eTOX

Newsletter

In This Issue

We are glad to celebrate the first year of the eTOX Newsletter. Many of our readers have provided valuable comments and we would like to express our gratitude for this feedback which helps us to continuously improve our Newsletter.

Season's Greetings
from the eTOX team,
with the best wishes for
a Happy and Fulfilling Year ahead!

data
ontologies
models

PROJECT NEWS

7th eTOX Consortium meeting in Basel

The 7th eTOX Consortium meeting was held in Basel in November. Two members of the Scientific Advisory Board attended the meeting who praised the advances of the project, and participated in the 3 workshops organized on Modeling, Use cases and Ontologies.

eTOX webinar at EPA CompTox Communities

The EPA Computational Toxicology Communities of Practices is a wide community of people interested in encouraging computational toxicology usage and exposure science in helping to implement EPA's mission of protecting human health and the environment. eTOX was presented in one of its monthly seminars, helping to raise the profile of eTOX in the USA.

Call to Explore New Scientific Opportunities

IMI JU launched a call aiming ongoing IMI projects to reinforce their capacities in view of promising results deserving additional investigations. eTOX has submitted a proposal in the framework of this call, which is primarily intended to expand the project in a number of areas and extend its duration. The proposal has received full endorsement of EFPIA-RDG and will now undergo a peer-review evaluation by independent experts.

KEYNOTE

An external perspective on eTOX
Message from the Former Group R&D Director, Welcome and Director General ABPI: Prof Trevor M Jones

Preclinical studies to evaluate the safety of putative candidates for drug development is an essential and critical step in the long and expensive process from drug discovery to the market.

Failure during late stage development –and especially if the product is launched– is costly in both human and financial terms and so the determination of which candidate compounds are suitable for continuing investment is a major critical parameter for innovative pharmaceutical companies.

Given the complexity of animal and human physiology in both healthy and disease states, it is probable that for the foreseeable future, interpreting data from whole animal pharmacology and toxicology will remain the prime, although still limited, means of making value judgments on the acceptability of such candidates for further development. In recent years, the emergence of reliable cell based assays has supplemented both traditional *in vitro* methodologies and biochemical assays to add further insight for such decisions. In the future, our understanding of the interpretation of genomics, proteomics and (eventually) epigenomics will add further knowledge to this difficult yet vital task.
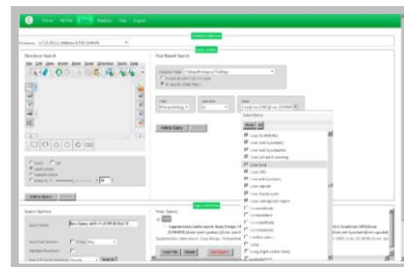
The eTOX project, by developing expert systems for integrating Bioinformatics and Chemoinformatics to predict toxicities, will add a further dimension to our current armamentarium to enable the decision process. The project has made good progress and it is especially gratifying to see positive results in the work on ontologies which are central to a common understanding and use of the data that will emerge as the project progresses. The commitment of the teams, both industrial and academic, involved in the project is testament to its likely future success which will be so important in bringing new medicines to the patients we all serve.

- Mid November 2012, Lhasa Limited launched the **third release of the Vitic Nexus eTOX database**, with 170 structures (65 confidential) linked to 1806 study design records collected from Bayer, Boehringer, Esteve, GlaxoSmithKline, Novartis, Pfizer and UCB.

- Ending November 2012, EMBL launched the **third release of the ChOX database**, a chemogenomics platform based on data from ChEMBL database, containing: 411 toxicology-linked targets; 169,216 distinct compounds and 672,684 activities gathered from 11,264 publications.

- An **eTOXsys** query task force was defined to identify possible query scenario and to support the design of a user friendly query interface. Bayer, Molecular Networks, Novartis and Sanofi partners collaborate to evaluate typical use cases formulated by different EFPIA partners of the consortium.

- In a pilot study with Bayer partner collaboration, Molecular Networks successfully installed the **eTOXsys virtual machine** and ran a copy of the **eTOXsys** server on a computer behind the company firewall. Thus, the general feasibility of the **eTOXsys** plan for deployment to the EFPIA companies has already been proven.
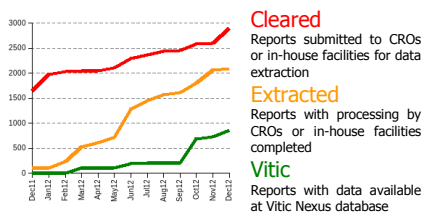
Vitic Nexus database

eTOX predictive system

REPORT-O-METER 2904

After 1 year of reports processing, 2/3 of the total of currently cleared reports have successfully completed the CROs data extraction, and data from 1/3 have been already included following the Vitic Nexus eTOX database schema.

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-(LJMU): Assessing toxicological data quality: basic principles, existing schemes and current limitations. Przybylak KR, et al. *SAR QSAR Environ Res.* 2012;23(5-6):435-59.
- ARTICLE-(FIMIM): Automatic Filtering and Substantiation of Drug Safety Signals. Bauer-Mehren A, et al. *PLoS Comput Biol* 2012;8(4):e1002457.
- ARTICLE-(FIMIM): Human diseases through the lens of network biology. Furlong LI. *Trends Genet*. In press. doi: 10.1016/j.tig.2012.11.004.

UPCOMING EVENTS

- **24-25.01.13 |** Predictive Human Toxicity and ADME/TOX Studies. Brussels (Belgium).
  Information: http://www.mondialresearchgroup.com/index.php?whereTo=humt13
- **13-15.02.13 |** Integrated R&D Informatics and Knowledge Management Leveraging IT and Informatics to Enable Global Information Sharing. San Francisco, CA (USA). Information: http://www.triconference.com/mmtc_content.aspx?id=118870&libID=118818
- **10-14.03.13 |** The Society of Toxicology (SOT) 52nd Annual Meeting San Antonio, Texas (USA).
  Information: http://www.toxicology.org/ai/meet/am2013/am.asp
- **7-10.04.13 |** Biocuration 2013. Cambridge (UK).
  Information: http://www.ebi.ac.uk/biocuration2013/