FACULTY OF SCIENCE
Charles University

LABORATORY OF BIOMOLECULE STRUCTURE AND FUNCTION

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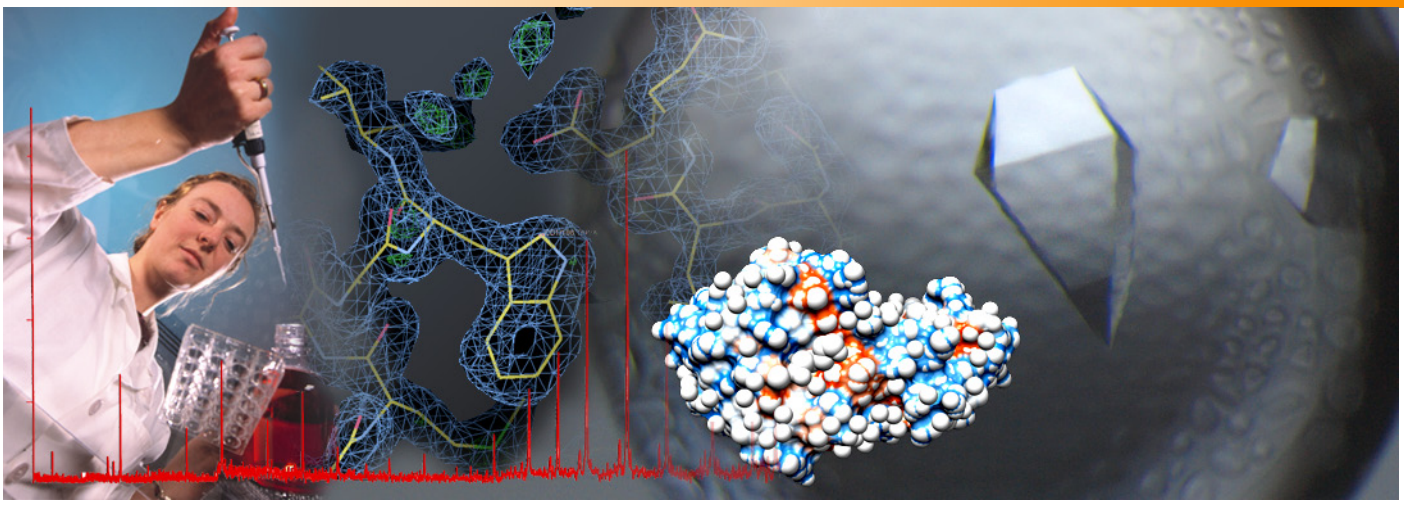

RESEARCH AREA & EXCELLENCE

Structure and function relationship of biomacromolecules: target biomolecule identification, isolation and characterization, biotechnologies dealing with recombinant proteins as therapeutic agents.

- *R*ecombinant protein expression and purification
- Structural biochemistry and biophysical characterization of proteins
- Structure of ligand-protein and multi-protein complexes
- Photo-initiated and chemical cross-linking, H/D exchange
- Mass spectrometry of biochemically interesting macromolecules
- Molecular modelling of biomolecules

Mission

Development and application of techniques for the structural description of clinical-relevant biomacromolecules and the understanding of their structure-function modulation.

KNOW-HOW & TECHNOLOGIES

Content of Research

The structural and functional characterization of proteins participating in cancer recognition, in xenobiotic biotransformation, in the regulation of cell processes, in biocatalysis and immunomodulation in their native conditions. Research of protein structure, protein-protein and protein-ligand/substrate interaction with the use of chemical cross-linking reagents, photo-initiated cross-linking, H/D exchange, photoaffinity labeling protein, determination of disulfide bridges, glycosylation and other post-translational modifications of proteins. Protein identification, structural determination and targeting by advanced techniques of mass spectrometry. Homology modeling, in silico ligand docking, molecular dynamics and interaction energy calculations.

Main Capabilities

Consultancy or collaboration within the fields of recombinant protein expression and purification (both in bacterial and in mammalian cell line expression systems) and protein characterization by various biochemical and biophysical techniques, e.g. sedimentation analysis in analytical ultracentrifuge, surface plasmon resonance, UV-VIS & CD spectroscopy, structure solution by protein X-ray crystallography or by advanced techniques of mass spectrometry.

EXPECTATIONS & OFFERS

Offers

We offer our expertise within a diverse range of issues broadly defined as protein biochemistry and biotechnology, protein structure solution or prediction, mass spectrometry and biomacromolecule analyses.

Requirements

We are looking for cooperation with academic partners as well as public and private organizations in the fields of recombinant protein expression and purification, protein characterization and binding assessment, protein structure determination, multi-protein complex mapping, molecular dynamic and protein structure modelling.

KEY RESEARCH EQUIPMENT

All equipment is operated by responsible persons: M. Šulc, M. Martínková, V. Martínek, P. Novák, P. Man, O. Vaněk, D. Kavan, P. Pompach, and P. Jeřábek.

- Analytical ultracentrifuge ProteomeLab XL-I
- Surface plasmon resonance workstation PLASMON-4
- HPLC/UHPLC and FPLC systems
- UV-VIS spectrophotometers, CD spectrophotometer
- Protein sequencer Procise 491
- Two photolysers emitting UV-light with maximum around 254 nm (100W) and 360 nm (500W)
- FT-ICR Bruker Solarix 12T and MALDI-TOF/TOF Bruker Ultraflex III mass spectrometer (partnership laboratory with Institute of Microbiology, v.v.i. ASCR)

PARTNERSHIPS & COLLABORATIONS

Academic partners: University of Texas, Houston, USA | Technische Universität Berlin, Germany | Institute for Molecular Science, Okazaki, Japan | National Institute of Molecular Studies, Okazaki, Japan | Loyola University, Chicago, USA | Georgetown University, Georgetown, USA

Public and Private sector: Zentiva, a.s. | Apronex, s.r.o.

Main Projects

- Innovative Technologies for the Identification and Optimization of the New Generation of Anti-Cancer Drugs (Charles University, UNCE 204025/2012, 2012–2016)
- Molecular mechanisms of intraprotein/interdomain signal transduction in model heme sensor proteins (Czech Science Foundation, 2015–2018)
- Harnessing soluble forms of NK cell receptors and their ligands for the generation of novel anticancer immunotherapeutics (Czech Science Foundation, 2015–2018)
- Mammalian microsomal cytochrome P450 interaction with redox partners – topology and structure-function relationships (Czech Science Foundation, 2012–2015)
- Interspecies comparison of nitrilases by using recombinant enzymes obtained by database-mining: their environmental impact and potential application (Czech Science Foundation, 2011–2014)
- Structural insight into *E. coli* protein WrbA, the founding member of a family of proteins implicated in defense of cells against oxidative stress (Czech Science Foundation, 2010–2014)
- Innovation voucher (with Zentiva, a.s., Prague city, 2013–2014)
- Molecular diagnostics of bacterial pathogens (with Apronex, s.r.o., Ministry of Industry and Trade, 2009–2013).

ACHIEVEMENTS

- Czech patent "Soluble form of mouse NK cell receptor NKR-P1A and means of its recombinant preparation" (PV 2010-132)
- Czech utility model "Active form of alfa-N-acetyl-galactosaminidase from filamentous fungi *Aspergillus niger*" (2012-26061).
- Jeřábek P et al.: Flexible docking-based molecular dynamics/steered molecular dynamics calculations of protein-protein contacts in a complex of cytochrome P450 1A2 with cytochrome b5. Biochemistry 53, 6695–705 (2014)
- Kádek A et al.: Aspartic protease nepenthesin-1 as a tool for digestion in hydrogen/deuterium exchange mass spectrometry. Anal Chem 86, 4287–94 (2014)
- Ptáčková et al.: The Application of an Emerging Technique for Protein–Protein Interaction Interface Mapping: The Combination of Photo-initiated Cross-linking Protein Nanoprobes with Mass Spectrometry. Int J Mol Sci 5, 9224–41 (2014)
- Stráňava M et al.: Introduction of water into the heme distal side by Leu65 mutations of an oxygen sensor, YddV, generates verdoheme and carbon monoxide, exerting the heme oxygenase reaction. J Inorg Biochem 140, 29–38 (2014)
- Bláha J et al.: Expression and purification of soluble and stable ectodomain of natural killer cell receptor LLT1 through high-density transfection of suspension adapted HEK293S GnTI- cells. Protein Expr Purif 109, 7–13 (2015)