Bioinformatics applied to proteomics

The aim of the course is to introduce participants into the main bioinformatic tools currently used in proteomics, i.e., strategies in protein identification, search engines, databases, as well as prediction of protein structure or protein PTMs. The course is divided into five parts:

- Introduction to Image analysis
- Mass spectrometry MALDI-TOF
- Mass spectrometry CID
- Data integration and analysis
- Prediction of protein function.

Location Facultad de Farmacia, UCM, pza Ramón y Cajal s/n 28040 Madrid Spain

Number of participants max. 20

Date April 3rd to 5th

Duration 3 Days

Organizer Proteored education and training group

Contact person Alberto Medina

Phone 91 585 45 40
e-mail jamedina@proteored.org

Contents

1. Part 1: Introduction and image analysis (Duration 1.30 hours)
   1.1 Motivation
   1.2 Introduction to the integration of proteomics into bioinformatics
   1.3 Principles of image analysis

2. Part 2: MALDI-TOF mass spectrometry (3 hours 30')
   2.1 Introduction
   2.2 MALDI-TOF mass spectrometry principles
   2.3 Peptide fingerprinting
   2.4 Processing the mass spectra
   2.5 Database searching using fingerprint data
   2.5.1 Databases
   2.5.2 Search engines
   2.6 Limitations of the technique

3. Part 3: CID mass spectrometry (3 hours)
   3.1 Introduction
   3.2 Fragmentation spectra principles
   3.3 Interpreting fragmentation spectra, classical methods
   3.4 Searching fragmentation spectra data against databases
   3.5 Useful tools
   3.6 De Novo sequencing. Main tools

4. Part 4: Data integration (4 hours)
   4.1 Introduction
   4.2 What is LIMS?
   4.2.1 License free tool (Garban)
   4.3 Data standards
   4.3.1 PEDRO
   4.3.2 Proteios
   4.3.3 HUPO PSI
   4.3.4 Ontologies
   4.4 Post-ID tools
   4.4.1 Searching information dynamically (PIKE)
   4.4.2 Graphic representation of data
   4.5 Future prospects

5. Part 5: Prediction of protein function (4 hours)
   5.1 Introduction
   5.2. Annotating by sequence homology
   5.3. New methodologies based on structure motifs
   5.4. De novo prediction
   5.5. Limitations and perspectives

Teaching Staff
Dr. Alberto Medina, Centro Nacional de Biotecnología, CNB-CSIC, Madrid
Dr. Alberto Paradela. Centro Nacional de Biotecnología, CNB-CSIC, Madrid
Dr. José Ramón Valverde. Centro Nacional de Biotecnología, CNB-CSIC, Madrid