

MINUTES

MedChem and structural biology: tools and strategies for hit and lead optimization in the One Health perspective
27-29/09/2023
Prepared by Sandra Gemma and Cecilia Pozzi (TS organizers)

1. LIST OF ATTENDANTS

Number	Name	Country
1.	Corfu Ioana Alexandra	IT
2.	Carvalho Maria Alice	PT
3.	Cintesun Sener	TR
4.	Ebiloma Godwin	UK
5.	Mahmutovic Vranic Sabina	BA
6.	Malpezzi Giulia	IT
7.	Santamaría Aguirre Javier	ES
8.	Stojanovski Stojmir	MK
9.	Tkachuk Oleh	IT
10.	Valiauga Benjaminas	LT
11.	Brogi Simone	IT
12.	Castagnolo Daniele	UK
13.	Mazzorana Marco	UK
14.	Roncaglioni Alessandra	IT
15.	Pozzetti Luca	IT
16.	Tassone Giusy	IT
17.	Tudino Valeria	IT
18.	Sandra Gemma (organizer)	IT
19.	Cecilia Pozzi (organizer)	IT

2. DESCRIPTION OF THE ACTIVITIES

Day 1. The first day of the event emphasized the interplay between the environment, humans, and animals in research, adhering to the "One Health" philosophy. The importance of computational methods and tools for chemical safety and sustainability assessment, regulatory compliance, Read Across, and the applicability of in silico tools for predicting toxicity were discussed. Practical sessions using VEGA software provided hands-on experience, enabling attendees to assess chemical compound characteristics and toxicities. The event fostered networking and collaboration opportunities among participants. Lectures were delivered by two invited speakers: Dr Alessandra Roncaglioni, Head of the Laboratory for Environmental Chemistry and Toxicology, IRFMN Milan and Prof. Brogi, Associate Professor of

Pharmacology at the Department of Pharmacy, University of Pisa (Italy) and by Dr Valeria Tudino, researcher in Medicinal Chemistry at the University of Siena
Trainees Corfu Ioana Alexandra, Tkachuk Oleh and Maria Alice Carvalho presented their research activities and interests through flash-presentations:



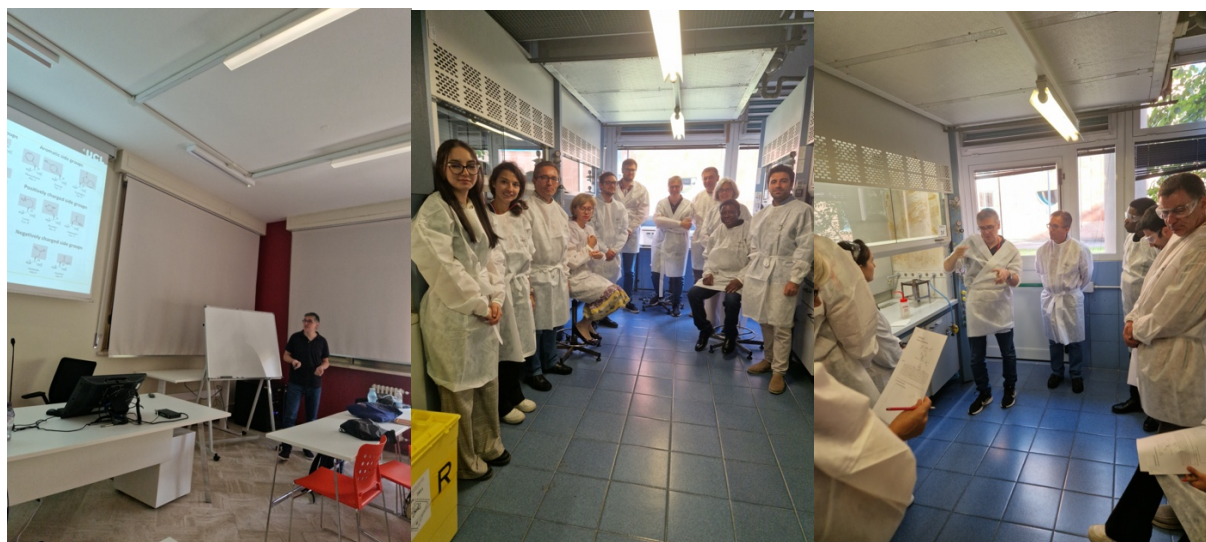
Day 2. The series of lectures and presentations covered various essential topics in the fields of medicinal chemistry and infectious disease research. These included the targeting of Trypanothione reductase in Leishmania parasites, the principles of Green Chemistry for sustainable drug development, the utilization of natural compounds in drug discovery, and the role of biocatalysis as a sustainable tool for medicinal chemists. Flash presentations by attendees highlighted innovative approaches to combat infectious diseases, emphasizing the interdisciplinary nature of the research. Overall, the discussions underscored the significance of sustainable and innovative strategies in advancing drug development and addressing infectious diseases. The practical section took place at the Chemistry Laboratory where the participants performed reactions catalysed by CALB. The attendees were organised in groups of two.

Lectures were delivered by Prof. Gemma (TS organizer), Dr Pozzetti, researcher in Medicinal Chemistry at the University of Siena, and Prof. Castagnolo (invited speaker), Associate Professor in Chemical Sustainability at University College London (UK) who also organized the practical activity

FLASH PRESENTATIONS FROM SELECTED TRAINING SCHOOL ATTENDEES

Giulia Malpezzi: Flavonoid-like compounds for treatment of Leishmaniasis

Javier Santamaria Aguirre: Nanotherapies against neglected tropical diseases caused by trypanosomatid parasites – fluoroquinolone and imidazoaxasole



Day 3. The activities of the third day focused on the structural characterization of biological macromolecules and the investigation of protein-ligand complexes for drug discovery purposes. In the morning session, the series of lectures started by a general overview on integrative structural biology and the application of various structural and biophysical techniques to investigate different aspects of a target. Then, the lectures focused on X-ray crystallography for structural and functional characterization of proteins, as isolated proteins or complexes with ligands or other macromolecules (proteins, DNA or RNA) and the application of this technique for drug discovery purposes. Different practical aspects were presented, opening a long discussion with the participants that were highly interested in this technique. The practical sessions performed during this third day focused on the analysis of structural models and of enzyme-inhibitor complexes, aiming to provide to the participants suitable tools exploitable for drug discovery purposes, and on performing a simple protein crystallization experiment. A final lecture was delivered at the end of the practical session, showing the facilities for integrative structural biology available at Diamond Light Source.

Lectures were delivered by Prof. Pozzi (TS organizer) and Dr. Mazzorana (invited speaker), structural biologist and beamline scientist at Diamond Light Source (UK). Prof. Pozzi and Dr. Mazzorana, together with Dr Tassone, researcher in Structural Biology at the University of Siena, organized the practical activities.



At the end of each day the Participants worked on the preparation of a Collaborative report to be published on the OneHealthDrugs website.