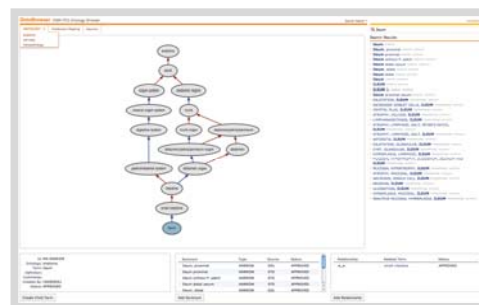


In This Issue

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- **Upcoming Events**

Have a look at the terminology harmonization tool: the OntoBrowser

A collaborative curation and browsing interface has been developed by Novartis to integrate into a single ontology the vocabularies used by the 13 different EFPIA partners in the project. First tests on mapping terms are under supervision of the curation team, who will consolidate them into a common ontology.



PROJECT NEWS

eTOX Mid-term Review at the IMI completed successfully

The mid-term review represents the main evaluation and assessment point for all IMI projects. Intensive preparatory efforts were therefore undertaken by a dedicated eTOX team for this review – with rewarding results: The external reviewers evaluated the eTOX project as being well conducted and advancing at a good pace. The ontology approach was highlighted as impressive having the potential to become a standard also for other projects and the progress made in overcoming the legal obstacles for data sharing was emphasized.

The valuable recommendations received will foster the work in the next months and will leverage the efforts of a well-united team towards achieving the aims of the project.

6th eTOX Consortium Meeting, Sweden

Our 6th Consortium Meeting in Gothenburg was a particular exciting one. For the first time the progress of the eTOX project really became tangible: all three pillars of the project, namely the public data collection (ChOX), the legacy report database (Vitic Nexus eTOX) and the prototype of the prediction system containing the first models (eTOXsys) were presented and are now accessible to all partners for testing and integration.

KEYNOTE

eTOX – From the Perspective of an SME

Message from Molecular Networks: **Christof Schwab**

Funded projects can play an important role for the business of an SME. Projects may have an impact on the business plan and on areas of activities, as it enables a small business entity with limited resources to explore areas and technologies which probably would not have been envisaged without external funding.

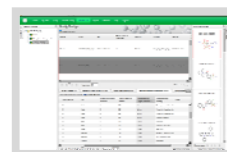


Molecular Networks has been involved in the eTOX project since the early planning phase. The multifaceted aspects in terms of scientific and technological challenges of the IMI project call fitted well with the expertise of the company, but they also offered the opportunity to gain new insights and knowledge in the area of toxicology in the early drug development process. Furthermore, the possibility to closely work together with pharmaceutical companies on a scientific level and to learn about their daily challenges is considered as a competitive advantage for an SME. However, there are also the benefits for large companies, such as the EFPIA partners in the eTOX consortium. An SME can flexibly, quickly and in an unbureaucratic way react to changes and challenges which arise during the course of a project. Work force can be rapidly re-assigned to newly emerging tasks or shifted to work packages that require more person months than originally planned due to their central role within the project. Thus, it was realized during the first year of the project, that the eTOXsys would be of critical importance and should be available as a prototype for testing by all partners as early as possible. In agreement with the ExCom members and the IMI authorities, Molecular Networks was able to quickly react and move manpower to the development of the eTOXsys to secure the progress and the success of the system. By March 2012, a first proof-of-concept version of the eTOXsys has already been established, presented and reported in year two of the project. Together with all partners, a stable version of prototype 1 of the eTOXsys has been optimised to user's needs, finalized and presented in the Mid-term review of the eTOX project.



ACHIEVEMENTS

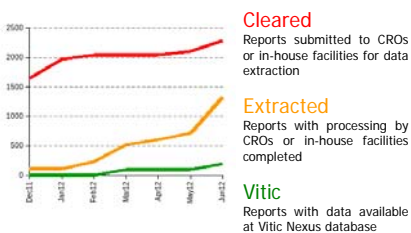
- Early April 2012, Lhasa Limited launched the first release of Vitic Nexus eTOX database, with 63 structures and data from the first 101 legacy reports submitted by Bayer Healthcare and Novartis.
- ESTEVE has already completed the in-house extraction data process for the total of their planned reports.
- A common tracking system on reports status has been defined to follow up the extraction data process on a monthly basis.
- Linked to the OntoBrowser, the OntoDB currently contains this total of preferred terms (PT) and synonyms (syn): Study design ontology (42 PT), Cell and tissue type ontology (1010 PT + 802 syn), Anatomy ontology (2907 PT + 1733 syn) and Histopathology ontology (844 PT + 3304 syn, with >10K synonyms to be labeled).
- EMBL presented a new release of the ChOX database in the 6th eTOX consortium meeting. This chemogenomic platform currently contains: 427 toxicology-linked targets, 175,401 distinct compounds and 705,415 activities gathered from 10,920 publications. The list of datasets available has been sorted by endpoint of interest to facilitate modelers in their modeling tasks.
- EFPIA partners together with the modelers team and the eTOXsys developers have defined a Model Taxonomy, that allows the organization of all models available from the eTOXsys Graphic User Interface in different categories taking into account the endpoint prediction addressed. Presumably, this taxonomy will evolve to host new types of predictions different from current needs.
- CT, DTU, FIMIM, IL, LJMU, LMD, MN, UNIVIE and VUA partners have already developed and fully documented a set of 59 models, from which 40 are available at the eTOXsys as web services. A Model-o-meter has been set up in order to provide monthly updates to consortium members on models status (developed, documented, available at eTOXsys and formally validated).



REPORT-O-METER

2289

EFPIA partners are progressing well with the data extraction and quality checks.



PUBLICATIONS

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

- ARTICLE-(UNIVIE): Fingerprint-based *in silico* models for the prediction of P-glycoprotein substrates and inhibitors. Poongavanam V., et al. *Bioorg. Med. Chem.* 2012, Mar 29. [Epub ahead of print].
- ARTICLE-(EMBL, LL, Novartis): Toxicology Ontology Perspectives. Hardy B., et al. *ALTEX*. 2012, 29 (2): 139-156.
- ARTICLE-(EMBL, LL, Novartis): Food for Thought... A Toxicology Ontology Roadmap. Hardy B., et al. *ALTEX*. 2012, 29 (2): 129-137.

UPCOMING EVENTS

- **21-25.7.12** | International Conference on Biomedical Ontology 2012, co-located with FOIS 2012, Graz (Austria). Information: <http://purl.org/icbofois2012/>
- **26-30.8.12** | 19th EuroQSAR, Knowledge Enabling Ligand Design, Vienna (Austria). Information: <http://www.euroqsar2012.org/>
- **2-6.9.12** | 22nd International Symposium on Medicinal Chemistry: Drug Safety: what toxic effects can be reasonably predicted. Information: <http://www.ismc2012.org/>
- **5-6.9.12** | 3rd International Lhasa Symposium on New Horizons in Toxicity Prediction, Downing College, Cambridge UK. Information: <http://www.lhasasymposium.com/>