Jiří Mareš

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. . . well motivated, results-oriented scientist with very good problem- solving skills in wide variety of problems in both experimental NMR and modeling of molecular systems. Due to his easy-going character, he is an excellent team-worker that can also work on his own initiative with very complicated subjects and, with resiliency, solve them. . .
Assoc. Prof. Perttu Lantto

Education and degrees

2004 **Ing. (M.Sc.)**, *Institute of Chemical Technology Prague, Chemistry*
2009 **Dr. sc. nat. (Ph.D)**, *University of Zurich, Chemistry*
2020 **Docent**, *University of Oulu, Nuclear magnetic resonance modeling*

Master thesis

title *Study of structure and interactions of structural proteins of retroviral capside*
supervisors Prof. Tomáš Ruml and Dr. Ing Michaela Rumlová
description Combining techniques of biochemistry, NMR, molecular modeling. First showing my unusual flexibility in tackling scientific problems.

Doctoral thesis

title *Structure, folding and interactions of membrane-associated biomolecules studied by NMR*
supervisors Prof. Oliver Zerbe
description Combining techniques of molecular biology, biochemistry, NMR, molecular modeling. As an example: developing of HPLC purification protocol for bacterial LPS, NMR to measure interactions with antibiotic peptide, molecular modeling → nearly 100 citations (including several patents) of the resulting study.

Experience

2009–2010 **Early scientist Swiss National Funds scholarship**, *University of Helsinki*
paramagnetic NMR (pNMR), based on theoretical advancements of prof. Juha Vaara, computational studies
2010–2012 **Marie Curie postdoctoral fellowship**, *University of Oulu*
"Computation of nuclear magnetic relaxation in paramagnetic systems"
2013–2018 **Post doctoral researcher**, *University of Oulu*
part of European pNMR network, received 2-years funding of Finnish cultural foundation: "Xe NMR molecular sensors modeling and design for medical applications"

2019–2021 **Post doctoral researcher**, *University of Oulu*, Faculty of medicine
Cardiac magnetic resonance imaging: development of contrast based on natural biomarkers, NMR/MRI modeling, finite-elements modeling of heart electromagnetic activity

2021–2023 **Post doctoral researcher**, *University of Oulu*, Faculty on natural sciences
Part of study of atmospherically-relevant surfactant solutions by NMR relaxation and diffusions modeling - myself mostly molecular modeling and relaxation modeling including polarization forcefield parameters optimization, full relaxation matrix approach, quadrupolar relaxation ...

2024– now **Senior scientist**, *University Vienna*, Division of Pharmaceutical Chemistry

Languages

English	Proficient
Finnish	Independent
Czech	Mother tongue
German, Polish	Passive

Computer skills

Microsoft, Mac Os	User level
Linux	Admin level
Programming	Python and some knowledge in ± decreasing order in: Matlab, Bash, Perl, Html, C , C++, Fortran

Skill matrix

■□□□□ basic knowledge
■■□□□ intermediate knowledge with some project experience
■■■□□ extensive project experience
■■■■□ deepened expert knowledge
■■■■■ expert / specialist

	Level	Skill	Years	Comment
Experimental	■■■□□	protein epxresion, purification	3	*Recombinant protein expression, HPLC purification, (assisted) use of standard analytic techniques like UV-VIS spectrometry, LC-MAS, MALDI-TOF*
	■■■□□	NMR	7	*Standard organic chemistry set of experiments, protein set, diffusion, relaxation: CPMG ..., $T_{1,\rho}$, CEST*
	■□□□□	MRI	1	*Measurements on Siemens clinical scanners, development of contrast techniques tested on brain and cardiac MRI, some experience with implementation of pulse sequences.*

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NMR analysis	Evaluation of measured data	6	*From standard techniques to detailed simulation/fitting of measured spectra, special experience with various situations of chemical exchange and relaxation.*
Computational	Molecular modeling	16	*First principles MD (DFT, XTB), biomolecular MD including non-standard molecules, recently focused on my own accurate forcefield development based on AMBER/CHARMM forcefield form and AMOEBA multipole & polarizable forcefield form with a special attention on non-bonding forces, applicable to variety of molecular systems and materials.*
	Quantum chemistry	12	*DFT, ab initio, multiconfigurational, open shell methods for energies, forces, frequencies, spectroscopies*
	NMR parameters and properties	12	*Quantum chemistry calculation of nuclear shielding, J-couplings, quadrupolar couplings, special focus on paramagnetic nuclear shielding, and its effect such as pseudcontact shifts and relaxation enhancement.*
	Spin dynamics simulation	3	*(Liouville-space) spin dynamics simulation, (Redfield) relaxation with thermalization, including systems with chemical exchange implemented in my own python code.*
	Numerical optimization	12	*Large set of numerical optimization techniques, with a special focus on Bayesian optimization, experience with machine learning based optimization - mostly gaussian processes.*
Outreach	Scientific writing and presenting	18	*Experience from many peer-reviewed scientific papers, grant applications, oral and poster presentations for scientific community and broader public.*
Leadership	Student guidance and teaching	10	*Guidance of numerous MSc. and PhD students, leading workshops and university course exercies.*
Other	Finite element analysis	2	*Some experience with fluid dynamics, fluid-solid interaction modeling and electromagnetic simulation using Elmer, NGsolve and Fenics.*

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■□□□□	CAD and CNC	3	*Experience with computer aided design using Rhino3D and OpenSCAD, implementation of reverse kinematics for milling tools and robotic arm, g-code generation, computer numerical control using LinuxCNC, experience with hardware building and wiring with stepper and servo control.*
■□□□□	Embeded system programing, computer visions	3	*Some experience with Arduino programing, ROS operating system, computer vision using openCV.*

Interests

Science It is so, science has been not only profession, but also my hobby much even before I joined university, as an example, I scored high repeatedly in national biology competitions at high school. Science is also a common topic for discussion with anyone similarly oriented.

Technology I learn to use Linux operating system in my free time, the same with programming, LaTeX, computer numerical control, finite element analysis, CAD design ...

Nature Nature has been the most important balance for my civilization-based activities, place where I often get most important new ideas in science, and where I meet people for example as paddling leader or scout leader.

Music Unfortunatelly, only in a form of listening now, but Piano and Cello playing used to be a dear hobby to me.

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