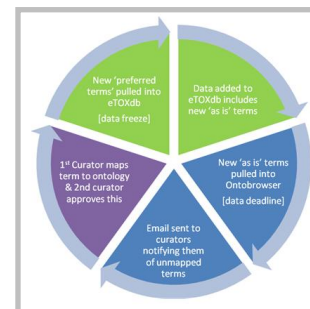


## In This Issue

- **Project news**
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## Have a look at the workflow for harmonization of Legacy reports Verbatim Terms

A common ontology is seen as key to integrating the public and private data and harmonising the terms used by the different EFPIA partners. New verbatim terms added to the eTOX database are passed to the Ontobrowser tool where the curation team (pathologists from Novartis, GlaxoSmithKline, Sanofi, and Pfizer; in collaboration with Lhasa and FIMIM) can then map them to the ontologies. A second pathologist with approval privileges then checks and confirms this mapping. The resulting preferred terms are then integrated back into the eTOX database so users can see both verbatim and preferred terms alongside each other.



## PROJECT NEWS

### 8<sup>th</sup> eTOX Consortium meeting in Copenhagen, Denmark

The 8<sup>th</sup> eTOX Consortium meeting was held in Copenhagen in April. At this meeting the four new public partners were welcomed and presented their contribution to ENSO (project extension). A member of the Scientific Advisory Board particularly remarked on the visible progress of the eTOX system. A first workshop on Sustainability was organized in order to set the scene towards the future of the project and the eTOX system.

### eTOX presented at DETECTIVE meeting in Slano, Croacia

eTOX project has been presented at the DETECTIVE summer school, June 13th. The overall aim of this project is to identify, develop and evaluate relevant biomarkers and surrogate endpoints *in vitro* that can be used for safety assessments and replacement of repeated dose toxicity testing in the field of cosmetics.

### Analysing the value of Public Private Partnerships (PPP)

The eTOX project has been selected by IMI-JU for an in-depth analysis of reasons of success and/or difficulties related to the outcome or deliverables of IMI projects. The study is led by the Katholieke Universiteit Leuven.

## KEYNOTE

### Shared Knowledge, Shared Progress

Message from Lhasa Limited Chief Executive officer: David Watson

Sharing data to increase knowledge is the fundamental basis upon which Lhasa Limited was founded in 1983. Given our role as 'honest broker' in the project, using Vitic as the repository for shared data aligns with our vision of being acknowledged and trusted by our members and the scientific community as the world leader for knowledge and data sharing in chemistry and the life sciences.



In providing the database that will be used to create novel *in silico* models, we are also contributing to the furthering of our charitable purpose i.e. the promotion of computer aided reasoning in this field. Our experience in the creation and development of consortia working in collaboration to deliver specific scientific outcomes suggests that it is not easy to create the balance between partners and tasks to optimise the potential for successful outcomes. The difficulties in this regard are increased when consortia have a mix of SME's, academic organisations and large corporate organisations, simply by culture and approach differences. The excellent progress made with the eTOX project is in no small part to the spirit of cooperation and collaboration that pervades every part of the project. *The willingness of all partners to work together to overcome obstacles for the greater good of the project, demonstrates the level of teamwork necessary to make success of consortia such as these, and in our opinion, it is this factor that supported the decision to award the ENSO extension to the project.*

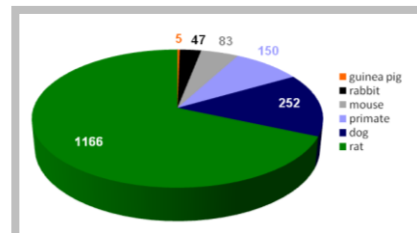
The important advances the eTOX team are working towards should provide future users with novel approaches for predictive models that will enhance their ability to bring new, safe medicines to the wider public. This will require the continued focus of our team for the next 4 years, building on the solid platform of the first 3, expanding the scope and volume of the data to be shared in order to maximise the impact of new models across the key endpoints of interest. We look forward to tackling the challenges of both the remainder of the existing project and the recently granted extension.



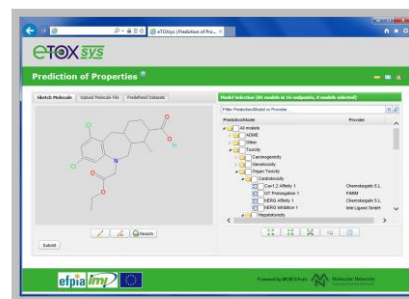
## ACHIEVEMENTS

- Mid May 2013, Lhasa Limited launched the **fifth release of the Vitic Nexus eTOX database**, with 537 structures (165 confidential) linked to 1,703 study records collected from Bayer, Boehringer, Esteve, GlaxoSmithKline, Lundbeck, Novartis, Pfizer, ROCHE, Sanofi, Servier and UCB legacy reports. In addition, it contains data from the **third release of the ChOX database** (162,287 substances and 701,181 records) and **OPEN TG GATES database** (170 substances and 304 records).
- The **eTOX database** contains preferred terms facilitating greatly searches conducted by modelers. Using the **OntoBrowser** tool, the curators reviewed and assigned to preferred terms over 1 million verbatim terms extracted from toxicology reports. Current coverage of verbatim by preferred terms is 97% for clinical pathology parameters, 98% for tissues/organs locations and 20% for microscopic findings.
- **Version 1** of the integration system, **eTOXsys**, was released to all partners along with the **eTOXsys central software management site** available to manage software issues, collect user feedback and feature requests for new versions, and compile documentation related with technical aspects. The proof-of-concept for the installation of **eTOXsys** behind the firewalls is in its final stage. Seven of ten companies have already a running system. Issues with the connections to the in-house **eTOX** databases are currently being fixed.

Vitic Nexus eTOX database 2013.2  
Study records/specie



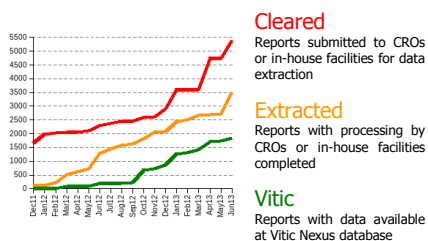
eTOX predictive system v1.0



## REPORT-O-METER

5392

After 1 year and a half of reports processing, all reports cleared by December 2011 form part of the Vitic Nexus eTOX database, and progressively new batches of reports enter in this process. Lessons learned from first steps are being helpful to accelerate the workflow.



## PUBLICATIONS

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

- ARTICLE-(DTU): HExpoChem: a systems biology resource to explore human exposure to chemicals. Taboureau O, Jacobsen UP, Kalhauge C, Edsgård D, Rigina O, Gupta R, Audouze K. *Bioinformatics* 2013; 29(9):1231-2.
- ARTICLE-(DTU): ChemProt-2.0: visual navigation in a disease chemical biology database. Kim Kjærulff S, Wich L, Kringelum J, Jacobsen UP, Kouskoumvekaki I, Audouze K, Lund O, Brunak S, Oprea TI, Taboureau O. *Nucleic Acids Res* 2013; 41(Database issue):D464-9.
- ARTICLE-(LJMU): Pragmatic Approaches to Using Computational Methods to Predict Xenobiotic Metabolism. Piechota P, Cronin M, Hewitt M, Madden JC. *J Chem Inf Model* 2013 May 29.

## UPCOMING EVENTS

- **20.07.13** | Bio-Ontologies 2013. Berlin (Germany). Info: <http://www.bio-ontologies.org.uk/home>
- **01-04.09.13** | EUROTOX13 meeting. Interlaken (Switzerland). Info: <http://www.eurotox2013.com/welcome.html>
- **09-13.09.13** | Practical Application of Toxicology in Drug Development. Edinburgh (United Kingdom). Info: [https://www.actox.org/meetCourses/patdd.asp?qoback=qde\\_1921622\\_member\\_249943171](https://www.actox.org/meetCourses/patdd.asp?qoback=qde_1921622_member_249943171)
- **10-13.09.13** | 11<sup>th</sup> European Congress of Toxicologic Pathology: A pathologists's view of animal models and *in-vitro* systems. Ghent (Belgium). Info: <http://www.eurotoxpath.org/meetings/index.php?id=congress2013>
- **27.09-02.10.13** | 2013 Annual Meeting of the North American Congress of Clinical Toxicology Hyatt Regency Atlanta (USA). Info: <http://www.clintox.org/meetings>
- **10-11.10.13** | 5<sup>th</sup> Open PHACTS Community Workshop. Amsterdam (The Netherlands). Info: <http://www.openphacts.org/community-workshops>