POZNAN UNIVERSITY OF TECHNOLOGY

EUROPEAN CREDIT TRANSFER AND ACCUMULATION SYSTEM (ECTS)

COURSE DESCRIPTION CARD - SYLLABUS

Course name
RNA structural bioinformatics [S2Bioinf2>RNA]

Course

Field of study Bioinformatics	Year/Semester 1/1
Area of study (specialization) –	Profile of study general academic
Level of study second-cycle	Course offered in Polish
Form of study full-time	Requirements compulsory

Number of hours

Lecture 15	Laboratory classes 15	Other 0
Tutorials 0	Projects/seminars 0	

Number of credit points

3,00

Coordinators	Lecturers
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Prerequisites

The person starting the 2nd-cycle studies should have attained the learning objectives defined for the 1st-cycle studies in the resolution of the PUT Academic Senate - the learning objectives are available at the website of the Faculty of Computing and Telecommunications. The student starting this module should have the basic knowledge about structural biology, theory of algorithms, programming, data bases and combinatorial algorithms. Moreover, he / she should be able to solve the fundamental problems in the area of programming and analysis of biological data. In addition, with respect to the social skills, the student should show such attitudes as honesty, responsibility, perseverance, curiosity, creativity, manners, and respect for other people.

Course objective

1. The transfer of knowledge concerning (i) algorithms and optimization methods used to solve fundamental problems of modern biology, biochemistry, and bioinformatics of RNA structures, and (ii) currently best tools for acquisition, storage, processing and analysis of biological data concerning nucleic acids. 2. The acquaintance of students with an architecture of most common tools used in RNA structural bioinformatics, including both, new and precursory projects. The emphasis is placed on pros and cons of the solutions, their limitations (mostly unknown to the typical users), technologies used in implementation, quality and accuracy of obtained results, their reliability and ways of evaluation and verification. 3. The development of students' skills in the area of mathematical modeling and solving computational problems of RNA structural bochemistry and biology using both, simple and advanced bioinformatic algorithms, in testing novel computational methods.

Course-related learning outcomes

Knowledge:
1. The student has an extended knowledge of the mathematical, statistical, optimization and artificial intelligence models used to represent structures of nucleic acid molecules on different levels of their architecture, their modeling, and analysis of processes involving these molecules.
2 The student knows methods, techniques and tools used in the process of solving complex tasks in the analysis of RNA structures, mainly of engineering nature.
3. The student knows an architecture and the functional details of the most popular structural data repositories and algorithms for structure processing (structure prediction, structure determination, structure evaluation and comparison, clustering, etc).
4. The student is familiar with issues in modeling and analysis of biological systems and structures based on theoretical foundations.
5. The student has a detailed knowledge of the design of structure prediction processes, structure comparison and structure modeling.
6. The student has a detailed, based on solid theoretical foundation, knowledge of research planning, optimization and efficient algorithms used in RNA structural bioinformatics; knows the most important (from the historical point of view) and most popular algorithms to compute and predict structures, search for common substructures, align structures.
7. The student knows the trends in development of computational methods for crucial problems of structural biology and biochemistry of RNA, and is aware of the approaches proposed for solving novel problems in structural bioinformatics.

Skills:
1. The student uses and interprets the information acquired from the literature concerning the general problems of RNA structural bioinformatics and from specialist journals (scientific publications in Bioinformatics, BMC Bioinformatics, Nucleic Acids Research, Nature Methods, etc; internet services and portals from the bioinformatics area); interprets and evaluates their contents.
2. The student is able to use advanced techniques and computational tools (e.g. GenBank, BLAST, RNA FRABASE, FARFAR, ModeRNA, RNAComposer, Vfold, RNAstructure, Eterna, mfold, RNAfold, RNAinverse)
for solving biological problems and can estimate their usefulness.
3. The student is able to apply knowledge from the area of biochemistry and related sciences to solve problems of RNA structural bioinformatics (for example, modeling, annotating, evaluating of structures).
4. Under the supervision of a teacher, the student can plan and solve research tasks (e.g. modeling of biomolecule structure with the use of bioinformatic tools, evaluating of RNA model quality and accuracy, clustering of structures based on their similarity) using the known computational methods.
5. The student applies mathematical methods as well as specialized IT techniques and tools to represent, process, and analyse structural data describing an architecture of nucleic acids on various levels of detail.
6. The student is able to design and develop computer software to solve selected structural bioinformatics problems using appropriate methods, techniques and tools.
7. The student prepares the presentation of obtained results in Polish and English (reports, multimedia presentations) and discusses them in the group.
8. The student can estimate the usefulness of new achievements of structural bioinformatics and biochemistry, especially in the area of processing and analysis of RNA structural data.

Social competences:

1. The student understands the necessity of learning (during the lectures students are introduced with the latest achievements of structural bioinformatics; students have the possibility to present an interesting subject concerning the latest solutions in the field).
2. The student can co-operate and work in a group (laboratory gives a chance to work in groups).
3. The student understands the necessity of reading the scientific and popular journals in order to gain and extend bioinformatics knowledge.
4. The student has a creative attitude in professional and social activities.

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Formative assessment
a) verification of assumed learning objectives related to lectures:
- answers to the questions regarding the material from previous lectures

b) verification of assumed learning objectives related to tutorials / laboratory classes:
- evaluation of the ability to perform the laboratory exercises
- evaluation of the report of the exercises (prepared partially during the laboratory and partially at home)
- evaluation of the exercises' execution during the laboratories.

Total assessment
a) verification of assumed learning objectives related to lectures:
- evaluation of the knowledge during the written test. The test is composed of 5 questions; the student can obtain 3 points for an answer to each question; 20% of the test is prepared as multiple choice questions; the remaining part has the form of an open questions; all questions concern the problems introduced during the lectures and practised during laboratory exercises. In order to get positive mark, one should obtain at least 8 points.
- discussion on the test results

b) verification of assumed learning objectives related to tutorials / laboratory classes:
- the verification of the skills and knowledge regarding the issues mentioned during the laboratories during the final written test
- the final evaluation is based on the weighted average, which includes the marks obtained for the projects, reports and activity during the laboratories.

Additional activities taken into account:
- discussion on the additional aspects of the topics,
- preparation of short presentation about a structural bioinformatics problem that was not presented by the lecturer,
- effectiveness knowledge gained during problem solving,
- remarks helping to improve the teaching materials or the teaching process.

Programme content

The program of the lecture encompasses the following issues. The first lecture generally introduces the subject, in particular it discusses the crucial issues of modern RNA structural bioinformatics, their proposed solutions, and their characteristics from the point of view of requirements, limitations and computational complexity. The second lecture introduces to the data bases of RNA structures. The students learn about selected, most popular structural repositories, data schemes, dabase architecture, interface applications, meta-languages defined to generate advanced queries and data formats used to save structural information. The succeeding lecture is devoted to the most popular models and formats proposed for RNA secondary structure representation, secondary motifs and the methods of their visualization. During the lecture, the students learn the methodology of mathematical modeling of structural data and issues, including their optimization for the following analysis of the problems and considering the completeness of modeled information. The forth lecture refers to the basic methods of secondary structure prediction. It presents the first, historical algorithms for RNA secondary structure prediction (the methods performance is shown based upon the selected cases) as well as the novel methods. Within the next lecture, the fundamental approaches to the tertiary structure modeling are discussed, including the general characteristics of the approaches, their drawbacks, advantages and usefulness. The selected modern methods for the RNA tertiary structure prediction are also presented. The sixth lecture is devoted to the algorithms for structural data comparison, similarity search, distance and similarity measures, and data clustering. Examples for using various similarity measures are presented for different types of structures, and the most popular modern tools that enable structure comparison and analysis are shown. The visualization of bioinformatic data is a subject of the next lecture. It introduces the basic information about computational graphics and visualization methods implemented in various bioinformatic tools. The final lecture is devoted to students' presentations: student pairs present the latest issues appearing in structural bioinformatics, due to their choice and interests.

Laboratory exercises are strictly related to the lectures. The lecture is a theoretical introduction, while the laboratory allows for hands-on exercises related to the introduced topics and for implementation of the own solutions for simple bioinformatic problems.

Laboratory has the form of seven 2-hour exercises in the computational lab. Students obtain tasks to be solved, thus, practising the issues discussed during the lectures and preparing to use the available tools and programming libraries. Additionally, during the laboratory exercises, the students implement their projects (partially during the laboratory, partially as a homework), which solve the selected combinatorial problems within the field of structural biology. The program of laboratory exercises encompasses the following issues. In the first class, students explore the canonical RNA secondary structure, learn about its storage formats and define possible motifs. As part of the project, they develop a format converter with a heuristic function for solving the pseudoknot order assignment problem and a tool for identifying structural motifs. Another class is devoted to tools for 2D RNA structure prediction based on single sequence and alignment. Students also learn how to compare secondary structures, collect data for analysis and implement comparison metrics. The next class focuses on non-canonical pairs and modules, or evolutionarily conserved 3D RNA motifs. Students identify the most common modules and create a tool to detect them in spatial structures. Another topic is the annotation of secondary structure based on 3D coordinates. Students learn classical geometric techniques, which they implement and test on a data set. The next class is about comparing 3D structures, where they learn the classical RMSD method and the angular MCQ measure, gaining the skills they need for their projects. The last two classes focus on molecular dynamics simulations. Students first learn the basics of running simulations, and then interpret the results. During the final class, they create a project that allows them to analyze structural issues on the basis of simulation trajectories, using the acquired knowledge for practical applications.

Course topics

The course covers topics related to obtaining RNA structure data through computational and laboratory experiments, processing structural data at various levels of detail, analyzing structural features, data visualization, topology classification, structure annotation, motif searching, reference-based and reference-free structure evaluation, detecting irregularities in structural models, and modeling structures with or without experimental data.

Teaching methods

1. Lectures: multimedia presentation, blackboard presentation illustrated with examples, multimedia show.
2. Laboratory classes: solving exercises, practical exercises, running computational experiments, discussion, group work, multimedia show, workshops, games, case study.

Bibliography

Basic:
1. J. Gu, P.E. Bourne, "Structural Bioinformatics"
2. P. Baldi, S. Brunak, "Bioinformatics: The Machine Learning Approach"
3. T. Schwede, M. Peitsch, "Computational structural biology. Methods and applications."

Additional:
Recent scientific publications from the area of structural bioinformatics.

Breakdown of average student's workload

	Hours	ECTS
Total workload	75	3,00
Classes requiring direct contact with the teacher	30	1,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	45	1,50