Chemoinformatics+ Summer School 2025

with COST21111 WORKSHOP

FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY – UNIVERSITY OF LJUBLJANA 30 JUNE – 4 JULY 2025

The Chemoinformatics+ Summer School 2025, held at the Faculty of Chemistry and Chemical Technology, University of Ljubljana (30 June – 4 July 2025), offers an intensive program of lectures, workshops, tutorials, and hands-on activities. It brings together students, educators, and researchers to explore cutting-edge topics in chemoinformatics, including AI, QSAR, and molecular modeling. A key part of the event is the **COST21111 Workshop**, focusing on the integration of chemoinformatics and ecotoxicology for sustainable drug discovery. This hybrid event features leading European experts and encourages collaboration across disciplines through keynotes, discussions, and practical demonstrations. Participants can join online or in person and engage in a vibrant scientific exchange.

Program Schedule

Monday, 30 June

Hackathon (Participants of Hackathon only)

Hackathlon moderators: Črtomir Podlipnik (University of Ljubljana); Gilles Marcou and Dragosh Horvath (University of Strasbourg); Marko Jukič (University of Maribor); Viet-Khoa Tran-Nguyen (University - Paris Cite)

Tuesday, 1 July

09:00 – 12:00

Mini Workshop – Didactics for Chemoinformatics

- How to create microMOOCs? (assist. prof. Črtomir Podlipnik – Hands-on Session)

- Task-Based and Project-Based Learning (prof. João Montargil Aires de Sousa)
- Problem Solving .OR. How not to sit on your brain? (prof. Dragosh Horvath)

9:00 – 14:00

Excursion of EMJM Chemoinformatics+ students to Novartis, Menges (EMJM Students only)

🔒 By invitation only – EMJM Chemoinformatics+ members and guests.

13:00 – 17:00

Chemoinformatics+ Boards (EMJM Chemoinformatics+ members only)

The following sessions are open to all registered participants of EMJM CSS 2025.

15:30 – 17:00 Registration

16:30 – 17:00 Opening Ceremony

17:00 – 18:00 Lecture 1: Prof. Alexandre Varnek (Strasbourg University) – *Artificial Intelligence: the Future for Synthetic Chemistry?*

18:00 – 20:00 Welcome Party

Wednesday, 2 July

9:00 – 12:00 EMJM CSS2025 - Wednesday's morning session - 4 plenary lectures

09:00 – 09:40 Lecture 2: Prof. Matija Strlič

09:40 – 10:20 Lecture 3: Prof. Pavel Polishchuk – *Multi-instance learning as a response to the complexity of molecular entities*

10:20 – 10:40 Coffee Break

10:40 – 11:20 Lecture 4: Prof. Hanoch Senderowitz – *Forensic Informatics: Using ML in Crime Scene Analysis*

11:20 – 12:00 Lecture 5: Prof. Marc Baaden

12:00 – 13:30 Lunch

9:00 – 12:00 EMJM CSS2025 - Wednesday's afternoon session - 1 keynote + 2 plenary lectures + Tutorial + Posters

13:30 – 14:10 Lecture 6: Prof. Martin Šicho – *De Novo Drug Design*

14:10 – 14:30 Keynote 1: Dr. Filip Cernatič (Chemical Institute - Ljublljana) - *Multi-elemental signal detection limits in laser ablation imaging techniques*

14:30 – 15:10 Lecture 7: Prof. Dmytro M. Volochnyuk (Enamine Ltd, Kyiv, Ukraine) *Chemoinformatic tools as an integrated part for creating new products and compound catalogs by CRO and chemical suppliers.*

15:10 – 15:30 Break

15:30 – 17:00 Tutorial: Prof. Gilles Marcou – *Compound Profiling using QSAR*

17:00 – 19:00 Poster Session

3–4 July 2025:

COST21111 Workshop: Integrating Chemoinformatics and Ecotoxicology for Sustainable Drug Discovery

Organised in collaboration with the Erasmus Mundus Chemoinformatics+ (EMJM) project, this hybrid event features leading experts in cheminformatics, toxicology, and sustainable drug discovery.

Online participation requires a two-step registration:

1. Create an account on the e-COST platform: www.cost.eu
2. Register for the workshop: Workshop Registration Form

Thursday, 3 July

9:00 – 12:30 EMJM CSS2025 - 4 plenary lectures, 1 keynote

09:00 – 09:40 Lecture 8: Prof. Igor Tetko (Helmholtz Munich) - *How to win challenges? Best practices for model development.*

09:40 – 10:20 Lecture 9: Prof. Thierry Langer (University of Vienna) - *Pharmacophore Methods for Rational Compound Design and Toxicity De-Risking.*

10:20 – 10:40 Coffee Break

Hybrid Session: One Health Drugs - COST21111

10:40 – 11:20 Lecture 10: Prof. Sheraz Gul

11:20 – 11:40 Keynote 2: Daniele Aiello (Modena University) - *A One Health-Driven Pipeline for the Discovery of Selective Calpain Inhibitors in Leishmania infantum*

11:40 – 12:20 Lecture 11: Prof. Maria-Paola Costi

12:20 – 13:30 Lunch

13:30 – 15:30 Activity for students

13:30 – 15:30 Restitution of Hackathon (EMJM Chemoinformatics+ students)

16:00 – 23:00 EMJM CSS2025 - Social Activities

16:00 – 19:00 Social Activity (Ljubljanica Boat Trip or Castle Visit)

19:30 – 23:00 Conference Dinner – The Place

Friday, 4 July

9:00 – 12:30 EMJM CSS2025 - 4 keynotes and 1 plenary speach

9:00 – 9:10 Keynote 3: Tieu Long Phan (Universität Leipzig) - *SynKit: A Comprehensive Cheminformatics Tool for Streamlined Manipulation and Analysis of Chemical Reaction Data*

09:20 – 9:40 Keynote 4: Dr. Said Byadi (Title Be Announced)

09:40 – 10:00 Keynote 5: Assist. Prof. Viet-Khoa Tran-Nguyen (University Paris Cite) *HERGAI strikes a ClassyPose? Mission: Possible! Two machine learning models for structure-based drug design — in style*

10:00 – 10:20 Keynote 6: Assoc. Prof. Marko Jukić (Title Be Announced)

10:20 – 10:50 Coffee Break

10:50 – 11:30 Lecture 12: Prof. Dragosh Horvath (University of Strasbourg) - *Docking – Between Myth and Reality: Lessons from Practice and Benchmarking*

11:30 – 12:15 Round Table – **CHEMOINFORMATICS: QUO VADIS?**

12:15 – 12:30 Closing Ceremony

12:30 – 14:00 Lunch

14:00 – 17:00 Afternoon session

14:00 – 15:00 Report from the Hackathon about work on Antiparasitic targets + discussion "What to do next?"

15:00 – 16:00 Podlipnik/Jukić Demonstration of using OCART (Orange tools for Chemoinformatics) for generation predictive toxicologic models.