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## PROJECT NEWS

### eTOXsys at EuroTox

Our end user platform -eTOXsys- has been presented at the Eurotox conference (52<sup>nd</sup> Congress of the Federation of European Toxicologists & European Societies of Toxicology) in Sevilla. The comprehensive overview of the system with the title "eTOXsys - An Integrated Platform for Profiling And Data Mining Across Multiple Databases and Prediction Models" presented the integrated platform, the database and the predictive modules. The poster also included the presentation of three use cases prepared by some of the EFPIA companies which demonstrate the value of the system in early drug safety assessment.

### eTOX – iPiE joint meeting

eTOX and iPiE will hold a joint meeting on Oct 7<sup>th</sup>, 2016 in Barcelona. The meeting particularly aims at analyzing the overlaps between both systems, collect and align user requirements as well as to open the debate around exploiting the benefits of the collaboration.

### The show will go on!

IMI2 has completed its evaluation of the NexGETS (Next generation translational safety) call. The call was developed by two eTOX EFPIA members and intends to combine preclinical data sharing with clinical data to assess translational safety. Project start is expected for the second half of 2017.

## eTOX Testimonials

*Towards the end of our project the editorial team of the Newsletter decided to pass the keynote floor to a few people, who heavily contributed to the success of eTOX behind the scenes...*

### TESTIMONIALS

*Martyna Pawletta, Nils Oberhauser, Oriol López Massaguer*

#### "How to count the value of the eTOX database?"

As the eTOX project is coming to an end, we can retrospectively summarize how processes have changed and what the value of eTOX is for Bayer. So what's the value of it? Is it even possible to count that? What I see in my daily life is that with every new use case and in-house example the interest and the acceptance within the toxicology department and even more so in the early research groups is growing. The database extends the search capabilities and certain *in silico* models can be used to prioritize compounds for further experimental investigations. The search results changed the way we communicate about safety hypotheses. That's the value of eTOX for me and Bayer.



#### Martyna Pawletta

*Bayer Pharma Aktiengesellschaft, Berlin*

#### "My One-Year Résumé"

When I joined the eTOX project about a year ago, I was fascinated by the ambitious goals of the project itself and the huge amount of data and effort that was contributed by the different eTOX partners. I was amazed how well a collaboration between competing pharmaceutical companies can work, even though much of the contributed data is still confidential. I am glad to be part of such an important and well-working project and that I can contribute by extracting data as well as by the maintenance and development of the "Data Quality Checks tool" for automatic inconsistencies detection in the extracted study data. The tool helped to improve the quality of the eTOX data significantly and regular feedback and suggestions from fellow WPO members help me to improve the program.



#### Nils Oberhauser

*Novartis Institutes for BioMedical Research (NIBR), Basel*

#### "Development of tools to obtain, integrate and transform data to build in silico toxicity models"

For several years I have been involved in the eTOX project, developing tools that extract, integrate and transform data for building *in silico* models. This project gave me the opportunity to work with people from a wide variety of disciplines; biologists, chemists, toxicologists and ontology experts from both public and private institutions. This environment allowed me to apply my background in computer science to develop together advanced methods for extracting and analyzing information in the complex area of *in silico* toxicology.



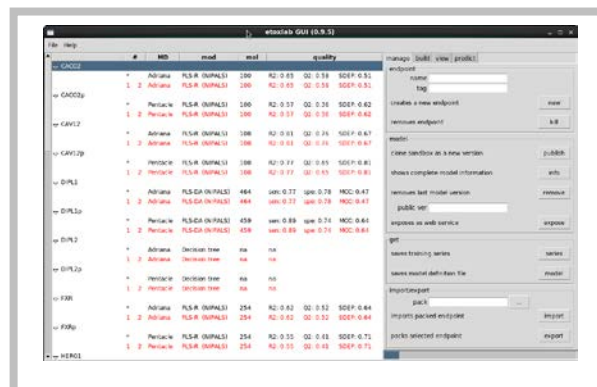
#### Oriol López Massaguer

*Research Program on Biomedical Informatics (GRIB) - IMIM/UPF, Barcelona*



## ACHIEVEMENTS

**eTOXlab GUI.** eTOXlab was designed to guarantee large consistency with respect to the location of the models within the filesystem of the Virtual Machines. Basic model maintenance operations (model creation, removal, export/import) are carried out using the eTOXlab manage module, either in command model or via the eTOXlab GUI. The model workflow enforced by the use of eTOXlab allows for easy maintenance of the models by producing new versions, but these never overwrite previously existing versions. Any published version will be kept in its original form unless it is explicitly removed. New versions of the same model are assigned new directories, thus keeping the collection of models well ordered.



## eTOX FINAL MEETING & SYMPOSIUM

After 7 years of achievements the eTOX project reaches its successful end and a **Final Consortium Meeting** will be held on the 28<sup>th</sup> and 29<sup>th</sup> of November 2016 in Basel, Switzerland, hosted by Novartis and co-sponsored by Bayer and Roche.

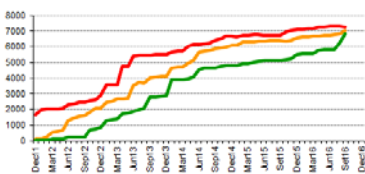
The meeting will be focused on the closing of the project, offering global presentations of the final tasks and activities as well as the presentation of posters. The agenda will include a scientific event closing the project in which technical discussions around toxicology are scheduled with the attendance of valued experts.

Additionally, the meeting will be marked by the lectures from two outstanding keynote speakers from the Innovative Medicines Initiative (IMI) office and from a renowned computational scientist from the U.S. Environmental Protection Agency (EPA).

## REPORT-O-METER

# 7244

The last packages of reports have been contributed to the **Vitic Nexus eTOX database**, in preparation of the final release before project finishes. Total of cleared reports decreased (7287 Jun2016 to 7244 currently) due to final rejection from legal departments.



**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 (NOVARTIS): [OntoBrowser: a collaborative tool for curation of ontologies by subject matter experts](#). Ravagli C, Pognan F, Marc P. *Bioinformatics 2016: btw579*.
- ARTICLE (FIMIM): [Combining machine learning, crowdsourcing and expert knowledge to detect chemical-induced diseases in text](#). Bravo A, Shu-Li T, Su A, Good B, Furlong L. *Database 2016: baw094*.
- ARTICLE (UNIVIE): [Subtle Structural Differences Trigger Inhibitory Activity of Propafenone Analogues at the Two Polyspecific ABC Transporters: P-Glycoprotein \(P-gp\) and Breast Cancer Resistance Protein \(BCRP\)](#). Schwarz T, Montanari F, Cseke A, Wlcek K, Visvader L, Palme S, Chiba P, Kuchler K, Urban E, Ecker GF. *ChemMedChem 2016;11(12):1380-94*.

## UPCOMING EVENTS

- 17-19.10.2016** | 6<sup>th</sup> Global Summit on Toxicology and Applied Pharmacology. Houston, Texas, USA. Info: <http://toxicology.global-summit.com/>
- 24-26.10.2016** | 7<sup>th</sup> Euro-Global Summit on Toxicology and Applied Pharmacology. Houston, Texas, USA. Info: <http://toxicology.global-summit.com/europe/>
- 6-9.11.2016** | 37<sup>th</sup> Annual Meeting of the American College of Toxicology. Baltimore, USA. Info: <http://www.actox.org/am/am2016/>