In This Issue

Picking Toxicology and Modelling Pockets
First eTOX Hackathon
(4-7th May 2015, Barcelona)

Early May, the first **eTOX Hackathon** was held in Barcelona hosted by FIMIM. This event had 30 participants from almost all consortium partners (3 toxicologists, 3 pathologists, 15 model developers and 9 data managers).

PROJECT NEWS

12th Consortium Meeting, Ware, UK

The meeting was hosted by GSK on June 22nd and 23rd. Key topics were verification procedures for the developed *in silico* models, SEND readiness of the eTOX database, and the sustainability of the system. Special attention was devoted to summarize the progress of the hackathon challenges and to plan the next steps for the integration of human safety information into eTOXsys.

iPIE collaboration

iPiE Executive Team attended the eTOX Consortium Meeting to discuss the data and software linkage of the two projects. A Memorandum of Understanding to establish the framework for collaboration is being under preparation and will be signed soon.

eTOX Website includes eTOX Tools

The eTOX website was updated to include the freely accessible eTOX Tools: eTOX Library, OntoBrowser, eTOXlab, LiMTox. A short description and the links to access the results developed in the framework of the project are accessible through:

http://www.e-tox.net/results.html

The **eTOX** Hackathon is a new initiative within the project designed as a hands-on exercise to promote collaborative best practices and team work across modelling and toxicology communities. Core of the exercise is the exploration of the collected **eTOX** data, consisting currently of more than 7,000 systemic toxicity reports corresponding to over 1,200 different non-confidential molecules. The cross-disciplinary group (chemists, biologists, pharmacists, toxicologists, pathologists, bioinformaticians, etc.) joined for a face to face meeting to analyse this amount of non-clinical toxicity data with read-across analysis and modelling purposes.

The event was organized around four challenges:
- *In vivo* hepatotoxicity modelling proof of concept
- From potency to risk
- Anemia model
- Open Challenge

The initial results obtained from each challenge will be translated into usable results within the project. Although our direct outputs were modest, all the participants felt that the experience was a positive one, enabling a forum to exchange ideas and methods as well as giving the participants a direct insight into the skill sets that our fellow collaborators hold.

Some highlighted experiences and conclusions as expressed on the flip-chart:

"A better understanding of the database. What we can model from the findings. The endpoints of interest to the toxicologists.

Face to face problem resolution and method/approach comparison.

Build up a challenge working group to improve the exchange of information.

We know better who to contact for the different problems we can encounter with the data. We go home with datasets."

"New ideas that I didn't expect came out from partners. New techniques, new viewpoints.

Good learning process also from failures. Good exchange between people/groups.

Found limitations of datasets and how to improve data combining datasets.
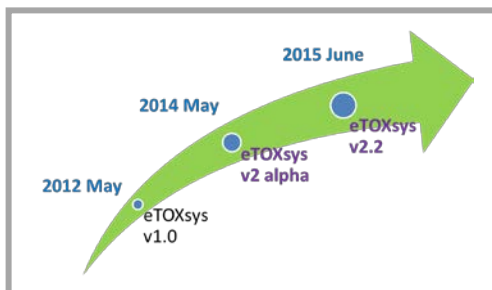
Better understanding of toxicologically relevant problems.

Being able to learn how other individuals approach eTOX data.

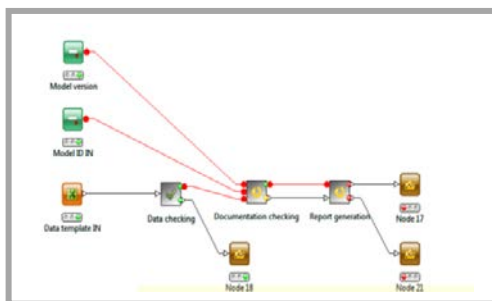*Some problems are common to everybody. Fixing them may have a great impact."*
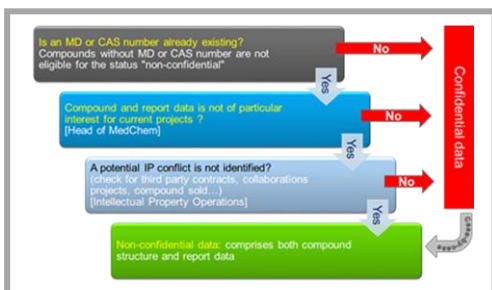
ACHIEVEMENTS

Mid June, the boxed eTOXsys v2.2 was deployed to the **eTOX** consortium partners. This version connects to the eTOX database 2015.1 and accesses the Fraunhofer ITEM RepDose database as well as all prediction models that are available as web services.

A hands-on session at the 12th eTOX consortium meeting was focused on the presentation of the new features of the system; to name a few: drag and drop molfiles/structures, Sub-string (partial) search in compound IDs, Export hit lists (SDFile), Display of similarity index, Export toxicity study tables, Use code lists of SEND code lists and harmonized terms into the common ontology.

The **Auto-verification Data workflow** was presented during the 12th consortium meeting. The verification process initially designed has been streamlined to optimize the verification task of all models in eTOXsys. The implementation of this workflow has several advantages, as it removes the need for an "external" verifier, speeds up the process and is sustainable for the future of the models development. The verification of all models is now paramount in **eTOX** and all modellers agreed to implement the auto-verification workflow.
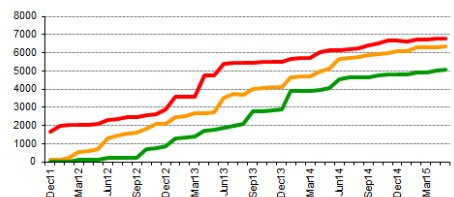

Bayer has revised its internal IP policy for data-sharing within **eTOX**. The revision not only speeds up the internal release process but more importantly results in a significant increase of compounds and reports accessible to all **eTOX** partners. At least 50% of extracted report data may now be shared with the partners.

REPORT-O-METER   6785

Currently, 5071 reports of the 6785 cleared for sharing within the consortium have finished the extraction data process and are available in the **Vitic Nexus eTOX database**.

Cleared Reports submitted to CROs or in-house facilities for data extraction
Extracted Reports with processing by CROs or in-house facilities completed
Vitic Reports with data available at Vitic Nexus database

PUBLICATIONS

A full list of publications is available on http://www.etoxproject.eu

- ARTICLE (FIMIM): DisGeNET: a discovery platform for the dynamical exploration of human diseases and their genes. Piñero J. et al. *Database* 2015:bav028
- ARTICLE (FIMIM): Integrative modeling strategies for predicting drug toxicities at the eTOX project. Sanz F. et al. *Mol Inf* 2015;34: 477–84
- POSTER (FIMIM): Implementation of new cardiac proarrhytmia safety paradigms in the eTOX prediction system. SOT 2015
- POSTER (MN): Comparative Data Mining Across Multiple Toxicity Databases Harmonized by eTOX Ontology to Test Hypotheses. SOT 2015
- POSTER (LL): Analysis of human and in vivo data for hepatotoxicity modelling. SOT 2015

UPCOMING EVENTS

- **12-16.07.2015 |** 41st Annual Summer Meeting. The Toxicology Forum 2015 Summer Meeting. Info: http://toxforum.org/

- **27-29.07.2015 |** 2nd International Conference on Health Informatics and Technology. Valencia, Spain. Info: http://healthinformatics.conferenceseries.com/

- **24-26.08.2015 |** 4th Global Summit on Toxicology. Philadelphia, USA. Info: http://goo.gl/uWOxPp

- **05-06.10.2015 |** Stratified medicine and prevention of adverse drug reactions. Edinburg, UK. Info: http://www.bps.ac.uk/meetings/BTS_BPS