

CEIPEX MU TOPIC 10

Položka / Field	Obsah / Content
NAME	prof. RNDr. Radek Marek, Ph.D.
NAME OF THE RESEARCH GROUP	Structure of Biosystems and Molecular Materials
CEIPEX RESEARCH TOPIC LEVEL2	Advanced instrumentation and methods for materials characterization (development of methods & modelling)
TOPIC No. 1	Pushing the Frontiers of Magnetic Resonance Spectroscopy for Biotechnology and Materials Engineering
ABSTRACT No. 1	Magnetic resonance (MR) spectroscopy represents one of the most powerful and versatile methods for structural analysis in biology, chemistry, and physics. While nuclear magnetic resonance (NMR) investigates the properties of atomic nuclei, electron paramagnetic resonance (EPR) investigates systems containing unpaired electrons. These two methods are closely interconnected in the NMR spectroscopy of paramagnetic substances, commonly referred to as paramagnetic NMR spectroscopy (pNMR). The development of pNMR methods depends not only on advances in instrumentation but also on the development of new concepts and methods for the prediction and interpretation of pNMR parameters. These parameters can currently be predicted using advanced relativistic quantum-chemical methods, in particular density functional theory (DFT). In biotechnological applications, it is necessary to account for the effects of molecular dynamics and the surrounding environment in theoretical predictions of paramagnetic systems. This can be achieved by combining machine-learning-based force fields, molecular dynamics simulations, and relativistic quantum-chemical methods representing the current state of the art. In materials research, it is necessary to account for solid-state conditions. For designed systems, this requires periodic DFT calculations including relativistic effects and different spin states. For a number of systems, it is also important to account for correlated motions and non-adiabatic effects in photochemically excited systems. Within the projects currently pursued in the area of paramagnetic NMR spectroscopy, we focus on the development of ruthenium-based anticancer metallodrugs and their carriers, as well as on the development of catalytic systems based on metal-organic frameworks.
CEIPEX RESEARCH TOPIC LEVEL2	Molecular Medicine: Molecular Oncology of Solid Tumors
TOPIC No. 2	Next-Generation Anticancer Therapies Based on Metallodrugs

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ABSTRACT No. 2	Cancer represents one of the most common causes of mortality worldwide. Consequently, considerable attention is devoted to the development of new cancer therapies and strategies for preventing the formation of metastases. Despite significant advances in biological therapies, including gene therapy, chemotherapy, and the modulation of biological processes using small therapeutic molecules, these approaches remain among the important tools for the treatment of these serious diseases. Metallo drugs, historically represented by cisplatin, constitute an established class of anticancer agents with considerable potential for further development. A detailed understanding of the molecular processes underlying their activity, transport, and release may enable the development of new metal-based therapeutic systems and molecular drug carriers. Our current research focuses on platinum-based systems involving platinum in oxidation states +II and +IV and their association with molecular carriers, including supramolecular host-guest complexes. A parallel research direction focuses on the development of migrastatic agents based on ruthenium complexes, which target processes associated with cancer cell migration and metastasis. Molecular carriers based on macrocyclic compounds and metallocages will be further developed by incorporating biovectors (targeting moieties) to improve the targeting of the therapeutic agents. Drug release at the target site is achieved either through spontaneous release mechanisms or by external stimuli, such as an external magnetic field. The development of these drug-carrier systems is carried out in collaboration with the Masaryk Memorial Cancer Institute.
WEBPAGE OF THE RESEARCH GROUP	https://www.ceitec.eu/structure-of-biosystems-and-molecular-materials/rg108