Colloquium: Bioinformatics

04. - 07. May 2026

DHEG136E (Showroom) | Data House, Sandgasse 36, Erdgeschoß

It is a pleasure to invite you to the colloquium for our Professorship in Bioinformatics at Graz University of Technology. The public part will be a short teaching sample at Bachelor's level in Biomedical Engineering, 5th semester in "Sequence-Read Mapping as part of the lecture Fundamentals of Bioinformatics", a scientific talk (titles below), and a discussion with the audience.

Coskuner-Weber Orkid

04. May 2026 | 09:00 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: From BioMatics to Drug Discovery: AI-Based Ensemble Generation, MaxEnt Refinement, Transient Pocket Detection, and Multiagent Reinforcement Learning

Abstract: Intrinsically disordered proteins and other highly dynamic biomolecular systems remain challenging targets for bioinformatics and drug discovery because their function often arises from heterogeneous conformational ensembles rather than from a single stable structure. In this talk, I will present an integrated computational framework that begins with BioMatics, a disorder-aware sequence analysis and multiple sequence alignment strategy designed to better capture the evolutionary and physicochemical characteristics of dynamic protein systems. Building on this foundation, I will discuss AI-based ensemble generation approaches that move beyond static structure prediction toward population-level modeling of biomolecular conformational landscapes.

A central component of this framework is the reconciliation of computationally generated ensembles with experiment through the Maximum Entropy (MaxEnt) method, which enables minimally biased refinement of ensemble distributions so that they remain consistent with experimental observables while preserving structural diversity. On the basis of these experimentally grounded ensembles, I will then describe computational strategies for identifying cryptic and transient pockets that are often invisible in static models but emerge dynamically across the ensemble and may provide new opportunities for therapeutic intervention.

Finally, I will show how ensemble-resolved pocket information can be coupled to fragment-based drug design using multiagent reinforcement learning, in which interacting AI agents explore, optimize, and prioritize fragment combinations against dynamic and disorder-dependent binding opportunities. Together, BioMatics, AI-based ensemble generation, MaxEnt refinement, transient pocket detection, and multiagent reinforcement learning define a unified bioinformatics framework for next-generation biomolecular modeling and drug discovery.

Bio: Prof. Dr. Orkid Coskuner-Weber was born in Remscheid, Germany. She studied at Middle East Technical University, where she received her B.S., at the Universität zu Köln, where she completed her Diplom in Chemistry, and later earned her Dr. rer. nat. at the Universität zu Köln in Germany. She also pursued further academic training through research visits at the Department of Physics, University of Amsterdam, and the Department of Chemical Engineering at UMIST in the United Kingdom.

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She worked for 12 years as a postdoctoral scientist and assistant professor at Johns Hopkins University, Stanford University, NIST, George Mason University, Georgetown University, and The University of Texas at San Antonio. During this period, she also built strong links between her research at NIST and academia. She later joined the Turkish-German University as an assistant professor, where she was subsequently promoted to associate professor and then to full professor of Molecular Biotechnology.

Her research spans bioinformatics, computational biology, biophysics, artificial intelligence, and dynamic biomolecular systems, with particular emphasis on intrinsically disordered proteins, ensemble modeling, and AI-driven drug discovery. She has published approximately 70 peer-reviewed scientific articles and 11 book chapters. Her work has been supported by funding from COST EU, DAAD, and BAP.

Hausser Jean

04. May 2026 | 14:30 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: Bioinformatics and Machine Learning to Identify Immunotherapy Targets from Single-Cell and Spatial Omics Data

Abstract: Single-cell and spatial transcriptomics offer unprecedented views of tissue biology, yet extracting the signals and genes that actually control cell behavior from these observational datasets remains an open problem. This gap matters: signals and genes that causally drive disease phenotypes are the therapeutic targets pharma needs to develop disease-modifying drugs, in oncology, neurodegeneration, and metabolic disease. Existing approaches identify correlative signatures but cannot reliably distinguish drivers from passengers, limiting their translational utility.

My lab develops bioinformatics and machine-learning methods that exploit transcriptional heterogeneity - within tissues, across individuals, and over disease stages - as natural experiments to identify phenotype-controlling genes and cell interactions. I will briefly outline our overall research program, including Niche-Phenotype Mapping (NIPMAP, Nature Communications 2023), which uses ecological niche theory to decode spatial tissue organization.

The core of the talk will focus on Tissue Dynamics Inference (TIDYI), a recent method that infers absolute cell proliferation and death rates from single-cell RNA-seq snapshots, revealing tissue dynamics previously inaccessible from experimental measurements alone. I will conclude with our research vision and how it connects to BIOINFO, BioTechMed Graz, and the Cori Institute.

Bio: Jean Hausser leads the Computational Cancer Immunology group at Karolinska Institute, Stockholm. He trained in computer science at the University of Karlsruhe, completed his PhD at the University of Basel, and did postdoctoral work with Uri Alon at the Weizmann Institute (systems biology) and Johanna Joyce at the Ludwig Institute Lausanne (tumor immunology). His lab develops bioinformatics and machine-learning methods to identify immunotherapy targets from single-cell and spatial omics data, with a translational focus on solid tumors and an active interest in spin-off development.

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Mohorianu Irina

05. May 2026 | 09:00 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: RoSignOL (Robust Signature of Life).
Or How biology demanded new computational approaches.

Abstract: The vast amount of data and the rapid diversification of assays led to numerous (not always converging) hypotheses. The lack of golden standards realigned computational optimisation to robust, biological interpretations. To underline the importance of machine learning and data mining applied to bioinformatics challenges, I will focus on clustering, a fundamental step for processing single-cell and spatial assays (across modalities e.g. transcriptomics, epigenetics, proteomics/ metabolomics). The limitations of theoretical clustering approaches can be addressed with fuzzy community-based clustering. The FAIR-ness of approaches and datasets is enhanced with framework for studying the dynamics of gene regulatory networks.
The talk will focus on the ClustAssess framework and the flufftail one, centred on GRN dynamics.

Bio: IM's background in Computer Science was streamlined after finishing a CS BSc in Iasi, Romania, towards Machine Learning and Data Science (applied to Bioinformatics). During her PhD, she studied small non-coding RNAs (sRNAs), first in plants, then in animal systems. Soon after completing the first year of post-doc (working on D Melanogaster), she was awarded a BBSRC grant (as a Researcher Co-I). She started integrating mRNA and sRNA expression and became interested in Gene Regulatory Networks.
IM leads the Core Bioinformatics group (CSCI and IMS) comprising PhD students, research assistants and interns with an interest in data analysis and method development for high-throughput sequencing datasets. With her group, she is actively developing RoSignOL (Robust Signature of Life).
URL for the group: https://github.com/Core-Bioinformatics

Finotello Francesca

05. May 2026| 14:30 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: Bioinformatic analysis of the tumor microenvironment to advance precision immuno-oncology

Abstract: Cancer immunotherapy has revolutionized cancer treatment, shifting the focus from directly targeting tumor cells to harnessing the body's immune system to fight cancer. However, durable responses are observed in only a minority of patients, and the determinants of therapeutic success remain poorly understood.

My research aims to translate this paradigm shift in oncology into bioinformatics by transforming tumor data into quantitative and interpretable descriptors of the tumor microenvironment and anticancer immunity, which can ultimately inform and advance cancer immunotherapy.

In this talk, I will illustrate how bioinformatic analyses of tumor multi-omics data can be used to quantify key facets of the tumor microenvironment, including its cellular composition and spatial organization, underlying molecular circuitry, and interactions between malignant and immune cells. These quantitative features can then be leveraged to derive interpretable

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biomarkers and predictive models of patient trajectories, providing a mechanistic rationale for improving precision immuno-oncology.

A particular focus will be placed on *in silico* deconvolution, a powerful approach that infers the cellular composition of the tumor microenvironment from transcriptomic data, thereby enabling the identification of clinically relevant cellular biomarkers. We specifically develop and optimize deconvolution methods to couple the robustness of bulk transcriptomics with the cellular resolution of single-cell technologies and the spatial context provided by spatial transcriptomics.

Finally, I will discuss emerging opportunities at the interface of bioinformatics and machine learning and AI, highlighting how integrative and holistic analyses of multimodal tumor data can extract clinically relevant insights from increasingly complex datasets and support the development of predictive models that anticipate therapeutic responses.

Bio: Francesca Finotello earned her PhD in Bioengineering in 2014 at the University of Padova, Italy. She is an Associate Professor at the Institute of Molecular Biology and Digital Science Center (DiSC) of the University of Innsbruck, Austria, where she leads the Computational Biomedicine group. Her research focuses on the bioinformatic analysis of bulk and single-cell multi-omics data and on the development of computational methods to inform precision and personalized medicine. Her group has a particular focus on cancer immunology and integrates bioinformatics, systems biology, and machine learning techniques to elucidate the mechanisms underlying tumor-immune cell interactions.

May Patrick

06. May 2026 | 09:00 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: Translational Bioinformatics: Integrating Genomics and Multi-Omics for Precision Medicine

Abstract: High-throughput sequencing and multi-omics technologies have transformed biomedical research, yet translating these data into mechanistic insight and clinical applications remains a major challenge. In this talk, I will present my work on integrative bioinformatics approaches that combine genomics, multi-omics data, and clinical phenotypes to better understand complex diseases.

I will highlight three key areas: (i) large-scale genetic studies in neurological diseases, including the contribution of rare and common variants; (ii) pathway-based and polygenic risk approaches that enable patient stratification and have been validated in patient-derived cellular models; and (iii) integrated multi-omics and microbiome analyses to capture system-level disease processes.

Finally, I will outline future perspectives in translational bioinformatics, focusing on integrative data analysis and interdisciplinary collaboration at the interface of life sciences and medicine.

Bio: Patrick May, Dr. rer. nat., is Senior Researcher and Head of Genome Analysis at the Luxembourg Centre for Systems Biomedicine. His research focuses on genomics, bioinformatics, and multi-omics data integration in neurological and complex diseases, with particular expertise in Parkinson's disease, epilepsy, and microbiome systems biology. He has led and contributed to numerous international consortia, including NCER-PD, ILAE Genomics, and Epi25, and has authored more than 200 peer-reviewed publications. His work spans large-scale sequencing analysis, variant

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interpretation, translational genomics, and precision medicine approaches linking genetic risk to molecular and clinical phenotypes.

Krueger Robert

06. May 2026 | 17:00 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß | Webex Meeting | https://tugraz.webex.com/tugraz-de/j.php?MTID=mbe111063ce895c9735f52af04e58cda9

Papst Martin

07. May 2026 | 09:00 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: Bridging the sequencing gap: decoding microbiomes with metaproteomics and metabolomics

Abstract: Microbes represent the unseen majority of life on Earth, driving global biogeochemical cycles and impacting human health and well-being through the human microbiome. At the same time, microbial pathogens and antibiotic resistance pose an increasing global threat, underscoring the need for systems-level understanding of microbes and their ecosystems. While next-generation DNA sequencing has transformed microbiome research, it is largely limited to describing the genetic potential. In contrast, recent advances in mass spectrometry now enable functional characterization of complete microbiomes at the metaproteome and metabolome levels. Although these developments are milestones in microbiome research, our ability to interpret such data has not kept pace with instrumental progress. As information density increases, extracting deep molecular and mechanistic insights remains a major bottleneck. This talk demonstrates advancements in computational mass spectrometry that provide deep mechanistic insights into complex microbiomes of engineered ecosystems and shows how de novo metaproteomics overcomes reference database constraints and ensures transparent and reproducible data. Finally, the talk showcases how chemistry-informed discovery uncovers carbohydrate epitopes and their biosynthetic routes in these microbes, which opens avenues for the development of novel vaccines and antimicrobials.

Bio: Martin Pabst is an Associate Professor at Delft University of Technology, working at the interface of bioinformatics, biochemistry, and microbial ecology. His research focuses on developing next-generation mass spectrometry and computational frameworks to characterize microbial ecosystems at the metaproteome and metabolome levels.
After studying Chemistry at the University of Vienna, he completed a PhD in biological mass spectrometry at BOKU Vienna. He then moved to ETH Zurich for a postdoctoral and lecturer position, and subsequently gained experience as a Group Leader at a pharmaceutical spinout company from UCL in Cambridge, UK. With over a decade of experience across academia and industry, he is also active in early-stage innovations. He recently co-founded ProteoT, a spinout from TU Delft focused on food metaproteomics and database solutions, now part of the BiotechBooster ecosystem. He serves on several boards, including the Dutch Society for Mass Spectrometry.

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Stoeger Thomas

07. May 2026 | 14:30 | Showroom (DHEG136E) | Sandgasse 36, Erdgeschoß

Title: Connecting the Dots in Biomedical Data:
Toward Integrated, Trustworthy, and Epistemically Aware Bioinformatics

Abstract: Biomedical data is abundant — but systematically distorted. The order in which discoveries are made is non-random, AI systems inherit and entrench the biases of the literature they learn from, and large fractions of published findings fail to replicate across cohorts and contexts. Addressing these distortions requires more than better algorithms: it requires computational frameworks that treat provenance, uncertainty, and evidence reliability as first-class components of biomedical analysis.
This talk presents a research program built around that premise, illustrated through two case studies and a forward-looking program for TU Graz. The first describes ongoing work constructing a comprehensive, expert-supervised curation of the Proteostasis Network (3,052 genes, 150+ data sources), which is being used to ask whether proteostatic changes in aging are truly specific to aging or reflect more general biological processes — a question only approachable by integrating across datasets with minimal historical path-dependence. The second describes a completed document intelligence platform developed for the NIH's History of Genomics Program, which integrates heterogeneous document types — handwritten notes, proposals, meeting records, spreadsheets — with biological and bibliometric data to reveal the processes behind strategic scientific decisions. Building on these foundations, the talk outlines three interconnected research thrusts for Graz: provenance-aware multi-omics integration, mechanistic and translational models that connect omics-derived features to clinically meaningful outcomes across disease contexts, and epistemically aware AI systems that reason not just over data but over the reliability of the evidence landscape itself.

Bio: Thomas Stoeger is a computational biologist and bioinformatician at Northwestern University. He trained in developmental biology at the IMBA in Vienna (lab of Jürgen Knoblich) and completed a PhD combining novel algorithm development, massive-scale computation, and cell biology at the University of Zurich, where his dissertation was awarded the annual prize for best PhD in the Sciences. His current research spans multi-omics integration, document intelligence, and epistemically aware AI, unified by a focus on how systematic distortions in biomedical information shape what science discovers and what it misses. He builds information tools and knowledge resources that serve double duty: as instruments for studying how science itself works, and as foundations for first-order biomedical discovery. His recent research has appeared in Nature Aging, PNAS, JCI, eLife, and Nucleic Acids Research, with further work in press at Nature Communications.

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