

Dear "member" of the OpenTox community:

With great pleasure I am looking back at our OpenTox Euro meeting in Dublin. I really think it was a great meeting with many excellent talks and productive discussions and I hope that you now see yourself as part of OpenTox. My special thanks goes especially to the group participating in the working group discussions on the first day. Even if we had some virtual meetings before, I see this date as the real starting point of the working group activities. What was planned as four separate meetings ended up to be one meeting of the complete group since we directly recognized that the topics of the four working groups are extremely interlinked. There is need for strong interactions with the AOP activities led by Clemens Wittwehr (WG2) in two directions: 1) Data from the OpenTox community should be made available to verify APOs and 2) information from AOPs should be included in OpenTox modelling tools. This is only possible with standardized data/metadata (WG3, Thomas Exner) and extended APIs (WG1, Christoph Helma). All this has then to be provided in a user-friendly environment (WG4, Tim Dudgeon). The following discussion showed that there are many different opinions and demands on interoperability and standards. To get all these into one working model is definitely not an easy task. To approach it, two main goals for the near future were proposed:

1) Documenting the past: Unfortunately, the openTox developments are very fragmented at the moment. To change that, Tim volunteered to generate an overview of existing OpenTox services. You can find more details in his E-mail below. Besides the services, which resulted from the OpenTox projects and its successors, we are also welcoming all suggestions for services, which should be linked to OpenTox. Especially, the input from Yanli Wang (PubChem) was extremely helpful in this respect and we are looking forward to a fruitful cooperation.

2) Planning for the future: Even more important than file format standards for the data and metadata are quality standards of the data. Only if we can judge the quality of the data, we can decide if we want to use them in modelling or if it is acceptable for regulatory purposes. But already these two applications demand for different information stored as metadata. Is it possible to design a infrastructure, which stores all data/metadata, so that it can easily be retrieved and included in decision making or converted to reports like REACH and SEND? To find this out, use cases or better backbones of uses cases will be developed and analyses regarding their demands on the data formats. In Dublin some more volunteers were identified:

- a) Clements: Data for regulatory purposes
- b) Christoph, Thomas: Datasets for tox prediction
- c) Thomas, Joh Dokler (Douglas Connect) (and Yanli Wang): Data exchange using PubChem as most important example
- d) Roland Grafström, Hristo Alajdov, Clements, Thomas: Interacting and modelwith AOPs
- e) Ignacio Gonzalez Suarez (PMI): standards for high contents screening

Maurice Whelan (EC) pointed us to the successful use of use cases in the SEURAT-1 program including ToxBank and ask us to take a look at them, which we definitely will. To cover even more opinions, IO would like to ask you to propose additional use cases. These don't have to be fancy but just describe your daily life --> How do you use tox related data and what information you need or would like to see associated with this data. Just a short draft of the work flow is enough highlighting the problems in current datasets. I will create a doodle (additional invitation will follow soon) to find a date for a follow-up virtual meeting end of this month in which the use cases can be discussed.

Thanks again for all the valuable input on the working groups.

Thomas