Sveučilište u Rijeci
University of Rijeka

BIOtech
Odjel za biotehnologiju
51000 Rijeka, Radmile Matejčić 2
Tel. +385 51 584 550
Fax. +385 51 584 599
e-mail: ured@biotech.uniri.hr

Detailed curriculum for the course:

Laboratory apprenticeship – Design of short catalytic peptides and peptide assemblies

Academic year: 2020/2021

Program: Biotechnology for the Life Sciences (1st year)

Course code: EBLS105

ECTS points: 12

Language of the course: English

Teaching hours: 280 hours (all practical work)

Pre-requisites: Successful completion of BLS103 "Introduction to Laboratory Work and Safety"

Course leader and contact information:
Title and name: Doc. dr. sc. Daniela Kalafatovic
Address: Odjel za biotehnologiju, O-810
E-mail: daniela.kalafatovic@biotech.uniri.hr

Time period: 1st March - 16th April 2021
or
19th April – 4th June 2021

Teaching staff: Course leader:
Doc. dr. sc. Daniela Kalafatovic

Associates:
Patrizia Jankovic, Mag. Pharm. Inv.

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Reading:

Frederix, P. W. J. M.; Scott, G. G.; Abul-Haija, Y. M.; Kalafatovic, D.; Pappas, C. G.; Javid, N.; Hunt, N. T.; Ulijn, R. V.; Tuttle, T., *Exploring the sequence space for (tri-) peptide self-assembly to design and discover new hydrogels*. Nat. Chem. 2015, 7 (1).
Lampel, A.; Ulijn, R. V.; Tuttle, T., *Guiding principles for peptide nanotechnology through directed discovery*. Chem. Soc. Rev. 2018, 47 (10), 3737–3758.
Wei, G.; Su, Z.; Reynolds, N. P.; Arosio, P.; Hamley, I. W.; Gazit, E.; Mezzenga, R. *Self-assembling peptide and protein amyloids: from structure to tailored function in nanotechnology*. Chem. Soc. Rev. 2017, 46 (15), 4661–4708.
Woolfson, D. N.; Mahmoud, Z. N., *More than just bare scaffolds: towards multi-component and decorated fibrous biomaterials*. Chem. Soc. Rev. 2010, 39 (9), 3464–3479.
Duncan, K. L.; Ulijn, R. V. *Short Peptides in Minimalistic Biocatalyst Design*. Biocatalysis 2015, 1 (1), 67–81.
Maeda, Y.; Javid, N.; Duncan, K.; Birchall, L.; Gibson, K. F.; Cannon, D.; Kanetsuki, Y.; Knapp, C.; Tuttle, T.; Ulijn, R.V.; Matsui, H. *Discovery of Catalytic Phages by Biocatalytic Self-Assembly.* J. Am. Chem. Soc. 2014, 136 (45), 15893–15896.
Lengyel, Z.; Rufo, C. M.; Korendovych, I. V., *Preparation and Screening of Catalytic Amyloid Assemblies*. Methods Mol Biol. 2018, 1777, 261–270.
Rufo, C. M.; Moroz, Y. S.; Moroz, O. V.; Stöhr, J.; Smith, T. A.; Hu, X.; Degrado, W. F.; Korendovych, I. V., *Short peptides self-assemble to produce catalytic amyloids*. Nat. Chem. 2014, 6 (4), 303–309.
Kalafatovic, D.; Mauša, G.; Todorovski, T.; Giralt, E., *Algorithm-supported, mass and sequence diversity-oriented random peptide library design.* J. Cheminform. 2019, 11 (25), 1–15.

Additional articles, specific to each student's research, may be assigned by the course leader.

Course description:

Artificial enzymes have attracted tremendous interest in recent years and several approaches to mimic biological catalysts have been proposed. One approach is to create minimalistic catalysts based on peptides and their assemblies. Peptides are increasingly investigated in biomedical applications due to their inherent biocompatibility, biodegradability, low toxicity of metabolites and because they are the building blocks of life. Short peptides can self-assemble into nanostructures, which often results in new emerging functions, not seen with their constituent monomers. One such function is catalytic activity. Little is known about the principles that govern the catalytic activity of short peptides at the sequence level. From previous studies it is evident that the residues that make up the sequence and the order in which they appear are important.

In this project (financially supported by the Croatian Science Foundation- HRZZ), we want to combine machine learning with experimental validation to develop a more efficient and economical approach compared to unguided experimental evaluation. We aim to discover patterns in existing data and accelerate the discovery of new catalytic peptides within a relatively small number of experiments. The overall objective is to determine whether we could use machine learning to efficiently predict the catalytic activity of short peptides and understand what are the key features that govern this process. We aim to reveal how peptide sequences are

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responsible for catalysis with the scope of evolving them to more complex systems, through self-assembly or tandem peptide repeats, to reach function. In our approach we aim to encompass the entire spectrum from fundamental understanding of peptide sequences and their ability to catalyse reactions to eventual societal benefit of discovering minimalistic versions of enzymes able to be used in everyday life. The successful outcome of this project will result in a strategy able to explore broad sequence and structural spaces for future discoveries.

During this course, students will spend 8 weeks conducting laboratory work in Dr. Kalafatović's research group. This will begin with basic training in the peptide synthesis and various analytical techniques. This teaching will occur in a "mentorship" situation, with two students being taught at a time. As the skills of the students develop, they will then begin to perform research experiments, using these techniques, to gain novel insight into the research field of design of short catalytic peptides and peptide assemblies.

After completion of the course, students will then have the option of continuing their research as a **Research Project** under the mentorship of Dr. Kalafatović or in a different research group of choice.

Learning outcomes:

Students will gain an in-depth theoretical knowledge of the study of peptide nanotechnology through peptide synthesis and characterization. In addition, the students will receive an insight into the application of machine learning methods to peptide design with the aim of searching for function (i.e. catalytic activity). This will come through reading on the subject, discussion with the course leader/mentor and other members of the research group, as well as first-hand experience in the laboratory.

Practically, students will gain significant practical experience at synthesizing peptides, analysing their quality and purity using chromatography techniques, often coupled to mass spectrometry for identification purposes. Options for performing AFM imaging, participation in database building and learning basic machine learning methods will also be available. This will be obtained through guided training, and reinforced through using the techniques to perform genuine research experiments. In this way, the skills learned should become relevant to the students in a research context.

Through work in a research environment, students will also have an opportunity to hone their soft research skills, including searching the academic literature, critical review of papers, experimental design and analysis, and writing of scientific reports.

Requirements, methods of assessment and evaluation:

Students are required to perform work in the laboratory for the duration of the course, as indicated in "Schedule of Classes" below. They will engage fully in the day-to-day activities of the work group, including observing the work of others, engaging in research work of their own, and performing other tasks required for running the laboratory. They are required to keep a laboratory book/journal of their work, written in English, in a

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manner that is understandable to their supervisor. They will also engage in scientific discussions, lab meetings and/or presentations of their work to the same degree as other members of the research group. They will work at all times in a safe manner, as defined in the course "Introduction to Laboratory Work & Safety" plus any additional safety measures that apply to members of this laboratory.

Students will receive continuous assessment from the mentor/course leader who will meet with and teach the students on a regular basis. In this way, the student will both be assessed, and receive continuous feedback concerning their work. At the end of the course, the mentor will submit a report on their work and progress at the end of the course. The mentor's report, and accompanying grade, will account for 50% of the student's grade for the course.

Additionally, at the end of the course, the student will submit a short report (approximately 3 pages), detailing the area that they worked in, the experiments they performed, any results they obtained, and skills that they learned and used. This report will then be assessed by the mentor and one other member of faculty, who will together agree on a grade for the remaining 50% of the course.

Qualification and grades (according to the *University of Rijeka Study Regulations*):

The following grades will be awarded based on the final score:

Percentage score	ECTS grade	Numerical grade
90% to 100%	A	Excellent (5)
75% to 89.9%	B	Very good (4)
60% to 74.9%	C	Good (3)
50% to 59.9%	D	Satisfactory (2)
0% to 49.9%	F	Unsatisfactory (1)

The final grade is based on the sum of percentage points accumulated during the course. Passing grades are excellent (5), very good (4), good (3) and satisfactory (2).

Schedule of classes:

Daily, from 9:00-12:00 and 13:00-17:00, every weekday, either from 01.03.2021 to 16.04.2021, or from 19.04.2021 to 4.06.2021 (excluding national and University holidays). All work will be performed in laboratories O-149 and O-276, unless otherwise indicated by the course leader/supervisor. Variations in exactly which hours are worked can be made with the agreement of the course leader/supervisor. Some laboratory time may be replaced with private study and background reading, subject to the requirements of the research performed, and with the agreement of the course leader/supervisor.

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Additional information:

Academic integrity

Students are required to respect the principles of academic integrity, and refer to the documents: *Ethics Guidelines of the University of Rijeka* and the *Ethics Guidelines for Students*.