# Computational

# Approaches to

# Polypharmacology

## Concept

Participants will benefit from keynote lectures and hands-on training sessions given by leading experts from industry and academia in the areas of library design, polypharmacology, virtual screening, fragment-based, chemoinformatics and computer-aided design methodologies that support multi-target paradigms in drug discovery.

## MuTaLig COST Action Committee

Stefano Alcaro, Chair (Italy) Fernanda Borges, Vice Chair (Portugal) João Carlos Ferreira Ribeiro (Portugal) Danijel Kikelj (Slovenia) Eugenio Gaudio (Switzerland) Sharon D. Bryant (Austria) Hanoch Senderowitz (Israel) Maria Laura Bolognesi (Italy) Mu.Ta.Lig. COST ACTION CA15135 www.mutalig.eu http://www.mutalig.eu/training-schools/ Maurizio Botta, (Italy) Rita Guedes (Portugal) Anna Artese (Italy) Holger Stark (Germany) Claire Schoemake (Malta) Christa Muller (Germany) Lucia Forzi (COST-Belgium) Svetlana Voinova (COST-Belgium)

#### COST

The mission of the European Cooperation in Science and Technology (COST) is to contribute to Europe's research and innovation capacities by enabling breakthrough scientific developments leading to new concepts and products. It is a unique platform where European researchers can jointly develop their initiatives across all scientific disciplines. (www.cost.eu).





# 1<sup>st</sup> MuTaLig COST Action Training School

CA 15135

# 8-10 February 2017

Vienna, Austria



# Program

## **Confirmed Speakers**

Peter Ertl (Novartis) Thierry Langer (Universität Wien) Marie-Louise Jung (Prestwick Chemical) Gerhard Ecker (Universität Wien) Hanoch Senderowitz (Bar Illan University) Peter Ettmayer (Boehringer Ingelheim) Rita Guedes (University of Lisbon) Andrea Danani (IDSIA) Stefan Kubicek (CeMM) Francesco Ortuso (University Magna Græcia di Cantazaro)

### **Training Sessions**

Participants will experience exciting lectures by experts from industry and academic research in the area of library design & screening followed by hands-on training sessions using computeraided design approaches to provide a foundation for applying *in silico* approaches to design and discover multi-target ligands that will support the development of the MuTaLig Chemotheca.

#### **Topics:**

Library building, profiling & filtering: 3D-pharmacophore modeling, virtual screening, docking, ligand profiling, chemoinformatics, QSAR, & fragment based compound design methods.

#### Trainers

Sharon D. Bryant (Inte:Ligand, Austria) Hanoch Senderowitz (Bar-Ilan University, Israel) Thierry Langer (University of Vienna, Austria) Avi Yosipof (Bar-Illan University, Israel)

#### Language

#### The official language of the training school will be English. No simultaneous translation will be provided.

#### Local Organizing Committee

Sharon D. Bryant (Inte:Ligand) Thierry Langer (Universität Wien) Goekhan Ibis (Inte:Ligand) Daniela Krizan (Universität Wien)

# Logistics

### Registration

Website: http://www.mutalig.eu/training-schools/ Inquiries: mutalig.vienna.training.school@gmail.com \*Limited places available. Register early using the registration form that can be downloaded from the website.

### Transportation

Vienna International Airport: (www.viennaairport.com)
City Airport Train (CAT): Direct train from airport to Vienna Center (Wien Mitte/Landstrasse) with connections to U<sub>4</sub> & U<sub>3</sub> metro lines. Costs €12 one-way. (www.cityairporttrain.com/en/home).
S-Bahn (Rail Connection): S7 train from Airport to Wien Mitte

Costs € 3.90 one-way (www.oebb.at/en/)

Vienna Public Transport: www.wien.gv.at/english/transportationurbanplanning/public-transport/

#### Venue

University of Vienna UZA2 Pharma Center Althanstrasse 14 1090 Vienna, Austria

### Accessibility

Tram D: (Liechtenwerderplatz-Augasse) Tram D: (Althanstrasse) Metro Lines: U4 or U6 (Spittelau) Bus: 35A (Spittelau)

