Minutes of the OpenTox working group meeting on 12 Nov. 2015

The meeting started with the announcement of the next OpenTox meeting. It will take place on 11 April 2016 as a satellite workshop to the Pan-American Conference for Alternative Methods (April 12-14, 2016) to hosted at John Hopkins in Baltimore. The plan is to use this day for presentations and workshops on the working group activities similar to the first day of the OpenTox Euro 2015 Dublin meeting. We plan also have an open room space during the Pan-American Conference, where the results and demos of OpenTox implementations and services will be presented to interested people from this larger audience. Everyone, who would like to present a hands-on tutorial, database or software application, is very welcome.

Then the 7 use cases proposed during the OpenTox Euro meeting in Dublin and at the general assembly of the OpenTox Association were discussed:

1) Data for regulatory purposes
2) Datasets for tox prediction
3) Data exchange using PubChem as most important example
4) Interacting and modelling with AOPs
5) Standards for high content screening
6) Data integration approaches for OpenTox
7) Use cases for specific endpoints from generation of data to regulation

The main goal was to prioritize use cases and to form subgroups starting the work on these. Roland Grafström expressed in an E-mail before the meeting that his group is not able to work on use cases this year. Therefore, the use case 4 was postponed (please see also the attached more detailed description of this use case from Clemens Wittwehr). Regarding its extreme importance, work will still be performed with respect to the integration of data from AOP-KB into the OpenTox framework. Starting point is a project proposal offered by the JRC (Clemens) for the development of an XML-schema to describe AOPs. This should be used for the development of new AOPs but also to access the information form AOP-KB e.g. to be included in modelling. The call is attached to these minutes and is also available on the OpenTox website. OpenTox will try to be involved in these developments in a consulting role.

The participants of the meeting then expressed their interest in the remaining use cases. It became clear that large overlap exists between different use cases and that some are only more specific versions of others. Since this was also reflected in the participants wanting to join specific use cases. Therefore, it was decided to build subgroups for three topics:

1) Data for specific endpoints from generation to regulation (use case 5 and 7): This subgroup will protocol the data flow for two specific endpoints: transcriptomics and high contents screening. The first workflow is relatively well-established and the needed steps are more or less known. Nevertheless, there currently is no accepted automatic protocol and the manual steps performed are time-consuming, error-prone and sometimes not reproducible and, thus, not fit for regulatory purposes. The second workflow is even more complicated, since here not even the data/metadata, which has to be shared is well defined as highlighted by Ignacio Gonzalez Suarez in his talk at OpenTox Euro 2015 in Dublin.
   Initial subgroup members: Ignacio, Ahmed Abdelaziz, Michael Dellarco (by E-mail), Thomas Exner, (Andreas Karwath)

2) Data for modelling and data integration (use cases 2, 3, and 6): (Minimal) data/metadata quality standards will be defined for modelling, since trustworthy models can only be developed on the basis of retraceable/reproducible data. The second task will then be to incorporate additional data sources. Prioritization of these will include considering the quality standards. One most important source is PubChem and the involvement of Yanli Wang in the subgroup guarantees good progress in this direction.
   Initial subgroup members: Christoph Helma, Andreas Karwath, Ahmed Abdelaziz, Joh Dokler
3) Regulatory reporting (use case 1, see also attached description from Clemens): Even if this is already partly covered by the first topic, the specific demands of regulatory reports justify an additional subgroup on this topic. Main question to be answered here is how to prepare and handle data so that it can be directly used for reporting in the different formats (REACH, SEND, OCED harmonized templates, …).
   Initial subgroup members: Clemens, Thomas

The three subgroups will now start their "independent" work. I created three doodle polls to find dates for the first meetings (all times are given in CET). I hope that these can be used to find dates for more regular meetings. And I also hope that many people will join the initial members given above. Additional to the use cases, there is still the demanding task to collect all available OpenTox services, make them more easily deployable and to adapt the APIs to new demands (e.g. AOP modelling). The next steps to accomplish this will be discussed in a separate meeting hosted by Tim Dudgeon.

1) Endpoints: http://doodle.com/poll/p4bxb3kvs2hdqv6q
2) Modelling and integration: http://doodle.com/poll/nzer3igsa2c6cpnf
3) Reporting: http://doodle.com/poll/3424ar3zvcs44ger
4) API and deployment (WG 1 and 4): http://doodle.com/poll/g84ccnraymtzt4za

Thank you very much for all the engagement and effort you invested already in the OpenTox idea and I hope that we can continue this journey together.

Best regards.

Thomas Exner