

## **GBS 747 - Special Topics (Structural Bioinformatics) – CRN 43202**

### **Purpose:**

The purpose of this course is to provide an introduction to main topics in computational structural biology/structural bioinformatics. Specifically, the participants are exposed to practical use of standard web available resources and tools for the analysis and comparison of macromolecular three-dimensional structures. A successful participation includes the development and implementation of computational tools and/or pipelines for large-scale studies in structural bioinformatics. 3.00 Credit hours

**Instructor:** Emidio Capriotti, PhD

**Levels:** Graduate

**Schedule Types:** Lecture

**Type:** Class

**Time:** 10:00 a.m. – 1:00 p.m.

**Days:** Mondays, Tuesdays, Thursdays and Fridays

**Where:** West Pavilion Conference Center, Room G.

**Date Range:** April 8 - May 2, 2014

Graduate Biomedical Sciences (GBS 747) Program and Pathology (PAT 727)

### **Course Attributes:**

Tuition Joint Health Science

### **Rationale and history:**

More efficient high-throughput sequencing techniques are expanding exponentially the knowledge about the ensemble of proteins expressed by living organisms. At the same time, the determination of their three-dimensional (3D) structure is still requiring expensive and time-consuming experiments. During the last few decades, the effort of the scientific community allowed the crystallization of thousands of proteins, which have been resolved at atomic level. Currently the Protein Data Bank (PDB), the largest repository of protein structures, contains more than 88,000 macromolecular 3D structures. The computational analysis of this huge source of information revealed that during the evolution protein structure is more conserved than sequence. This finding constitutes the basic assumption behind most of the available bioinformatics algorithms for protein structure prediction. Thus, structure information collected in the PDB has been successfully used to predict the 3D structure of new proteins.

According to this scenario the course will summarize recent findings in the field of computational structure biology/structural bioinformatics focusing on the rationale behind the implementation of the methods that enabled the most significant breakthroughs. In the “Big Data” era a solid training in the computational analysis of experimental molecular biology data is key delivering high quality research in biomedical sciences.

### **Organization:**

This course is organized as a hands-on training for graduate students, faculty and computational staff. A limited number of slots are made available for Pathology residents, fellows and graduate students with research interests in understanding the molecular basis of disease. In the first part of the course an introduction about the computational skills required to perform basic tasks in structural bioinformatics will be provided. The course will mainly focus on the study of protein three-dimensional structures. The protein folding is the process responsible

for the formation of the native structure. It is a hierarchical process that requires different level of organization. First, the interactions that stabilize the native protein structure will be summarized. The different level of structural classification and the related web available databases will be presented. In addition, structural information available on the PDB (Protein Data Bank) will be extracted and used to perform protein structural analysis. After that, a broad overview of the structural prediction tools will be provided. The attention will be focused on the algorithms for the prediction of the secondary structural elements and more complex methods for tridimensional prediction. The three main approaches for protein structure prediction (comparative modeling, threading and *ab-initio*) and the differences between will be discussed. Algorithms for structural evaluation and comparison will be also introduced to evaluate the predicted protein three-dimensional structures.

Further details and information about the course and the lectures will be made available at <http://cmb.path.uab.edu/training>.

**Evaluation:**

Evaluation is based on class participation and project development. The attendees are required to present their implemented projects at the end of the course.

**Additional Information:**

- Cap class at 15 students
- Lecture Course
- Interview with course master before accepted in class
- Grading: letter grade
- Cross link PATH course with GBS and open to all 8 themes
- Must drop class within first week
- Attendees should bring their personal laptops (preferably Mac or Linux) to the class.