



Training School

Rational drug discovery based on computational modelling, high-throughput virtual screening, image-based screening technologies, lead optimisation, structure-relationship activities (SAR) analysis

10-12th of July

PROGRAM

10 July, 2023:

- 08:30 – 09:00** Registration of participants
- 09:00 – 09:15** Opening: L. Monteiro Rodrigues (CBIOS Director),
Patrícia Rijo – Local organizer
Chiara Riganti (Action Chair)
- 09:15 – 13:00** **Session #1** Romano Silvestri, Sapienza University of Rome (Italy)

“The Wnt/ β -catenin pathway as a target in drug discovery of CRC agents”

Niamh O’Boyle, Trinity College, Dublin, Ireland **online**
The role of medicinal chemistry in the drug discovery process

Mariano Storaniuolo, University “Federico II”, Naples, Italy **online**
The Wnt/beta-catenin pathway

Romano Silvestri, Sapienza University, Rome, Italy **in presence**
The Wnt/beta-catenin pathway as a target in drug discovery of CRC agents

Antonio Coluccia, Sapienza University, Rome, Italy **in presence**
The virtual screening approach looking for bioactive molecules. NHERF1 as easy study

13:00 – 14:00

Lunch break

14:00 – 17:30

Hands-on #2 Romano Silvestri & Antonio Coluccia, Sapienza University of Rome (Italy)

Trainer: Romano Silvestri & **co-Trainer:** Antonio Coluccia

- Hands-on case study: The course provides an introduction on basic knowledge to use in the drug design and discovery process with focus on the Wnt/beta-catenin pathway.

Romano Silvestri in presence

Synthesis of a beta-catenin targeting compound

Antonio Coluccia in presence

Molecular modeling of a beta-catenin targeting compound

11 July, 2023

"DNA-encoded chemical libraries from lead discovery to targeted therapeutics"

Trainers: Gabriele Bassi & Nicholas Favalli, Philochem

09:00 – 13:00

Session #1 Gabriele Bassi & Nicholas Favalli, Philochem

13:00 – 14:00

Lunch break

14:00 – 17:30

Hands-on #2 Gabriele Bassi & Nicholas Favalli, Philochem

- Hands-on case study: "Small molecule ELISA for the measurements of affinity constants of targeted therapeutics"

12 July, 2023

Trainer: Thomas Efferth (Germany) & Wolfgang Link (Spain)

09:00 – 11:00

Session #1 Thomas Efferth, Johannes Gutenberg University

Mainz, Germany

"The anticancer activity of nerium oleander leaf extract"

11:00 – 12:00

Session #2 Wolfgang Link, Instituto de Investigaciones Biomédicas Alberto Sols, CSIC-UAM Spain

"Principles of Cancer Treatment and Anticancer Drug Development"

Topics: High content screening, counter screening strategies, analysis of mode of action, structure activity relationship (SAR) analysis, Potency analysis, Target deconvolution

14:00 – 17:30

Lunch break and closing remarks.