Workshop on

Bioinformatics Approach in Enzymology: Molecular Structure and Data Analysis

Dokuz Eylül Üniversitesi, 2 to 6 June 2014

Your instructor:
Angel Herráez, PhD
University of Alcalá (Spain)
angel.herraez@uah.es

Brief outline of the workshop

Workshop plan

- Schedule to follow
- We will be flexible – please ask, or comment what your needs are
- Aim: you should prepare a mini-project to be presented on Friday
- Website with our outline and materials bit.ly/DEU2014
- 2 parts:
  - Use of molecular visualisation to study enzyme-ligand
  - Tools to study enzyme kinetics data

Section 1 (Monday-Tuesday)

- Presentation of resources for molecular structure
- Getting the Jmol software: download
- Starting to use Jmol
  - Loading files
  - Top menu bar
  - Mouse
  - Pop-up menu
  - Capturing images
  - Saving results
- Using the console and scripting

Section 2 (Tuesday-Wednesday)

- More practice about Jmol scripting, specifically those commands suitable for the binding site
  - Polarity
  - Surfaces, pockets and cavities
  - Ligand contacts with the enzyme
- Specific examples of enzymes with alternative ligands

Section 3 (Wednesday)

- Presentation of molecular displays
  - Method 1: standalone files
    - "Molecular scenes" prepared and saved in advance, loaded into Jmol application.
  - Method 2: using Proteopedia as the platform for presentation
  - Method 3: using webpages as the means to present – built using the "Jmol Export to Web" module

Section 4 (Thursday)

- Simulations for testing the meaning of kinetic parameters – graphically, Michaelis-Menten plot and transformed plots
- The use of nonlinear regression for fitting experimental data directly to Michaelis-Menten equation.

Section 5 (Friday)

- Reinforcing whatever was left or raised interest
- Presentations by the workshop attendants