ELIXIR CZ Artificial Intelligence in Life Sciences I
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Stanislav Mazurenko, Masaryk University, Brno

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Stanislav Mazurenko received his Ph.D. in applied mathematics and cybernetics from Lomonosov Moscow State University in 2013. He then joined the protein engineering group Loschmidt Laboratories at Masaryk University to work on data analysis and modelling of protein thermal denaturation. He is a co-author of the CalFitter web server and the FireProt^{DB} database. In 2018, he completed a one-year stay at the University of Liverpool, working in nonlinear optimization. He now leads a team in Loschmidt Laboratories, focusing on machine learning, automation, and data analysis in protein engineering. This is a fascinating area of research at the interface of biochemistry, biophysics, computer science, and mathematics. The team's goal is to delve into protein data to gain insights into the underlying biophysical mechanisms and create better tools for the design of improved protein variants. Those enhanced variants are then used in numerous applications, from healthcare – stem cells, Alzheimer's disease, stroke – to the food industry and environmental protection.

Thomas Evangelidis, IOCB Prague

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Thomas Evangelidis is a Senior Researcher in the Institute of Organic Chemistry and Biochemistry (IOCB) in Prague and CEITEC in Brno. He has >12 years of experience in novel method and software

development for protein-ligand binding affinity prediction and NMR structure determination, for which he combines notions from Chemoinformatics, Machine Learning, and Quantum Chemistry. He is currently starting a spin-off company named "Alffinity", which will provide software and computational services for Molecular Binding Affinity prediction by AI and 4D NMR structure determination.

Thomas obtained his PhD in Computation Medicinal Chemistry & NMR from the Dept. of Pharmacy, University of Athens, Greece & Central European Institute of Technology (CEITEC), Brno, Czech Republic. He continued in CEITEC for a 2-year post-doc on 4D-NMR protein structure determination. In 2018 he also joined IOCB, where he develops new methods for protein-ligand binding affinity prediction by Semiempirical Quantum Mechanics calculations.

Jan Švec, University of West Bohemia, Pilsen

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Jan Švec obtained a Phd. in 2013 at the University of West Bohemia in Pilsen, since then he has been working as a researcher at the NTIS Research Centre of the University of West Bohemia in the field of natural language processing and speech recognition. He specializes mainly in applied research in the field of applications of artificial neural networks and related technologies. He teaches courses in Internet technologies and voice dialogue systems. He is also an employee of the university spin-off company SpeechTech s.r.o.

David Hoksza, Charles University, Prague

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David Hoksza received his master's degree in computer science from the Faculty of Mathematics and Physics (FMP) at Charles University where he also defended his PhD thesis focused on similarity search in protein structure databases. Between the years 2010 and 2017, he was working as an assistant professor at the Department of Software Engineering of FMP where he co-founded the bioinformatics study program. At the same time he was also involved in teaching and research at the Czech Technical University and at the University of Chemistry and Technology, Prague. Between 2017 and 2020 he has been employed as a research associate in the bioinformatics core of Luxembourg Centre for Systems Biomedicine, Université du Luxembourg. He is interested in the development of efficient algorithms in the area of structural bioinformatics and data visualization. He has been involved in projects involving mostly protein and RNA structure with the occasional excursions to the fields of cheminformatics (ligand-based virtual screening, exploration of chemical space), computational genomics (analysis of MinION data), and systems biology (visualization and analysis of molecular networks).

Ekaterina Grakova & Antonín Kunka, IT4Innovations, Technical University of Ostrava & Masaryk University

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Ekaterina Grakova, Ph.D., is a female young researcher, who concentrates her research interest to the development of optimization methods suitable for the analysis of dynamic data and its spatial information. Solving the optimization of traffic with the help exact, heuristics and metaheuristic algorithms with the usage of HPC. Testing of the routing results with the help of implemented methods. Her research interest also includes the search for optimal parameter setting for the algorithm we created using the hyperparameter search method implemented in HyperLoom pipeline. She participates in the realization of the projects: NPU II - National Programme of Sustainability project „IT4Innovations excellence in science" (Investigator), Personalized Medicine - Diagnostics and Therapy TN01000013 (Investigator).

Antonin Kunka is a graduate student in Loschmidt laboratories at Masaryk University Brno. He graduated in Biochemistry and is currently finishing Ph.D. studies in Microbiology. Antonin is focused on experimental aspects and the structural basis of protein stability. His former projects include deciphering the unfolding mechanisms of computationally stabilized proteins, development of software tool Calfitter for global analysis of protein temperature-denaturation experiments, and stabilization of model protein by rational design. For the past two years, Antonin has been studying the aggregation of medically relevant proteins/peptides, e.g. amyloid-beta, and its modulation by small molecules and other proteins. He is also developing the protein aggregation predictor in collaboration with the IT4Innovations.

Konstantinos Tripsianes, CEITEC - Central European Institute of Technology, Masaryk University

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Dr. Tripsianes is a top expert in biomolecular NMR developing tools and software to streamline NMR structural studies and integrate NMR data to synergistic structural approaches. He explores and synthesizes ideas and techniques from fields as diverse as biochemistry, molecular biophysics and computer science to understand molecular recognition mechanisms associated with human health (hereditary diseases, cancer, aging). He has co-authored 28 publications (h-index=14) in international high-impact journals, such as *Science, Nat Struct Mol Biol*, *Nat Commun*, etc.