Chemoinformatic Tools, Compound Databases and Data Management Platforms

9 October 2023

14:00-17:00 CEST

online

Workshop of the COST Action CA21111

One Health drugs against parasitic vector borne diseases in Europe and beyond

OneHealthdrugs

The event is open to PhD, young innovators and senior scientists from both academia and pharma.

Description

High quality data on compound properties and activities form the backbone of the daily work for many members of the COST Action OneHealthdrugs. Chemoinformatics tools, compound repositories and data management platforms play an essential role in providing access to vital compound information and facilitating the analysis of compound properties for modelling of drug targets and developing compounds as potential drug candidates against parasitic diseases. The aim of this workshop is to introduce knowledge in using various chemoinformatics tools, accessing and navigating compound databases, and efficiently managing chemical data through data management platforms.

Programme

14:00 - 14:10 **Welcome**
Ulrike Wittig (Heidelberg Institute for Theoretical Studies, Germany)

14:10 - 14:20 **Introduction to COST Action**
Maria Paola Costi (University of Modena, Italy)

14:20 - 14:50 **Open data resources for drug discovery at EMBL-EBI**
Andrew Leach (European Bioinformatics Institute, UK)

14:50 - 15:20 **The European Lead Factory: 10 years of collaborative drug discovery**
Vera Nies (Lygature, Netherlands)

15:20 - 15:50 **Chemography applications to drug design: from (ultra)large libraries analysis to de novo design of molecules and reactions**
Alexandre Varnek (University of Strasbourg, France)

15:50 - 16:10 **Probes & Drugs portal: a hub for the integration of high-quality bioactive compound sets**
Ctibor Škuta (CZ-OPENSCREEN: National Infrastructure for Chemical Biology, Institute of Molecular Genetics of the Czech Academy of Sciences, Czech Republic)

16:10 - 16:30 **Integrating the ATC Database and Structural Analysis for Computational Repurposing of Drugs with Antiparasitic Potential**
Marcus M.K. Nielsen (Technical University of Denmark, Roskilde University, Denmark)

16:30 - 16:50 **High resolution chemical imaging of surfaces using infrared spectroscopic photo-induced force microscopy (PiF-IR) and its requirements for data analysis**
Maryam Ali (Friedrich Schiller University Jena, Germany)

The event registration requires two steps :
1) create an e-COST account in the www.cost.eu and
2) register here: https://forms.gle/suEmNKCje5SVLyqc8