Master in Biomedicine

Subject Name: Advanced Bioinformatics

(Free election matter)

Credits: 3; 30 hours

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Teachers: Gabriel Pons, Josep Lluís Gelpí, Fco Javier Luque, Xavier Barril, Axel Bidon-Chanal

Program: All classes will be attended on Informatic laboratories, thus each student will work with a personal computer

1. Introduction to advanced Bioinformatics.

Basic Bloc
(specially intended for students with low background in bioinformatics)

2. Sequence databases and sequence comparison. Blast and multiple alignments. Functional prediction. Prosite

3. Three-dimensional Structures, PDB files, molecular visualization. structural motifs

"Target discovery" Bloc

4. Genome sequencing and annotation: different strategies for sequencing, assembly and functional annotation of genomes, ENCODE; genomic browsers: ENSEMBL, UCSC

5. Genome variability: approaches to detect and analyze varibility in humans (SNPs, CNVs, etc...), 1000 genomes, dbgap,

6. Inherited diseases: Mendelian or complex disease. Mendelian (citogenetics, linkage analysis) . Complex diseases (personalized medicine, GWAS)

7. Somatic genomic variations and disease (Whole Genomes, exomes, methods for somatic variant calling, exemple cancer genomics, other diseases)

8. Expression analysis and disease (RNAseq, arrays)

9. Epigenomics

10. Personalized medicine (future perspectives)

Advanced Pharmacological strategies Bloc

11. Introduction

12. Bioinformatics and drug discovery. Pharmaceutical research: current challenges. Computer-assisted drug design. Parameters to be optimizad in drug design. What areas are implicated in drug design?. Integration of computational tools. Designing cascade of assays.

13. Drug-likeness of compounds. Pharmacodynamics and pharmacokinetics. ADME properties. Toxicity. ADMET predictors. Filtering of databases. Binding kinetics.

Ligand-based drug design

14. Quantitative structure-activity relationships (QSAR). Molecular basis of the ligand-receptor interaction. Biological and physico-chemical descriptors. Ligand-receptor complementarity: concept of pharmacophore. Molecular similarity. Molecular fields and 3D-QSAR: COMFA and COMSIA.

15. Strategies for searching new candidates. Chemoinformatics: virtual and real libraries. Combinatorial chemistry: a tool for molecular diversity.

Structure-based drug design

16. Protein Structure and Ligand Binding. Protein structure and potential energies. Protein-ligand energy landscape. Homology Modeling. Druggability.

17. Docking. Receptor-based drug design. Prediction of binding sites. Flexibility of ligand and receptor. Scoring functions. Screening of virtual libraries. Analysis of ligand-receptor interactions and complex refinament. Prediction of relative binding affinities

Bibliography

Baxevanis, A.D. and Oullette, B.F Francis. ***Bioinformatics.*** A practical guide to the analysis of genes and proteins. 3rd edition. Wiley. 2005

Gu, J. and Bourne, P. E. ***Structural Bioinformatics***. 2nd edition. Wiley Blackwell 2009

Luque, F. J., Barril, X ***Physico-Chemical and Computational Approaches to Drug Discovery***.. (eds). RSC Drug Discovery 2012

Gohlke, H. (ed). Wiley VCH ***Protein-Ligand Interactions***. Methods and Principles in Medicinal Chemistry Series, Vol. 53,. Weinheim 2012

Tutorials at:
http://www.expasy.org
http://www.ebi.ac.uk
http://www.ncbi.nlm.nih.gov
http://www.pdb.org