SEMESTER B

1. Computational Analysis of Biomacromolecular Sequences

Coordinator: Prof. S. Hamodrakas

Lecturers: Prof. S. Hamodrakas | Assoc. Prof. G. Rodakis | Dr. I. Almyrantis | Dr. V. Promponas

Compulsory Module

Semester: B

Syllabus:

- **Introduction:** DNA and protein sequences
- **Sequence similarity search algorithms:** Sequence homology and similarity and their importance, dynamic programming algorithms, Global Alignment and Needleman & Wunch algorithm, Local Alignment and Smith & Waterman algorithm, Calculation of alignment's statistical significance, Importance of Identity matrixes, gaps and penalties, Heuristics methods for similarity searches in databases (BLAST, FASTA etc).
- **Multiple sequence alignment:** Multidimensional dynamic programming algorithms, Heuristic methods for multiple sequence alignments (HMMER, SAM, HMM-Pro etc), phylogenetic trees and multiple alignments
- **Discovery of patterns and periodicities in protein and DNA sequences**
- **Prediction algorithms based on protein and DNA sequences:** Empirical statistical methods, Clustering, Neural networks, Hidden Markov Models, Genetic algorithms. Applications of the above mentioned methods for:
    - Secondary structure prediction of proteins and RNA
    - Prediction of Transmembrane segments and their orientation in proteins
    - Gene finding in DNA sequences
    - Multiple sequence alignments using Hidden Markov Models (HMMER, SAM, HMM-Pro etc)
    - Sequence clustering in families

2. Computational Analysis of Biomacromolacular Structures

Coordinator: Prof. E. Iliopoulos

Lecturers: Prof. S. Hamodrakas | Prof. E. Iliopoulos | Dr. M Vlasi | Dr. N. Papandreou

Module: Compulsory

Semester: B

Syllabus:

- Introduction - Biomolecular structures - Determination methods
- Fold recognition
- Fitting (Anteposition) of stereo structures

- Comparative homology modeling - Threading
- Modelling of protein structures by molecular mechanics and molecular dynamics.
- Protein-Ligand docking - Drug design
- Protein-protein structural recognition (docking)
- Structure quality evaluation methods - Methods for stereochemical structure checks

3. Programming Languages and Software Tools in Bioinformatics II

Coordinator: Prof. S. Hamodrakas

Lecturers: Prof. S. Hamodrakas | Dr. V. Promponas

Compulsory Module

Semester: B

Syllabus:

PART I The JAVA programming language

- Classes and Objects, Java foundation classes, Applets and Applications, Topics in Graphical User Interface design, Distributed computing, JavaBeans, JAVA applications in Bioinformatics - the BIOJAVA project

PART II The perl programming language

- Scalar variables, lists, arrays, strings. Flow control structures. Subroutines, Associative arrays (hashes). Input/output. Pattern matching with regular expressions. Perl applications in Bioinformatics - the BIOPERL project.

4. Molecular Recognition - Molecular Diseases - Structural Drug Design

Coordinator: Prof. I. Iliopoulos

Lecturers: Prof. S. Hamodrakas | Prof. I. Iliopoulos | Dr. M Vlasi | Dr. V. Oikonomidou

Compulsory Module

Semester: B

Syllabus:

- **Structural elements of biomolecules:** Size and environment of biomolecules
- **Biomolecular interactions:** Protein-protein interaction types, Protein-DNA interaction types

- **Molecular recognition:** Binding and dissociation constants, Binding energy, A molecular recognition example, Entropy terms in complex creation, Degrees of molecular recognition - high fidelity recognition, Evolution and molecular recognition, Interactions of proteins and nucleic acids.
- **Energetic analysis of interactions:** Molecular mechanics, Introduction to the methodology of "ab initio" protein folding, the empirical function of energy, energy minimization, energy surface, Enthalpy and entropy, Molecular dynamics.
- **Protein folding - molecular chaperones:** New approaches for protein folding with or without intermediate states, The value of molecular topology, Molecular chaperones.
- **Biological membranes and membrane proteins:** Composition and structure of biological membranes, membrane proteins, Membrane protein structure, Families of membrane proteins, Channels and receptors.
- **Cellular Translocation of proteins:** The endoplasmic reticulum function, protein targeting and signal sequences, protein translocation in mitochondria, chloroplasts and the nucleus.
- **Drug design:** Methodology, Drug design based on target?s structure, Problems - Resistance of infectious diseases and cancer against therapeutic agents.
- **Chemical signal transduction:** Usual molecular mechanisms for signal transduction, Hormones, Neurotransmitters, Signal transduction in membranes and cytoplasm, Steroid hormones and their receptors. Feromones.

5. Methodology of Research

Coordinator: Prof. S. Hamodrakas

Lecturers: Prof. S. Hamodrakas | Prof. L. Margaritis | Prof. E. Moudrianakis | Assoc. Prof. G. Rodakis | Prof. I. Iliopoulos | Lecturer G. Goulielmos

Compulsory Module

Semester: B

Syllabus:

- General issues
- Science, Scientific Field and Scientific Research
- Biological research.
- Ethics in scientific research and specifically in biological sciences
- Bioinformatics and moral dilemmas. The role of a bioinformatician in different stages of a project.
- Writing, evaluating and publishing the results of scientific research in the academic press (journals, conferences etc).
- Choosing the appropriate journal (Sources, Information, Instructions to authors, peer review system, journal evaluation)
- Type of Articles (review, letters etc). Scientific paper format (Abstract, Introduction, Materials and Methods, Results, Discussion).
- Assessment of a submitted paper through the peer review system. Answering reviewer?s comments.
- Applications.