UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

UNIVERSITÀ DI PARMA

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

RegioneEmilia-Romagna

Università degli Studi di Ferrara

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Parma, 29th August – 30th September 2022

Program

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations,

Artificial Intelligence, Biophysical methods

The Course

- The **University of Parma**, in collaboration with the Universities of **Bologna**, **Ferrara** and **Modena e Reggio Emilia** and with the support of the **Medicinal Chemistry Division** of the **Italian Chemical Society**, is organizing the first edition of the Advanced School in Drug Research and Development entitled "***Integrating Structural and Biophysical Data in Drug Discovery in the AI Era***".
- The School is offered to **PhD students and professionals** interested in achieving a firm grasp of the latest developments of **computer-aided drug design** and **biophysical methods** in drug discovery.
- The Summer School will provide an **international** and **multidisciplinary** environment, in which participants will meet **experts** from **industry** and **academy** to exchange views, share ideas and work on real-world case studies.

The School is divided into three stages

- An **on-line warm-up** stage, in which the participants will be provided with material (documents and case studies from the literature) regarding the contents of the core lessons.
- A **core-lesson** stage in **presence**, with **face-to-face seminars and lessons** held by international experts from academia and industry. Seminars will be followed by **workshop sessions**, that will give the participants the opportunity to get hands-on training through experimental practices.
- **An on-line collaborative working** with a follow-up stage, in which the participants will have the opportunity to face problems like those investigated and solved during the practical workshops.

INFORMATION

Please write to pharmasummerschool@unipr.it

or visit https://www.pharmasummerschool.unipr.it

Program of the School

Monday Aug 29 **WARM-UP**	Tuesday 30 **WARM-UP**	Wednesday 31 **WARM-UP**	Thursday Sep 1 **WARM-UP**	Friday 2 **WARM-UP**	Saturday 3	Sunday 4 **WELCOME DAY**
Monday 5 **CORE LESSONS**	Tuesday 6 **CORE LESSONS & WORKSHOP** Schrödinger	Wednesday 7 **CORE LESSONS & WORKSHOP** acellera®	Thursday 8 **CORE LESSONS**	Friday 9 **CORE LESSONS & WORKSHOP** TECAN.	Saturday 10	Sunday 11
Monday 12	Tuesday 13	Wednesday 14	Thursday 15 **COLLABORATIVE WORKING** Schrödinger	Friday 16 **COLLABORATIVE WORKING** acellera®	Saturday 17	Sunday 18
Monday 19	Tuesday 20	Wednesday 21	Thursday 22 **FLASH PRESENTATION**	Friday 23 **FLASH PRESENTATION**	Saturday 24	Sunday 25
Monday 26	Tuesday 27	Wednesday 28	Thursday 29	Friday 30 **ROUND TABLE**	Saturday Oct 1	Sunday 2

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations,

Artificial Intelligence, Biophysical methods

Welcome Day - 04/09/2022 (Aula Magna - Palazzo dell'Università - Parma)

13.45 **Registration of the Participants**

14.30 **Greetings and Presentation of the School**

14.55 **Mini Symposium "***Drug Design and Discovery in Academia and Industry***"**

15.00 **Prof. Marco Mor** – Università di Parma
Integrating Cheminformatics and Simulations in Drug Discovery

15.30 **Dr. Elisa Uliassi** – Università di Bologna
Multi-Target Drug Discovery

16.00-16.30: coffee-break

16.30 **Prof. Maria Paola Costi** – Università di Modena e Reggio Emilia
Integrating Chemical Biology and Drug Discovery.

17.00 **Prof. Stefano Manfredini** – Università di Ferrara
Translational Research in Academia: From Lab bench to Spin-Off Company

17.30 **Dr. Maurizio Delcanale** – Chiesi Farmaceutici
Present and Future Challenges in the Drug Discovery Process

18.00 **Concluding Remarks**

20.00 **Welcome Dinner**
Ristorante Gallo d'Oro - Parma

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations, Artificial Intelligence, Biophysical methods

Day I - 05/09/2022 (Centro San Elisabetta – Campus Universitario – Parma)

9.00 - 10.30: **Dr. Martin Walsh** – Diamond Light Source

Diamond Light Source: Contributions to SARS-CoV-2 Biology and Therapeutics

10.30 – 11.00: coffee break

11.00 – 12.30: **Dr. Garrett Morris** – University of Oxford

De Novo Drug Design Using AI and Docking

12.30 – 14.30: lunch

14.30 – 16.00: **Prof. Giulio Rastelli** – Università di Modena e Reggio

Refinement and Rescoring of Docking and Virtual Screening Results

16.00 – 16.30: coffee break

16.30 – 18.00: **Dr. Marco De Vivo** – Istituto Italiano di Tecnologia

Implementing Molecular Dynamics in Structure-based Drug Design

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations, Artificial Intelligence, Biophysical methods

Day II - 06/09/2022 (Centro San Elisabetta – Campus Universitario – Parma)

9.00 - 10.30: **Prof. Andrea Cavalli** – Università di Bologna & Istituto Italiano di Tecnologia

Thermodynamics and Kinetics of Drug-Target Interactions

10.30 – 11.00: coffee break

11.00 – 12.30: **Dr. Anna Bochicchio & Dr. Mila Krämer** – Schrodinger

Lead Optimization with Free-Energy Methods

12.30 – 14.30: lunch

14.30 – 18.00: **Dr. Anna Bochicchio & Dr. Mila Krämer** – Schrodinger

Workshop I

Schrödinger

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations, Artificial Intelligence, Biophysical methods

Day III - 07/09/2022 (Centro San Elisabetta – Campus Universitario – Parma)

9.00 - 10.30: **Prof. Gerhard Ecker** – University of Vienna

Transporter Informatics and Computational Toxicology - from QSAR to Machine Learning and beyond

10.30 – 11.00: coffee break

11.00 – 12.30: **Dr. Maciej Majewski** – Acellera

Machine Learning Methods in Drug Design

12.30 – 14.30: lunch

14.30 – 18.00: **Dr. Maciej Majewski** – Acellera

Workshop II

acellera®

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations, Artificial Intelligence, Biophysical methods

Day IV - 08/09/2022 (Centro San Elisabetta – Campus Universitario – Parma)

9.00 - 10.30: **Dr. Edoardo Fabini** – Evotec UK

The Role of Biophysics in the Early Phases of Drug Discovery

10.30 – 11.00: coffee break

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

Drug-Target interactions by Mass-Spectrometry

12.30 – 14.30: lunch

14.30 – 16.00: **Prof. Jesus Angulo** – CSIC, Seville

Drug-Target Interactions by High-Resolution Solution-State NMR Spectroscopy

16.00 – 16.30: coffee break

16.30 – 18.00: **Prof. Helena Danielson** – Uppsala Universitet

The Use and Significance of Biosensor-based Methods in the Early Phases of Drug Discovery

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations, Artificial Intelligence, Biophysical methods

Day V - 09/09/2022 (Centro San Elisabetta – Campus Universitario – Parma)

9.00 - 10.30: **Dr. Mara Colzani & Dr. Nicola Vettore** – Tecan

Fluorescence and Luminescence Technologies to Characterize Drug-Target interaction

10.30 – 11.00: coffee break

11.00 – 12.30: **Prof. Antonio Macchiarulo** – Università di Perugia

The (WONDER)land of Microscale Thermophoresis: Principles, Applications and Opportunities

12.30 – 14.00: lunch

14.00 – 18.00: **Tecan Scientists**

Workshop III

TECAN

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations,

Artificial Intelligence, Biophysical methods

Social Activities

Monday 5th Sept
Aperitivo in Via Farini
Meeting place: *Piazza Garibaldi*

Tuesday 6th Sept
Town walk & Aperitivo in Parco Ducale
Meeting place: *Piazza Garibaldi*

Wednesday 7th Sept
Salumi Dinner
Meeting place: *Artusi la Salsamenteria*

Thursday 8th Sept
Aperitivo in Piazzale Santa Croce
Meeting place: *Parco Ducale*

INFORMATION

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

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Società Chimica Italiana
Divisione di Chimica Farmaceutica

Keywords

Drug design, Free-energy simulations, Artificial Intelligence, Biophysical methods

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
- Dr. Sara Zambernardi – Università di Parma
- Dr. Francesca Ferlenghi – Università di Parma
- Prof. Federica Vacondio – 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
- Dr. Valentina Raimondi – Tecan

INFORMATION

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

Advanced School in Drug Research and Development

"Integrating Structural and Biophysical Data in Drug Discovery in the AI era"

Acknowledgements

Regione Emilia-Romagna

Società Chimica Italiana
Divisione di Chimica Farmaceutica

acellera®

Schrödinger

TECAN.

JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING