STSM REPORT

Title ***Hits and leads chemical space and collection in freely available databases.***

Description of the work carried out during the STSM

Aim of the STSM. **The main goal of the planned STSM** was to discuss and write the outline of the first draft of the manuscript entitled "Hits and leads chemical space and collection in freely available databases". This is in line with the below reported objectives:

Main expected results and their contribution to the progress towards the Action WGs objectives (either research coordination and/or capacity building objectives) and deliverables. The output of your STSM will be:

a) the STSM contributes to a deliverable described in the MoU of the Action:
D4_Web resource - Coordination of compound libraries resources. M24 (WG1) .
b) It will respond to the following goal for WG1 in the first year: **Setup of the web-platform for compounds database (FAIRDOM) [WG1]**
c) It will respond to the following goal for WG2 in the first year (2022-2023):
   - **Setup a collection process for the chemical structures of compounds previously synthesized/available from different projects of the COST participants [WG2]**
   - **Definition of criteria for compounds to be included into the database [WG1 + WG2]**

A parallel aim was to develop contacts with stakeholder not yet connected with OneHealth*drugs* Action to improve the quality of the activities performed, to broaden the concepts about the impact of ecotoxicity principles in drug discovery and to increase the probability to have an impact on the practical approach to a drug discovery process specifically including the One Health good practice; foster the collection and coordination of data and information about compound design and finally to give a perspective use of the retrieved structural information for the design of novel hits and leads.

The **work performed** during my scientific visit was based on a metadata analysis of the existing approaches to database building. Discussion about how to organize the metadata research work to identify scaffolds and compounds that can be of interest for medicinal chemists working in the field of antiparasitic drug discovery. Coordinating the work among Ulrike Wittig, WG1 Leader and Theodora Calogeropoulou and myself to achieve the objectives.
We had some meetings focused on database compounds exploitation. Commercial/ non-commercial and in house. We will describe the existing databases and the in house database and how the compounds are encoded

- We also discussed about how we can encode the internal compounds in the database, which properties to include in the database.
- Consideration should be given to how to extract the information from the different database and how to elaborate the information directly in the database. Some chemoinformatic tools should be adopted.
- Scaffold based approach: this is one of the most relevant means of analysis of the overall data available. This can give a strong support to perspective medicinal chemistry work.
- Finally, the potential of retrieving compounds from in house databases upon proper collaboration agreement among the groups that own these.
- Ecotox studies should be part of the profiling activity and encoded properties.