OpenTox

OpenTox USA 2013

29 October

North Carolina Biotech Center

Raleigh-Durham

Barry Hardy (Douglas Connect)

OpenTox

ToxBank

Thank you -

For organising ...

For preparing ...

For coming ...

For overcoming shutdown paralysis ...

For being open to participating in new developments and adventures ...

OpenTox

OpenTox

Source: Baily Ed, U.S. Fish and Wildlife Service

Islands

Knowledge-Oriented Framework

Tacit

Tacit

Tacit

Knowledge Sharing: Discussions

Socialisation

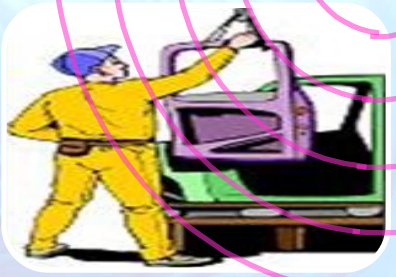
Externalisation

Explicit

Knowledge Creation from R&D: Data, Codes

Acceptance

Learning: Apply Models



Internalisation

Combination

Knowledege Combination: Predictive Models

Tacit

Explicit

Explicit

Explicit

OpenTox

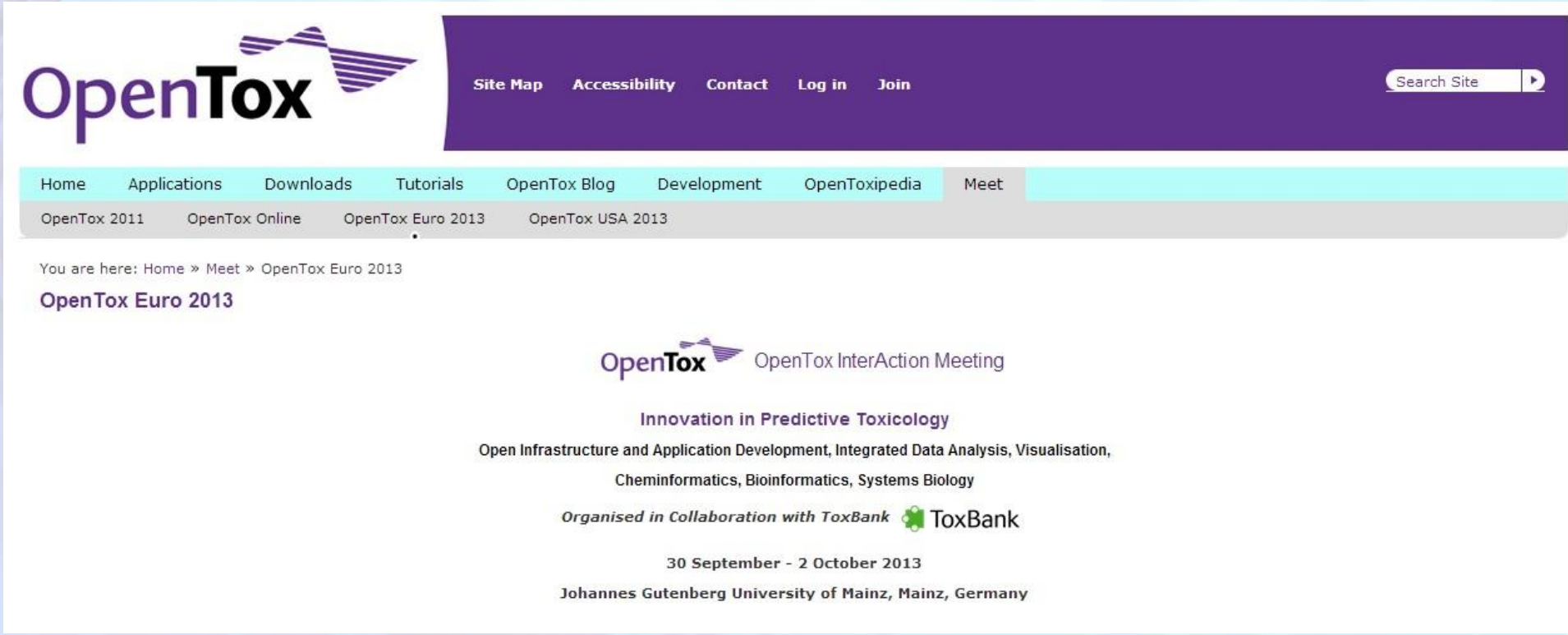
Based on Nonaka & Takeuchi, The Knowledge Creating Company, 1995

Knowledge Sharing

OpenTox

18M

OpenTox Euro 2013



What is OpenTox?

We are an Open Knowledge Community!

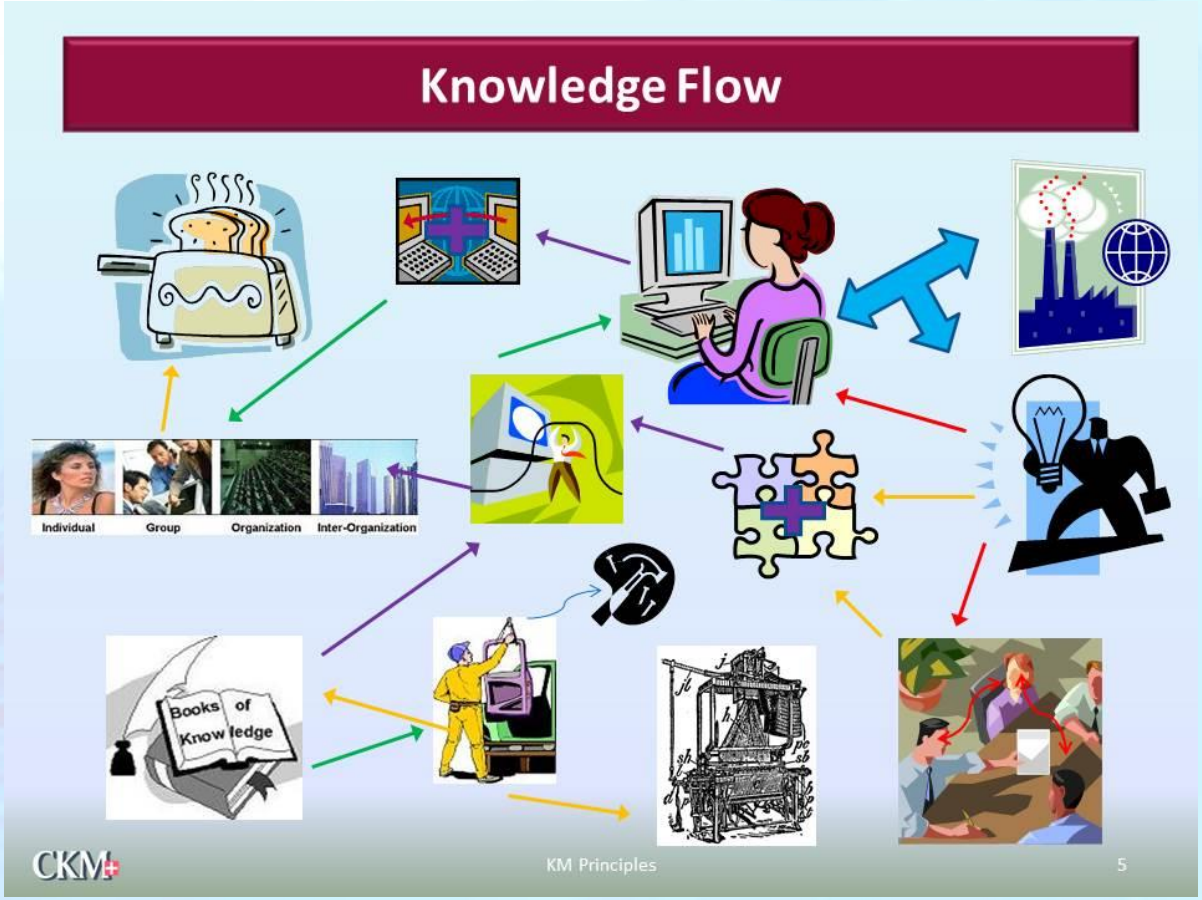
We collaborate, solve problems and create the best solutions we can together.

We learn from each other .. and enjoy it.

We accelerate knowledge flow & innovation.

Supported by a 21st Century Computer Science for Predictive Toxicology and Safety Assessment that we develop together

Goals for next year for OpenTox
- Implement Expanded Data Foundation
(based on Consensus Open Specifications)
- Leverage Foundation for Applications and Impact
- Develop Scientific and Business Ecosystem
Accelerate Knowledge Flow



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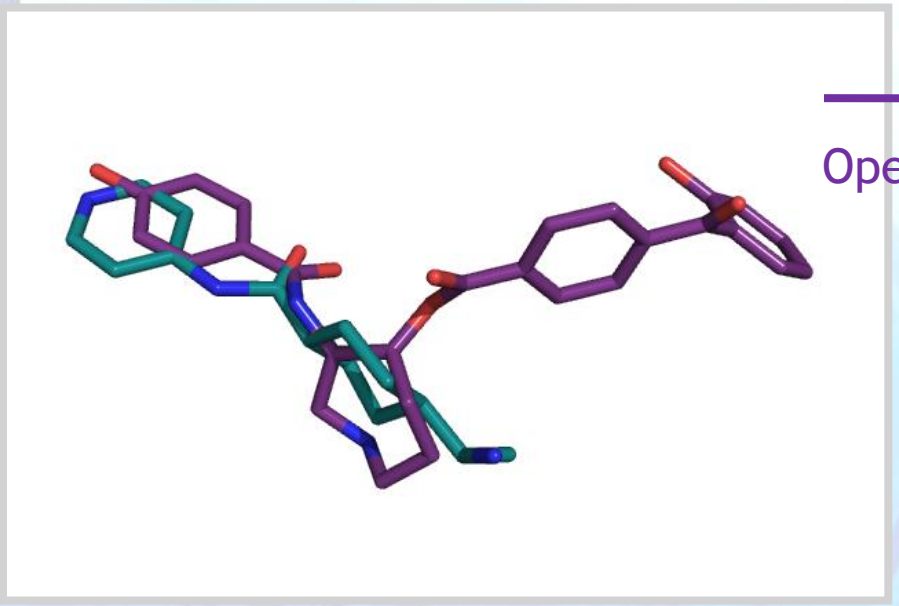
Predictive Toxicology Challenge & Use Case

Input Structure



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Out – Toxic or Not?

- LD50
- Liver Toxicity
- Secondary Metabolites
- Bioavailability
- Mutagenicity
- Carcogenicity
- ReproductiveToxicology
- Skin Irritation
- Aqua Toxicity
- Combined predictions for arrays of mutiple end points

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Challenges to Interoperating Resources & Applications

- Database silos
- Missing information
- Varying quality
- Hard to integrate data
- Hard to integrate models
- No common framework
- Lack of consensus on working standards
- Lack of validation
- Complex subject
- Application difficult
- Lack of transparency
- Interdisciplinary collaboration

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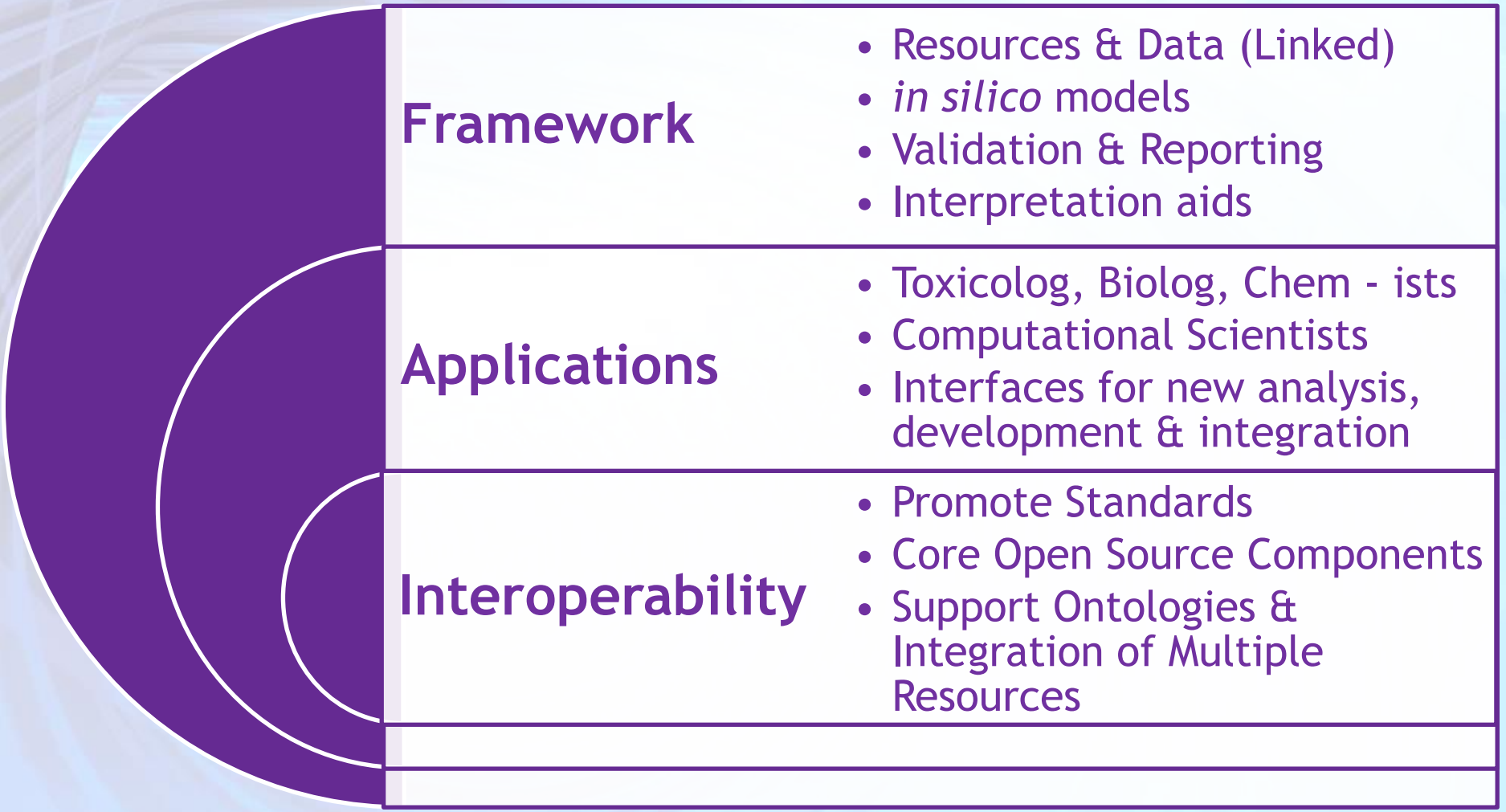
OpenTox is an Integrating Framework



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Interacting Components create Solutions

Adaptor Solution in Jeddah, 2008

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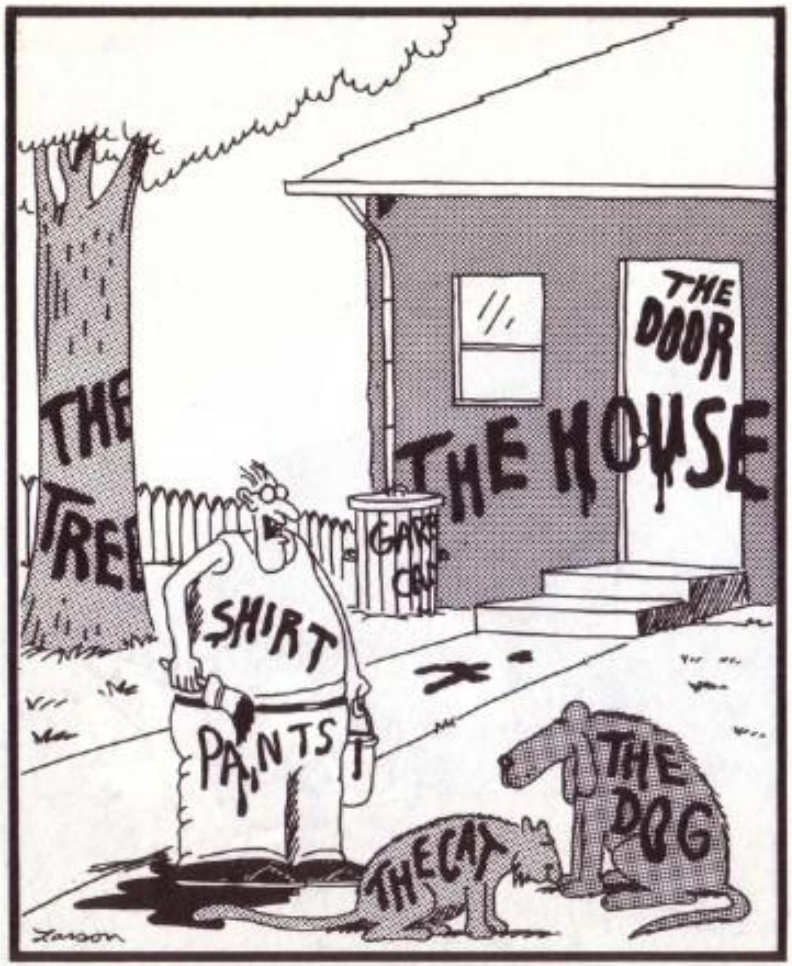
Semantic Reflections



"Now! ... *That* should clear up a few things around here!"

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OpenTox committed to creating a Semantic Web for Predictive Toxicology (*with its API 1.1 development in 2009*)

Linked Data is a term used to describe the exposing, sharing, and connecting of data on the Semantic Web using:
URIs a generic means to identify entities in the world
HTTP a simple yet universal mechanism for retrieving resources
RDF a generic graph-based data model with which to structure and link data

Linked Data needs:

1. Provision of a URI that describes a Data Resource
2. Use of HTTP to retrieve useful data from the URI
3. A Data Format described with standardised semantics (so relationships are enabled) e.g. RDF
4. Data should provide links to other Data (through URIs)

Linked Data approach can also be applied to other resource types e.g., for algorithms or models as done in OpenTox… Linked Resource approach enables Knowledge Creation, Combination and Analysis

DBpedia = Linked Data approach applied to Wikipedia

OpenTox

The OpenTox Framework (reported 2010)

Collaborative development of predictive toxicology applications
Journal of Cheminformatics 2010, 2:7 doi:10.1186/1758-2946-2-7

Barry Hardy, Nicki Douglas, Christoph Helma, Micha Rautenberg, Nina Jeliazkova, Vedrin Jeliazkov, Ivelina Nikolova, Romualdo Benigni, OlgaTcheremenskaia, Stefan Kramer, Tobias Girschick, Fabian Buchwald, Joerg Wicker, Andreas Karwath, Martin Gutlein, Andreas Maunz, Haralambos Sarimveis, Georgia Melagraki, Antreas Afantitis, Pantelis Sopasakis, David Gallagher, Vladimir Poroikov, Dmitry Filimonov, Alexey Zakharov, Alexey Lagunin, Tatyana Gloriozova, Sergey Novikov, Natalia Skvortsova, Dmitry Druzhilovsky, Sunil Chawla, Indira Ghosh, Surajit Ray, Hitesh Patel and Sylvia Escher

Open Access publication available at
www.jcheminf.com/content/2/1/7

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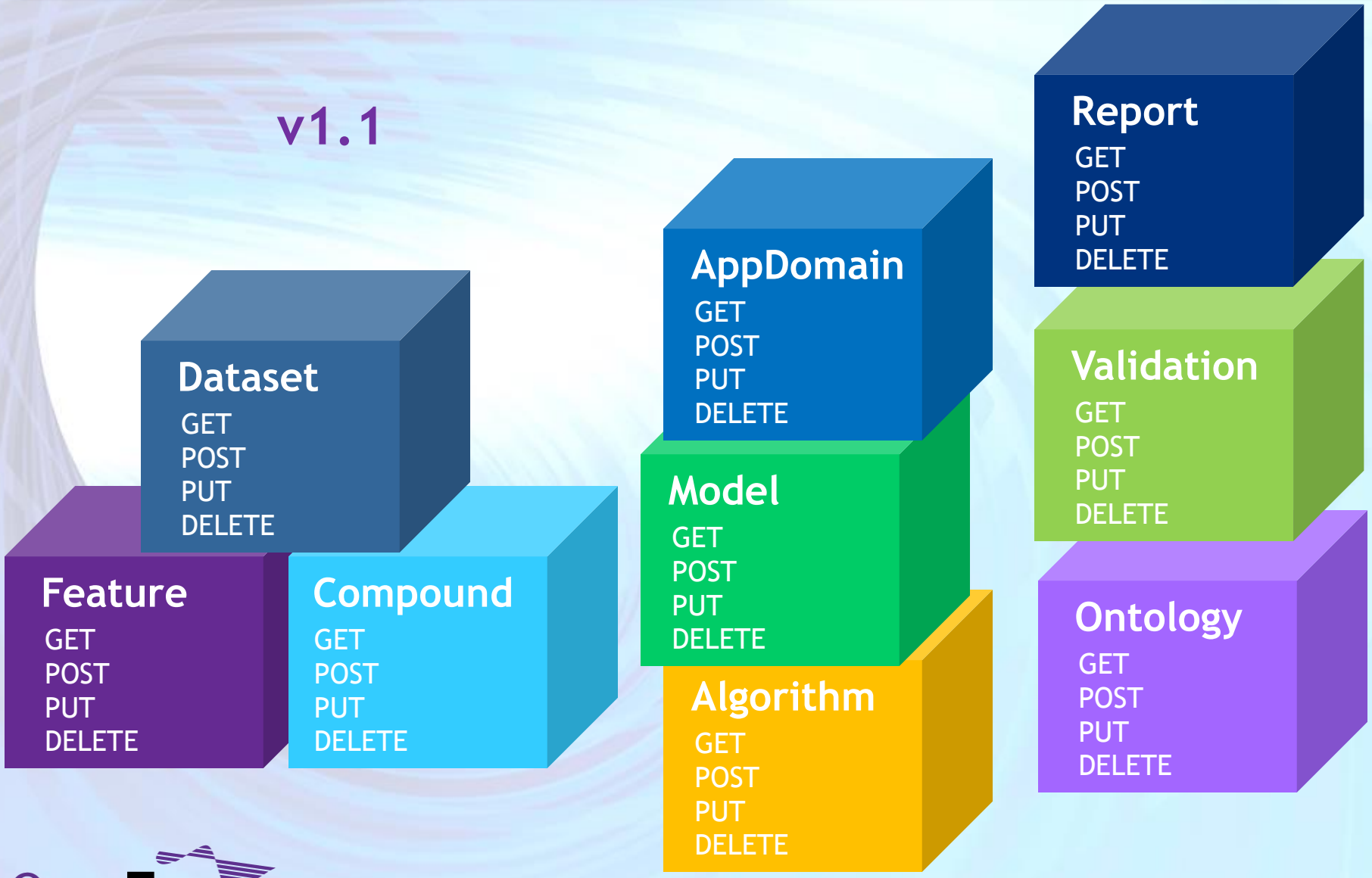
Overview of Application Programming Interfaces



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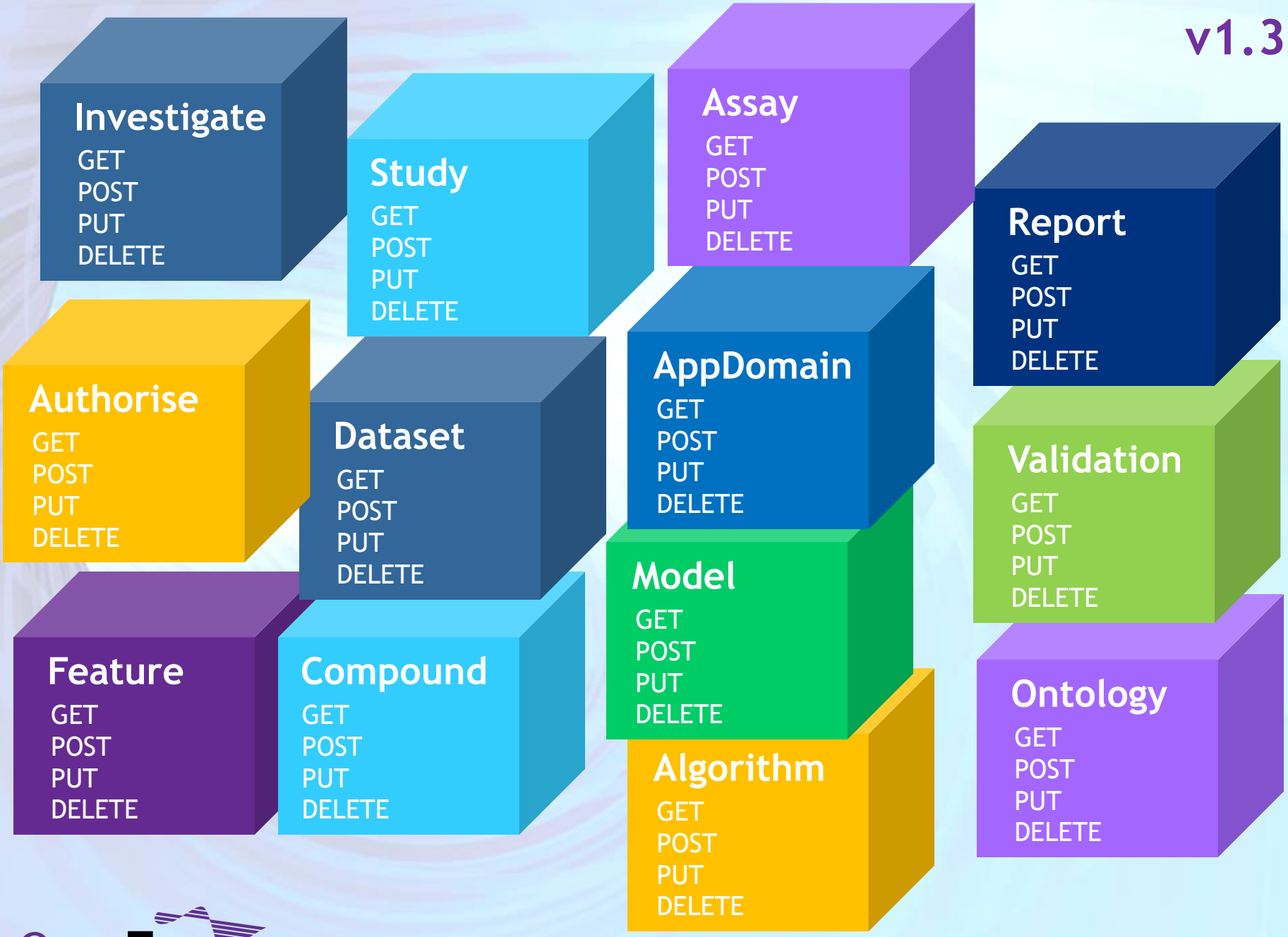
v1.3?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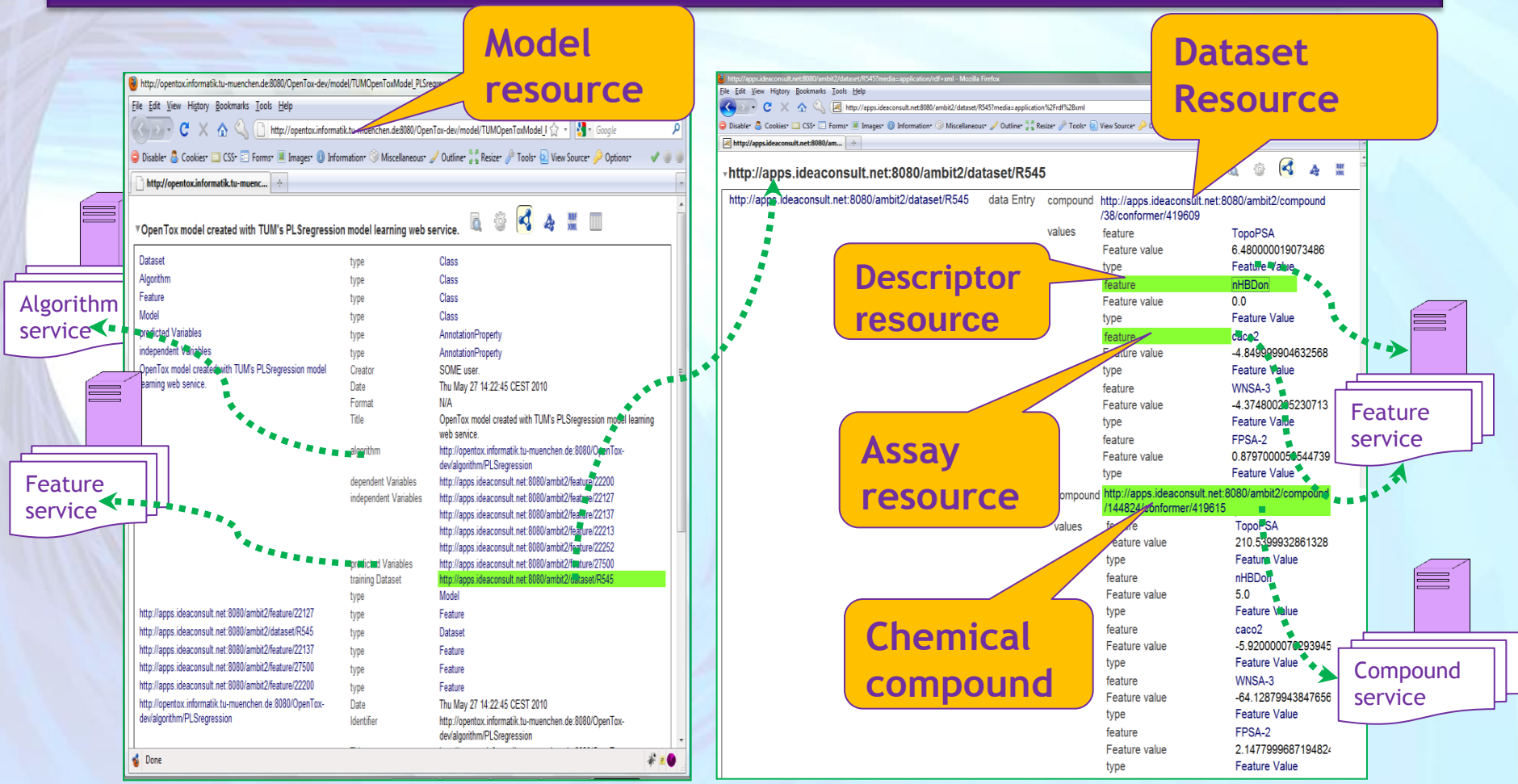
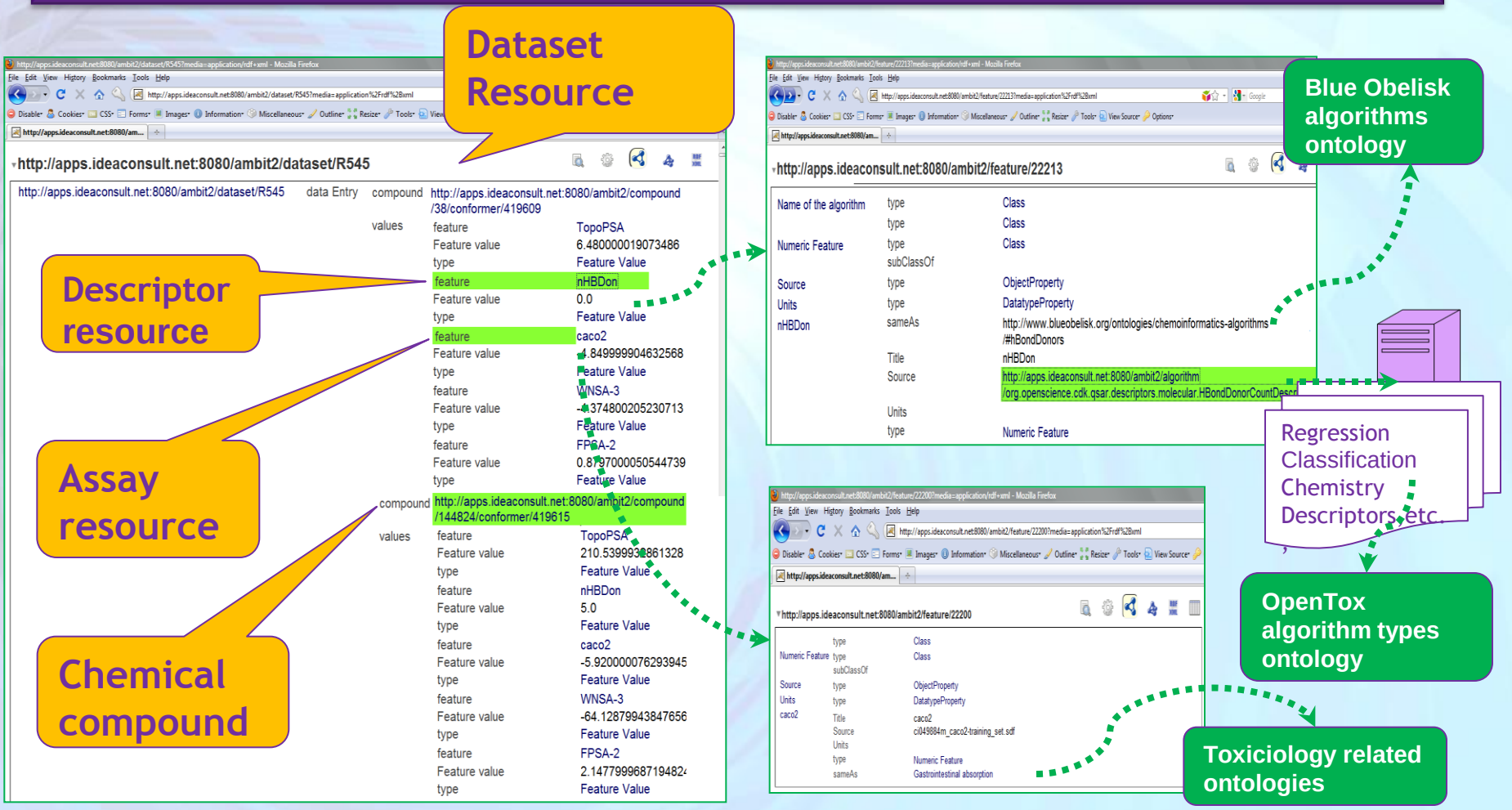
OpenTox

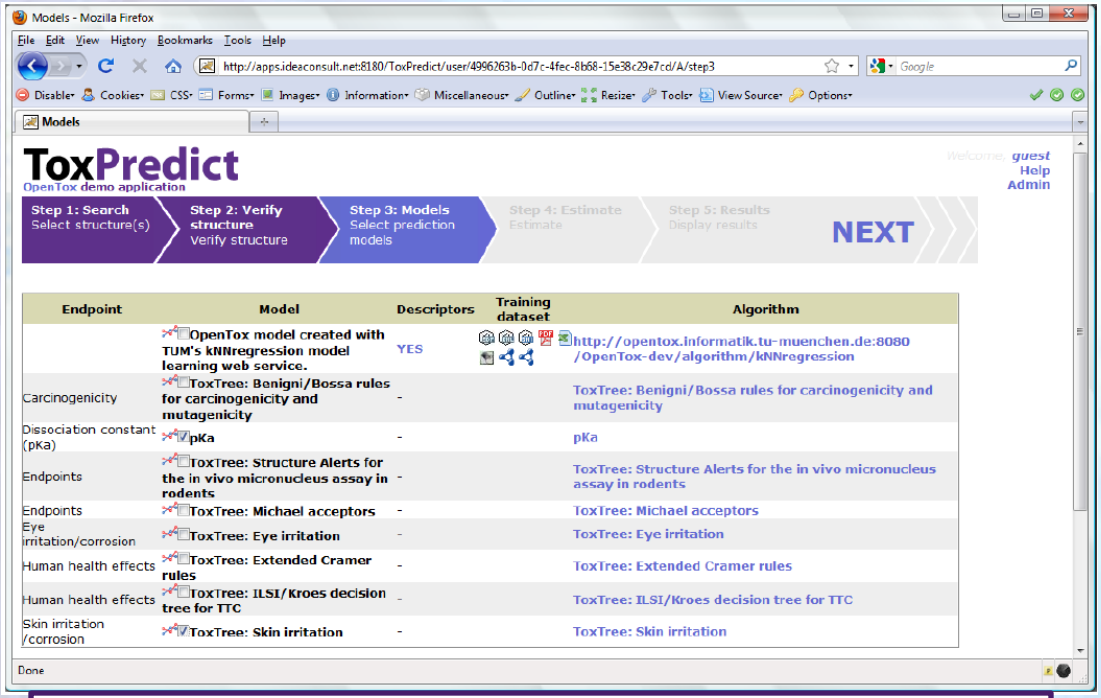
Linked resources: Compound, Algorithm, Model, Dataset, Features



Linked resources:
Compound, Algorithm, Model, Dataset, Features



Prototyping demonstrated …



Simple building of predictive toxicology applications based on well-established methods and databases

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First AXLR8 Meeting ...

Simple building a

applications

methods and

Distributed applications, integrating wide range of data, models, prediction methods

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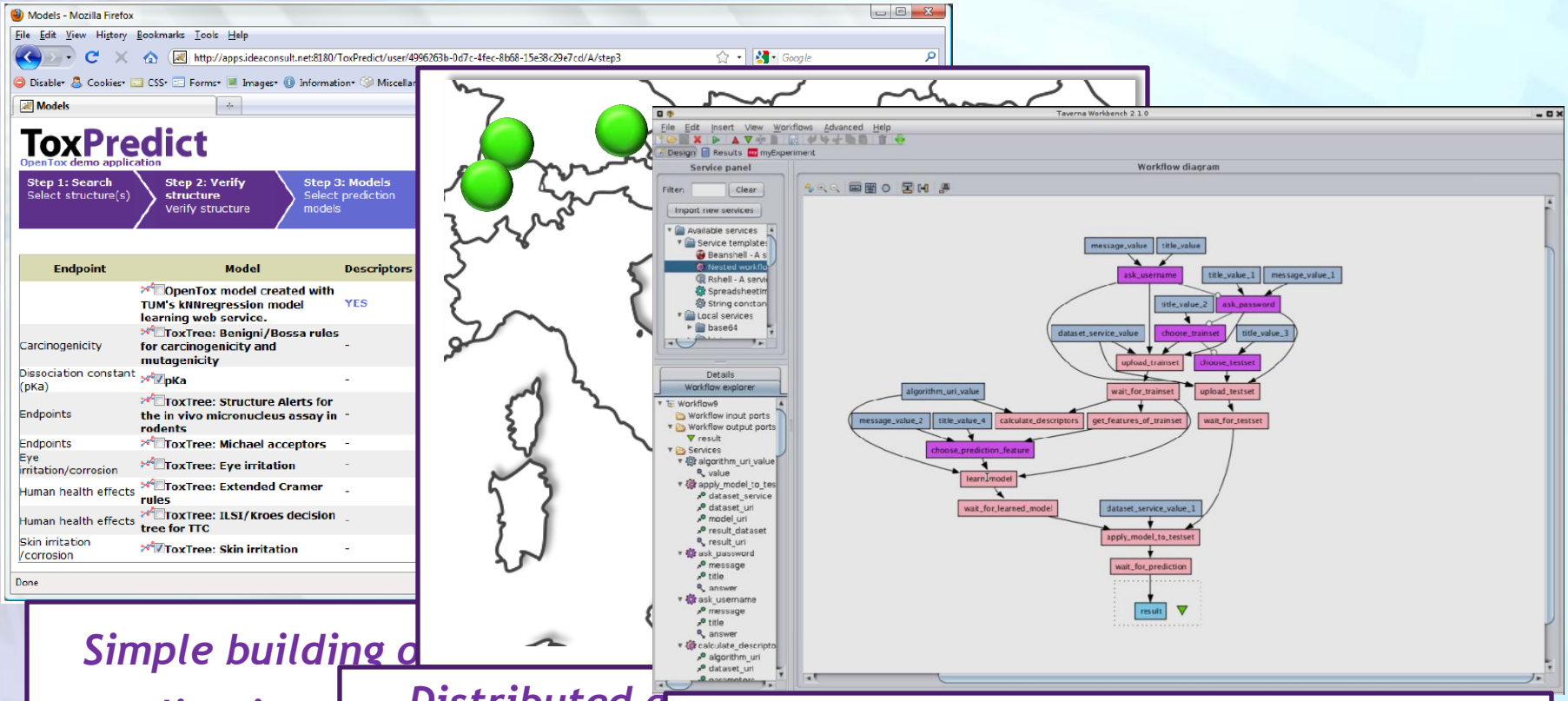
Spring 2010 …



Simple building a… applications … methods and …

Distributed a… wide range o… methods

Integration into workflow systems for computational biology

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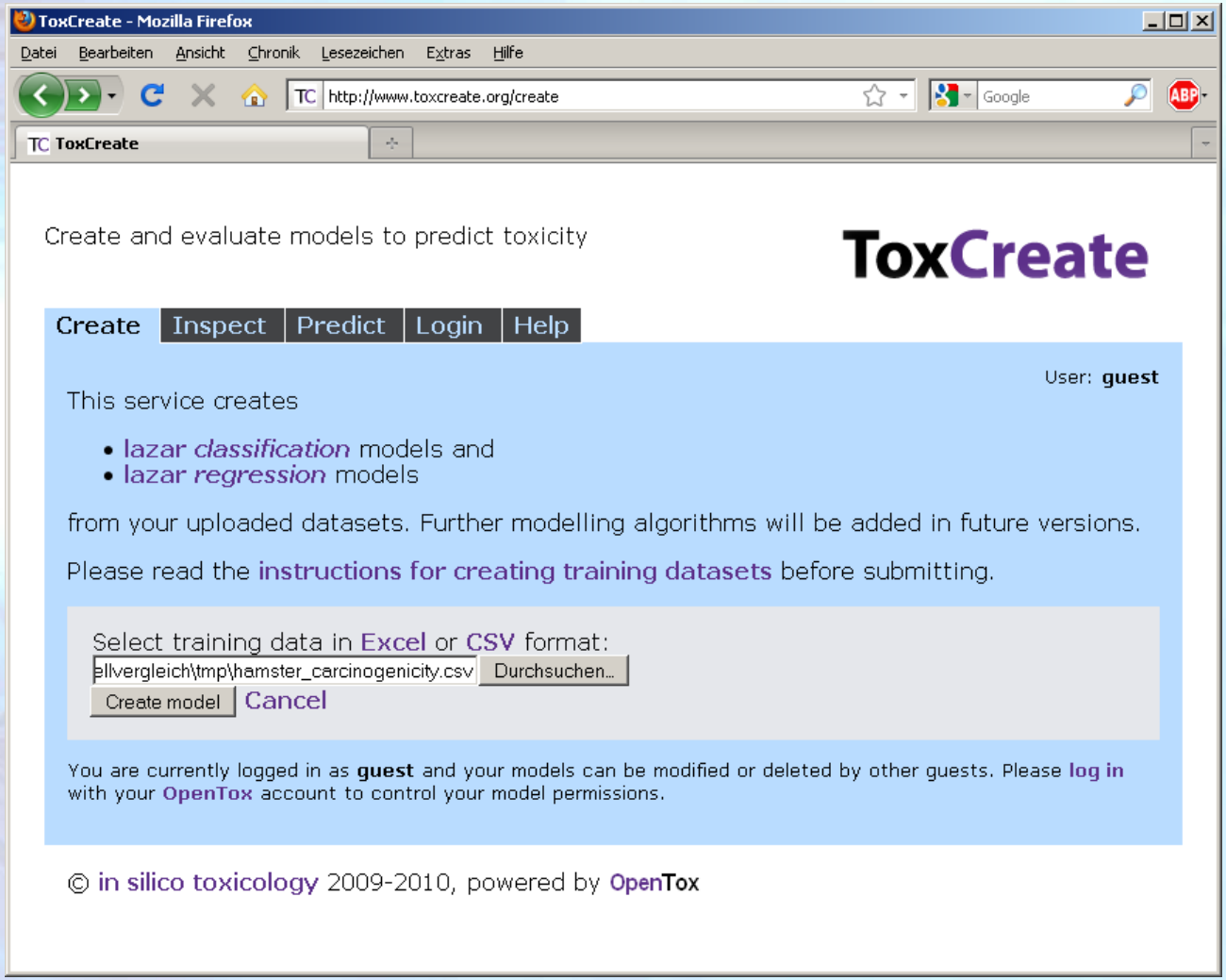
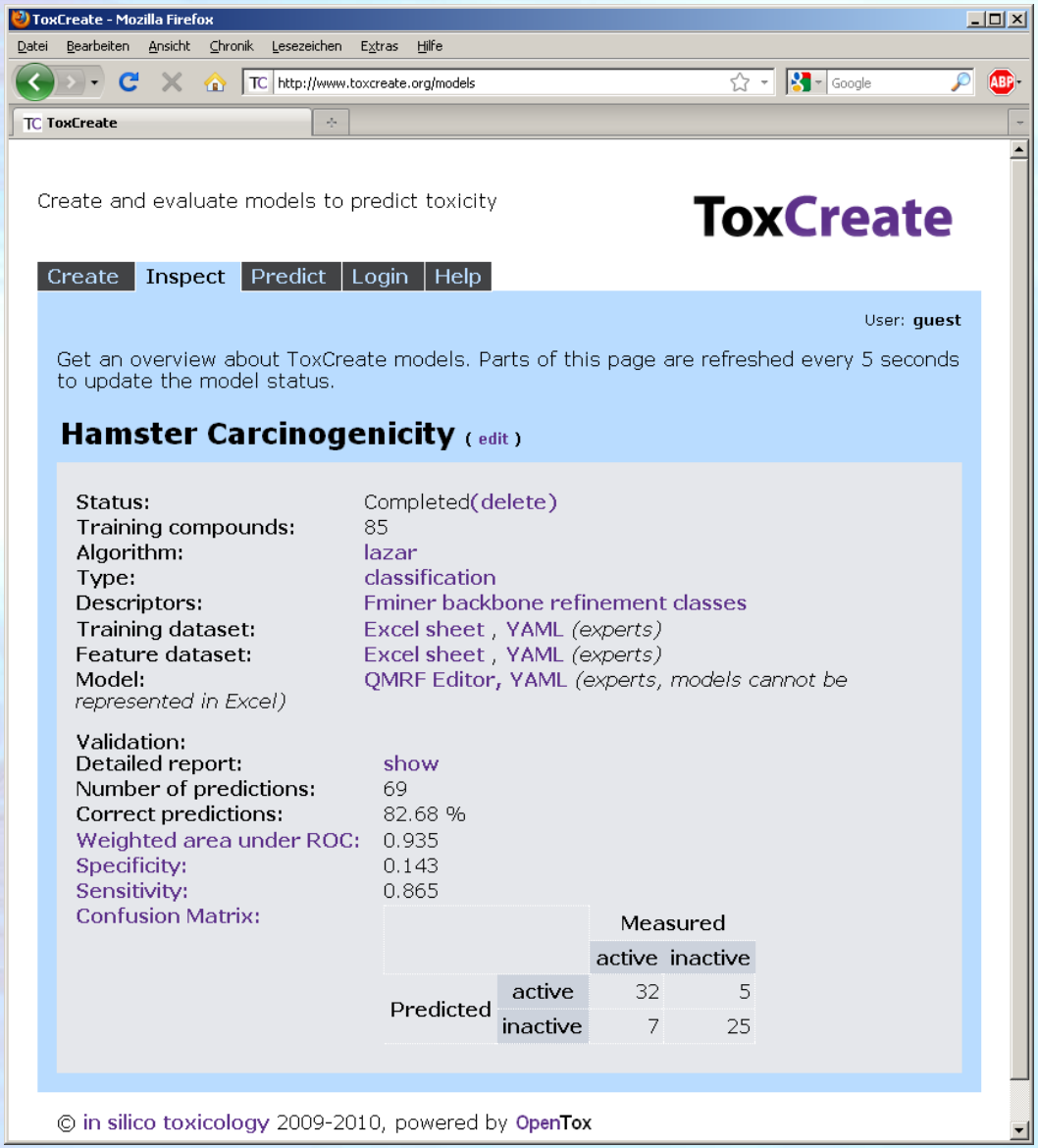
ToxCreate - (Q)SAR Model Building application



Developed by In Silico Toxicology

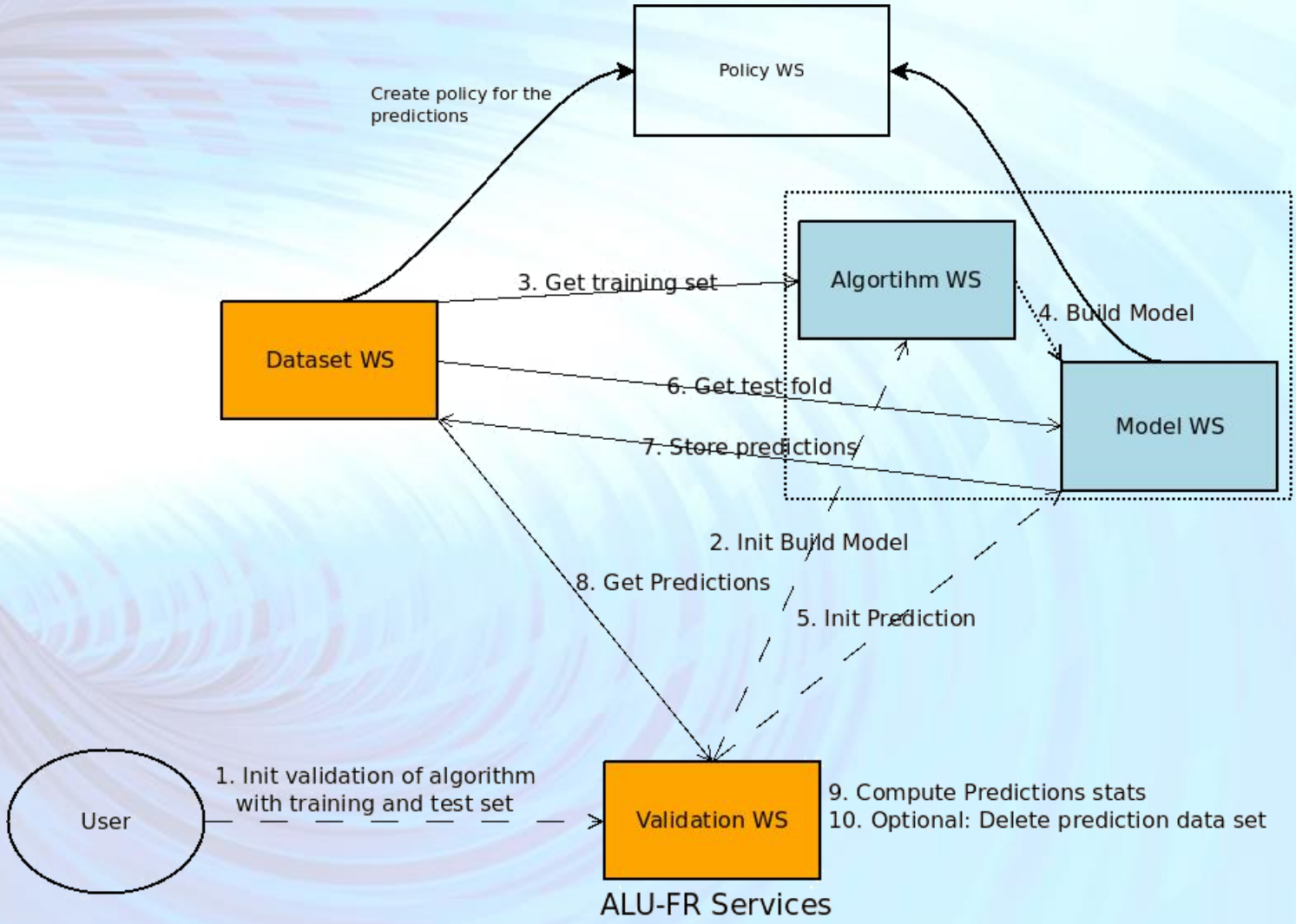
ToxCreate – (Q)SAR Model Results



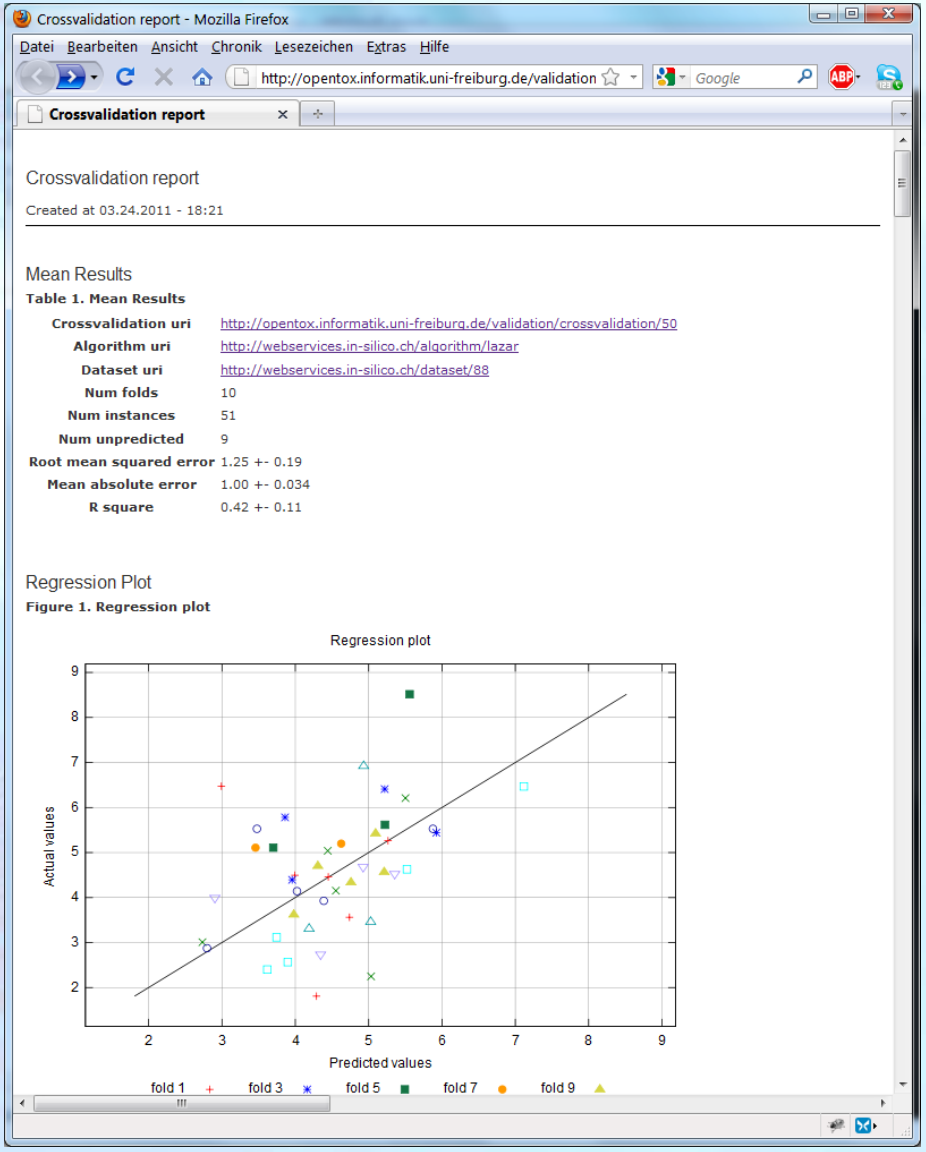
	OECD Principle	OpenTox addresses Validation Principles by...
1	Defined Endpoint	providing a unified source of well defined and documented toxicity data with a common vocabulary
2	Unambiguous Algorithm	providing transparent access to well documented models and algorithms as well as to the source code
3	Defined Applicability Domain	integrating tools for the determination of applicability domains during the validation of prediction models
4	Goodness-of-fit, robustness and predictivity	providing scientifically sound validation routines for the determination of errors and confidences
5	Mechanistic interpretation (if possible)	integrating tools for the inference, correlation or prediction of toxicological mechanisms and the recording of opinions and analysis in reports

OpenTox

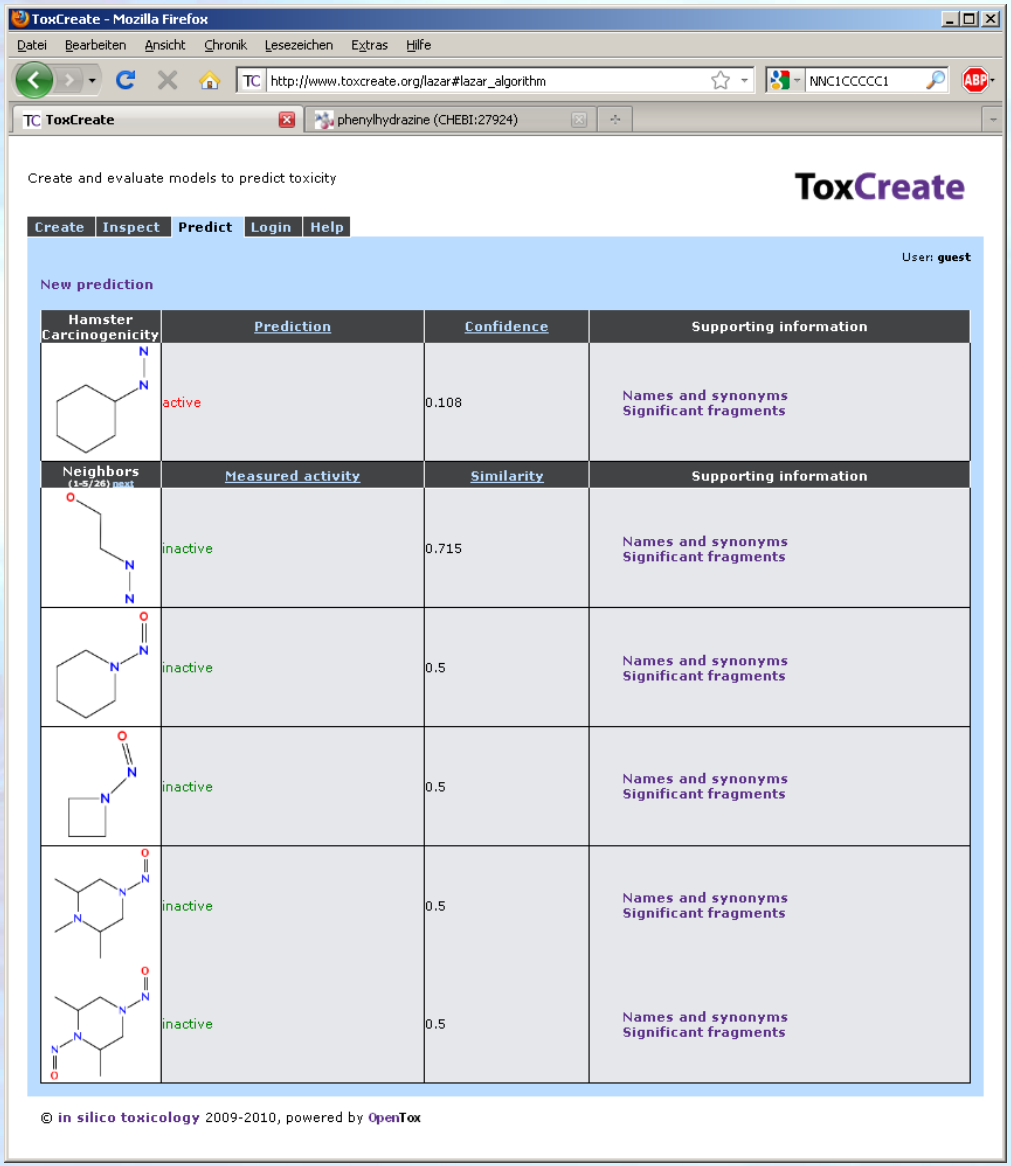
Validation within OpenTox



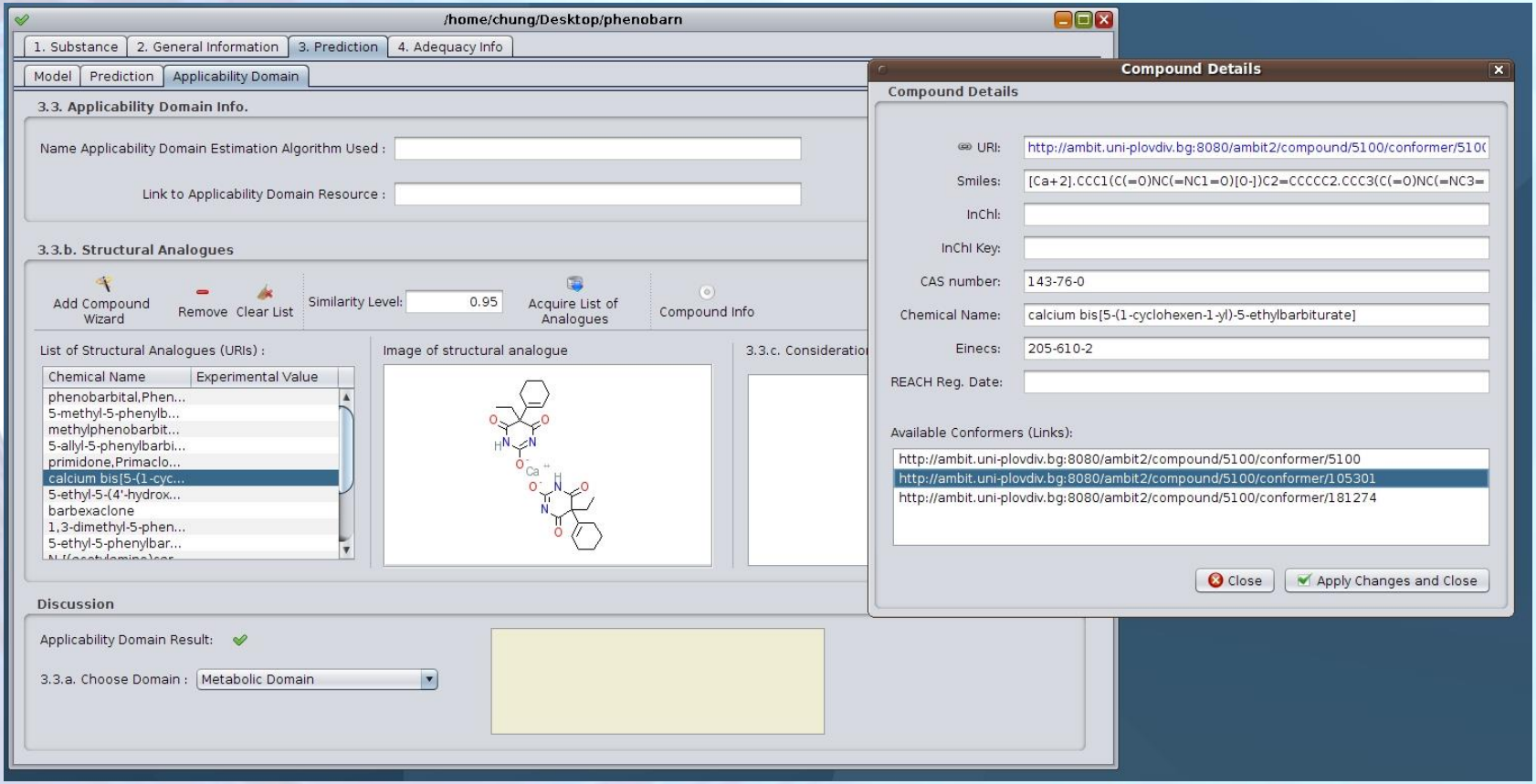
ToxCreate – linked to Validation Service



ToxCreate - Confidence, Supporting Information



QPRF Reporting (Qedit)



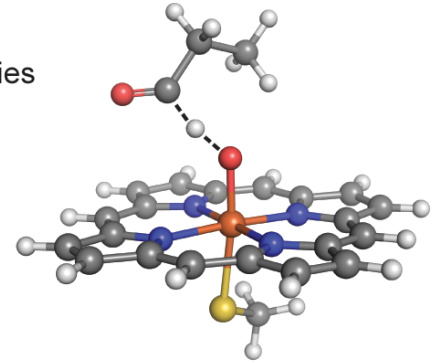
Application by Pantelis Sopasakis (NTUA)

SMARTCyp Service for Predicting Metabolites

Atom Reactivity Library

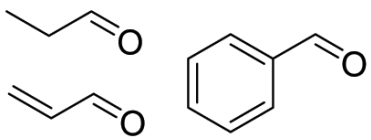
A. Calculate Quantum Chemical Reference Energies

Calculate transition state energies using density functional theory



B. Define SMARTS Rules

Group calculations by fragments and calculate average energies

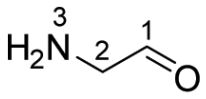


[CX3H1](=O)[#6]

40.2 kJ/mol

SMARTCyp

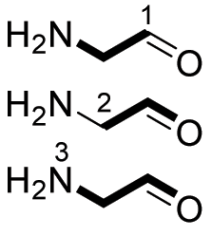
1. Assign Energies By SMARTS matching



Atom	SMARTS	Energy
1	[CX3H1](=O)[#6]	40.2
2	[CX4][N]	39.8
3	[N^3][H1,H2]	54.1

2. Compute Accessibility Descriptor

$A_i = Maxbonds_i / Maxbonds_{all}$



$A_1 = 2 / 3 = 0.67$

$A_2 = 2 / 3 = 0.67$

$A_3 = 3 / 3 = 1.00$

3. Compute Score and Rank Atoms

Score, S = E - 8A
Lowest score gets rank 1

$S_1 = 40.2 - 8*0.67 = 34.84$

$S_2 = 39.8 - 8*0.67 = 34.44$

$S_3 = 54.1 - 8*1.00 = 46.10$

Atom 1 - Rank 2

Atom 2 - Rank 1

Atom 3 - Rank 3

SMARTCyp - developed by Patrik Rydberg, University of Copenhagen

www.farma.ku.dk/index.php/SMARTCyp/7990/0/

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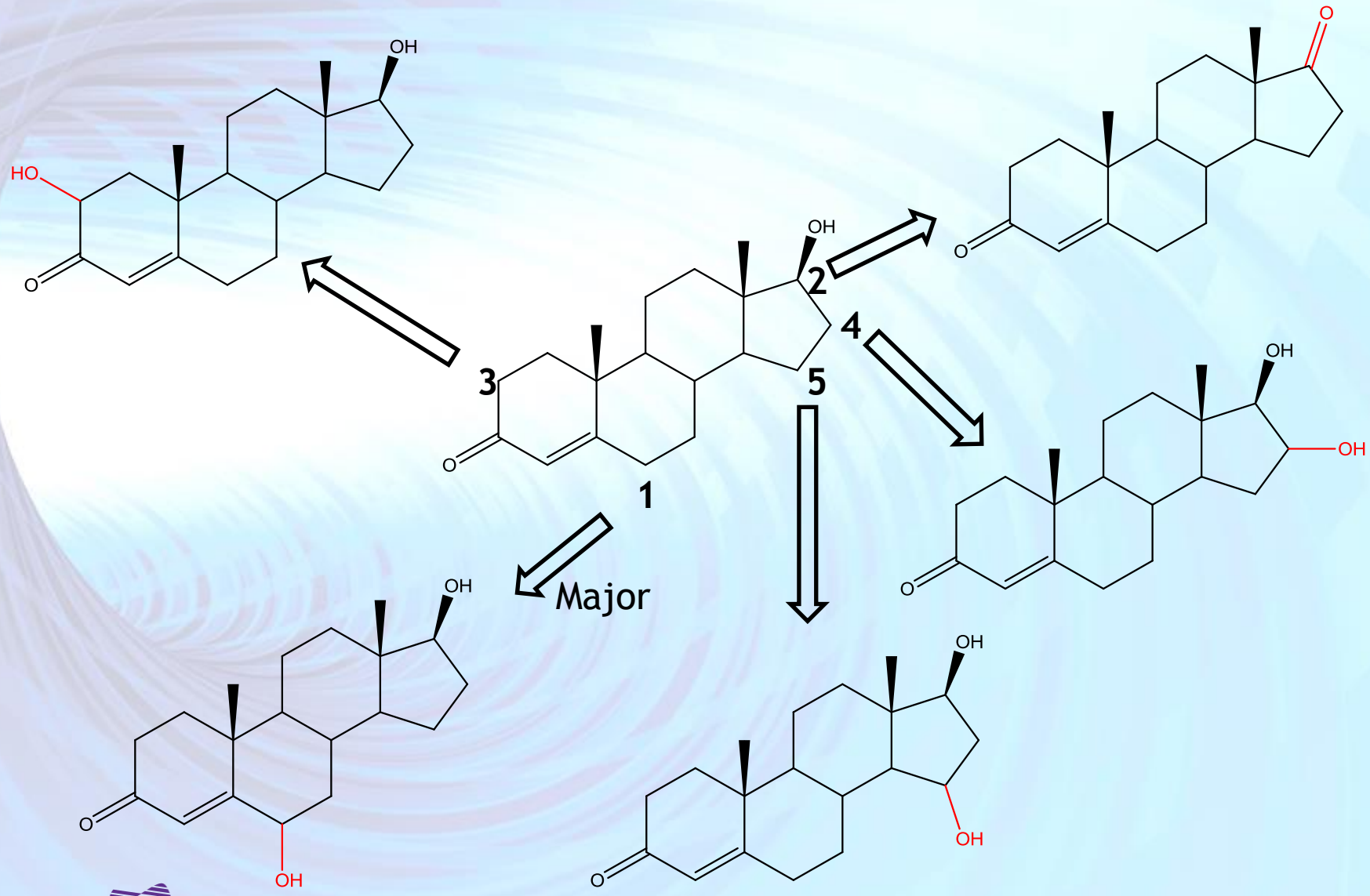
SmartCYP Prediction of Testosterone Metabolites



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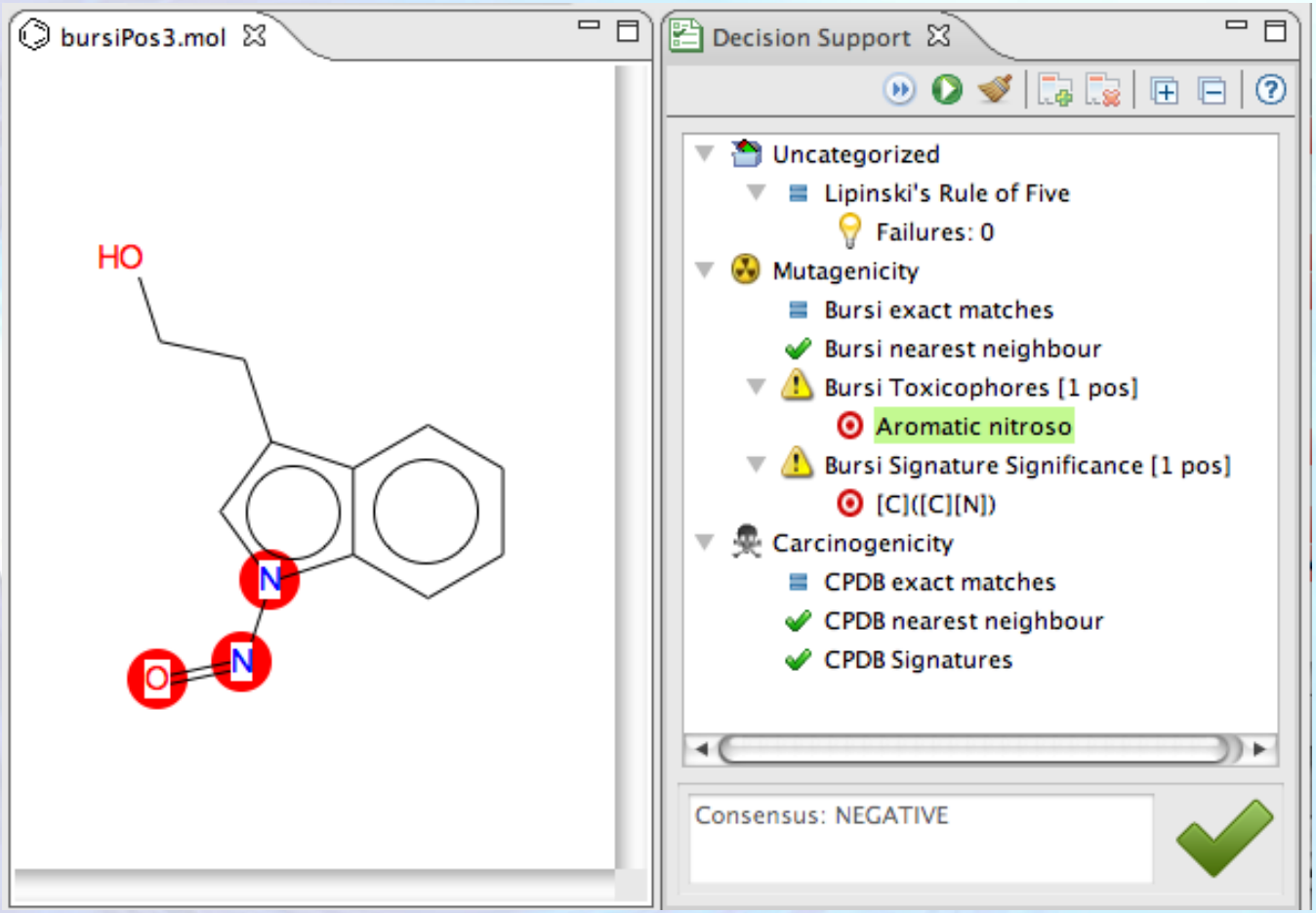
Bioclipse Visualisation Workbench - OpenTox



Collaboration with Ola Spjuth and Egon Willighagen

OpenTox

Bioclipse-OpenTox Integration – See Application example in Chapter in Open Source Software in Life Science Research: Practical Solutions to Common Challenges in the Pharmaceutical Industry and Beyond (Woodhead Publishing Series in Biomedicine) edited by Lee Harland and Mark Forster (30 Oct 2012)

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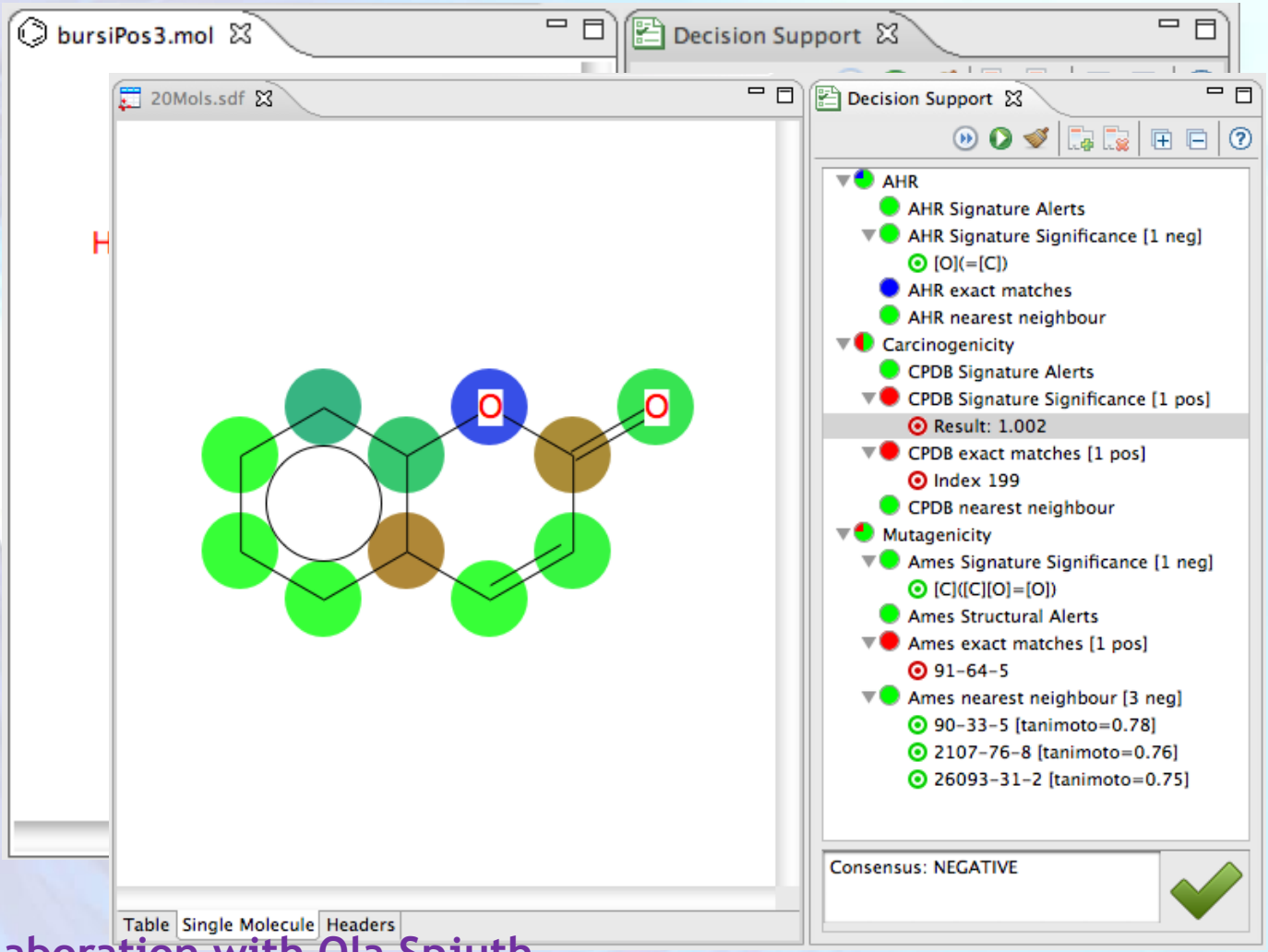

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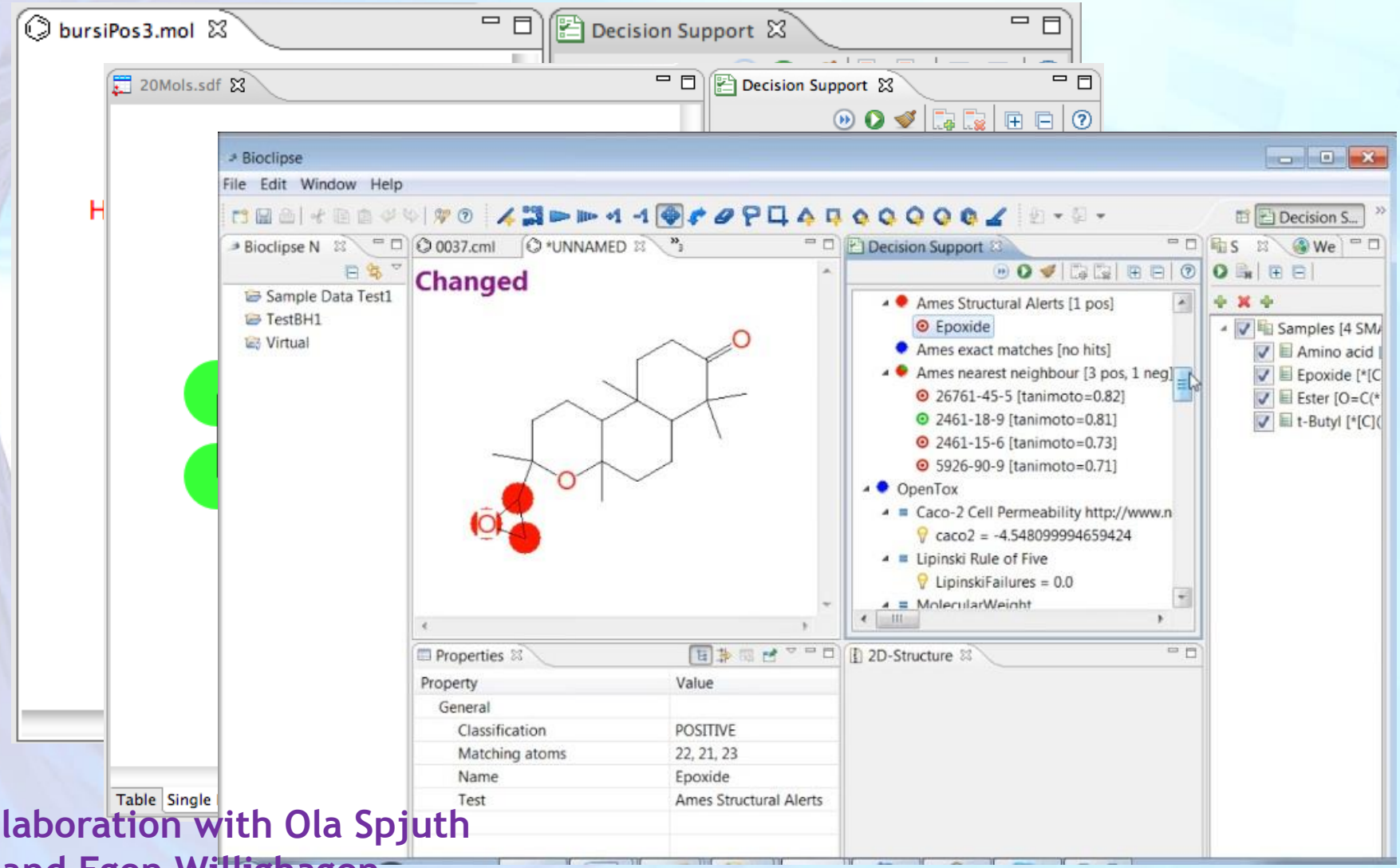

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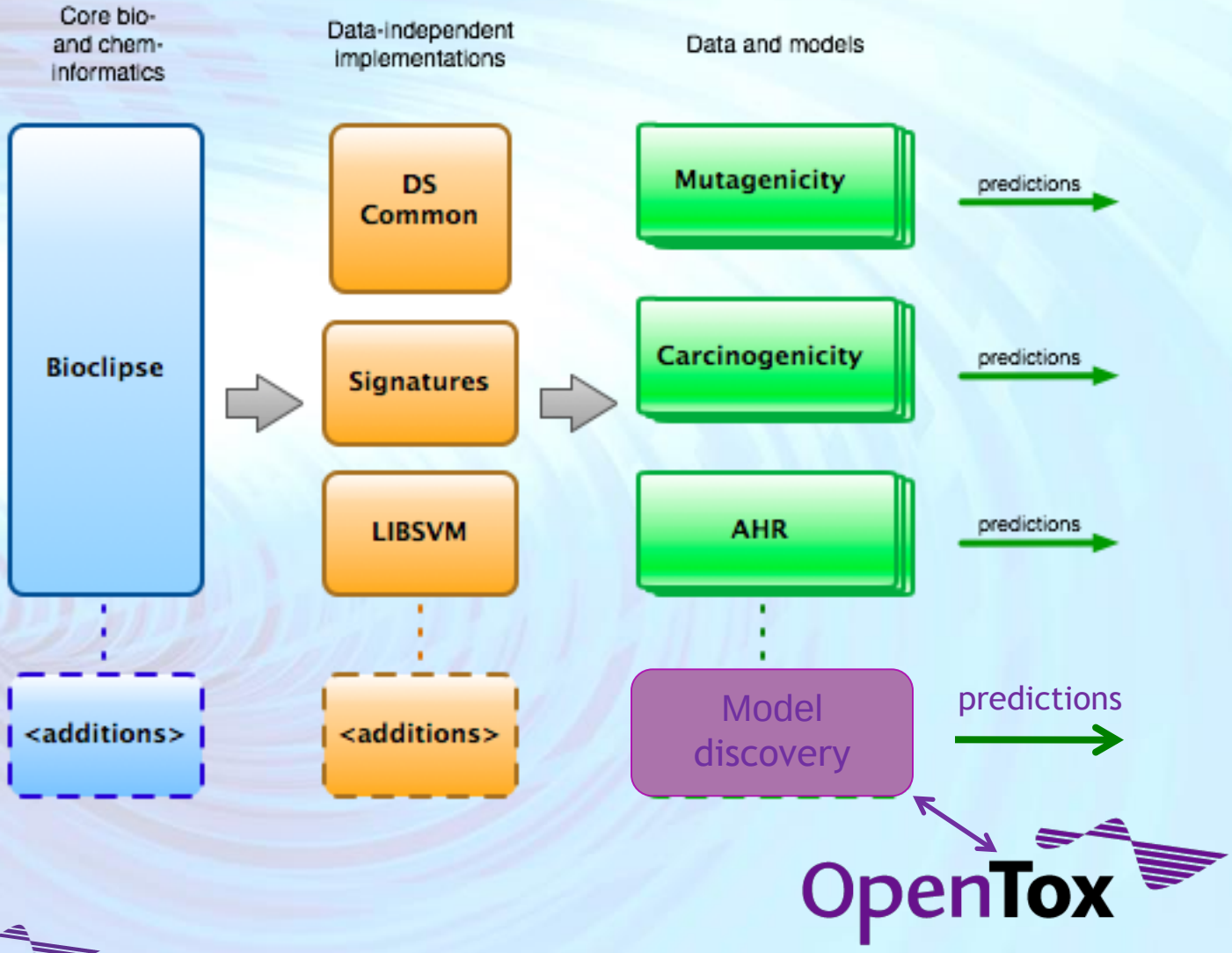
Bioclipse - OpenTox Interoperation



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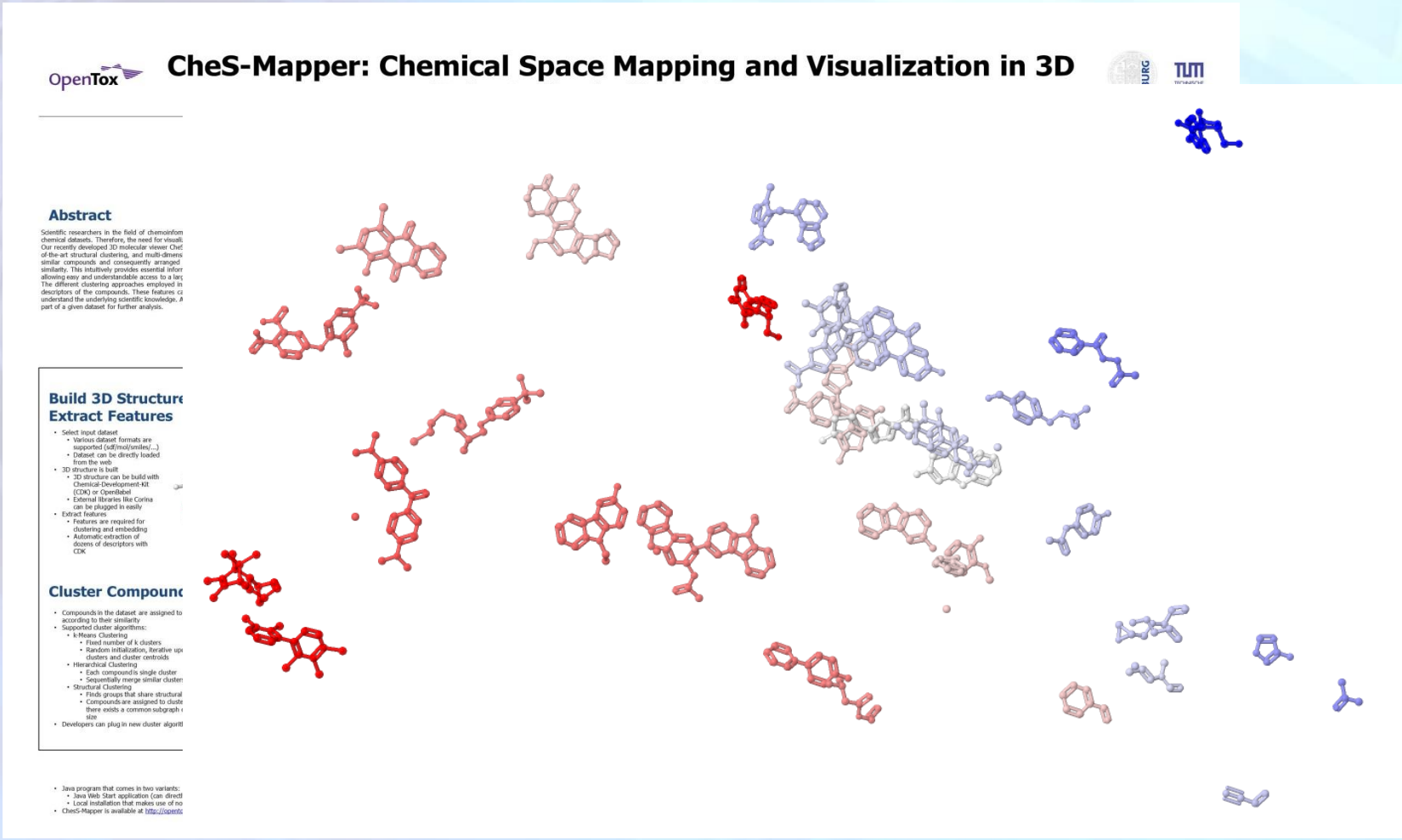
Visualisation of chemical feature-based categories



Definition of Ontology

In computer science and information science, an ontology formally represents knowledge as a set of concepts within a domain, and the relationships between those concepts. It can be used to model a domain and support reasoning about concepts.

In theory, an ontology is a "formal, explicit specification of a shared conceptualisation". An ontology provides a shared vocabulary, which can be used to model a domain, that is, the type of objects and/or concepts that exist, and their properties and relations.

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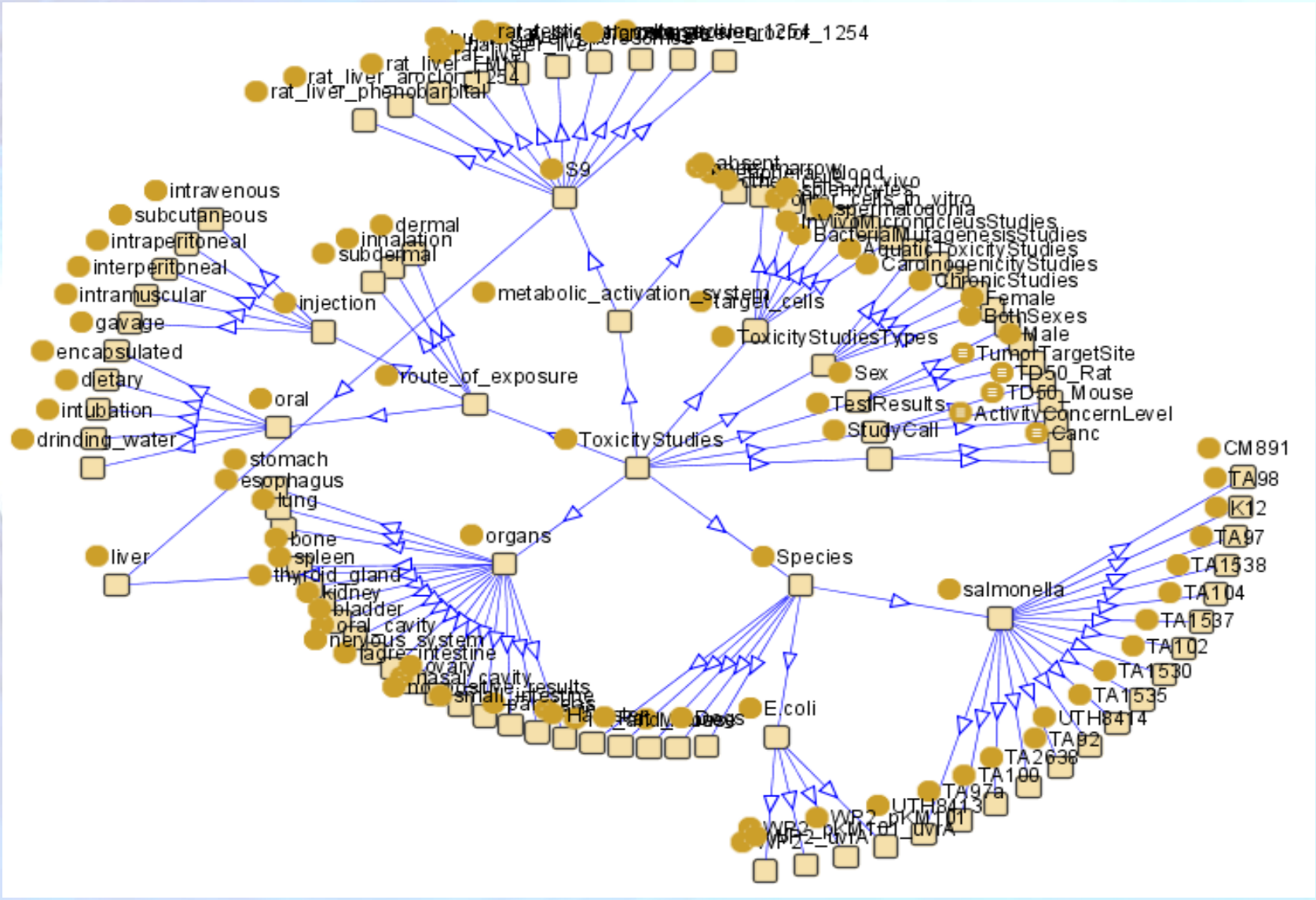
en.wikipedia.org/wiki/Ontology_information_science

Toxicological Ontology: graphical representation



Toxicology Ontology Developments and Roadmap

- See perspectives and roadmap published in A Toxicology Ontology Roadmap ALTEX 29(2), 129- 137 and Toxicology Ontology Perspectives 139 - 156 (2012)
- Available online in Open Access mode from www.altex.ch
- Barry Hardy (Douglas Connect and OpenTox), Gordana Apic (Cambridge Cell Networks), Philip Carthew (Unilever), Dominic Clark (EMBL-EBI), David Cook (AstraZeneca), Ian Dix (AstraZeneca & Pistoia Alliance), Sylvia Escher (Fraunhofer Institute for Toxicology & Experimental Medicine), Janna Hastings (EMBL-EBI), David J. Heard (Novartis), Nina Jeliazkova (Ideaconsult), Philip Judson (Lhasa Ltd.), Sherri Matis-Mitchell (AstraZeneca), Dragana Mitic (Cambridge Cell Networks), Glenn Myatt (Leadscope), Imran Shah (US EPA), Ola Spjuth (University of Uppsala), Olga Tcheremenskaia (Istituto Superiore di Sanità), Luca Toldo (Merck KGaA), David Watson (Lhasa Ltd.), Andrew White (Unilever), Chihae Yang (Altamira)

Based on Proceedings from the Toxicology Ontology Roadmap Workshop
EMBL-EBI Industry Programme Workshop
16 -17th November 2010, Hinxton, UK

Weight of Evidence

"An evidence based approach involves an assessment of the relative values/weights of different pieces of the available information that have been retrieved and gathered in previous steps. To this end, a value needs to be assigned to each piece of information. These weights/values can be assigned either in an *objective* way by using a formalised procedure or by using expert judgement. The weight given to the available evidence will be influenced by factors such as the quality of the data, consistency of results, nature and severity of effects, relevance of the information for the given regulatory endpoint.
One definition for weight of evidence is: 'the process of considering the strengths and weaknesses of various pieces of information in reaching and supporting a conclusion concerning a property of the substance.'
Within the REACH legislation, the so-called weight of evidence approach is a component of the decision-making procedure on substance properties and thus an important part of the chemical safety assessment.»

ECHA echa.europa.eu/documents/10162/13655/pg_report_weight_of_evidence_en.pdf

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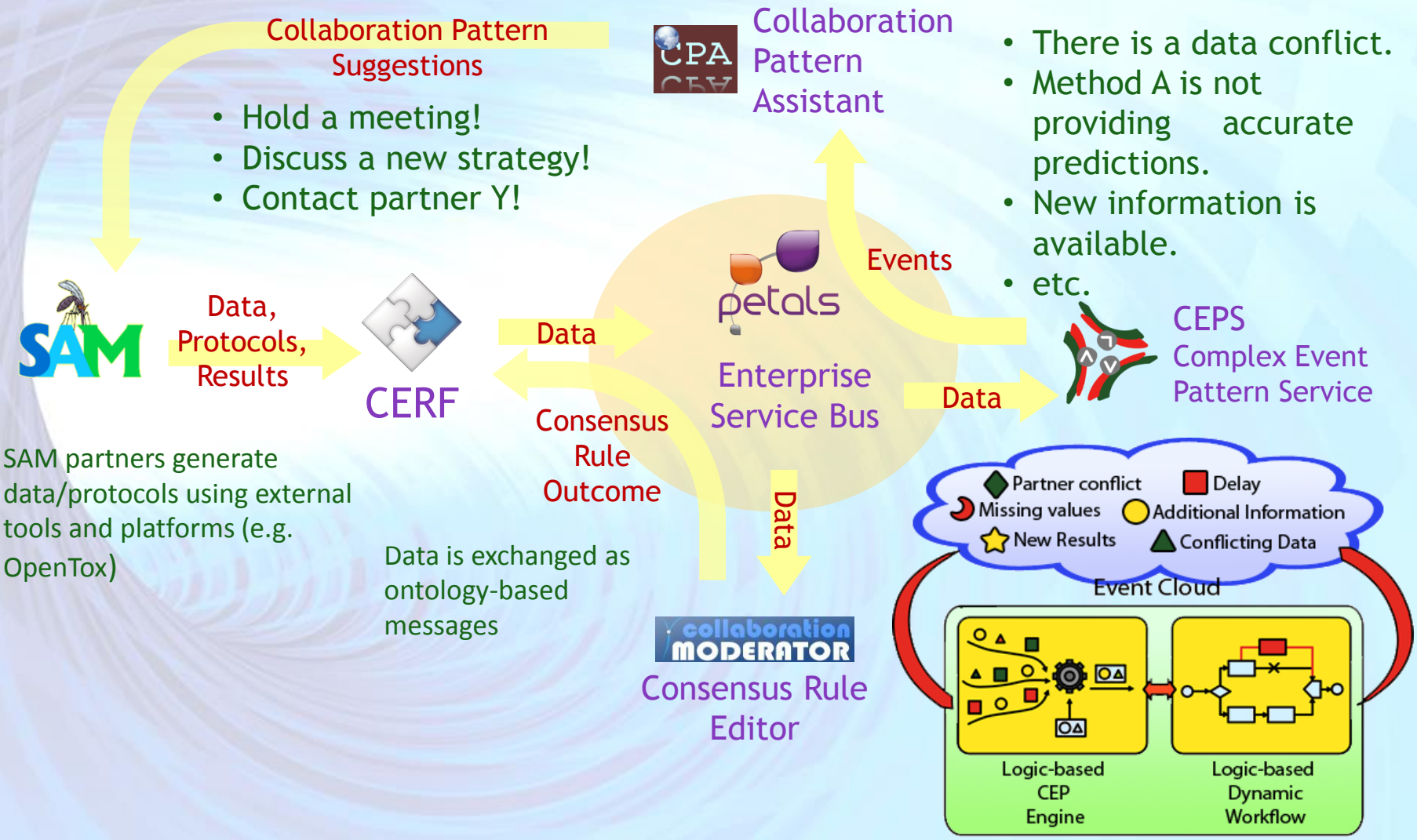
Event-driven Collaboration Architecture



SAM partners generate data/protocols using external tools and platforms (e.g. OpenTox)

Data is exchanged as ontology-based messages

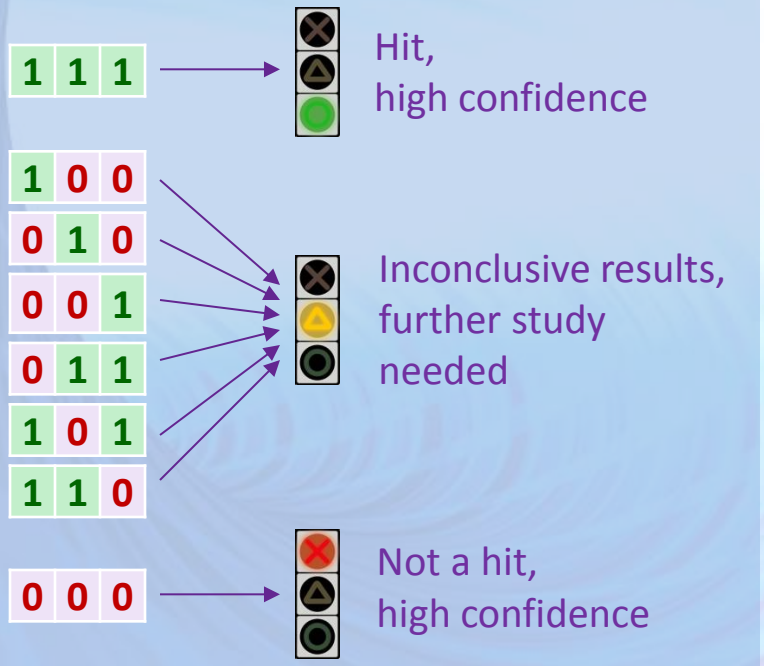
Hardy and Affentranger, Drug Discovery Today. 2013 Jul;18(13-14):681-6.

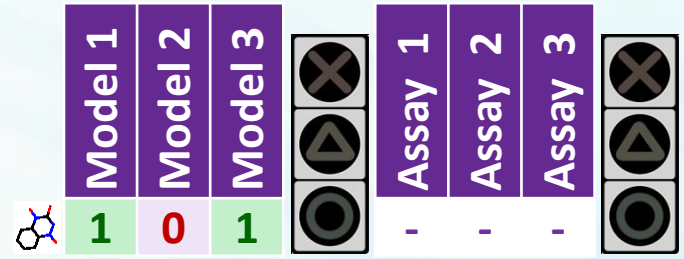
Event Driven Weight of Evidence

collaboration MODERATOR

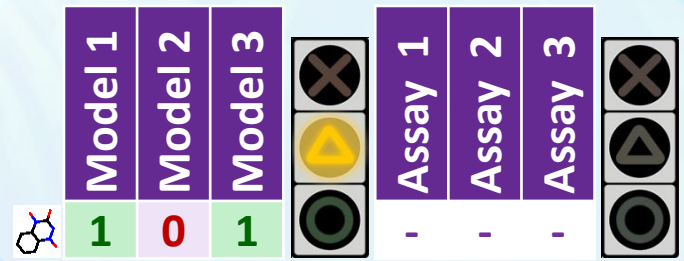
Consensus Rule Editor

Recommendation Rules:





Synergy



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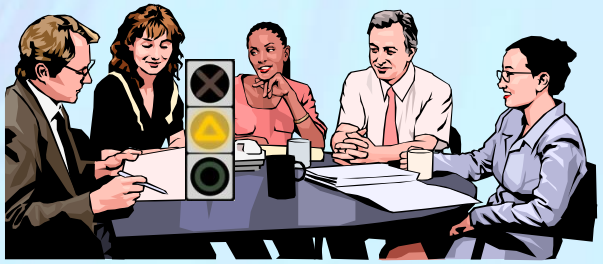

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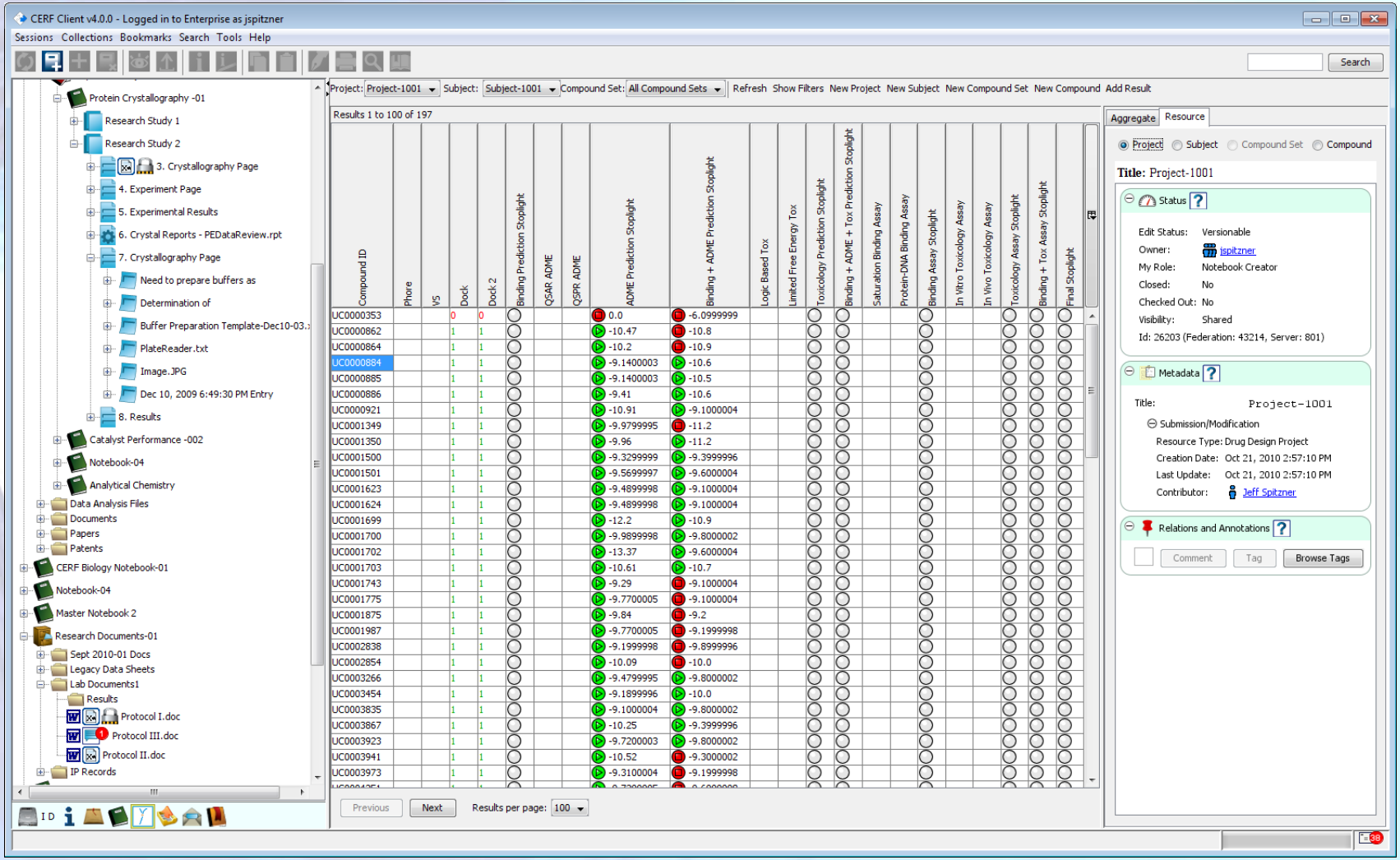
Event-driven Weight of Evidence



[Hardy and Affentranger, Drug Discovery Today. 2013 Jul;18(13-14):681-6.]

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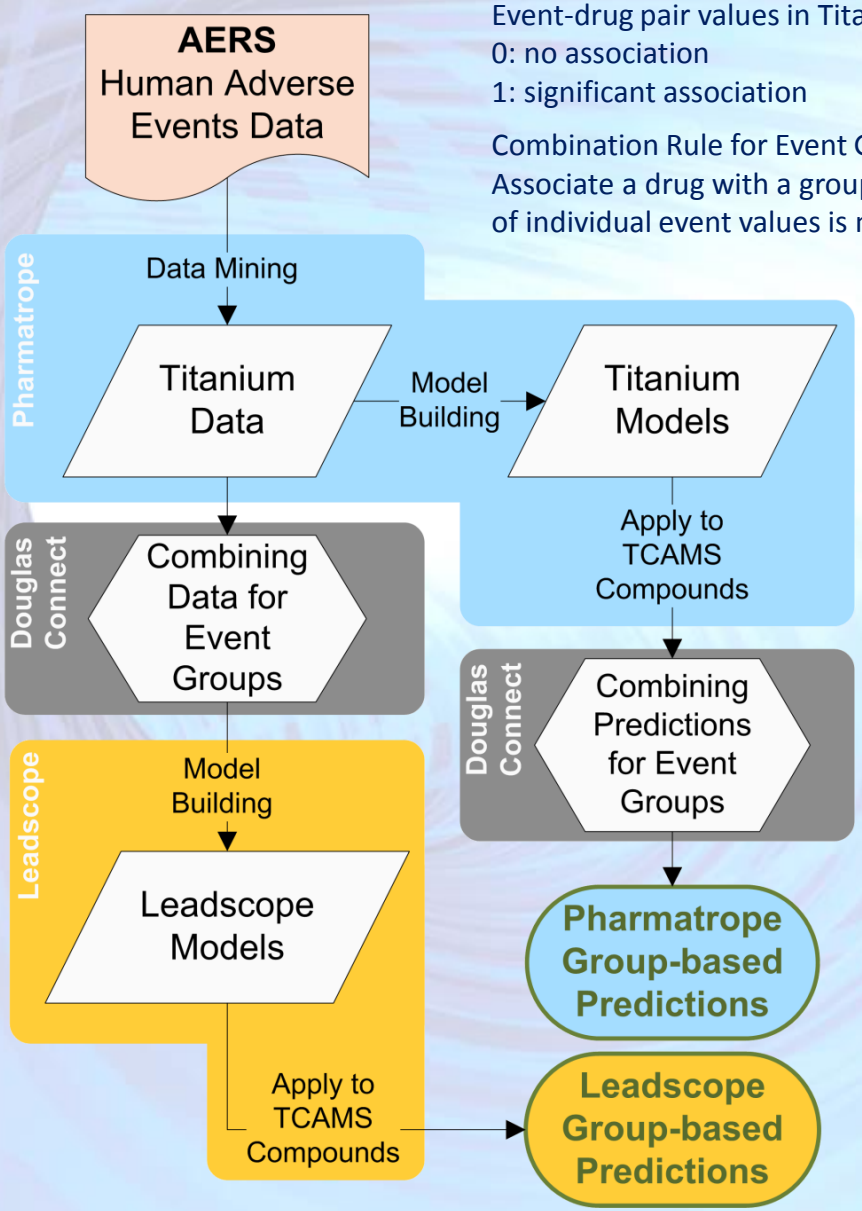
Need for Ontology

A Weight of Evidence requires

A common open public toxicology ontology supporting the review process, the capturing of the results and their synthesis into applications supporting decision-making and judgement.

OpenTox

Human Adverse Events Data



Event-drug pair values in Titanium Data:
0: no association
1: significant association

Combination Rule for Event Groups:
Associate a drug with a group if the sum of individual event values is non-zero

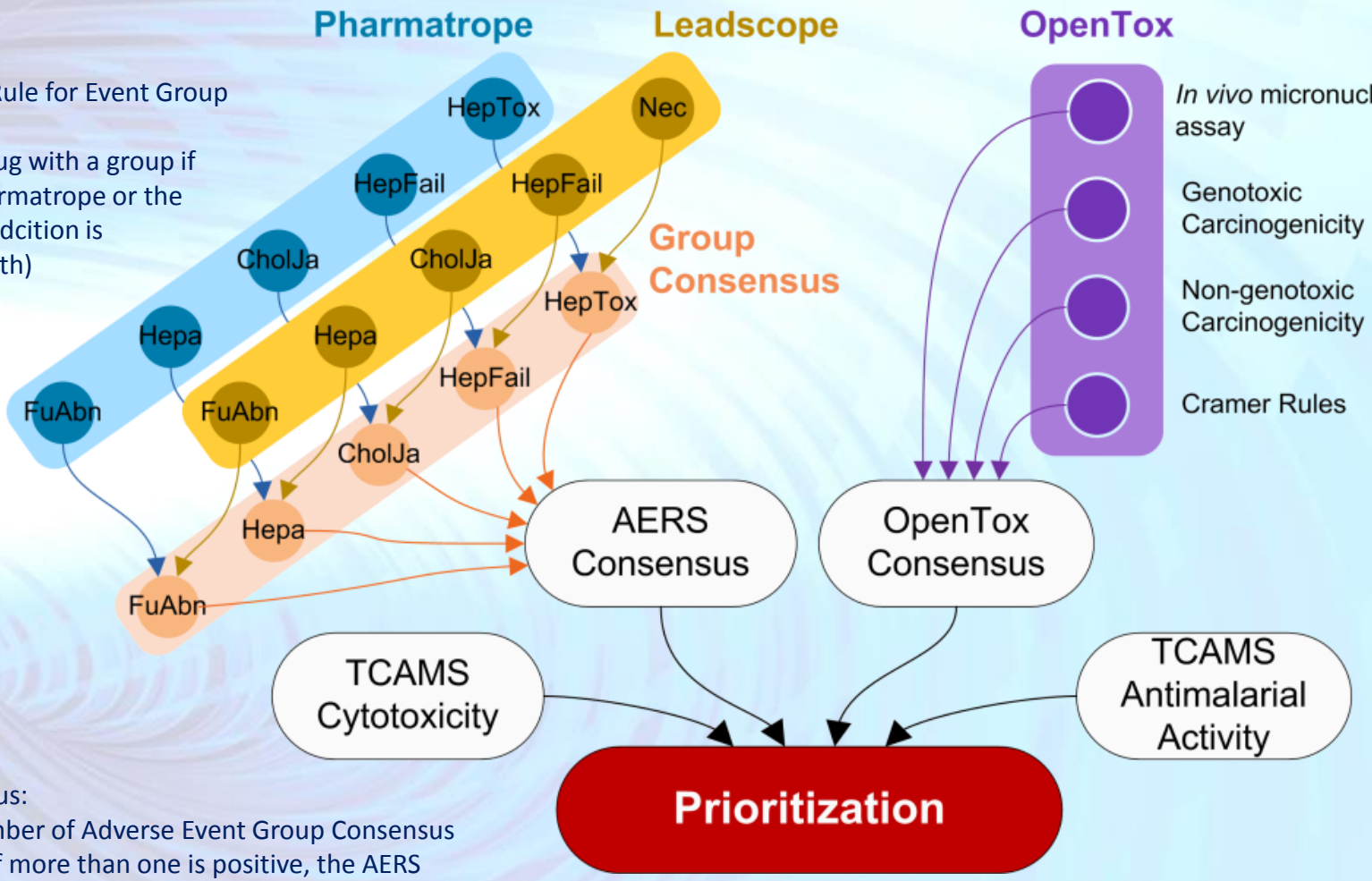
Event-drug pair values in Titanium Predictions:
0 : no association (0)
0.35-0.4 : non-significant association (0)
> 0.4 : significant association (1)

Combination Rule for Event Groups:
Associate a drug with a group if the sum of individual event values is larger of equal to 0.4.

Adverse Event Groups	Group Name
Hepatic function abnormal Liver disorder	**FuAbn**
Hepatic necrosis	**Nec**
Cytolytic hepatitis Hepatitis Hepatitis acute Hepatitis toxic	**Hepa**
Cholestasis Jaundice Hepatitis cholestatic jaundice cholestatic Yellow skin	**CholJa**
Hepatic failure Hepatitis fulminant Acute hepatic failure Hepatorenal failure	**HepFail**
Hepatotoxicity Hepatomegaly Hyperbilirubinaemia Hepatosplenomegaly	**HepTox**

Combining Predictions and Experimental Data

Combination Rule for Event Group Predictions:
Associate a drug with a group if either the Pharmatrope or the Leadscope predcition is positive (or both)



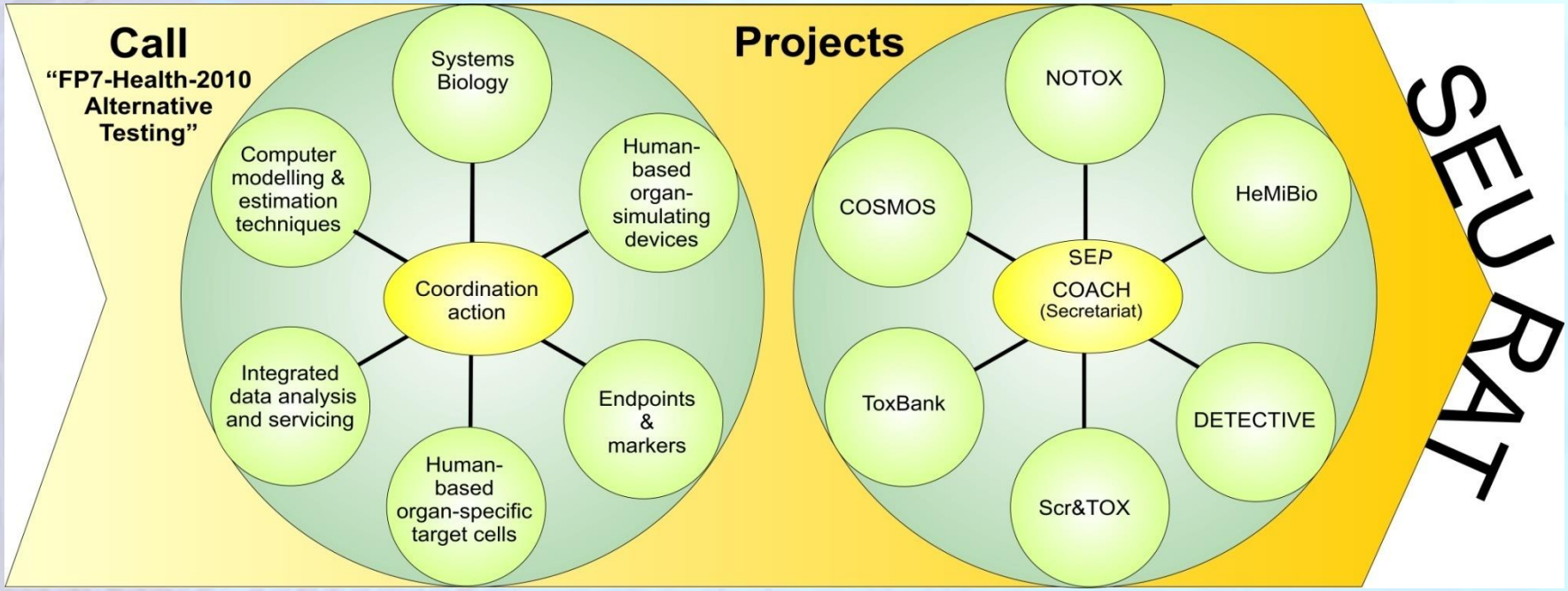
AERS Consensus:
Count the number of Adverse Event Group Consensus associations. If more than one is positive, the AERS Consensus is positive.

OpenTox Consensus:
Negative if both carcinogenicity and the micronucleus assay predictions are negative, OR if the Cramer Rule classification is Class I. Positive otherwise.

TCAMS Cytotoxicity:
Positive if > 30% growth inhibition at 10 µM.

TCAMS Antimalarial Activity:
Positive if > 80% growth inhibition of P. Falciparum DD2 at 2 µM.

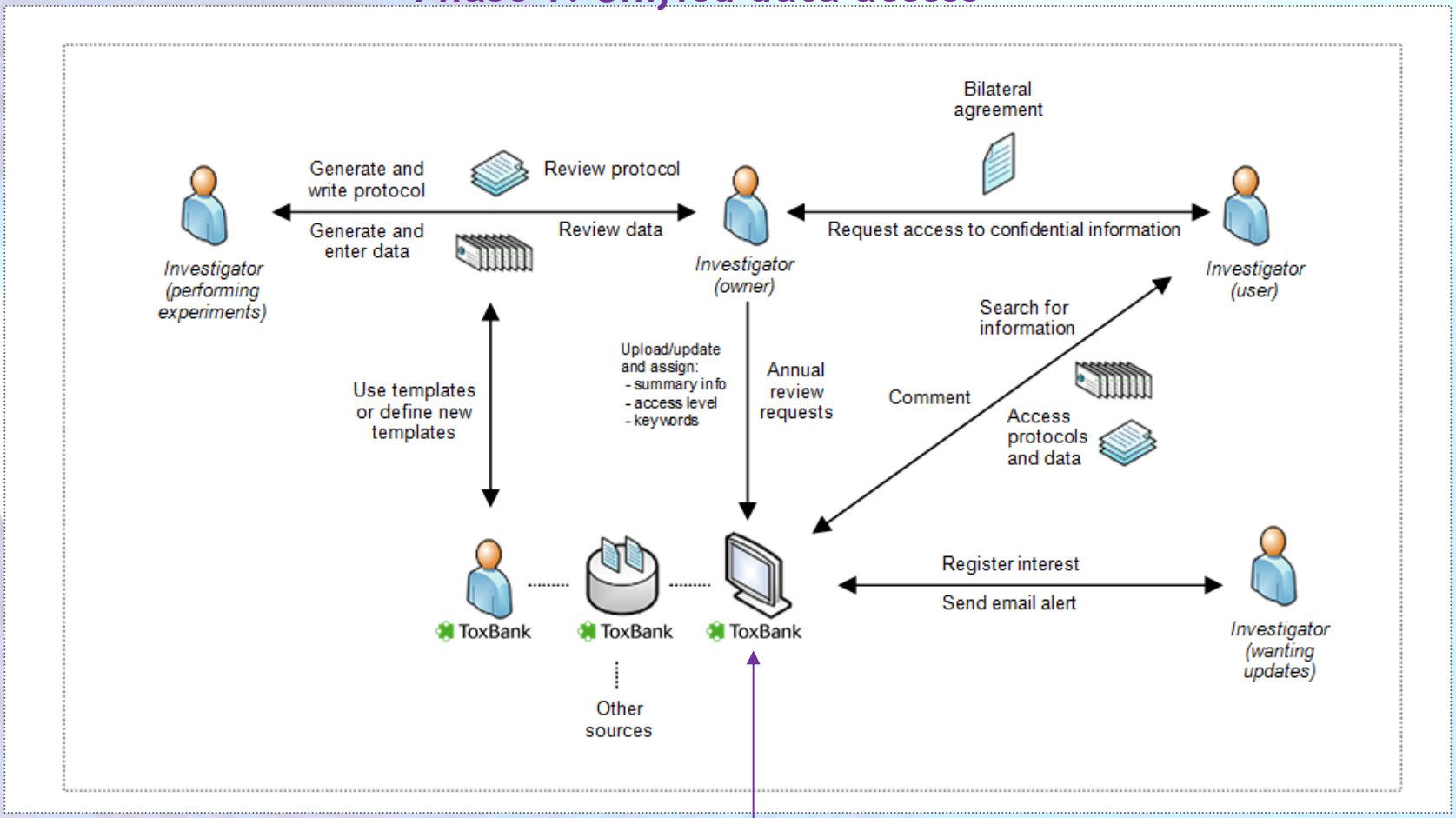
The Building Blocks of SEURAT-1



~ 70 research groups from European Universities, Public Research Institutes and Companies (more than 30% SMEs)

Outline of the ToxBank Data Warehouse

Phase 1: Unified data access



Phase 2: Integrated data analysis

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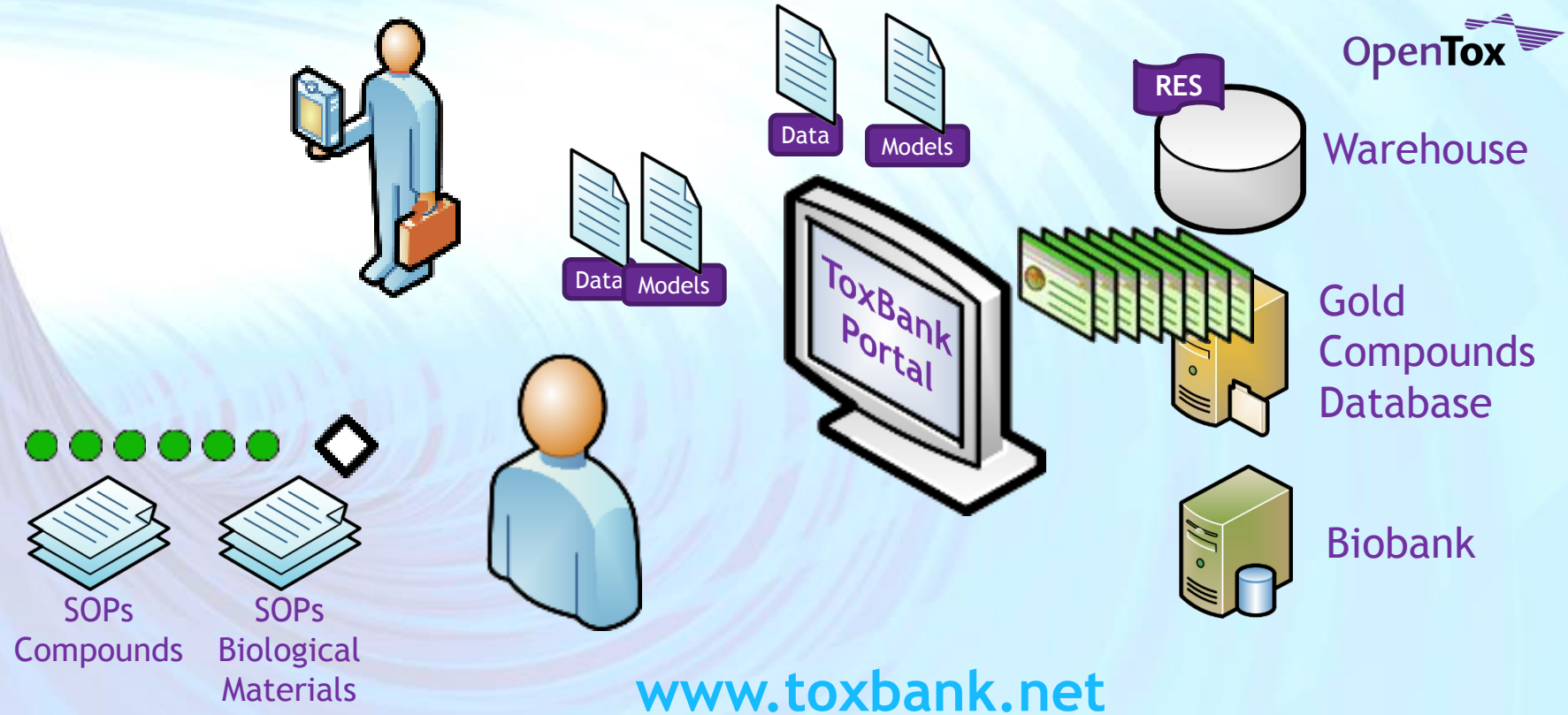
ToxBank Infrastructure System Vision

Users access compounds, biological materials, data and models for experimental planning and integrated analysis of experimental results



www.toxbank.net

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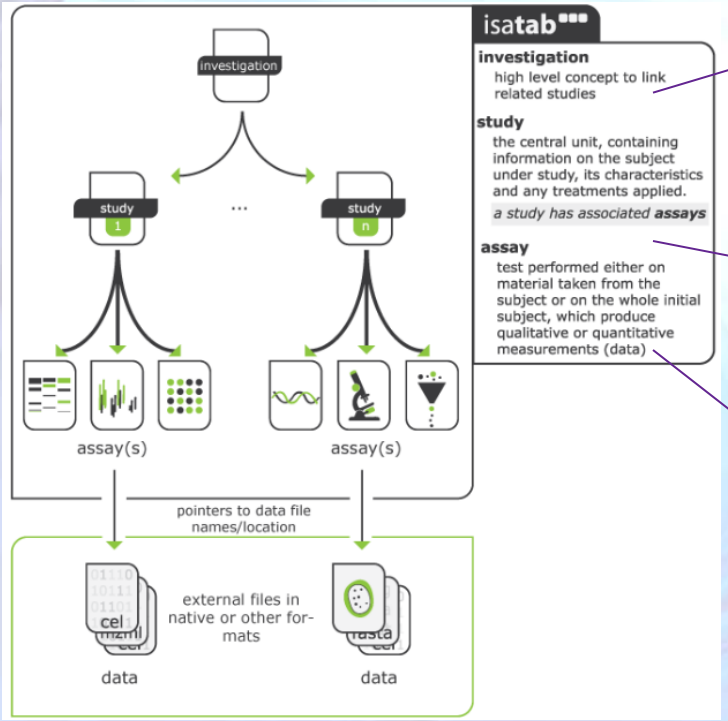
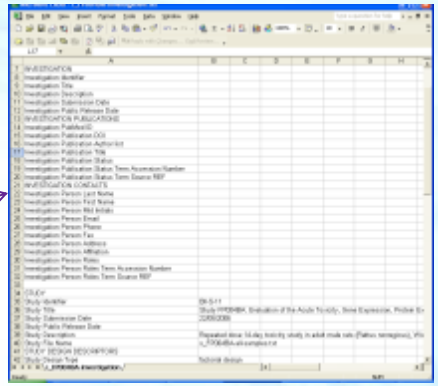
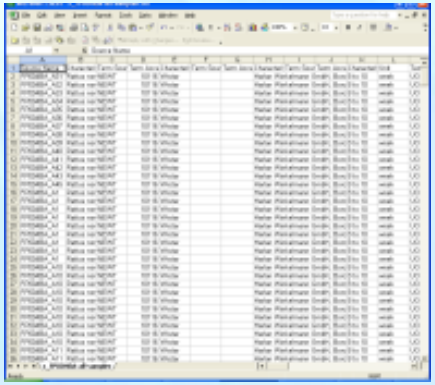
ISATab archives are created for each investigation

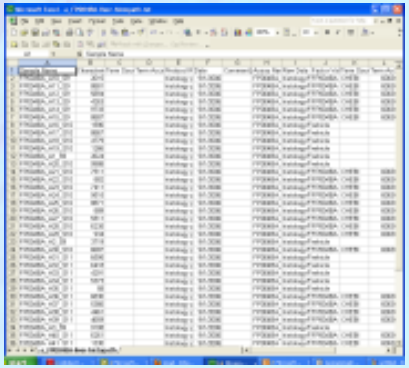




Overall investigation design and information (i... files)



Study description (s... files)



Test results (a... files) with links to data table or native file (e.g. CEL files)

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SEVENTH FRAMEWORK PROGRAMME

ToxBank integrates systems biology concepts into toxicological assessment

Pekka Kohonen,[a] Emilio Benfenati,[b] David Bower,[c] Rebecca Ceder,[a] Michael Crump,[c] Kevin Cross,[c] Roland C. Grafstrçm,[a] Lyn Healy,[d] Christoph Helma,[e] Nina Jeliazkova,[f] Vedrin Jeliazkov,[f] Silvia Maggioni,[b] Scott Miller,[c] Glenn Myatt,[c] Michael Rautenberg,[e] Glyn Stacey,[d] Egon Willighagen,[a] Jeff Wiseman,[g] and Barry Hardy*[h];

[a]Karolinska Institutet, Institute for Environmental Medicine, Molecular Toxicology,Stockholm, Sweden; [b], Istituto di Ricerche Farmacologiche Mario Negri, Milan, Italy; [c] Leadscope, Columbus, USA; [d] National Institute for Biological Standards and Control, Potters Bar, UK; [e]In silico toxicology, Basel, Switzerland; [f]Ideaconsult, Sofia, Bulgaria; [g]Pharmatrope,Wayne, USA; [h]Douglas Connect, Zeiningen, Switzerland.

Conclusions - *great potential to contribute to*

- ❖toxicity evaluation based on **Mode-of-Action**
- ❖**decreased need for animal experiments**

Systems toxicology - *principles*

Understanding the **toxicological interactions** in *biological systems under compound challenges*

Based on developments in **high-throughput biology**

- ❖ *'Omics* profiling: *gene expression, proteins, metabolites and others*
- ❖ *cell-based screening:* High-Throughput and High-Content analyses

Risk assessment carried out primarily using

- ❖ *in vitro*
- ❖ *In silico* methods

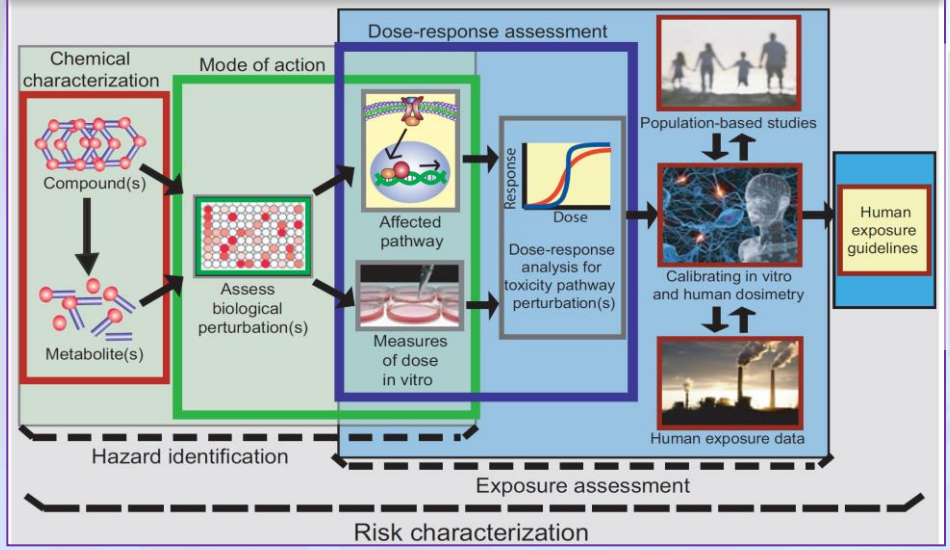


Figure 1. Multiple tools will be, **step by step**, implemented into an **innovative toxicity testing** strategy based on **mode-of-action**.

Kohonen P. et al. The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. Molecular Informatics. 17 JAN 2013, DOI: 10.1002/minf.201200114.

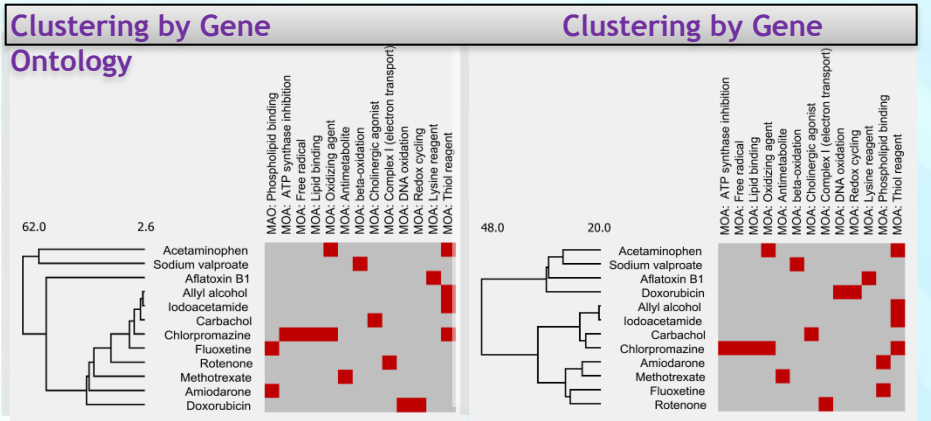


Figure 2. Clustering of ToxBank Gold Compounds by **biological similarity** using chemical-genome links from Comparative Toxicogenomics Database (CTD). Compounds with similar Mode-of-Action cluster together.

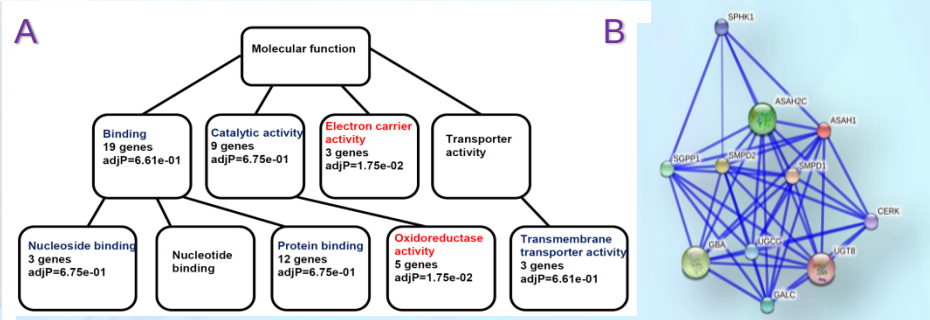
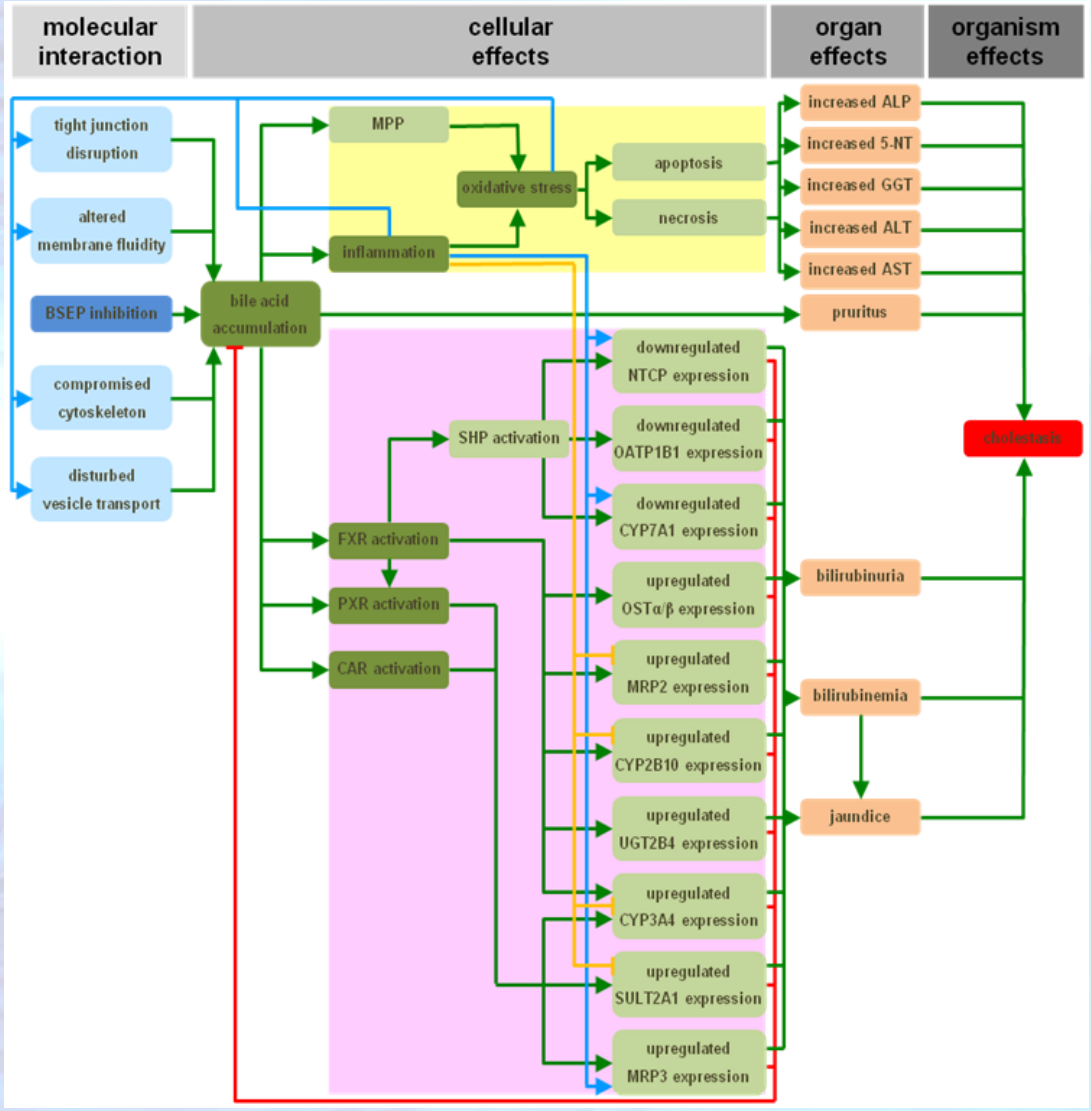


Figure 3. A) Enriched gene ontology (GO) categories of genes associated with the oxidizing agent mode-of-action (MOA) B) Protein-protein association network around the Asah1 protein Associated with phospholipid binding MOA.

ToxBank builds *databases and data management solutions* to aid in **systems toxicology-based** risk assessment

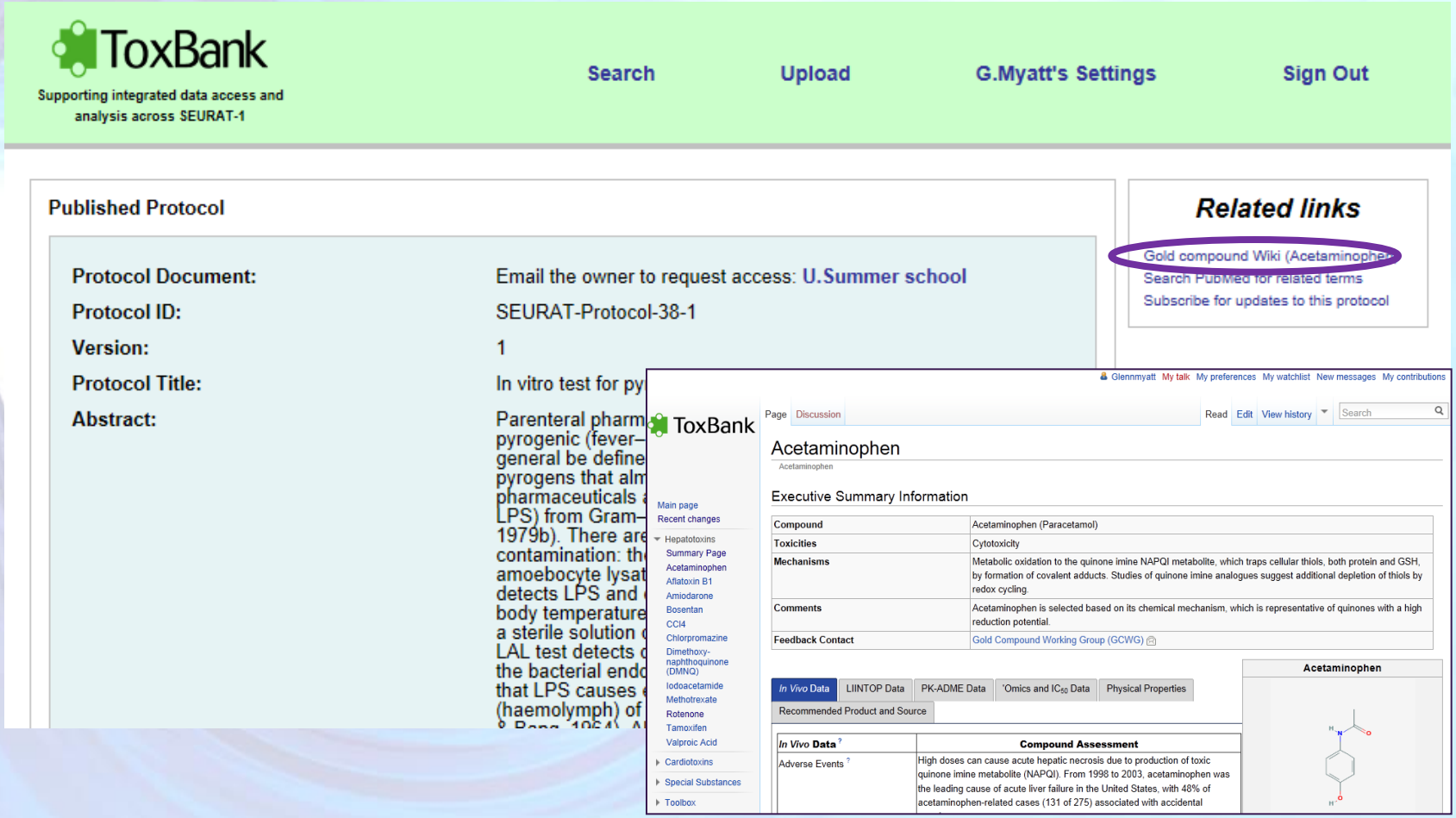
Cancer- och Allergifonden
cancer - allergi - miljö
Cosmetics Europe
the personal care association
ToxBank
Seventh Framework Programme
Karolinska Institutet
Anno 1810
IMM Institute of Environmental Medicine
Institutet för Miljömedicin

Adverse outcome pathway (AOP) : drug-induced cholestasis



Vinken M., Landesmann B., Goumenou M., Vinken S., Shah I., Jaeschke H., Willett C., Whelan M., Rogiers V. (2013) Development of an adverse outcome pathway from drug-mediated bile salt export pump inhibition to cholestatic liver injury. *Archives of Toxicology*: submitted .

New data may be combined with reviewed community data on reference compounds



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wiki.toxbank.net

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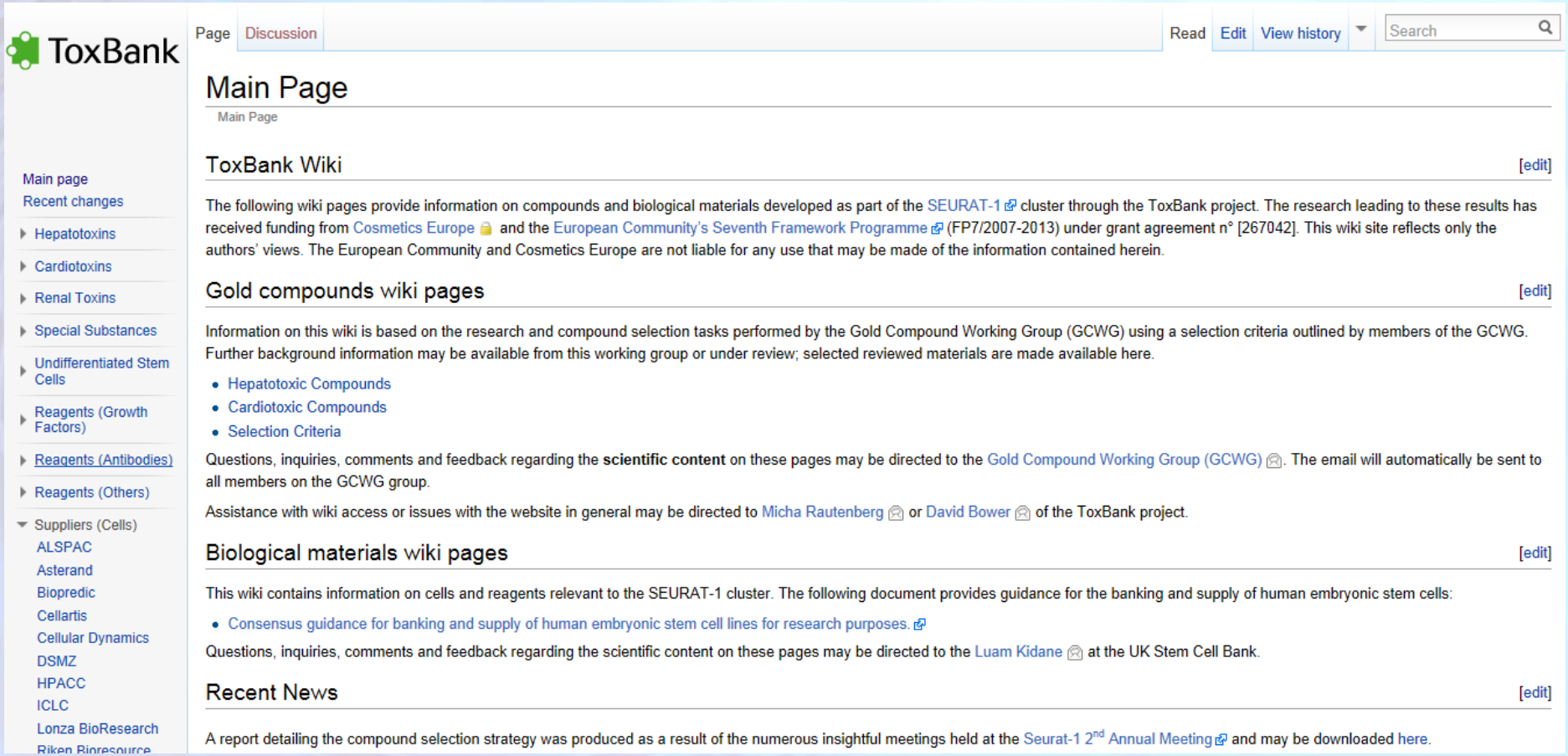
ToxBank Wiki Reference Information Resource



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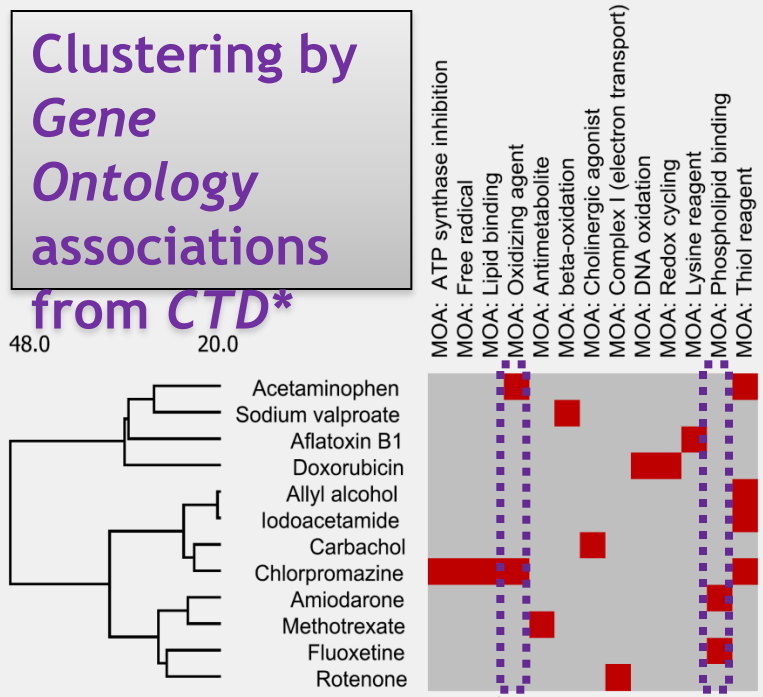
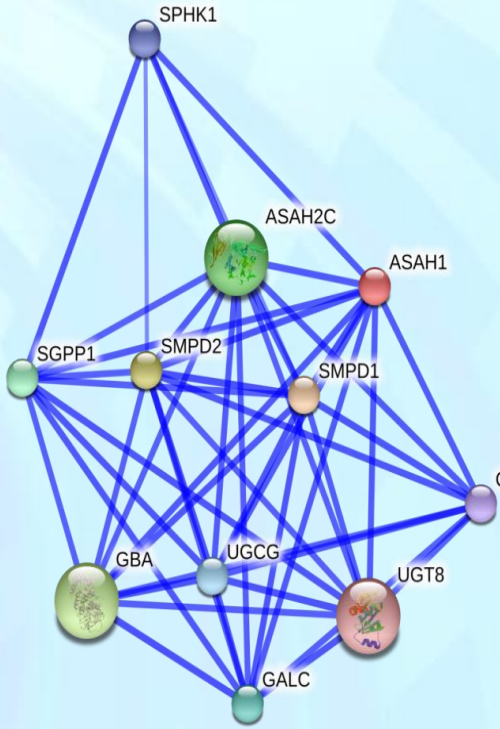
Public Data Analysis

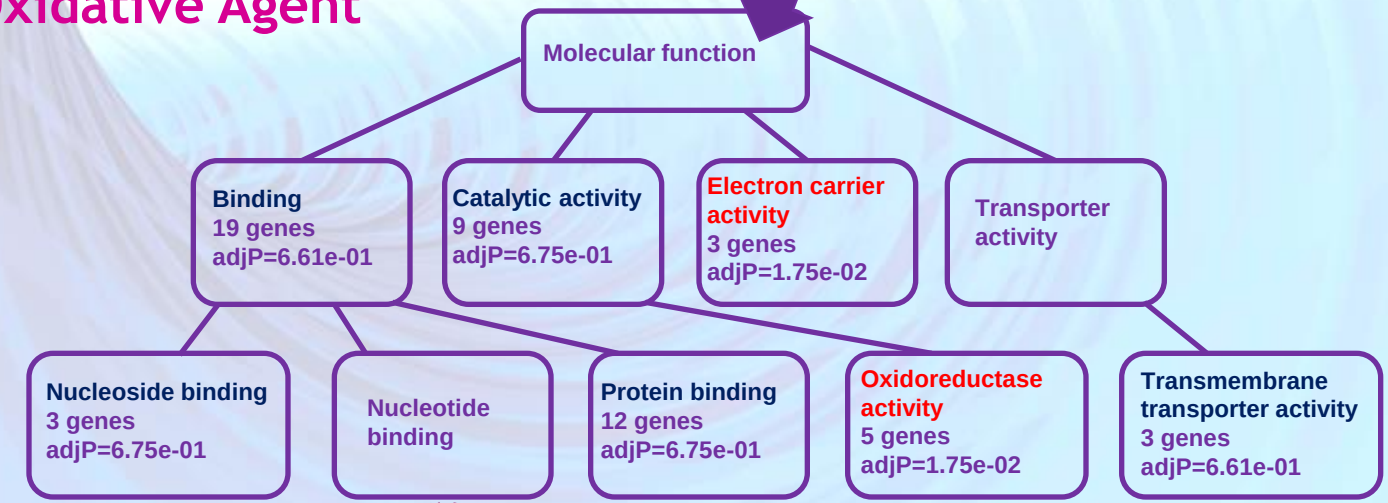
Clustering by *Gene Ontology* associations from *CTD**



Phospholipid Binding



Oxidative Agent



**CTD = Comparative Toxicogenomics Database (www.ctd.org)*

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Karolinska Institutet

Kohonen P. et al. The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. Mol. Inf.17 JAN 2013.

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http://onlinelibrary.wiley.com/doi/10.1002/minf.201200114/full

The ToxBank Data ... | 53BP1 clone 19

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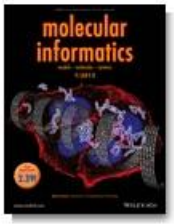
The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing

Pekka Kohonen[1], Emilio Benfenati[2], David Bower[3], Rebecca Ceder[1], Michael Crump[3], Kevin Cross[3], Roland C. Grafström[1], Lyn Healy[4], Christoph Helma[5], Nina Jeliazkova[6], Vedrin Jeliazkov[6], Silvia Maggioni[2], Scott Miller[3], Glenn Myatt[3], Michael Rautenberg[5], Glyn Stacey[4], Egon Willighagen[1], Jeff Wiseman[7], Barry Hardy[8,*]

Article first published online: 17 JAN 2013

DOI: 10.1002/minf.201200114

Issue



Molecular Informatics

Special Issue: Advances in Computational Toxicology

Volume 32, Issue 1, pages 47–63, January 2013

Additional Information **(Show All)**

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Abstract | Article | References | Supporting Information | Cited By

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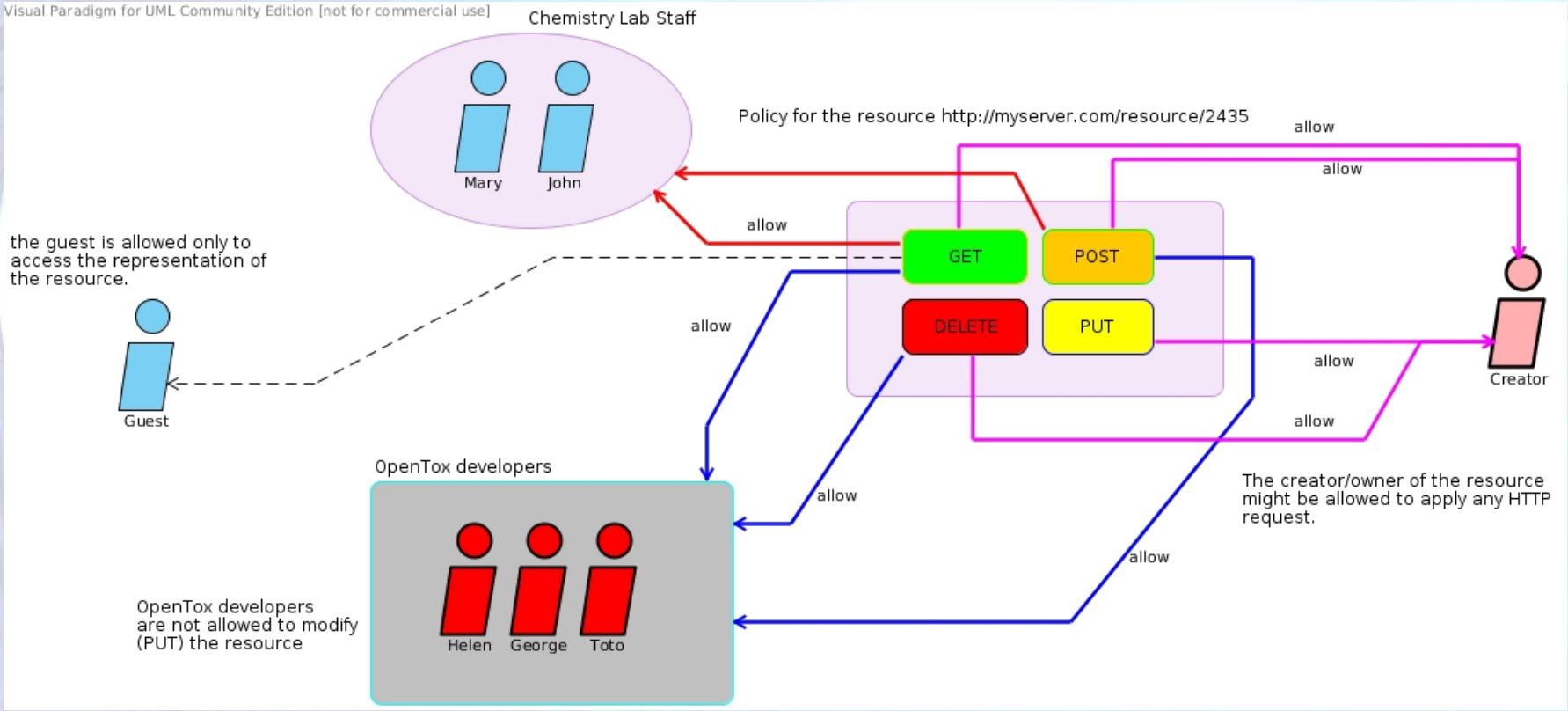
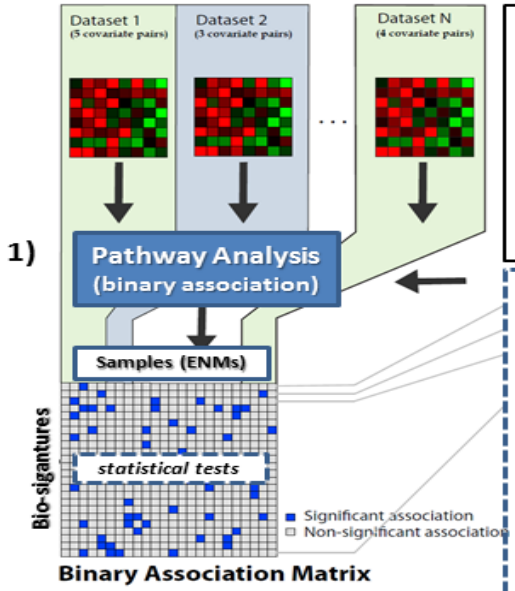
Security



Use Open Standards on Resources but with extensive Authorisation and Authentication facilities accompanied by confidential data policies. e.g. *Validation against Confidential Data Case implemented Spring 2011*

OpenTox

eNanoMapper starting 2014: OpenTox/ToxBank applied to Nano



Data origins

I. **Cells/tissues:** Data on cells treated with ENMs (*e.g. gene expression, metabolomics, high-throughput cellular assays*)
II. **Particles:** Omics data on corona composition (*e.g. proteomics of plasma proteins bound to ENMs*)
III. **Chemical/structural descriptors:** NanoQSAR (e.g. *UM/KI NanoWiki*)

Examples of data providers

A. **eNanoMapper** (e.g. *UM/KI NanoWiki)*
B. **Public Sources** (*e.g. NanoMiner, ArrayExpress*)
C. **EU NanoSafety Cluster (NSC)** Projects (*e.g. NanoSolutions)*
D. **U.S.-EU nanoEHS** (e.g. cellular assay activity data)

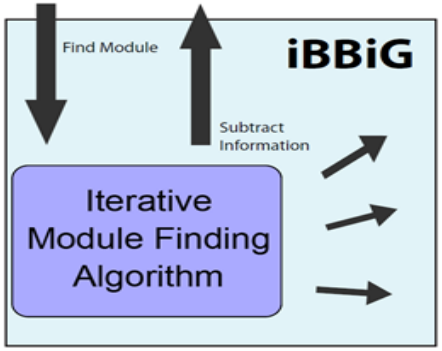
Bio-Signatures

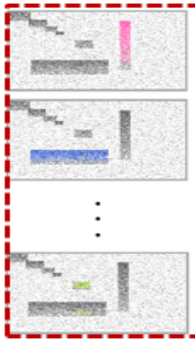
- ***WikiPathways, KEGG, GO,MsigDB***
- ***Toxicity pathways***
- ***Cellular activity assays***

Statistical tests

- **Gene Set Enrichment Analysis (GSEA)** *(e.g. gene expression)*
- **Over-Representation Analysis (ORA)***(e.g. corona proteins)*
- ***Z-scores*** *(e.g cellular activity)*

1) Process the data **into binary matrix**
2) Iterative class/module finding to **group nanoparticles**
3) Testing modules for **covariate enrichment**
4) Classes/modules of ENMs are constructed to enable **biological read-across**





+

3)

Data Covariates (*e.g. UM/KI NanoWiki*)

A. **Particle, Structural** (*e.g. shape, size, band gap*)
B. **Particle, covalent surface modifications** (*e.g. functional groups*)
C. **Particle, bound entities** (*e.g.* corona composition*)*
D. **Phenotypic data, cell level** (*e.g. apoptosis, ROS production, MTT assay, etc. cellular activity assays)*
E. ***Phenotypic data, organism / organ level*** (*e.g. lung fibrosis)*

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What is the African vision for the environment? What can predictive toxicology methods do to progress it?

OpenTox Workshop, SETAC Africa, 2011

www.setac.org/event/africa-2013

OpenTox

OpenTox Workshop with 90 Participants in Rhodes

Rhodos, Greece
Sept. 2010
OpenTox 3rd meeting

EuroQSAR 2010

ca. 90 participants engaged in using a variety of OpenTox applications

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OpenTox InterAction Meeting 2011

Innovation in Predictive Toxicology

Modeling, Applications, REACH, Risk Assessment

9-12 August, 2011
Technical University of Munich, Germany

Ca. 80 attendees participated in workshop, knowledge cafés, conference, poster session

More Information at:
www.opentox.org/meet/opentox2011

There will be OpenTox 2014 workshops and meetings...!

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Upcoming OpenTox Meetings

September 2014 – Athens, Greece

November 2014 – John Hopkins, Baltimore

September 2015 – Dublin, Ireland

October 2015 – Miami beach, Florida

Discussing a first OpenTox Asia...

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Collaborating Partners

Douglas Connect, Switzerland (Coordinator)

In Silico Toxicology, Switzerland

Albert Ludwigs University Freiburg, Germany

Ideaconsult, Bulgaria

National Technical University of Athens, Greece

Istituto Superiore di Sanità, Italy

Fraunhofer Institute for Toxicology & Experimental Medicine, Germany

Technical University of Munich, Germany

David Gallagher, UK

Institute of Biomedical Chemistry of the Russian Academy of Medical Sciences, Russia

Seascape Learning & JNU, India

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in silico toxicology

Karolinska Institutet

Leadscope®

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UK StemCellBank

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ISTITUTO DI RICERCHE FARMACOLOGICHE

UK Stem Cell Bank, NIBSC-HPA

Ideaconsult Ltd

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