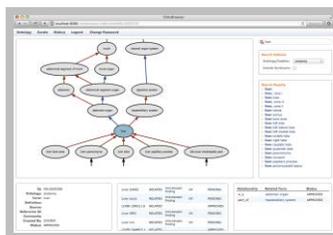


In This Issue

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Just Released: *OntoBrowser* and *eTOXlab* on Open Access*!

The eTOX consortium is glad to announce the publication of these software packages.



Novartis developed the *OntoBrowser* to support the generation of a common ontology aimed at harmonization/standardization of the *eTOX database terminology*.



FIMIM developed the *eTOXlab* to support the generation and implementation of *predictive models* into the *eTOXsys*.

*See access details in page 2

PROJECT NEWS

6th eTOXsys user meeting, Berlin

The 6th eTOXsys User Meeting hosted at Bayer premises on February, 26th 2015 marked a cornerstone in the development of the front-end query and prediction system. The eTOXsys v2.0 was successfully installed and intensively tested by more than two-thirds of the EFPIA partners. An intensive hands-on session resulted in valuable and constructive feedback, identification of feature requests and bug-fixes. Companies can now implement complex searches behind their own firewalls.

eTOX SAB enlarged

A new expert has been recently incorporated in the Scientific Advisory Board of eTOX consortium. Dr. Peter Kasper is Director and Professor at the Federal Institute for Drugs and Medical Devices (BfArM) in Bonn, Germany, where he serves as toxicologist in preclinical safety sciences. As an expert in Genetic Toxicology, he has profound knowledge in *in silico* prediction systems and is thus a valuable addition to the existing SAB members.

KEYNOTE

The role of eTOX project in the sustainable business of computational toxicology tools and solutions

Message from Dr. Chihae Yang, Molecular Networks Managing Director

Computational toxicology has made strong advances during the last decade, thanks in no small part to important regulatory initiatives such as REACH, the 7th Amendment for Cosmetics, and ICH M7 (genotoxic impurities). The real need to solve real problems presents genuine opportunities for an SME, where a focused direction is required to maximize the use of available resources.



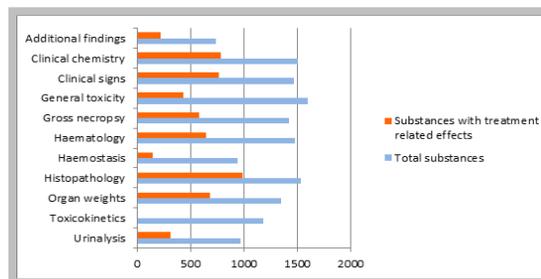
The IMI **eTOX** project is at the center of this advancement of science and technology, and importantly this project includes a sustainability component to enable the development of commercial products. In contrast to traditional US routes of top-down dissemination through national centers, publicly funded European projects reach the grass roots across a broad economic spectrum of public institutions, academia, and R&D industry, including SMEs. There are many examples of public projects in Europe creating useful computational tools and web applications. Although the scope and specialization of these vary widely, to a certain extent these public projects deliver a similar workflow: a database to find information and test hypotheses, and a platform to allow both human and machine learning and extraction of knowledge leading to predictions. Whilst the core idea is similar, the implementations differ greatly due to their individual strengths, focus, and constraints. This disparity of technology and lack of a common design often impedes and discourages the integration of tools from different sources. Furthermore, maintaining and supporting a system of such diverse and non-connected subsystems is challenging once the project is successfully delivered at the end. Many of the players now recognize that it is time to pay attention to the sustainability of these tools and solutions beyond the project period. *The science and technology that eTOX creates through its unique ontology-driven database approach and prediction models distributed at experts' sites is a concept that many computational solution providers have already recognized as a promising way to go.* Although technically demanding, the **eTOX** project has made huge strides in establishing distributed databases and knowledge providers through **eTOXsys** and **eTOXlab** within and across firewalls of defined communities. In addition to this strategic design achievement, the sustainability project of **eTOX** must play an exemplary role. Although the economic impact of EU investments is first realized through the funding of projects, the larger and ultimately more important impact will benefit from a business perspective that emphasizes the sustainability of project outcomes.



ACHIEVEMENTS

- In January, Lhasa launched **the tenth release of the Vitic eTOX database** containing 1791 substances associated with 6105 preclinical studies. The majority of the treatment related findings in the database are histopathological (992 substances) with liver being the most common organ affected (576 substances). The database also includes toxicokinetic related data (i.e., Cmax, AUC, Tmax) for a significant number of substances (1182 substances).
- In terms of **enhancing data sharing**, Bayer has recently revised its data sharing policy for **eTOX**. As a consequence, Bayer will significantly increase the rate of non-confidential data visible for all partners. This revision will result in an increase from 11 to 44% of the compound structures. With regard to report data, 50% of all extracted data sets will become visible to all partners of the project.
- This month, Novartis published **OntoBrowser** as an open source software project. The source code was released under the [Apache License Version 2.0](#) and is available on **GitHub** (<http://github.com/Novartis/ontobrowser>). Consortium members are free to download and deploy the tool within their own environments; and to modify it to meet their own specific requirements. The release includes an [installation guide](#) to facilitate installation.
- This month, FIMIM published **eTOXlab** as an open source flexible modeling framework. It was developed for supporting models predicting the biological properties of chemical compounds (e.g. QSAR models) in production, and provides predictions as web services. This software consists of a collection of object-oriented Python modules with methods mapping common tasks of standard modeling workflows and is available on **GitHub** (<https://github.com/manuelpastor/eTOXlab>). The ensemble eTOXlab-VM constitutes a portable, self-contained prediction engine that can be easily distributed and installed. Read their [article](#) for details of functionality.

Vitic Nexus eTOX database 2015.1

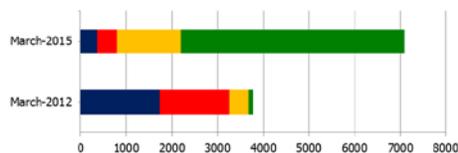


REPORT-O-METER

6740

Currently, 4908 reports of the 6740 cleared for sharing within the consortium have finished the extraction data process and are available in the **Vitic Nexus eTOX database**.

Since we had the first reports collected in the database (101^{Mar12}), the total number of reports under **eTOX** process has almost doubled (3782^{Mar12}, 7098^{Mar15}). The graph below shows the current distribution of reports by their status.



Planned Reports awaiting for clearance
Cleared Reports under submission to CROs or in-house 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): [Extraction of relations between genes and diseases from text and large-scale data analysis: implications for translational research](#). Bravo A. *et al. BMC Bioinformatics* 2015;16:55.
- ARTICLE (CNIO): [CHEMDNER: The drugs and chemical names extraction challenge](#). Krallinger M. *et al. J Cheminform* 2015;7(Suppl 1):S1.
- ARTICLE (CNIO): [The CHEMDNER corpus of chemicals and drugs and its annotation principles](#). Krallinger M. *et al. J Cheminform* 2015;7(Suppl 1):S2.
- ARTICLE (FIMIM): [eTOXlab, an open source modeling framework for implementing predictive models in production environments](#). Carrió P. *et al. J Cheminform* 2015;7:8.
- ARTICLE (EMBL): [Chemical databases: curation or integration by user-defined equivalence?](#) Hersey A. *et al. Drug Discov Today: Technologies* 2015; Available online 11 March 2015. *In press*.
- ARTICLE (LJMU): [Ensuring Confidence in Predictions: A Scheme to Assess the Scientific Validity of In Silico Models](#). Hewitt M. *et al. Adv Drug Deliv Rev* 2015. Available online 18 March 2015. *In press*.

UPCOMING EVENTS

- **19-22.04.15** | BTS Annual Congress 2015. Solihull (UK). Info: <http://goo.gl/ttWn0v>
- **19-24.04.15** | KESA 2015. The International Workshop on Knowledge Extraction and Semantic Annotation. Barcelona (Spain). Info: <http://www.iaia.org/conferences2015/KESA.html>
- **23-26.04.15** | 8th International Biocuration Conference. Beijing (China). Info: <http://biocuration2015.tilsi.org/>
- **5-6.05.15** | 9th Drug Design & Medicinal Chemistry Conference. Berlin (Germany). Info: <http://goo.gl/PLUrtD>