; analysis of genome evolution and variation; molecular biology databases.
- **Structural Bioinformatics**  
An introduction to experimental methods used in determining the structure of biomolecules, protein structure prediction and biomolecular systems simulation.
- **Systems Biology**  
The description of biological networks and protein and metabolic gene network modelling. Emphasis in both topological aspects of networks and their dynamical behavior.
- **Pharmacoinformatics**  
Molecular library management and virtual screening, computer assisted drug design and quantitative modelling of structure-activity relationships (QSAR and 3D-QSAR).
- **Biomedical Computing**  
Clinical and healthcare information systems, biomedical imaging analysis, studying genotype-phenotype relationships and IT support systems for healthcare decision making.

# BACKGROUND HISTORY

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## Teaching facilities

The building, which completes the complex of which Hospital del Mar is part, had been built in 1991, taking advantage of the celebration of the 1992 Olympic Games, to house the Municipal Institute of Medical Research (IMIM), which was accredited by the International Olympic Committee (IOC) as an antidoping laboratory.

This narrow, 10-metre wide building measures 140 m in length and is arranged in the shape of a circumferential arch upon the axis of the pavilions that form the Hospital rooms. The renovation of the building for university purposes dates from 1998, the year in which it accommodated the new Biology studies. It was carried out by architects Josep Benedito, Frederic Crespo and Ramon Valls. The renovated surface area totals 3,350 m<sup>2</sup>.

At present, studies belonging to the field of health sciences are taught here. This building together with the Barcelona Biomedical Research Park (PRBB), form the [University's Mar campus](#).



Databases are free  
accessible in internet

Programs are Open Source

SBI = Structural Biology

upf. Universitat Pompeu Fabra Barcelona

Web map Other languages Campus Global

Search...

## Master in Bioinformatics for Health Sciences

Home > Student Experiences

- Presentation
- Syllabus
- Professors
- Master Thesis
- Student Experiences
- Schedules
- Teaching facilities
- Practical information

### Student Experiences

**Miquel Duran (2012):** "As a trained organic chemist and mathematics enthusiast, I had to bear the frustration of not seeing a direct impact of my work on the lives of people. Through the Master's in Bioinformatics, I was smoothly introduced into timely biological problems, and aided in recycling my previous knowledge into cutting-edge research"

**David Mosén (2011):** "The Master in Bioinformatics was a great opportunity to apply what I learnt during my engineering degree in Computer Science to an exciting and constantly evolving field. On top of that, the demanding courses and the knowledge from a heterogeneous group of students were extremely rewarding. Still, I had time to have fun and enjoy the picturesque Barceloneta quarter"

[www.vives.org](http://www.vives.org)

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# ONLINE MATERIAL

## Structural Bioinformatics Lab



RESEARCH PROGRAMME ON BIOMEDICAL INFORMATICS



UNIVERSITAT POMPEU FABRA



Parc de Salut MAR Barcelona

Institut Hospital del Mar d'Investigacions Mèdiques

Home Research Members Courses

### Main Menu

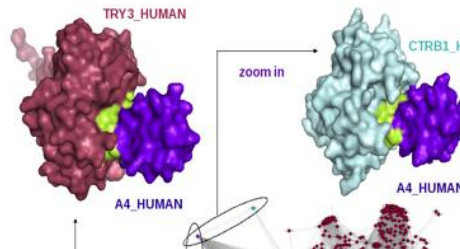
- ▶ [Home](#)
- ▶ [Research](#)
- ▶ [Members](#)
- ▶ [Courses](#)

### Structural Bioinformatics Lab

The Structural Bioinformatics Laboratory (SBI) is integrated in the Research Programme on Biomedical Informatics (GRIB), which is affiliated with the Pompeu Fabra University (IMIM-Hospital del Mar), and it is located at the Barcelona Biomedical Research Park.

Our lab is dedicated to conduct state of the art research in Computational Bioinformatics. Our research lines include:

- Fold prediction
- Protein docking
- Function prediction and annotation
- Description of the dynamical properties of biomolecules



## Structural Bioinformatics Lab



RESEARCH PROGRAMME ON BIOMEDICAL INFORMATICS



UNIVERSITAT POMPEU FABRA



Parc de Salut MAR Barcelona

Institut Hospital del Mar d'Investigacions Mèdiques

Home Research Members Courses

### Main Menu

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- ▶ [Research](#)
- ▶ [Members](#)
- ▶ [Courses](#)
- ▶ [M. Sc. students projects](#)
- ▶ [Undergraduated students projects](#)

### M. Sc. students projects (2009-2010)

- [Chaperones and chaperonins](#) - Marta Bleda and Xavier Lucas [PPT file].
- [G protein-coupled receptors](#) - Javier Prado and Ramon Guixà [PPT file].
- [Hedgehog family](#) - Oriol Senan, Alexandros Pittis and Amadís Pagès [PPT file].
- [Coagulation serine proteases](#) - Daniel Costa, Leo Rib and Oscar Mora.

### M. Sc. students projects (2008-2009)

- [DcpS family](#) - Salvador Jesús Capella Gutiérrez, Juan Ramón Meneu Hernández and Rut Carolina Morata Gil [PPT file].
- [AIM2 homology modeling](#) - Dmitry Repchevsky [PDF file].
- [Cys-loop family](#) - Isabel Fernández and Elena Escubedo [PDF file (part 1)][PDF file (part 2)].

### M. Sc. students projects (2005-2006)

- [Alcohol dehydrogenase](#) - Iñaki Martínez de Ilarduya, Lorena Pantano Rubiño and Albert Mascarell Creus [PPT file].
- [Nuclear receptors](#) - Ferran Briansó, Elisenda Feliu and Núria Queralt [PDF file].
- [SH2 domain](#) - Núria Bonifaci and Francesc Estanyol [PPT file].
- [TIM barrel](#) - Teresa Páramo, Miguel Hernández and Diana Garzón [PPT file].

<http://sbi.upf.edu>

# SELECTING A COURSE TO BE IN ENGLISH

- ◆ **01** Material, sources and experience from the master
- ◆ **02** International teachers: Jana Selent (Germany), Gianni de Fabritiis (Italy)
- ◆ **03** Mathematical language, programming languages and IT terms
- ◆ **04** High percentage of the course are practices and seminars with computers
- ◆ **05** Presentations of students are in English, in order to evaluate oral competences

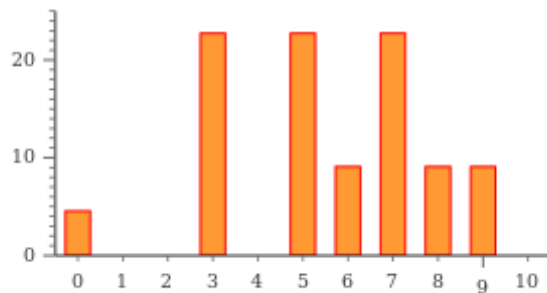
## ***IN SITU***

- ◆ **01** Questions by the students are accepted in English, Catalan or Spanish
- ◆ **02** Individual help in practices can be in English, Catalan or Spanish
- ◆ **03** Questions of essay are in English and Catalan
- ◆ **04** Answers in essay are accepted in English, Catalan or Spanish

# THE RESULTS: 2011-2015

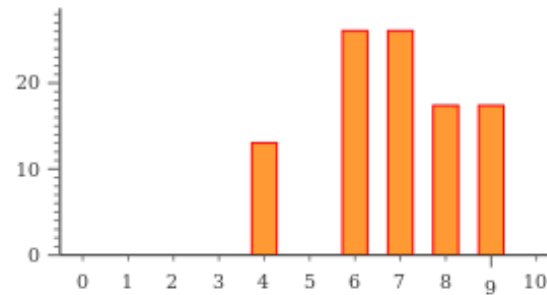
2012

P4 : L'assignatura en el seu conjunt



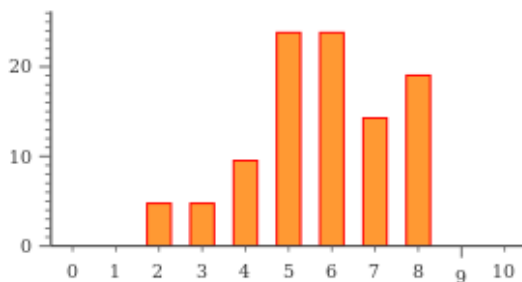
2013

P4 : L'assignatura en el seu conjunt



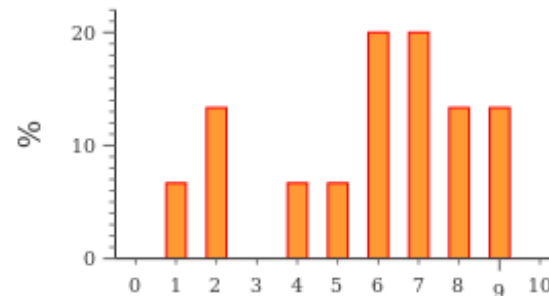
2014

P4 : L'assignatura en el seu conjunt



2015

P4 : L'assignatura en el seu conjunt



Degree of satisfaction of the students with the course of Structural Biology

# THE RESULTS: 2012

Selected comments from the students

2011-2012 (first year). **99% negative** comments for having the course in english

*Crec que és una assignatura bastant complicada i el fet de fer-la en anglés augmenta el seu grau de dificultat considerablament.*

I think this is a difficult course and having it in English considerably increases its difficulty

*Per una banda, el fet de l'idioma ha sigut una mica limitant. La nova normativa de tot en anglés (a BE) ha suposat un repte; i mentre **en activitats com el treball m'ha semblat una oportunitat**, trobo que limitaven molt les classes teoriques ja que no s'entenien be les explicacions.*

On the one hand, the language has been a little impairment. The new rule of having all the lectures (of SB) in English was a challenge, while **for activities such as the presentation this was an opportunity**, I think it was a handicap to understand the explanations on the lectures of theory



# THE RESULTS: 2013

Selected comments from the students

2012-2013 (second year). Only **40% of negative** comments blamed the language

*És una assignatura complicada, i el fet de que sigui en anglés ho fa encara més.*

This is a complicated course, and being in English makes it worst

*Estic d'acord que l'anglés en ciència i en general actualment és imprescindible, però trobo que fer TOTA l'assignatura en anglés no és necessari.*

I agree that English in science, and in general nowadays, is essential, but I think that having the whole course in English was not necessary

# THE RESULTS: 2014

Selected comments from the students

2013-2014 (**third** year). Many **positive** comments on having lectures in English, Complaints on the choice (structural biology) and the English level of the teachers

*Sens dubte algun, l'anglès és l'idioma de les ciències i per aquest motiu no trobo malament fer algunes assignatures de la carrera en aquest idioma*

I have no doubts that English is the language for sciences. Therefore, it's OK to have some subjects of Biology in English.

*Entenc que és angoixant trobar-te amb una assignatura que de per si complicada, a més sigui en anglès.*

It's stressing to have one of the most complex subjects in English.

*No entenc com l'assignatura més difícil de la carrera estigi en anglès, el qual no és l'idioma que dominen els profes*

I don't get how the most difficult subject of Biology is in English, which is not the native language of the teachers

*Crec que aquesta assignatura hauria de ser en català o castella, ja que els professors són d'aquí*

I think this subject should be in Catalan or Spanish, because the teachers are local

# THE RESULTS: 2015

Selected comments from the students

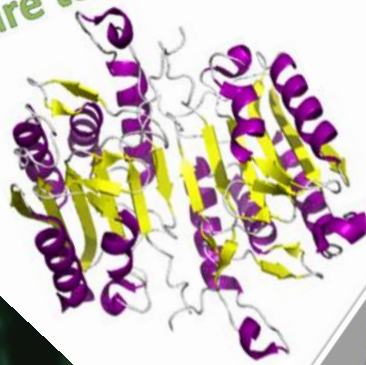
2015-2016 (last year). Still complaints on the choice (structural biology), potential **discouragement to make questions?**

*El fet de ser en anglés disuadeix de fer preguntes a les classes teòriques per vergonya (m'incloc), i has de pressionar força al professor, preguntant-li en català o castellà, per que et respongui enj algun d'aquests dos idiomes*

English in the lectures of theory discourages the students to ask in class. We have to insist by questioning in Catalan or Spanish in order to get an answer in either of both.

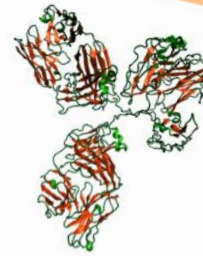
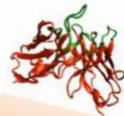
# EXAMPLES

## Structure to death: CASPASES



## IMMUNOGLOBULINS

Few conformations for amount of diversity

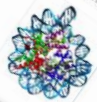


Maria Bargués, Marta Jarque and Sara Martínez

## STRUCTURAL BIOLOGY OF THE PROTEASOME

## THE NUCLEOSOME

Structural Biology Project  
Natalia Barbó, Ivan Bilazunco, Miran Bravo, Anis Garcia



## DNA polymerases

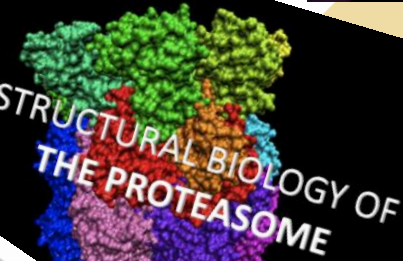
Natalia Cuiell  
Laura Domingo  
Joan Gil  
Javier Sebastián  
Structural biology 2014



## STRUCTURAL BIOLOGY OF THE PROTEASOME

Ricard Argelaguet  
Clàudia Fontserè  
Silvia Galan

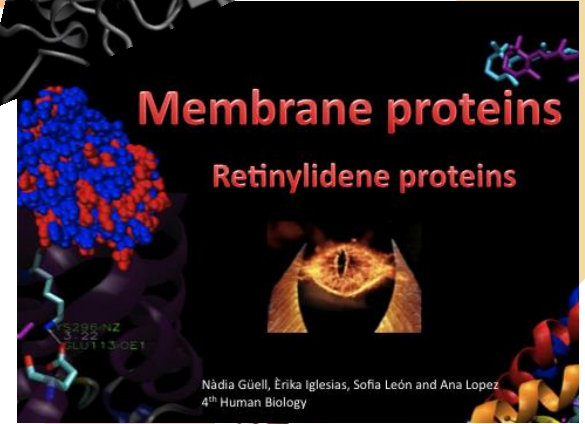
UPF  
11/03/2014



## Membrane proteins

## Retinylidene proteins

Nàdia Güell, Èrika Iglesias, Sofia León and Ana Lopez  
4<sup>th</sup> Human Biology



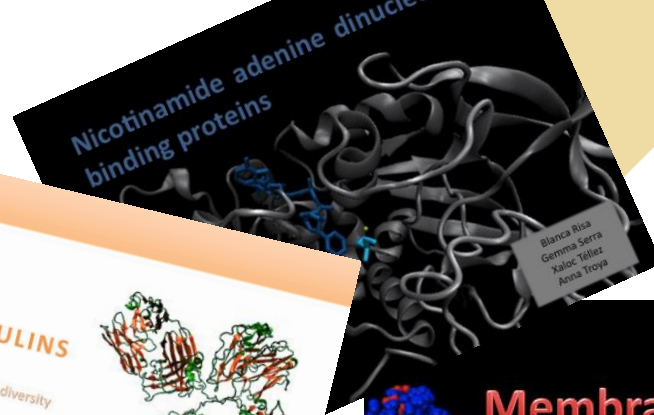
## The Ubiquitylation System

Prieto M, Riquelme A, Urbina L, Vives A  
Structural Biology 2014



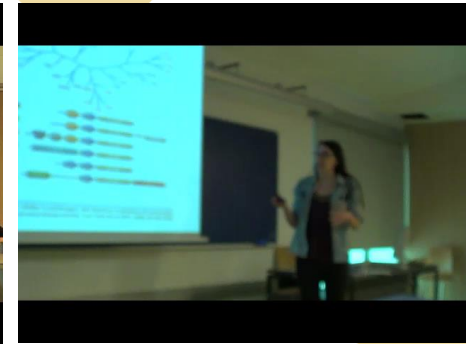
## Nicotinamide adenine dinucleotide binding proteins

Blanca Riza  
Gemma Serra  
Xaloc Tellez  
Ariana Troya

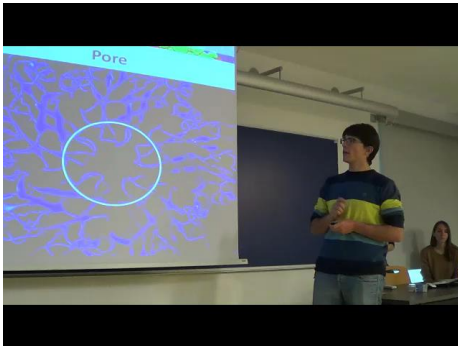
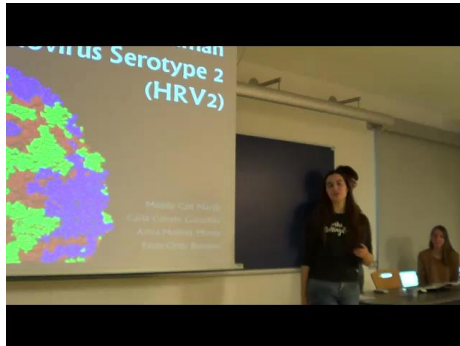


# EXAMPLES

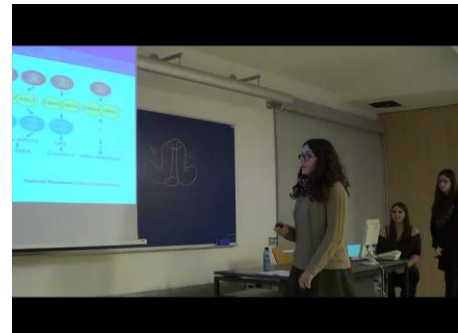
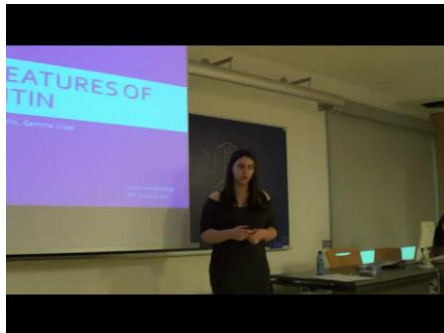
## Tyr-Kinase SRC



## Virus capsides (HRV2)



## Ubiquitins



# FÒRUM VIVES

Obrint **marcs**  
d'**intercanvi i reflexió**  
des de la **universitat**

**Xarxa Vives**  
d'universitats 

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Universitat Abat Oliba CEU. Universitat d'Alacant. Universitat d'Andorra. Universitat Autònoma de Barcelona. Universitat de Barcelona. Universitat de Girona. Universitat de les Illes Balears. Universitat Internacional de Catalunya. Universitat Jaume I. Universitat de Lleida. Universitat Miguel Hernández d'Elx. Universitat Oberta de Catalunya. Universitat de Perpinyà Via Domitia. Universitat Politècnica de Catalunya. Universitat Politècnica de València. Universitat Pompeu Fabra. Universitat Ramon Llull. Universitat Rovira i Virgili. Universitat de Sàsser. Universitat de València. Universitat de Vic · Universitat Central de Catalunya.