



UNIMORE
UNIVERSITÀ DEGLI STUDI DI
MODENA E REGGIO EMILIA



**UNIVERSITÀ
DI PARMA**



ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA



Advanced School in Drug Research and Development

*“Enzyme Inhibition at the boundary between
Chemical Biology and Drug Discovery”*

Parma, 4th September – 29th September 2023

Program



**Università
degli Studi
di Ferrara**



Advanced School in Drug Research and Development

*“Enzyme Inhibition at the boundary between
chemical Biology and Drug Discovery”*



Keywords

Drug design, Enzymes

Covalent inhibition, Chemical Biology

Welcome Day - 10/09/2023 (Aula Magna - Palazzo dell'Università - Parma)

13.45: Registration of the Participants

14.30: Gabriele Costantino – *Università di Parma*
Welcome at the Università di Parma

14.45: Laura Scalvini – *Università di Parma*
Presentation of the Advanced School in Drug Research & Development

15.00: Maria Laura Bolognesi – *Università di Bologna*
Chimeric molecules in drug discovery

15.45: Giorgio Colombo – *Università di Pavia*
The Dynamics of Molecular Design

16.30: coffee-break

17.00: Gianluca Sbardella – *Università di Salerno*
Integrating Biophysical Methods in Medicinal Chemistry

17.45: Daniele Pala – *Chiesi Farmaceutici - Parma*
Computational Chemistry in Drug Discovery

18.30: Concluding Remarks

20.00: Welcome Dinner



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Day I - 11/09/2023

(Sala Congressi Plesso Aule delle Scienze – Campus Universitario – Parma)

9.00 – 10.30: **Richard Lonsdale** – *GlaxoSmithKline (GSK)*

Structure-based discovery of enzyme inhibitors

10.30 – 11.00: coffee break

11.00 – 12.30: **Marco Mor** – *Università di Parma*

Models for the discovery of covalent enzyme inhibitors

12.30 – 14.30: lunch

14.30 – 16.00: **Maria Paola Costi** – *Università di Modena & Reggio Emilia*

*Integrating Chemical Biology in the discovery of the dissociative inhibitors
of Thymidylate synthase accelerating protein degradation*

16.30 – 18.00: **György Keserű** – *Budapest University of Technology*

Covalent fragment approaches in drug discovery



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Day II - 12/09/2023

(Sala Congressi Plesso Aule delle Scienze – Campus Universitario – Parma)

9.00 – 10.30: **Marco De Vivo** – *Istituto Italiano di Tecnologia*

DNA processing enzymes in chemical biology and drug discovery

10.30 – 11.00: coffee break

11.00 – 12.30: **Vicent Moliner** – *Universitat Jaume I*

Enzyme catalysis and inhibition of cysteine proteases

12.30 – 14.30: lunch

14.30 – 16.00: **Andrea Cavalli** – *Università di Bologna*

*Integration of computational chemistry & biophysical methods
in Drug Discovery*

16.30 – 18.00: **Zoe Cournia** – *Biomedical Research Foundation, Academy of Athens*

Using FEP to predict binding poses and relative binding affinities



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Day III - 13/09/2023

(Sala Congressi Plesso Aule delle Scienze – Campus Universitario – Parma)

9.00 – 10.30: **Adrian Mulholland** – *University of Bristol*

Enzyme catalysis and inhibition at the basis of AMR

10.30 – 11.00: coffee break

11:00 – 12:30: **Giulio Rastelli** – *Università di Modena e Reggio Emilia*

Drug design based on Integration of different databases

12.30 – 14.00: lunch

14.00 – 15.00: **Alice Panzeri; Jonas Kaindl**– *Schrödinger*

Taking chemical space exploration from hit identification to lead optimization: de novo design with AutoDesigner

15.00 – 18.00: **Alice Panzeri; Jonas Kaindl**– *Schrödinger*

Workshop





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Day IV - 14/09/2023

(Sala Congressi Plesso Aule delle Scienze – Campus Universitario – Parma)

9.00 – 10.30: **Sofia Oliveira** – *University of Bristol*

Allosteric communication between drug targets revealed by non-equilibrium simulations

10.30 – 11.00: coffee break

11.00 – 12.00: **Elisa Donati; Franck Chevalier** – *Acellera*

Computational tools to investigate allosteric agents

12.30 – 14.00: lunch

14.00 – 17.00: **Elisa Donati; Franck Chevalier** - *Acellera*

Workshop





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Day V - 15/09/2023

(Sala Congressi Plesso Aule delle Scienze – Campus Universitario – Parma)

9.00 – 10.30: **Manuela Bartolini** – *Università di Bologna*

Analytical approaches for the in vitro characterization of the mode of inhibition of new active compounds

10.30 – 11.00: coffee break

11.00 – 12.30: **Barbara Pioselli** – *Chiesi Farmaceutici*

Structure, Dynamic and Function: the paradigm of chemical biology inspected by mass spectrometry

12.30 – 14.30: lunch

14.30 – 18.30: **Flash presentations** (12 participants)

18.00 – 18.30: *Closing remarks*



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Scientific Committee

- Prof. Alessio Lodola (Chair) – Università di Parma
- Dr. Laura Scalvini (Chair) – Università di Parma
- Prof. Maria Laura Bolognesi – Università di Bologna
- Prof. Maria Paola Costi – Università di Modena e Reggio
- Prof. Stefano Manfredini – Università di Ferrara

Organizing Committee

- Prof. Alessio Lodola – Università di Parma
- Dr. Laura Scalvini – Università di Parma
- Dr. Rossana Di Marzio – Università di Parma
- Gian Marco Elisi – Università di Parma
- Francesca Galvani – Università di Parma

Advisory Committee

- Prof. Marco Mor – Università di Parma
- Prof. Silvia Rivara – Università di Parma
- Dr. Frank Chevalier – Acellera
- Dr. Rita Podzuna – Schrödinger

INFORMATION

Please write to pharmasummerschool@unipr.it
or visit <https://www.pharmasummerschool.unipr.it>



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How to apply

The School is addressed to scientists with a background in drug sciences, including PhD students and professionals from industrial environment. The participants will be selected on the base of their CV and research project in which they are currently involved. The registration procedure for the selection will start the **20th February 2022** and will end the **30th April 2022** at 12 am (CET).

Documents required for the perspective students

The candidates will need to provide by e-mail (pharmasummerschool@unipr.it) the following information:

- Curriculum vitae (in English – max1-page A4 format)
- Research Project (in English – max1-page A4 format)
- Tax Code (if any) and a front-back copy of a valid identity document

Selection procedures

Admission to the School is subjected to a positive judgment by the Scientific Committee based on the evaluation of the applications. Only the first 25 candidates will be admitted. Successful applicants will be notified by e-mail within 10 working days after the deadline and provided with information to complete the registration.

Registration fee

Thanks to Regione Emilia-Romagna* the participation to School is offered at the reduced fee of 180,00 euros and include **attendance to all sessions, accommodation, welcome dinner, social dinner, coffee breaks.**

**The school is funded by the “Progetto di alta formazione in ambito tecnologico economico e culturale per una regione della conoscenza europea e attrattiva (n.1625/2021)” promoted by Regione Emilia-Romagna.*



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