

### WORKSHOP 1

## Applications of computational AI/ML in peptide research with a roadmap to peptide drug and material development.

| 10:00 - 12.00 | ML approaches  |
|---------------|--|
|               | Moderators: <b>Emel Adaligil</b> , Genentec and <b>Ewa Lis</b> , Koliber Bio   |
|               | <b>Ved Srivastava</b> , Perpetual Medicines<br>Roadmap to peptide drug development in AI Era   |
|               | <b>Ewa Lis</b> , Koliber Bio<br>Introduction to Machine Learning   |
|               | <b>Goran Mauša,</b> University of Rijeka<br>Breaking misconceptions in applying machine learning to peptides materials   |
|               | <b>Hirokazu Tamamura</b> , Tokyo University<br>Development of anti-HIV agents targeting HIV-Gag proteins using in silico<br>screening                              |
| 12:00 - 13:30 | Lunch  |
| 13:30 - 15:30 | Practical session  |
|               | <b>Marko Njirjak and Erik Otovic,</b> University of Rijeka<br>Overcoming antibiotic resistance: a machine learning pipeline for antimicrobial<br>peptide discovery |
| 15:30 - 16:00 | Coffee Break   |
| 16:00 - 18:00 | Demo / practical session   |
|               | <b>Tatjana Braun and João Rodrigues</b> , Schrödinger<br>Peptide and Macrocycle Design using Schrödinger's Computational Modeling<br>Platform                      |

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|               | MD / structure-based approaches   |
|---------------|---|
| 09:00 - 10:30 | Moderators: <b>YuShan Lin</b> , Tuffts University and <b>Marco Pagliai</b> , University of Florence |
|               | YuShan Lin, Tuffts University   |
|               | Molecular Dynamics intro and talk   |
|               | Sereina Riniker, ETH Zurich   |
|               | Structure-based design  |
| 10:30 - 11:00 | Coffee Break  |
| 11:00 - 12:00 | Leonardo de Maria, Astra Zeneca   |
|               | Generative models for peptide therapeutic optimization  |
|               | Marko Babic, University of Rijeka   |
|               | Effects of cluster analysis inputs for peptide self-assembly and aggregation                        |
|               | simulations.  |
| 12.00 - 12.30 | Close of workshop   |

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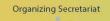
Florence, Italy- 2024



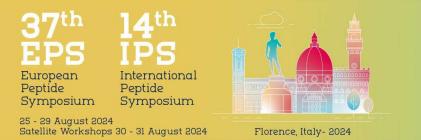
## WORKSHOP 2

## Embracing innovation and sustainability in peptide synthesis

| FRIDAY 30 August 2024 |   |
|-----------------------|---|
| 10:00 - 11:15         | Wendy Hartsock, AralezBio<br>Opening  |
|                       | <b>Fernando Albericio,</b> University of KwaZulu-Natal <i>A History of Peptide Synthesis Part 1</i>   |
|                       | <b>Stephen Kent</b> , University of Chicago<br>A History of Peptide Synthesis Part 2  |
|                       | <b>Timothy Reichart</b> , Hampden-Sydney College<br>Group Discussion  |
| 11:15 - 11:50         | Innovation in Synthesis   |
|                       | Jonathan Collins, CEM<br>Challenging the Norms of Peptide Synthesis   |
|                       | <b>Timothy Reichart</b> , Hampden-Sydney College <i>Folding-assisted ligation</i>   |
|                       | Timothy Reichart, Hampden-Sydney College<br>Group Discussion  |
| 12:00 - 13:30         | Lunch   |
| 13:30 - 14:20         | Sweet Science: Glycans in peptide science   |
|                       | <b>Mattan Hurevich,</b> The Hebrew University of Jerusalem<br><i>Glycan and peptide synthesis: differences, parallels and crossover of ideas</i>                                    |
|                       | <b>Baptiste Aussedat,</b> Chemitope Glycopeptide<br>Building Bridges: The Intersection of Peptide and Glycan Chemistry in<br>Glycopeptide Innovation                                |
|                       | <b>Timothy Reichart</b> , Hampden-Sydney College<br>Group Discussion  |
| 14:35 - 15:25         | Sustainability in Peptide Science Part 1  |
|                       | <b>Luísa Aguiar</b> and <b>Robert Zitterbart</b> , Gyros Protein Technologies<br>Green innovation on trial: How to improve the ecological impact of your<br>peptide synthesis today |
|                       | Timothy Reichart, Hampden-Sydney College<br>Group Discussion  |







| 15:30 - 16.00 | Coffee Break  |
|---------------|---|
| 16:00 - 16:20 | <b>Fabian Hogenkamp, Florence Genet</b> and <b>Łukasz Frankiewicz</b> , PeptiSystems<br>Flowthrough SPPS with integrated PAT – sustainable technology to reduce PMI<br>and make smart process decisions |
|               | Timothy Reichart, Hampden-Sydney College  |
|               | Group Discussion  |
| 16.30 - 18:00 | Fernando Albericio, University of KwaZulu-Natal   |
|               | 1st Panel Replacing reagents in SPPS (DMF, Fmoc, TFA, DCM); replacing SPPS?   |

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| SATURDAY      | SATURDAY 31 August 2024  |  |
|---------------|--|--|
|               | Spotlight on LPPS  |  |
| 9:00 - 9:25   | Wendy Hartsock, AralezBio<br>Opening   |  |
|               | Markus Löeweneck, Senn Chemicals AG<br>Advantages and strategies for successful implementation of LPPS                                     |  |
|               | Wendy Hartsock, AralezBio<br>Group Discussion  |  |
|               | Sustainability in Peptide Science Part 2   |  |
| 09:30 - 10.20 | <b>Stephen Kent</b> , University of Chicago<br>Fundamental Aspects of SPPS and Native Chemical Ligation for Efficient Peptide<br>Synthesis |  |
|               | <b>William Lubell</b> , Université de Montréal<br><i>N- to C-Peptide Synthesis is Arguably the Future for Sustainable Production</i>       |  |
|               | Wendy Hartsock, AralezBio<br>Group Discussion  |  |
| 10:30 - 11.00 | Coffee Break   |  |
|               | Innovations in Peptide Science Part 2  |  |
| 11:00 - 11:20 | Philip Dawson, Scripps Research Institute<br>Chemical manipulation of immobilized macromolecules   |  |
|               | Wendy Hartsock, AralezBio<br>Group Discussion  |  |
|               | Stephen Kent, University of Chicago<br>2nd Panel The future of the solid support. What will replace ChemMatrix?                            |  |
| 11:30 - 12:30 | Stephen Kent, University of Chicago<br>Challenges from the audience  |  |
|               | Wendy Hartsock, AralezBio<br>Close of Day 2  |  |

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#### **WORKSHOP 3**

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Peptide

Symposium

## Navigating entrepreneurship and technology transfer in peptide discovery and development

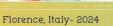
| FRIDAY 30 Au  | FRIDAY 30 August 2024   |  |
|---------------|---|--|
| 10:00 - 10:15 | Opening<br>Giorgia Giovannetti, University of Florence<br>Ines Neundorf, University of Cologne  |  |
| 10:15 - 12:00 | Marco Pierini, Maria Raffaella Martina and Fosca Errante, University of Florence   Bernadett Simon, University of Cologne   Technology Transfer strategies in the University of Cologne and University of Florence. Insight on peptide discovery and development. |  |
| 12:00 - 13:30 | Lunch   |  |
| 13:30 - 14:00 | <b>Stefano Pegoraro,</b> Bachem<br>Market Intelligence in the era of anti-obesity peptide therapeutics - A CDMO<br>perspective  |  |
| 14:00 - 14:30 | <b>Charlotte Ungerth</b> , RELIFE<br>Definisse Key Peptide 1 - a true breakthrough innovation in anti-ageing<br>treatments  |  |
| 14:30 - 15:00 | <b>Ved Srivastava</b> , Perpetual Medicines<br>Peptide-Drugs for Metabolic Disease: From Innovation to Market   |  |
| 15:00 - 15:30 | Aphrodite Kapurniotu, TU Munich and Jürgen Bernhagen, LMU Munich Peptide drugs for cardiovascular diseases  |  |
| 15:30 - 16:00 | Coffee Break  |  |
| 16:00 - 16:30 | Stefania Colarusso, IRBM<br>Our journey as peptide drug hunters at IRBM   |  |
| 16:30 - 17:00 | <b>Ikuo Fujii</b> , Osaka Metropolitan University<br>Post-antibody drugs: Generation of a novel class of drug modalities based on<br>molecular-targeting helix-loop-helix (HLH) peptides  |  |
| 17:00 - 17:30 | <b>Meritxell Teixido</b> , Gate2Brain<br>Gate2Brain entrepreneurial journey towards patients  |  |
| 17:30 - 18:00 | <b>Michael Chorev</b> , Mellitus LLC<br>Challenges in developing a novel diagnostic test for diabetes based on CD59 as<br>a disease relevant biomarker  |  |

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25 - 29 August 2024 Satellite Workshops 30 - 31 August 2024





| SATURDAY 31 August 2024 |   |
|-------------------------|---|
| 9:00 - 9:30             | <b>Rina Aharoni</b> , Weizmann Institute of Science<br>The story of the peptide-copolymer Glatiramer Acetate (Copaxone) in the<br>treatment of multiple sclerosis: from Bench to Bed side |
| 9:30 - 10:00            | <b>István Mándity</b> , Semmelweis University & HUN-REN Research Centre for<br>Natural Sciences<br><i>Success and pitfalls in drug research in academia</i>                               |
| 10:00 - 10:30           | <b>Richard Moakes</b> , Birmingham University<br>Novel anti-scarring eye drops: a view from bench to bedside  |
| 10:30 - 11:00           | Coffee Break  |
| 11:00 - 12:30           | Round Table discussion<br>István Mándity, Aphrodite Kapurniotu, Jürgen Bernhagen  |
| 12:30                   | Closing remarks and end of workshop   |

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