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Proteins - sequences, structures, comparison and evolution

Course description:

The whole course is principally anchored in protein bioinformatics and divided into two parts: (i) theoretical information (7 hours of lectures) and (ii) practical exercises (8 hours of lectures). In the first part of the course, the primary molecular-biology sequence and protein structure databases will be described, such as GenBank and UniProt as well as Protein Data Bank. Then, proteins as basic building blocks of living matter will be presented in a detail with emphasis on their structure, stability, evolution and design. A special method, the so-called Hydrophobic Cluster Analysis (HCA), for comparison of highly diverged protein sequences, will be introduced together with the basic principles of BLAST (Basic Local Alignment Search Tool), the tool used for, e.g., assigning a potential function for a hypothetical protein or for genomes mining. The second part of the course will be entirely devoted to practical exercises. First, students will get acquainted with protein sequences (i.e. GenBank and UniProt), followed by protein structures (i.e. the Protein Data Bank) – mainly on how to retrieve the data from those databases and how to work with them. This means to perform sequence alignments, to identify conserved sequence regions, to calculate an evolutionary tree, to display a protein structure, to make structure predictions via modelling and to superimpose protein structures. Each exercise is designed in an effort to lead the student to a final evaluation of achieved results and drawing his/her own conclusions.

Syllabus of the lecture subjects (enlisted):

Theoretical information (lectures 1-7):

1. Sequence databases – GenBank (EMBL-ENA/DDBJ) and UniProt (SwissProt/TrEMBL).
2. Hydrophobic Cluster Analysis method and the BLAST tool – basic facts and examples.
3. Protein structure database – Protein Data Bank (PDB).
4. Proteins – characterization, amino acids, peptide bond and protein backbone.
5. Structure of proteins – levels of protein structure (alpha-helices, beta-sheets, motifs, domains).
6. Prediction of protein structure – methods and approaches.
7. Stability and stabilization of proteins – denaturation, thermostable and cold-active enzymes.

Practical exercises (lectures 8-15):

8. Basic analysis of amino acid sequences of proteins; part I. Retrieving sequences from databases; preparing the input file for aligning; working with the alignment file.
9. Basic analysis of amino acid sequences of proteins; part II. Determining the consensus length and sequence identity (similarity); calculating and displaying the evolutionary tree.
10. Analysis of a protein family using the BLAST tool; part I. Performing the BLAST search; downloading the results and their preliminary analysis.

11. Analysis of a protein family using the BLAST tool; part II. Step-by-step analysis of BLAST results focused on identifying relevant members of a protein family.

12. Work with the PDB file of a protein. Retrieving the structure co-ordinates of a protein from PDB; manipulating and displaying the protein structure.

13. Prediction of a protein tertiary structure; part I. Performing the homology modelling using various servers (SwissModel, Phyre); downloading the results and their preliminary analysis.

14. Prediction of a protein tertiary structure; part II. Detailed analysis of individual protein models; identifying protein templates; overall evaluation of obtained results.

15. Comparison of protein tertiary structures. Preparing structural data for analysis; performing the structural superimposition (MultiProt server); displaying and comparing the overlaps.

Termin	Dzień tygodnia	Godzina	Miejsce
21.10.2019	**Poniedziałek**	**9.15 – 12.00**	**Minicentrum Konferencyjne WCH**
22.10.2019	**Wtorek**	**9.15 – 12.00**	**Minicentrum Konferencyjne WCH**
23.10.2019	**Środa**	**9.15 – 12.00**	**Sala komputerowa 109 (Chemia C)**
24.10.2019	**Czwartek**	**16.15 – 19.00**	**Sala komputerowa 109 (Chemia C)**
25.10.2019	**Piątek**	**13.15 – 16.00**	**Sala komputerowa 109 (Chemia C)**