COURSE DESCRIPTION CARD - SYLLABUS

Course name

BEYOND THE DOUBLE HELIX: COMPUTING STRATEGIES FOR COMPLEX BIOLOGICAL ARCHITECTURES [S5ITIT>PPH]

Course

Proposed by Discipline –	Year/Semester 2/4
Level of study Doctoral School	Course offered in English
Form of study full-time	Requirements elective

Number of hours

Lecture	Laboratory classes	Other
4	0	0
Tutorials	**Projects/seminars**	
0	0	

Number of credit points

1,00

Coordinators	Lecturers
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Prerequisites

Knowledge: Familiarity with fundamental concepts in algorithms and data structures is expected. A basic understanding of or interest in data visualization principles is beneficial. No prior background in biology or bioinformatics is required. Skills: The ability to independently search for scientific literature. Social competencies: An intellectual curiosity and readiness to engage with complex problems from an interdisciplinary perspective.

Course objective

This course is designed to introduce PhD students to the intricate and fascinating challenges presented by non-canonical nucleic acid structures. Through the instructor's research on RNA pseudoknots and G-quadruplexes as primary case studies, the course will illustrate how advanced algorithms, mathematical modeling, and custom visualization techniques are developed and applied to understand complex biological architectures. The ultimate goal is to showcase the field of structural bioinformatics as a promising area for innovative computational research.

Course-related learning outcomes

Upon successful completion of this course, graduates will:

- Understand current research challenges and the latest computational approaches for analyzing non-

canonical RNA and DNA structures. [P8S_WG/SzD_W01]
- Grasp the principles of algorithmic, mathematical, and visualization methodologies that can be applied to solve complex problems in related fields. [P8S_WG/SzD_W03]
- Be able to synthesize information from scientific literature across multiple disciplines (such as computer science, biology, and mathematics) to comprehend complex problems. [P8S_UW/SzD_U01]
- Critically assess the suitability and limitations of various computational approaches for specific scientific problems. [P8S_UW/SzD_U02]
- Be prepared to appreciate and integrate knowledge from diverse fields to address novel scientific challenges. [P8S_KK/SzD/K03]

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

A short test covering the key concepts presented during the lecture will be administered at the end of the course. A score of over 50% is required to pass.

Programme content

This course goes beyond the traditional double helix to explore the computationally rich domain of complex nucleic acid structures. It begins by highlighting RNA's structural versatility and the challenges associated with representing its secondary structures, particularly focusing on the topologically complex arrangements known as pseudoknots. We will discuss the formal problem of classifying pseudoknots by their order, presenting novel algorithms and Mixed-Integer Linear Programming (MILP) formulations developed to address this challenge.

In the second part of the course, we will shift our focus to G-quadruplexes (G4s), which are four-stranded structures that play significant biological roles. We will examine their structural diversity from a bioinformatics perspective and introduce a systematic framework for their classification and visualization. Throughout the course, we will emphasize how abstract computational and mathematical concepts can be applied to develop practical tools that enhance biological understanding.

Course topics

1. RNA structure
2. Pseudoknots
3. Heuristics and MILP formulation
4. Exhaustive enumeration
5. Quadruplexes
6. Classification and analysis
7. Summary and future directions

Teaching methods

- Lectures supported by a multimedia presentation.
- Demonstrations of specialized software tools and web servers.
- Case study analysis of key research findings.

Bibliography

Basic

Neidle, S. (2008). Principles of nucleic acid structure (1st ed). Elsevier ; Academic Press.

Staple, D. W., & Butcher, S. E. (2005). Pseudoknots: RNA Structures with Diverse Functions. PLoS Biology, 3(6), e213. https://doi.org/10.1371/journal.pbio.0030213

Spiegel, J., Adhikari, S., & Balasubramanian, S. (2020). The Structure and Function of DNA G-Quadruplexes. Trends in Chemistry, 2(2), 123–136. https://doi.org/10.1016/j.trechm.2019.07.002

Advanced:

Adamczyk, B., Zurkowski, M., Szachniuk, M., & Zok, T. (2023). WebTetrado: A webserver to explore quadruplexes in nucleic acid 3D structures. Nucleic Acids Research, 51(W1), W607–W612. https://doi.org/10.1093/nar/gkad346

Zurkowski, M., Zok, T., & Szachniuk, M. (2022). DrawTetrado to create layer diagrams of G4 structures. Bioinformatics, 38(15), 3835–3836. https://doi.org/10.1093/bioinformatics/btac394

Zok, T., Kraszewska, N., Miskiewicz, J., Pielacinska, P., Zurkowski, M., & Szachniuk, M. (2022). ONQUADRO: A database of experimentally determined quadruplex structures. Nucleic Acids Research, 50(D1), D253–D258. https://doi.org/10.1093/nar/gkab1118

Zok, T., Popenda, M., & Szachniuk, M. (2020). ElTetrado: A tool for identification and classification of tetrads and quadruplexes. BMC Bioinformatics, 21(1), 40. https://doi.org/10.1186/s12859-020-3385-1

Zok, T., Badura, J., Swat, S., Figurski, K., Popenda, M., & Antczak, M. (2020). New models and algorithms for RNA pseudoknot order assignment. International Journal of Applied Mathematics and Computer Science, 30(2), 315–324. https://doi.org/10.34768/amcs-2020-0024

Popenda, M., Miskiewicz, J., Sarzynska, J., Zok, T., & Szachniuk, M. (2020). Topology-based classification of tetrads and quadruplex structures. Bioinformatics, 36(4), 1129–1134. https://doi.org/10.1093/bioinformatics/btz738

Antczak, M., Popenda, M., Zok, T., Zurkowski, M., Adamiak, R. W., & Szachniuk, M. (2018). New algorithms to represent complex pseudoknotted RNA structures in dot-bracket notation. Bioinformatics, 34(8), 1304–1312. https://doi.org/10.1093/bioinformatics/btx783

Breakdown of average student's workload

	Hours	ECTS
Total workload	25	1,00
Classes requiring direct contact with the teacher	4	0,00
Doctoral student's own work (literature studies, preparation for laboratory classes/tutorials, preparation for tests/exam, project preparation)	21	1,00