

# Workshop

## Bioinformatics Tools for Protein Structure, Disorder and Interaction Analysis

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November 21st-23rd, 2017 9:00 - 18:00 hrs  
Universidad Nacional de San Martín and IIB-INTECH

### Organizers:

*Toby Gibson (EMBL, Heidelberg) and Lucía Chemes (IIB-UNSAM)*

**Course description:** Cellular signaling is carried out by dynamic multi-molecular complexes that may coalesce, split apart, relocate, gain and lose individual regulatory proteins. The state of these complexes can be switched by post translational modifications, and once the signal has been transmitted and complexes are no longer needed, they can be fully dismantled. Despite their central importance, for the most part these regulatory complexes are poorly understood. A protein's modular architecture determines the types of interactions it can establish. Many of these interactions are mediated by flexible or “natively unstructured” regions that code important functions through modular elements termed “linear motifs”. This Workshop will present a variety of bioinformatics tools that can be used to explore a protein's functional architecture as a tool towards predicting and testing its possible functions and interactions.

### Teaching team:

Toby Gibson (EMBL, Heidelberg)  
Lucía Chemes (IIB-UNSAM)  
Hugo Samano (EMBL, Heidelberg)  
Nicolás Palopoli (UNQ)  
Juliana Glavina (FCEN, UBA)

### Speakers:

Toby Gibson (EMBL, Heidelberg)  
Lucía Chemes (IIB-UNSAM)  
Gonzalo de Prat Gay (FIL, IIBBA)  
Ignacio Sánchez, (FCEN, UBA)

## SCHEDULE

<b>Tuesday, November 21<sup>st</sup></b>
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9:00-9:30 am: Registration at IIB
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9:30 am-12:30 pm. Course Intro (Aula 2 IIB)

9:30-10:15 am: **Welcome.** Presentation of teachers and students.

10:15-11:00 am: **Course Introduction** - Lucia Chemes.

**Coffee Break 11:00-11:30 am at IIB**

11:30-12:30: Lecture by Toby Gibson. Title: *warm up and experimental tips*.

**12:30-1:30 pm: Lunch on own**

1:30-3:00 pm: Practical Session 1: Protein databases and related annotation resources (UNIPROT, Pfam). Aula LC4, Edificio Tornavías

**Coffee Break 3-3:30 pm**

3:30-5 pm: Practical Session 2: Tools and resources for the analysis of the structural architecture of a protein (PDB, InterPro, TMHMM). Aula LC4, Edificio Tornavías

<b>Wednesday, November 22<sup>nd</sup></b>
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9:00-11:00 am: Practical Session 3: Analysis and prediction of intrinsically disordered regions (JPred, IUPRED, Anchor, Disprot, MobiDB). Aula LC2, Edificio Tornavías

**Coffee break 11-11:30 am at IIB**

11:30hs-12:30hs: Lecture by Toby Gibson. Title: *Complexity of PPIs*. (Auditorio IIB)

**12:30-1:30 pm: Lunch on own**

1:30 - 3:30 pm: Practical Session 4: Understanding linear motifs & intrinsically disordered regions (ELM, SLiMSearch, ProViz). Aula LC4, Edificio Tornavías

**Coffee Break 3:30-4pm**

4:00-6:00 pm: Practical Session 5: Revealing interactive features in protein multiple sequence alignments with Jalview. Aula LC4, Edificio Tornavías

<b>Thursday, November 23<sup>rd</sup></b>
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9:00-10:45 am: Talks (Auditorio IIB)

Ignacio Sánchez. Talk title: *Bioinformatics approaches to the study of IDPs*.

Gonzalo de Prat Gay. Talk title: *Experimental investigation of IDPs*.

**Coffee break 10:45-11:15 am at IIB**

11:15-1:15 pm: Practical Session 6: Visualizing protein structures and interaction interfaces with UCSF Chimera. Aula LC2, Edificio Tornavías

**1:15-2:00 pm: Lunch on own**

2:00-3:15 pm: Practical Session 7: Protein association networks with STRING. Protein networks (Reactome/KEGG). Aula LC4, Edificio Tornavías

**Coffee Break 3:15-3:45 pm**

3:45-5:00 pm: Practical Session 8: Practical with you own protein and QA session. Aula LC4, Edificio Tornavías

5:00-5:30 pm: Discussion and feedback.
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## SCHEDULE

	TUESDAY 21	WEDNESDAY 22	THURSDAY 23	
09:00 AM	9:00-9:30 <i>Arrival and Registration</i>	<b>PRACTICAL SESSION 3 (LC2)</b> 9:00 - 11:00 AM  Analysis and prediction of intrinsically disordered regions  <i>JPred</i> <i>IUPRED</i> <i>Anchor</i> <i>Disprot</i> <i>MobiDB</i>	<b>TALKS (Auditorio IIB)</b> 9:00 - 10:45 AM  <b>TALK 1</b> <i>Bioinformatics approaches to the study of IDPs</i> <i>Ignacio Sánchez</i>  <b>TALK 2</b> <i>Experimental investigation of IDPs</i> <i>Gonzalo de Prat Gay</i>	
09:15 AM	<b>WELCOME: IIB Aula 2</b> 9:30 - 10:15 AM		<b>PRACTICAL SESSION 6 (LC2)</b> 11:15 - 1:15 AM  Visualizing protein structures and interaction interfaces  <i>UCSF Chimera</i>	
09:30 AM	Presentation of teachers and students. Aula 2 IIB			
09:45 AM				
10:00 AM				
10:15 AM	<b>LECTURE 1: COURSE INTRODUCTION</b> 10:15 - 11:00 AM			<i>Coffee Break</i> 10:45 - 11:15 AM (IIB-INTECH)
10:30 AM	Lucia Chemes			
10:45 AM				
11:00 AM				
11:15 AM	<i>Coffee Break</i> 11:00 - 11:30 AM (IIB-INTECH)			<b>PRACTICAL SESSION 7 (LC4)</b> 2:00 - 3:15 PM  Protein association networks <i>STRING</i>  Protein networks <i>Reactome/KEGG</i>
11:30 AM	<b>LECTURE 3</b> 11:30 - 12:30 PM  <i>Complexity of PPIs</i> Toby Gibson  (Auditorio IIB)			
11:45 AM				
12:00 PM				
12:15 PM	Toby Gibson	<i>Lunch on own</i> 1:15 - 2:00 PM		
12:30 PM	<i>Lunch on own</i> 12:30 - 1:30 PM			
12:45 PM				
01:00 PM				
01:15 PM				
01:30 PM		<b>PRACTICAL SESSION 1 (LC4)</b> 1:30 - 3:00 PM	<b>PRACTICAL SESSION 8 (LC4)</b> 3:45 - 5:00 PM  Practical with you own protein and QA session.	
01:45 PM	<b>PRACTICAL SESSION 4 (LC4)</b> 1:30 - 3:30 PM  Understanding linear motifs & intrinsically disordered regions  <i>ELM</i> <i>SLiMSearch</i> <i>ProViz</i>			
02:00 PM		<b>PRACTICAL SESSION 5 (LC4)</b> 4:00 - 6:00 PM  Revealing interactive features in protein multiple sequence alignments  <i>Jalview</i>		
02:15 PM				
02:30 PM				<i>InterPro</i> <i>RCSB-PDB</i> <i>TMHMM</i>
02:45 PM				
03:00 PM				
03:15 PM	<i>Coffee Break</i> 3:00 - 3:30 PM	<i>Discussion and feedback</i>		
03:30 PM	<b>PRACTICAL SESSION 2 (LC4)</b> 3:30-5:00 PM  Tools and resources for the analysis of the structural architecture of a protein			
03:45 PM				
04:00 PM				
04:15 PM				
04:30 PM				
04:45 PM				
05:00 PM				
05:15 PM				
05:30 PM				

AULAS LC2 y LC4: Tornavias

CAMPUS MAP

