



**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, 4<sup>th</sup> September – 29<sup>th</sup> 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: **Adrian Mulholland** – *University of Bristol*

*Enzyme catalysis and inhibition at the basis of AMR*

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

*DNA processing enzymes in chemical biology & drug discovery*



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**Day III - 13/09/2023**

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

9.00 – 10.30: **Zoe Cournia** – *Biomedical Research Foundation, Academy of Athens*

*Using FEP to predict binding poses and relative binding affinities*

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 Kandl**– *Schrödinger*

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

15.00 – 18.00: **Alice Panzeri; Jonas Kandl**– *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](mailto: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 **20<sup>th</sup> February 2022** and will end the **30<sup>th</sup> April 2022** at 12 am (CET).

### Documents required for the perspective students

The candidates will need to provide by e-mail ([pharmasummerschool@unipr.it](mailto: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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