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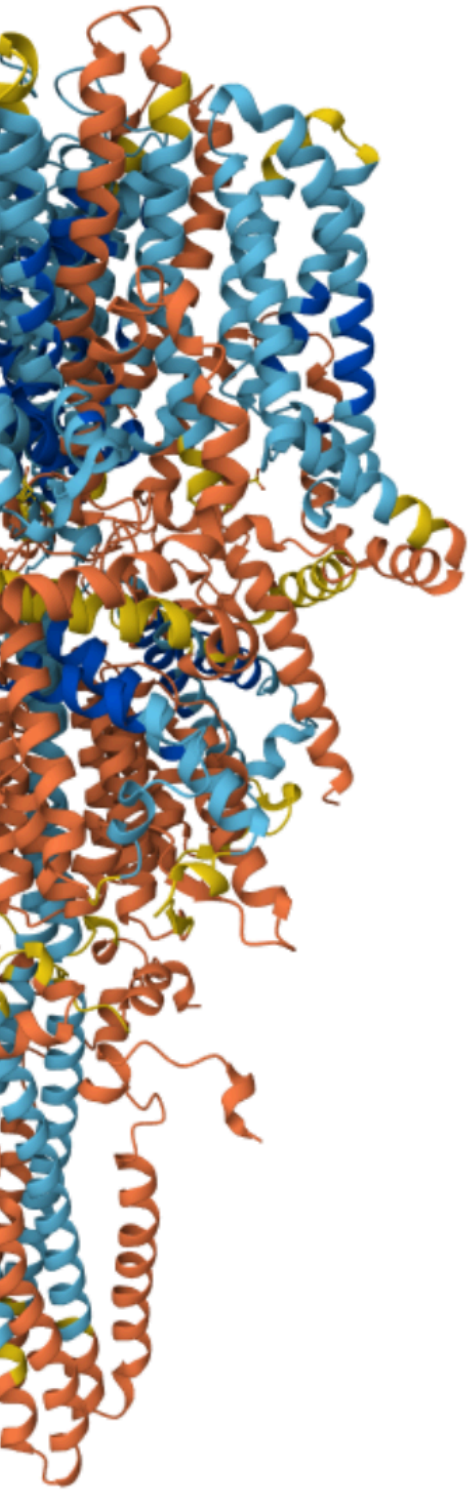
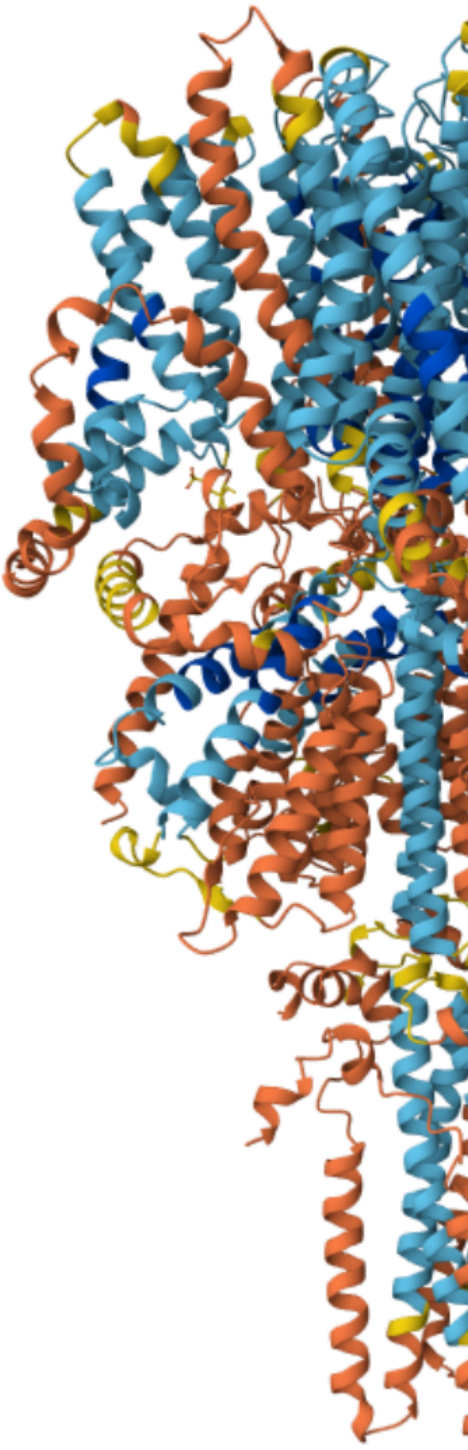
INSTITUTE OF MOLECULAR AND TRANSLATIONAL MEDICINE

9th Advanced in Silico Drug Design workshop 2026





Olomouc

26th – 30st January 2025

9ADD

Book of Abstracts

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AURORA

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9ADD workshop (26.1.2024 – 30.1.2024) is focused on using in silico tools and approaches in drug design. We cover both structure-based drug design (molecular docking, molecular dynamics, structural bioinformatics tools) and ligand-based drug design (QSAR, pharmacophores, deep learning) with lectures and on-hand tutorials.

Welcome to Olomouc! Karel Berka and Pavlo Polishchuk

Invited Lecturers

- Thierry Langer (UniVie, Vienna)
- Alexandre Varnek (Uni Strasbourg)
- Hanoch Senderowicz (Bar-Ilan University)
- Johannes Kirchmair (UniVie, Vienna)
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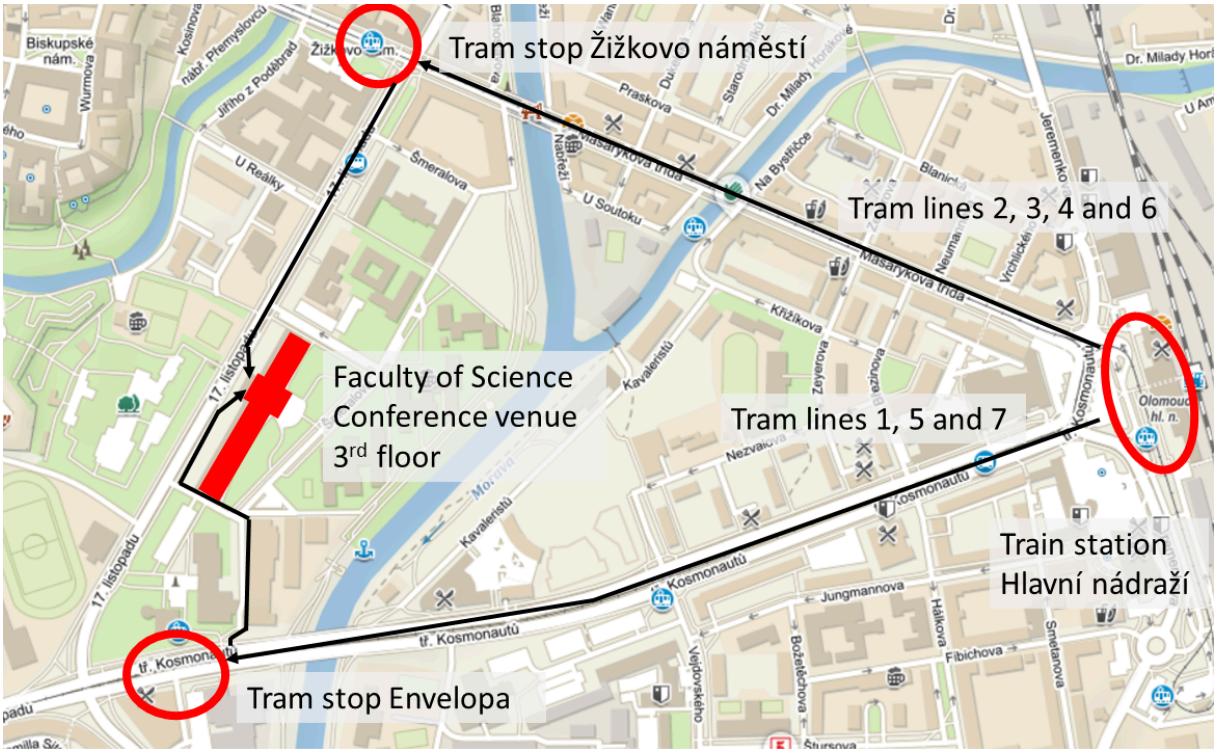

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Faculty building in Google Street View

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Poster Abstracts

HIV-1 RT Inhibitor Design via Generative AI, Screening, and MD

Damilola Bodun

Universite Paris Cite

The era of generative AI in drug design is here, and in this study, we applied a generative AI model to design potential non-nucleoside inhibitors of HIV-1 reverse transcriptase (RT). RT converts viral RNA into DNA, facilitating viral integration into a host's genome. Inhibiting RT is therefore critical in combating HIV-1. Using the REINVENT prior model, we fine-tuned it with classified RT inhibitors (pIC50 > 8.5) from ChEMBL, generating over 6000 compounds. These compounds underwent rigorous filtering, including classification by a Message Passing Neural Network (MPNN), PAINS filtering, pharmacophore modeling, structure-based screening, MMGBSA scoring, and ADMET prediction. We identified five top-performing compounds, which demonstrated superior docking scores (≤ -13.22 kcal/mol) and binding free energies (MMGBSA dG Bind ≤ -77.48 kcal/mol) compared to the reference ligand (-8.42 kcal/mol). Further ADMET predictions and Molecular dynamics simulation at 500 ns revealed that these compounds had better drug-like properties and comparable stability at the active site compared to the reference ligand. These findings suggest that the identified compounds are promising candidates for further in vitro validation to confirm their therapeutic potential against HIV-related proteins. This study highlights the transformative role of AI-driven drug discovery in addressing HIV drug resistance.

Bioactive chemicals from Urtica dioica L. in silico profile for breast cancer

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1. Muğla Sıtkı Koçman Univ., Dept. of Mol. Biol. & Genet., TR

2. Istanbul Tech Univ., MBG-Biotech Prog., TR

Breast cancer is the most common malignancy among women and is strongly associated with genomic instability and defective DNA repair mechanisms. The tumor suppressor proteins BRCA1 and BRCA2 play crucial roles in repairing DNA double-strand breaks and maintaining genomic integrity. Mutations or functional deficiencies in these proteins critically contribute to breast cancer development. Plant-derived natural compounds, due to their low toxicity and diverse biological activities, are promising candidates for novel anticancer strategies. Urtica dioica L. (U. dioica), known for its antioxidant and anticancer properties, is rich in phenolic compounds. In this study, potential interactions between U. dioica compounds and BRCA1/BRCA2 proteins were investigated using in silico molecular docking methods. Protein structures of BRCA1 (PDB ID: 1T15) and BRCA2 (PDB ID: 1N0W) were retrieved from the Protein Data Bank. Ligands were prepared with AutoDock Tools 1.5.6, and docking simulations were performed using AutoDock Vina. Binding poses were analyzed using PyMOL and Discovery Studio Visualizer. The U. dioica compound apigenin hexoside exhibited strong binding affinities (−7.5 kcal/mol for BRCA1 and −8.4 kcal/mol for BRCA2) and formed hydrogen bonds with residues SER1655, LEU1657, ASN1678, THR1700, and LYS1702 in BRCA1, and HIS294, SER296, THR297, and ARG299 in BRCA2. These results suggest that U. dioica-derived flavonoids may effectively interact with BRCA1 and BRCA2, potentially influencing DNA repair pathways and serving as natural inhibitor candidates for breast cancer treatment.

Keywords: Breast cancer, in silico, molecular docking, U. dioica

Pharmacophore-Based Drug Activity Prediction

Joanna Ceklarz, Agnieszka Wojtuch, Krystyna Waniová, Wim Dehaen, Tomasz Danel, Martin Šícho

UCT Prague

JU Cracow

Pharmacophores are molecular representations containing information about steric and electronic features necessary for biological activity of drugs. They are used by medicinal chemists to identify and visualize important fragments and generalize between groups with similar functionalities. Therefore, using pharmacophores as representations of molecules for Graph Neural Network (GNN) training is an interesting prospect which has been largely unexplored, yet. We compare performance of selected GNNs trained on pharmacophore representations of molecules with those trained on conventional atomic representations, as well as with a baseline model. Then, we investigate how those models compare when trained on datasets of varied sizes, and on ones containing different numbers of clusters of molecules. Finally, we use GNN-specific xAI methods that have been developed to answer questions about both feature and structural importance of functional groups in known bioactive compounds. In our case study, pharmacophore features attributed with the highest importance for the activity were directly compared with protein-ligand crystal structures, where interactions described by the pharmacophore models of molecules are experimentally revealed. The results helped us to identify areas for further improvement in our molecular featurization – some areas experimentally recognized as important for function were not encoded with appropriate features when default feature definitions were applied. Interestingly, we found that different GNN models rely on overlapping, yet not identical, pharmacophore features when making predictions, while all being in partial agreement with experimental data.

MD observations of binary interactions of small molecules in aqueous solution

Milana Dejaková

University of Chemistry and Technology, Prague, CZ

When a medication is taken, the overall behaviour and bioavailability inside the body are determined by its pharmacological and physicochemical properties. Pharmacological characteristics, such as the mechanism of action and pharmacokinetics of the formulation, are relatively well understood. On the other hand, the physicochemical characteristics of individual compounds remain less explored due to the complexity of experimental measurements. Mentioned properties, including permeability and hydrogen-bond donors and acceptors, are typically examined individually for each active pharmaceutical ingredient. However, in reality, drugs are often administered in combination, which raises questions about their mutual interactions. Do these molecules form clusters that slow their absorption in the body? Are there any interactions that enhance each other's transport? As these processes are difficult to study experimentally, this work employs molecular dynamics simulations to answer these questions. The aim is to study binary interactions between commonly prescribed drugs to explore their behaviour.

Advancing Evaluation of Molecular Generators

Valeriia Fil, Daniel Svozil

University of Chemistry and Technology Prague

Molecular generators are widely used to explore chemical space and propose novel compounds with desired properties. However, their evaluation remains challenging due to the structural diversity and large scale of generated molecules. Moreover, commonly used benchmarks often fail to reflect the primary goal of molecular generation: the discovery of novel biologically active compounds.

In this work, we employ scaffold-based metrics to assess a generator's ability to recover biologically relevant scaffolds that are absent from the input data. These metrics were applied to several molecular generators, including Molpher and DrugEx. Among the evaluated methods, the DrugEx Graph Transformer achieved the highest scaffold recall and demonstrated strong scaffold hopping capabilities.

Our results highlight that scaffold-based evaluation provides a more biologically meaningful perspective on molecular generator performance and can support the development of more effective virtual libraries for drug discovery.

Study of the quality of the description of protein-DNA interactions

Lukáš Gibala, Petr Jurečka

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The aim of this work was to compare the SPC/E water model with the newer TIP4P-D model, which was developed to provide a more accurate description of protein systems, and to evaluate how these models influence the hydrophobic effect in protein–DNA complexes. Molecular dynamics simulations of protein–DNA complexes were performed and analysed in terms of structural stability and the formation of hydrophobic contacts. The results show that TIP4P-D describes the strength of the hydrophobic effect more accurately than SPC/E. This indicates that TIP4P-D offers a more realistic representation of hydrophobic interactions in protein–DNA complexes, consistent with its behaviour previously observed in simulations of isolated proteins.

StreaMD: a tool for high-throughput automated molecular dynamics simulations

Aleksandra Ivanova[1], Olena Mokshyna[2], Pavel Polishchuk[1]

1. Palacky University Olomouc

2. Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences

Molecular dynamics (MD) simulations and binding free energy calculations are widely used in computational chemistry and molecular biology. In the study we present StreaMD tool for automate molecular dynamics simulations. The tool prepares multiple systems and replicas, starts or extends MD simulations, performs trajectory analysis, computes MMG(P)BSA binding free energies, along with protein-ligand interaction analyses. The pipeline supports diverse systems, such as protein, protein-cofactors, protein-ligand, and protein-ligand-cofactors complexes in explicit water environments. By utilizing the Dask Python library, the tool supports parallelization and distributed computing across a network of servers via SSH connections independent from a particular scheduler. The tool enables GPU-accelerated computations, offering a substantial reduction in processing time. For validation, we ran 10 ns simulations and calculated the GBSA energies by using the final 5 ns of the 10th ns trajectory for 624 complexes sourced from the Greenidge dataset, 166 molecules of human β-secretase 1 (UniProt ID: P56817), 63 molecules of human α-thrombin (UniProt ID: P00734), and 51 molecules of bovine trypsin (UniProt ID: P00760).

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic through INTER-EXCELLENCE II LUAUS23262, the e-INFRA CZ (ID:90254), ELIXIR-CZ (LM2018131, LM2023055), CZ-OPENSCREEN (LM2018130, LM2023052) grants and by European and Regional Fund project ENOCH (No. CZ.02.1.01/0.0/0.0/16_019/0000868).

Machine learning for scalable molecular dynamics

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Despite advances in experimental and computational methods, protein design remains challenging, with only a small fraction of designed sequences proving functional. Machine learning has improved sequence generation for desired folds, but many designs still lack natural enzyme-like activity [1]. Incorporating protein dynamics into ML-based design is a crucial yet unresolved issue, as such data are both costly to compute and complex to interpret. The reliability of ML-generated dynamics can be assessed by comparing them to classical MD simulations using established network-based metrics like the Shortest Path Map (SPM) and Dynamic Flexibility Index (DFI) [2,3]. In this work, we evaluate recent ML methods for generating protein dynamics within accessible time frames, focusing on their ability to recapitulate SPM and DFI statistics (Figure 1). We also explore how these descriptors can support the evaluation of novel designs and how DFI can scale across datasets and be integrated into ML frameworks, particularly those using evolutionary information, such as FireProtASR [4]. This integration may improve protein design by making models more dynamic and evolution-aware.

Non-canonical α/γ backbone conformations in DNA and protein-DNA complexes

Elizabeth Kolářová, Petr Jurečka

Palacky University Olomouc, CZ

Protein–DNA interactions modulate the conformational landscape of the phosphodiester backbone, frequently inducing significant structural perturbations such as bending, curvature, and the stabilization of energetically demanding, low-population noncanonical states. These interactions often promote the "north" C3'-endo sugar-pucker, facilitating localized B to A transitions that are critical for biological recognition. Accurate modeling of these effects depends on the force field: while bsc1, OL15, and OL21 reproduce canonical B-DNA well, they often underestimate A-DNA stability and protein-stabilized noncanonical states. OL24 improves upon these limitations by refining the deoxyribose pucker and χ torsion, providing a more balanced A/B equilibrium and better supporting protein-induced conformational changes, yielding simulations closer to experimental observations.

XGBoost-Based Docking Score Prediction with Atomistic Representations

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In this work, results of an atom-level descriptor approach, applied with an eXtreme Gradient Boosting (XGBoost) model, is presented, inspired by neural network models such as SchNet, where molecular properties are predicted as a sum of atomic contributions.

The model was trained on in-vivo dataset containing 59 884 molecules and tested on a large in-vitro dataset of 174 015 molecules. Both datasets were obtained from ZINC15 database. The predicted property was the docking score of ligands binding to the SARS-CoV-2 main protease (Mpro) binding cavity.

Atomic environments were represented using Smooth Overlap of Atomic Positions (SOAP) descriptors. The atom-level XGBoost model was evaluated in terms of prediction accuracy and classification performance and compared with a conventional XGBoost approach based on global molecular descriptors.

The results show consistent improvements in both regression and classification metrics. These findings suggest that combining atom-level descriptors with efficient tree-based learning algorithms provides a promising and computationally efficient alternative to traditional molecular-descriptor-based approaches for molecular property prediction.

Searching for CDK16 inhibitors in ultra-large chemical libraries

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Cyclin-dependent kinase 16 (CDK16), a member of the atypical CDK family, plays key roles in protein trafficking, vesicle transport, and non-canonical regulation of the cell cycle. Its overexpression and dysregulation are linked to tumorigenesis, cancer cell survival, and resistance to therapies, including radiotherapy and antimitotic drugs. Preclinical studies show that CDK16 inhibition reduces cancer cell proliferation and can sensitize tumors to treatment, highlighting CDK16 as a promising therapeutic target beyond CDK4/6. To identify CDK16 inhibitors, we used the Enamine REAL Database(~10 billion synthetically accessible compounds). Initially, de novo molecules were generated using the CReM-dock fragment-based, docking-guided approach. Compounds with favorable docking scores and predicted hinge-region interactions were then used as queries for similarity searches across the database using multiple molecular fingerprints. We investigated the impact of various generation scenarios and parameter settings on the efficacy of the proposed approach in retrieving promising hits from the Enamine REAL Database. Our findings indicate that structures generated from Enamine fragments during the initial stage yielded molecules with improved docking scores in the subsequent screening phase. Furthermore, Morgan fingerprints demonstrated superior performance in the similarity search step, effectively retrieving compounds with high docking scores and predicted binding affinity to the CDK16 hinge region. The compounds identified through this methodology were further evaluated using consensus docking to select the most promising candidates. Notably, the selected molecules exhibited a high degree of structural novelty relative to previously reported inhibitors and are considered strong candidates for experimental validation.

This work was supported by the Ministry of Education, Youth and Sports (LUAUS23262, LX22NPO5102 and e-INFRA CZ ID:90254).

Leveraging IAM-HPLC data to predict phospholipid affinity with Machine Learning

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Quantitative Structure–Retention Relationships (QSRR) remain an essential framework for elucidating the interactions between molecular structures and chromatographic systems. While recent advances in machine learning (ML) have substantially improved the predictive accuracy of QSRR models, this has often occurred at the expense of mechanistic interpretability. The present study addresses this challenge by integrating predictive performance with molecular-level insights for immobilized artificial membrane (IAM) chromatography.

A comprehensive dataset comprising over 2000 pharmaceutical agents, environmental toxicants, and drug candidates was tested using Valko's gradient IAM-HPLC methodology. For each compound, a broad spectrum of theoretical molecular descriptors was computed using the Chemicalize platform, encompassing lipophilicity indices (logP, LogD7.4), charge-related parameters, hydrogen-bonding capacities, polar surface area, molecular size and shape indices, geometrical and topological features, as well as descriptors reflecting molecular polarizability and refractivity.

An extensive screening of 40 regression algorithms identified the GradientBoostingRegressor as the most robust model (Q^2 = 0.81 on the test set), balancing predictive performance with mechanistic interpretability. SHAP (SHapley Additive exPlanations) analysis highlighted lipophilicity, isoelectric point, molecular polarizability, and charge distribution as dominant factors influencing IAM retention. Complementary t-SNE visualization revealed meaningful clustering within the chemical space, whereas applicability domain analysis ensured the reliability of predictions.

This study demonstrates that descriptor-based ML models can provide predictive accuracy comparable to advanced deep learning methods while preserving mechanistic interpretability, thereby offering a powerful tool for drug discovery, toxicological assessment, and chromatographic method optimization.

Predictive Modelling and Experimental Validation of Azo-Photoswitches in Diverse Solvents

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Photo switches are molecules that can alter their structure and properties in response to light exposure. The photochemically produced species are less stable and can be reverted to a more stable isomer by light or temperature. They have been utilized in various applications in medicines, leading to the development of an innovative discipline called 'Photo-pharmacology'. The maximum absorption wavelength (λmax) and the thermal half-life of the metastable isomer (t1/2) are the important properties that are tuned to design them. Among photochromic systems, azo derivatives are the simplest, valued for their fatigue resistance and straightforward synthesis, making them the most attractive class of molecular switches. However, discovering photoswitches is a tedious process. With advances in computational chemistry, quantum chemical calculations have become a popular approach for designing photoswitches. Yet, these methods are computationally expensive and often time-consuming. In the present work, we developed a machine-learning model for predicting the λmax and t1/2 of azo photoswitches. The datasets were compiled for both properties in multiple solvents to investigate the solvatochromic effects on the azo photo-switch behavior. We used simple 2D descriptors such as CircuS, Chyline, Linear, Morgan, RDKit fingerprints, Atom pairs, Avalon, and Torsion for modeling and property prediction along with associated physicochemical descriptors for solvent effects. The algorithm used for modeling is SVM. To validate the predictions of both models, we designed new azo photoswitches and compared the prediction results with experimental values. The interpretation of the model's applicability was made using the ColorAtom approach, which evaluates the contributions of each atom to the property. This allows us to see how the presence of different functional groups affect the predicted values and facilitate the rational design of new photoswitches.

Immune-Derived Antimicrobial Peptides from Granzymes

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Background:

Antimicrobial resistance (AMR) poses a critical threat to global health, necessitating the development of novel therapeutic strategies beyond conventional antibiotics. Cytotoxic immune effector proteins, such as granzymes (A, B, M) and granulysin, possess intrinsic antimicrobial activity and represent an underexplored reservoir for rational peptide-based drug discovery.

Methods:

Here, we present a computational framework for the systematic design and scoring of short antimicrobial peptides derived from granzyme A, B, M, and granulysin sequences. Using a sliding-window approach, peptide libraries were generated and evaluated through a multi-parametric scoring pipeline incorporating physicochemical and biophysical descriptors, including pH-dependent net charge, hydrophobic moment (α-helix), GRAVY index, aromatic residue content, aliphatic index, and Boman index. These features were standardized and integrated into an Advanced Toxicity Score (ATS) to prioritize peptides with optimal amphipathicity, cationicity, and predicted membrane activity.

Top-ranked peptides were subsequently subjected to structure-based molecular docking against essential proteins from drug-resistant bacterial pathogens to evaluate binding affinity, interaction profiles, and target specificity.

Results:

The pipeline efficiently identified high-scoring immune-derived peptides with favorable physicochemical properties consistent with antimicrobial activity. Preliminary docking analyses revealed strong and selective interactions with multiple bacterial targets implicated in survival, virulence, and resistance mechanisms.

Conclusion:

This integrative in silico-to-experimental strategy establishes immune effector proteins as a rational source of antimicrobial peptides and provides a scalable framework for peptide prioritization prior to wet-lab validation. The approach accelerates antimicrobial discovery while minimizing experimental burden and toxicity risk.

MolMeDB - Molecules on Membranes Database

Kateřina Storchmannová, Jakub Juračka, Dominik Martinát, Jindřich Lněnička, Václav Bazgier, Karel Berka

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Biological membranes serve as essential barriers that protect cells, playing a crucial role in cellular function and influencing the pharmacokinetics of drug-like small molecules. A small molecule can pass through membranes in two ways: via passive diffusion or actively via membrane transport proteins. A vast amount of data is available reporting interactions of small molecules and membranes and also interactions between small molecules and transporters.

MolMeDB (molmedb.upol.cz) is a free, comprehensive, and interactive database of interactions of small molecules with membranes.1 From the start, we have collected data about partitioning and penetration of the small molecules crossing biological membranes. Recently, we have expanded our area of interest to include interactions of small molecules with transporters and ion channels. Nowadays, more than 930,000 interactions for almost 500,000 molecules are available in MolMeDB.

The data within the MolMeDB is collected from scientific papers, our in-house calculations (COSMOmic/COSMOperm2), and obtained by data mining from several databases (e.g. ChEMBL3, PubChem4, or IUPHAR/BPS Guide to PHARMACOLOGY5). Data in the MolMeDB are fully searchable and browsable by name, SMILES, membrane, method, transporter, or dataset. Also, the database content is available via the REST API and the RDF model of MolMeDB (docs.molmedb.upol.cz).

pICkIT: Automated Analysis of Protein–Ligand Interactions

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pICkIT is an open-source Python library designed to automate the extraction, filtering, and analysis of protein–ligand interaction data from large structural datasets. The tool was developed to address the increasing need for efficient, scalable processing of interaction files generated by tools such as Arpeggio, whose datasets are often too large and complex for manual inspection. pICkIT provides a modular framework that integrates interaction parsing, automated summarization, dataset comparison, and publication-ready analysis, enabling researchers to rapidly identify meaningful interaction patterns across hundreds or thousands of complexes.

In its validation study, pICkIT processed hundreds of protein–ligand complexes, reducing hundreds of megabytes of raw interaction output to compact summary files while preserving key structural information. The library facilitates high-level tasks such as filtering by interaction type, quantifying residue-level contact frequencies, generating customizable heatmaps, and comparing interaction profiles across ligand series. By simplifying these steps, pICkIT accelerates workflows, QSAR model development, and structure-based drug design.

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Program

	Lectures	Aula lecture hall (3.001a/2.001)
	Tutorials	session 1 (room 3.002) – use classroom computers; installation on laptops possible
	Tutorials	session 2 (room 3.005) – use online tools or installation on personal laptops required
	Lectures	Lectures/Tutorials (5.007) - online tools or installation on personal laptops required
	Other	

Monday, January 26

10:00 - 12:00 Registration (2nd floor)
12:00 - 12:15 Opening of the workshop
12:15 - 13:00 Introduction to drug design (Prof. Karel Berka)
13:00 - 14:00 Introduction to chemoinformatrics (Prof. Johannes Kirchmair)
14:00 - 14:30 coffee break
14:30 - 15:00 PDB-Cat (Aleix Gimeno Vives)
15:00 – 16:00 Easy online access to molecular modelling tools with RowanSci (Corin Wagen)
16:00 - 17:00 Poster flash talks
17:00 - 19:00 Poster session (3rd floor)

Tuesday, January 27

8:45 - 9:45 Reaction informatics (Prof. Alexandre Varnek)	
9:45 - 10:45 Alphafoldology (Prof. Karel Berka)	
10:45 - 11:00 coffee break	
11:00 - 12:00 Quantum mechanics in Drug design (Dr. Martin Lepsik)	
12:00 - 13:00 lunch	
13:00 - 14:00 Substructure analysis in drug discovery (Dr. Peter Ertl)	
14:00 - 15:00 Pharmacophore (Prof. Thierry Langer)	
15:00 - 15:20 coffee break	
Session 1	Session 2
15:20 - 17:45 Pharmacophore tutorial (Prof. Thierry Langer)	15:20 - 16:30 RowanSci online platform and tools (Jonathon Vandezande)
	16:30 - 17:45 Online structural analysis – PrankWeb, MOLE, Autodock Vina (Dr. Marian Novotný, Anna Špačková)
18:30 Conference dinner (Kozlovna)	

Wednesday, January 28

8:45 - 9:45 From Classical Docking to AI-Enhanced Scoring (Dr. Federica Moraca)	
9:45 - 10:45 Application of drug design on plant protector (Prof. Hanoch Senderowitz)	
10:45 - 11:00 coffee break	
11:00 - 12:00 Why ML in Drug discovery is not (yet) a silver bullet (Dr. Semen Yesylevskyy)	
12:00 - 13:00 lunch	
Session 1	Session 2
13:00 - 15:00 Docking with EasyDock (Dr. Pavel Polishchuk)	13:00 - 15:00 Docking tutorial (Dr. Federica Moraca)
coffee break	
15:30 – 16:10 Introduction to molecular dynamics (Dr. Petr Stadlbauer)	
16:10 - 17:30 MD with StreaMD (Aleksandra Ivanova)	16:10 - 17:30 MD with OpenMMDL (Niklas Piet Doering, Dr. Valerij Talagayev)
18:20 - Excursion to the Institute of Molecular and Translational Medicine (IMTM)	

Thursday, January 29

8:45 - 9:45 Introduction QSAR modeling (Dr. Win Dehaen)	
9:45 - 10:45 Introduction to de novo design (Dr. Martin Sicho)	
10:45 - 11:00 coffee break	
Session 1	Session 2
11:00 - 12:00 Chemical space visualization (Dr. Martin Sicho)	11:00 - 12:00 The Orange toolbox for pipeline automation (Dr. Marko Jukic, Dr. Crtomir Podlipnik)
12:00 - 13:00 lunch	
13:00 - 15:00 QSAR tutorial in Python (Dr. Wim Dehaen)	13:00 - 15:00 QSAR tutorial with OCHEM online platform (Dr. Igor Tetko)
coffee break	
15:30 - 17:30 De novo design with CReM (Dr. Pavel Polishchuk, Guzel Minibaeva)	15:30 - 17:30 De novo design with DrugEx (Dr. Martin Sicho)

Friday, January 30

8:45 - 14:30 Ligand selection challenge (Dr. Pavel Polishchuk)
14:30 - 15:00 Presentations of winners

Challenge Overview

Participants will be provided with information about a biological target, including a set of compounds with known activity and a blind dataset consisting of confirmed active compounds and decoys. The blind dataset will contain approximately 3,500 structures. Registration of teams will be opened at the start of the workshop.

Objective

The goal of the challenge is to select 100 compounds from the blind dataset that maximize the number of true active hits. Only entries submitted within the designated challenge period (January 30, preliminary from 8:45 to 14:30) will be eligible for rewards. Nevertheless, submissions received after this period may be taken into account during the post-challenge evaluation.

Methods

Participants are free to use any computational approach or software tools, including but not limited to:

- Similarity search
- Pharmacophore modeling
- QSAR modeling
- Molecular docking

Teams and Submissions

- Participants may form teams of up to three members
- Teams may include on-site and remote participants
- Each team may submit up to 10 predictions
- Only the best-performing submission per team will be considered for scoring

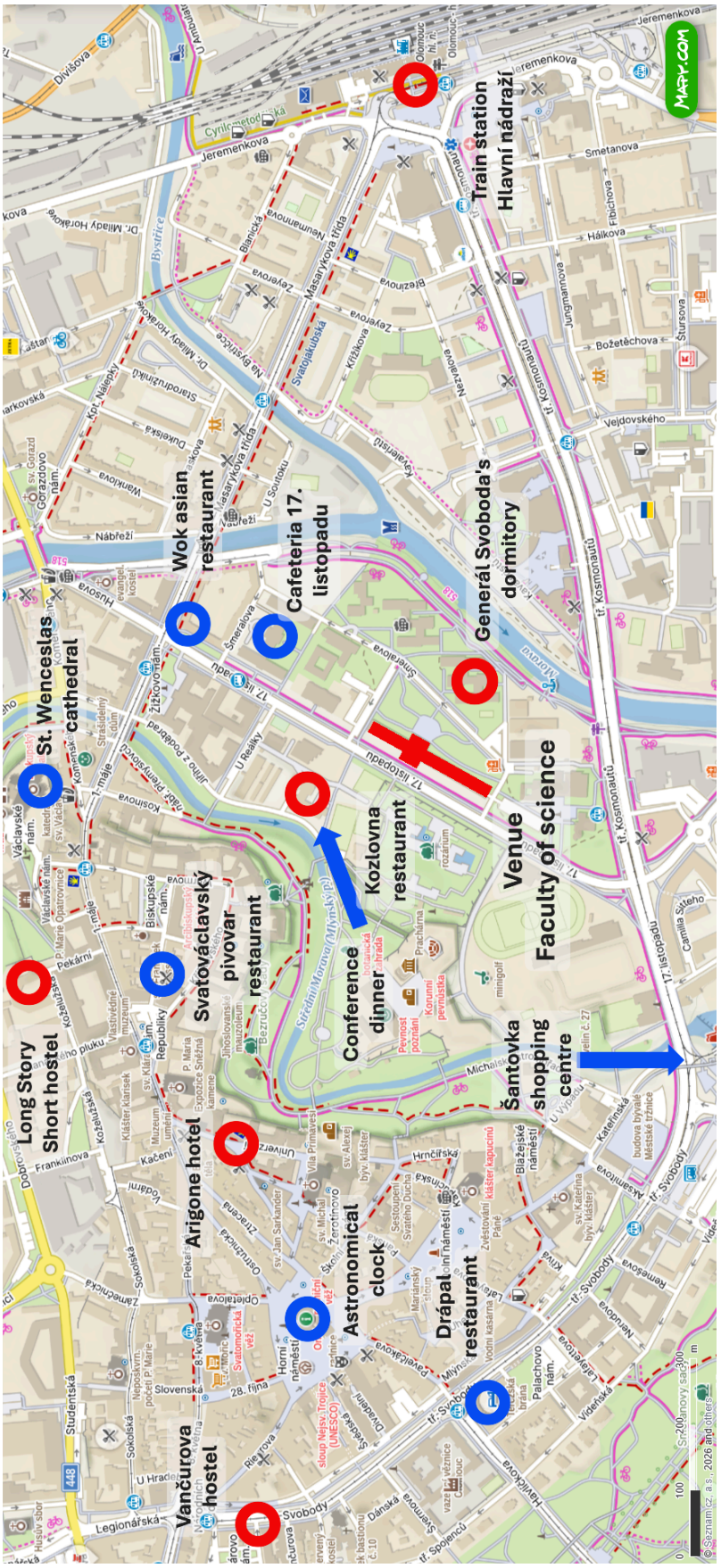
Evaluation and Awards

- On-site and remote teams will be evaluated separately
- A final leaderboard will identify the top three teams in each category, who will be awarded prizes provided by RowanSci
- The top three teams from both categories will be invited to prepare a short presentation (1–2 slides) describing their winning solution

Post-Challenge Prospective Validation

After the challenge concludes, predictions from the top-performing teams will be considered for compound purchasing and experimental validation.

Accomodations, restaurants, sights



Notes