



MUNDUS CHEMOINFO+



European Master in
Cheminformatics



**Université
Paris Cité**

Summer School in Chemoinformatics June 26th-28th 2023

Université Paris Cité

Organisers: A.C. Camproux, O. Taboureau & G. Marcou

Hackathon on Chemoinformatics

June 26th 2023

Location: Room 521 and 525, building Lamarck A, 35 rue Hélène Brion 75013 Paris

Welcome 8h30

Welcome of the students and distribution of the tasks.

Work the full day on the tasks.

Coffee, tea, juice and lunch box will be offer all along the hackathon

PS: A ½ day of preparation of the hackathon will be organized in visio conference with the students beginning of June in the aim to optimize the time of work during the hackathon.

End 20h00 – Refreshment at “la barge du CROUS”



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Symposium Summer school Chemoinformatics+ Scientific conference in chemoinformatics June 27th 2023

Location: Amphi Buffon, 15 rue Hélène Brion 75013 Paris

Welcome 8h30

G. Marcou: Presentation of the European Master chemoinformatics+

Session Chemoinformatics (chairs : Anne Claude Camproux, Olivier Taboureau, Hanoch Senderowitz)

8h50: Keynotes. Alexandre Varnek (Université de Strasbourg) – Cartography-driven molecular design.

9h30: Alexandre Borrel (Inotiv) – ChemMaps.com V2 – Exploring the Environmental Chemical Universe.

9h50: Brice Hoffmann (Iktos) - IA exploration in chemoinformatics.

Coffee break + session poster (10h10 -10h40)

10h40: Marc Baaden (Université Paris Cité) – Deep inside molecules – emerging trends in molecular modeling.

11h20: Loic Dreano (University of Helsinki) - Molecular contact in protein structure and ligand binding.

11h40: Manon Reau (Qubit) - Application of absolute binding free energy calculations to predict the binding modes and affinities of protein-protein inhibitors.

12h00: Paul Dupuyds (Medetia) – Machine learning classification for the identification of prostaglandin ligands.

Lunch Buffet – Session poster: 12h20-14:00

Session Molecular Modelling (chairs: Crtomir Podlipnik & Joao Aires de Sousa)

14h00: Keynotes. Thierry Langer (University of Vienna) - Next Generation Pharmacophore Modeling for Advanced Molecular Design and Risk Assessment.

14h40: Leslie Regad /Delphine Flatters (Université Paris Cité) – Structural exploration of HIV-2 protease to understand HIV-2 resistance against protease inhibitor.

15h00: Victor Reys (Université de Montpellier) – KinDock2: A web tool to predict protein-kinase inhibitors binding pose and affinities.

15h20: Bryan Dafniet (Université Paris Cité) - Network biology on adverse drug reactions.

Coffee break – Session poster: 15h40-16h30

16h30: Anne Goupil (Biovia Dassault System) - Exploring the Complementarity of Physics-Based Approaches and Deep Learning in Drug Design.

16h50: Dylan Serillon (WhiteLab Genomics) – Artificial intelligence as a tool for unraveling the potential of in silico-drug discovery.

17h10: Dhoha Triki (Novalix) - Chemoinformatics support for Drug Discovery projects

17h30: Minoletti (Sanofi) – AI-Driven Drug Discovery.

18h00 End of the symposium. Refreshment

20h00 Gala dinner (Dinner Cruise on the Seine)



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Paris Cité**

Symposium Summer school Chemoinformatics+

Young students – Industrial discussion

June 28th 2023

Location: Amphi Buffon, 15 rue Hélène Brion 75013 Paris

Welcome 9h

9h00 – 11h00: Presentations of the results obtained during the Hackathon by the students.

11h00 – 11h30: Coffee break

11h30-13:00: Time for discussions between students and industrials (Iktos, Givaudan,...)

End of the summer school 13h00 for students – Lunch Boxes will be proposed for the participants.

On afternoon:

- **A visit of Paris for students is organized.**
- **Meeting of the EMJM Chemoinformatics+ consortium members is scheduled**