EU-ToxRisk

An Integrated European 'Flagship' Program
Driving Mechanism-based Toxicity Testing and Risk Assessment
for the 21st Century

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AOP Workshop Report
The EU-ToxRisk AOP workshop took place from the 19th until the 22nd of September 2016. The event was hosted at the University of Vienna by the team of Prof. Gerhard Ecker. The four day event was structured around a two day introduction to the principles and practices of AOP development, which was followed up by two days of hands on training on data mining using the “OpenPHACTS” platform and KNIME software.

AOP training: The AOP training team from the OECD was represented by Mirjam Luijten (RIVM), Magdalini Sachana (OECD), Brigitte Landesmann (JRC) and Steven Edwards (US EPA). The OECD AOP training team focused on introducing the 40 participants from EU ToxRisk to the principles and best practices for AOP development and gave a short overview on weight-of-evidence analysis, which will be dealt with in more detail in the second part of the AOP training foreseen for next year. This theoretical information was immediately put into practice by working through a case study in small break-out groups. First the structure of the AOP was developed based on curated literature evidence and in a next step each group worked with the “AOP-Wiki” tool to practice entering an AOP to this communal work space. The OECD training team commented afterwards that they were impressed by the sound contributions from the audience and the lively and constructive discussions, even though many participants were new to the AOP concept. After the more general introduction to AOPs the link was also made to currently ongoing and planned future case studies in EU-ToxRisk. Mirjam Luijten highlighted the many ways in which the AOP Wiki can be searched for useful information; for example, one can search for existing AOPs related to organs of interest, search for shared key events that may form the basis of a future case study or search for AOPs that are lined to test compounds that are being used in EU-ToxRisk read-across case studies. The OECD AOP user’s handbook as well as the AOP Wiki are openly available resources that can be accessed here and here. Please note that a new version of the AOP Wiki will be launched before the end of the year.

Open PHACTS and KNIME training: Day three and four of the workshop were focused on data mining, which forms a crucial part in the development of AOPs as well as being more generally of use to the planning of experimental work. This portion of the course was attended by a smaller group of 20 people, made up mostly of PhD students and Post-Doctoral fellows. Gerhard Ecker’s group organized and led this portion of the workshop and was represented by Daria Goldmann and Daniela Digles. Following an introduction to the general functionalities of the KNIME software and the Open PHACTS extension the participants were split into small groups and worked through a series of 14 tasks and challenges that gradually increased in complexity. These hands-on tasks were aimed at giving all participants (with or without prior knowledge of this software) a working knowledge of basic functionalities and how the software can be explored further. Following these exercises the new expertise was immediately put to use by developing work flows to search different public data sources of interest to the EU-ToxRisk project, such as Tox21, diXa or TG-GATES. The workflows and challenges that were encountered in their development were then shared with the whole group and will be made available to all partners on the project internal SharePoint. It was clear to all that this is a very powerful tool and that some effort spent on learning how to use it will be well spent. Overall, the workshop participants provided very positive feedback on the workshop, even though for some advanced users of KNIME the introduction to the software was a bit too basic.

In conclusion, this workshop was a successful event that provided tools to workshop participants that will be useful for the duration of this project and beyond. In fact, it is already being discussed to hold a follow up workshop in the spring of 2017 with a focus on weight of evidence and AOP quantification as well as data extraction.