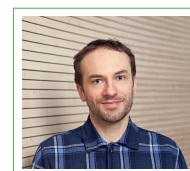


# Jiří Mareš

+358452618400

jiri.mares@iki.fi

<https://www.linkedin.com/in/jiri-mares-vienna>



*... 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 capsid*

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”

+358452618400 • jiri.mares@iki.fi

<https://www.linkedin.com/in/jiri-mares-vienna>

- 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

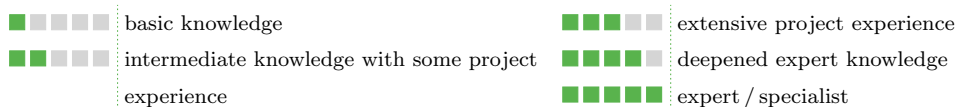
English Proficient  
 Finnish Independent  
 Czech Mother tongue  
 German, Polish Passive




## Computer skills

Microsoft, Mac Os User level  
 Linux Admin level

Programming Python  
 and some knowledge in  $\pm$  decreasing order in:  
 Matlab, Bash, Perl, Html, C , C++, Fortran

## Skill matrix



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

NMR analysis	■■■■■	Evaluation of measured data	6	<i>From standard techniques to detailed simulation/fitting of measured spectra, special experience with various situations of chemical exchange and relaxation.</i>
Computational	■■■■■	Molecular modeling	16	<i>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 &amp; polarizable forcefield form with a special attention on non-bonding forces, applicable to variety of molecular systems and materials.</i>
	■■■■■	Quantum chemistry	12	<i>DFT, ab initio, multiconfigurational, open shell methods for energies, forces, frequencies, spectroscopies</i>
	■■■■■	NMR parameters and properties	12	<i>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.</i>
	■■■■■	Spin dynamics simulation	3	<i>(Liouville-space) spin dynamics simulation, (Redfield) relaxation with thermalization, including systems with chemical exchange implemented in my own python code.</i>
	■■■■■	Numerical optimization	12	<i>Large set of numerical optimization techniques, with a special focus on Bayesian optimization, experience with machine learning based optimization - mostly gaussian processes.</i>
Outreach	■■■■■	Scientific writing and presenting	18	<i>Experience from many peer-reviewed scientific papers, grant applications, oral and poster presentations for scientific community and broader public.</i>
Leadership	■■■■■	Student guidance and teaching	10	<i>Guidance of numerous MSc. and PhD students, leading workshops and university course exercises.</i>
Other	■■■■■	Finite element analysis	2	<i>Some experience with fluid dynamics, fluid-solid interaction modeling and electromagnetic simulation using Elmer, NGsolve and Fenics.</i>

- 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.*
  
- Embedded 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, L<sup>A</sup>T<sub>E</sub>X, 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
Unfortunately, only in a form of listening now, but Piano and Cello playing used to be a dear hobby to me.