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Topics for the Janko Jamnik Doctoral Scholarship for Promising Early-Stage Researchers in Chemistry and Related Sciences for 2022

Topic Title	Short Content	Mentor	Department
Structure and dynamics of RNA in biomolecular condensates	Membraneless organelles or biomolecular condensates are formed by networks of specific proteins and RNAs. Due to dynamic and adaptable nature of condensates the process of their formation via phase-phase separation must be tightly controlled or it can lead to formation of pathological condensates. We aim to systematically explore how structure, dynamics and interactions of RNA are responsible for physical characteristics and biological role of RNA in various condensates, using *in vitro* reconstituted systems in combination with methods of structural biology.	Maja Marušič	D15/D12/D11
Increasing the rate of site-specific genome transgene integration using enhanced version of CRISPR/Cas system for therapeutic purposes	Viral delivery systems are mostly used for production of therapeutic relevant cells, e.g. CAR-T cells. The main drawback of viral mediated cells production is random integration process that can result in an insertional mutagenesis that can lead to oncogenic changes and abnormalities, also the final cell product can be less homogenous with lesser desired phenotype. To overcome that, site-specific targeted insertion is preferred, which could be accomplished by CRISPR mediated genome integration of transgenes. Nevertheless, the efficiency of HR is still quite low, therefore improvements of CRISPR orchestrated therapeutic cell generation should be introduced. We have developed enhanced version of CRISPR/Cas system that by utilizing modified DNA matrix can improve genomic integration. We believe that CRISPR/Cas mediated production of therapeutic cells will become the new gold standard of production of cells and could be extrapolated on treating all genetic diseases.	Duško Lainšček	D12/D11

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Modulating CAR-T cell cancer immunotherapy	CAR-T cell immunotherapy represent a revolutionizing highly efficient therapeutic option for treating various cancer, including lymphomas and leukemia. CAR-T cell immunotherapy is based on autologous transplantation of genetically modified cells, which kill cancer cells upon reinfusion into patient's body. We plan to implement versatile approaches of synthetic biology (signal and its pathway modification CRISPR/Cas usage etc.) in CAR-T cell immunotherapy for different cancers. With CAR-T cell modulation we want to make this therapeutic option more safe and controllable. Doctoral research will include various techniques, from confocal microscopy, cloning to testing *de novo* designed CAR-T cells in animal models.	Duško Lainšček	D12/D11
The origin of entropy	In environmentally important reactions in the atmosphere, entropy plays a decisive role. Thermodynamics of reactions in atmospheric aerosols, which are important environmental pollutants, will be studied theoretically (quantum molecular dynamics, statistical thermodynamics) and experimentally (photolysis with laser beam)	Matej Huš	D13/D04
Improving on catalysts with modelling	Modelling of chemical reactions and reactors has made tremendous progress in the past decade and enables the predictions of reaction mechanisms. Using this approach, we will computationally screen the periodic system and predict a better catalyst for nitrogen activation and expermientally test it.	Matej Huš	D13/D09
Theoretical description of photocatalysis	Photocatalysis is a promising approach in catalysis, where molecule in the excited state react differently than in the ground state. Using quantum chemical methods, we will describe chemical transformations of excited molecules on catalysts under illumination.	Matej Huš	D13/D01

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Active biodegradable foils with positive economic and environmental impacts	The research project includes studies of the utilization potential of the extracts of the invasive alien plant species, Japanese knotweed, to formulate novel, advanced, and active biodegradable foils for food packaging applications, which will provide the food with inherent active properties such as antioxidant and/or antimicrobial activity. Chemical characterization of the selected extracts as well as in-depth physicochemical studies of the formulated foils and the migration of the bioactive compounds from the foils into food and food simulants will be in the focus of the work.	Katerina Naumoska	L06 (D04) / D13
Development of photoswitchable ring-opening polymerization for 3D printing of synthetic polypeptides	Development of a novel system for photoswitchable polymerization to produce synthetic polypeptides. Good control over photopolymerization will allow 3D printing of polypeptide scaffolds for biomedical applications.	Petra Utroša	D07/D11
Biorefinery	Development and optimization of catalysts and processes for the efficient conversion of biomass into fibres and value-added chemicals will be crucial for the design and engineering of the first Slovenian biorefinery.	Miha Grilc	D13 & D10

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Development of a new method for understanding and improving the specificity of therapeutic RNAs	Antisense RNA technology is emerging as an effective tool for the treatment of genetic diseases. Understanding the specificity of antisense RNA binding to the target is critical for their safe and effective clinical application, which currently represents a large untapped potential. In the Ule lab, we have developed a hybrid version of the CLIP method that enables multiparallel assessment of therapeutic RNAs and quantification of the binding efficiency of individual antisense molecules to the target RNA. By complementing molecular and synthetic biology techniques, bioinformatics and modelling tools, and spectroscopy, the candidate will continue to develop a tool for optimisation and validation of therapeutic RNA molecules and lay the groundwork for their application.	Miha Modic	D11/D01/D12
The role of RNA interactions in the assembly of biomolecular condensates	Intracellular compartmentalization of RNAs determines their functionality within the cell. RNAs are often concentrated in phase-separated regions where they condense RNA binding proteins (RBPs) and network with other RNA molecules. The importance of the RBP-RNA and RNA-RNA interactions in condensate assembly remains poorly understood. By combining molecular modeling methods (D1 Praprotnik), new synthetic biology techniques, and omic-technologies (D11 Ule), the candidate will elucidate the architecture and principles of RNA condensate assembly, the importance of RNA-RNA and RBP-RNA interactions in phase separation of the condensates, and the effects of these interactions on the biological and pathological functions of the condensates.	Miha Modic	D11/D01

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Enhancing protein pores for use in nanobiotechnology	Biological pores are being already used as nanosensors to detect analytes in real time. Existing protein pores are further explored and optimized to improve specificity or discrimination between specific analytes. We are constantly searching for new pores and trying to determine their 3D structures and test their function in nanobiotechnological applications. Using high-throughput and in silico methods, we are trying to make them more suitable for specific detection systems and improve their detection properties.	Matic Kisovec	D11/D01/D04
Design of synthetic protein pores	To date, a number of 3D pore structures with different properties and specificities have been identified. Since each analyte (or group of analytes) requires a specific pore that is well suited for real-time detection, it would be beneficial to propose and test protocols for in silico design of protein pores with desired properties and also test the best candidates in the wet lab.	Matic Kisovec	D11/D01/D12
Synthesis and characterization of new metal-organic framework glasses	The recently discovered metal-organic framework glasses are only the fourth type of glass that can be prepared by melt-quenching, and the only one that is microporous without any post-synthetic modifications. Due to the large and accessible surface area and the ease of functionalization of their building units, they have exceptional application potential in many different fields (gas capture and separation, catalysis, energy storage, sensors, etc.). The search for new representatives of this interesting group of materials will be tackled by computational methods, followed by materials preparation and advanced structural characterization.	Andraž Krajnc	D09/D13

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Electrified epoxidation	Value-added raw material synthesis that is independent of intermittent nature of green energy. Induction catalysis and photo-thermo-catalysis enable on-demand production.	Janvit Teržan	D13/D09
Understanding the PEM fuel cell catalyst and their production at multiple scales	Fuel cells are devices that convert hydrogen and oxygen into clean electricity using a catalyst. With mass-commercialization of fuel cell technology, understanding of the catalyst both at the atomic/nanoscale as we production at high volume is essential. In this sense, both understanding of the catalyst properties, as well as reactor engineering in conjunction with multiscale modelling can provide the necessary tools to develop next-generation fuel cell catalysts at the required scale.	Andraž Pavlišič	D13/D10