OpenTox - An Open Interoperable Predictive Toxicology Framework

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12 April 2011

Current Methods for Computational Toxicology and Chemogenomics

BIO-IT, Boston, USA

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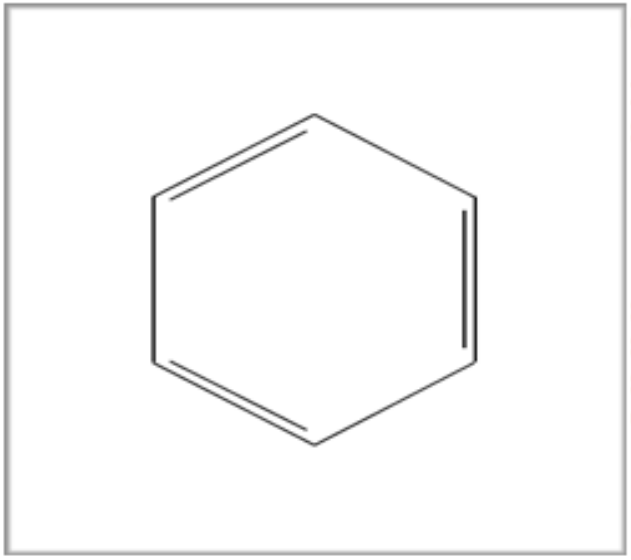
ToxPredict

OpenTox demo application

This page lists your ToxPredict workflow results for the structure(s) you have selected and the model prediction(s) you have chosen to run. You could also retrieve the ToxPredict report in various other formats, e.g. **SDF**, **CML**, **SMI**, **PDF**, **CSV**, **ARFF**, **RDF/XML** or **RDF/N3**.

Download as



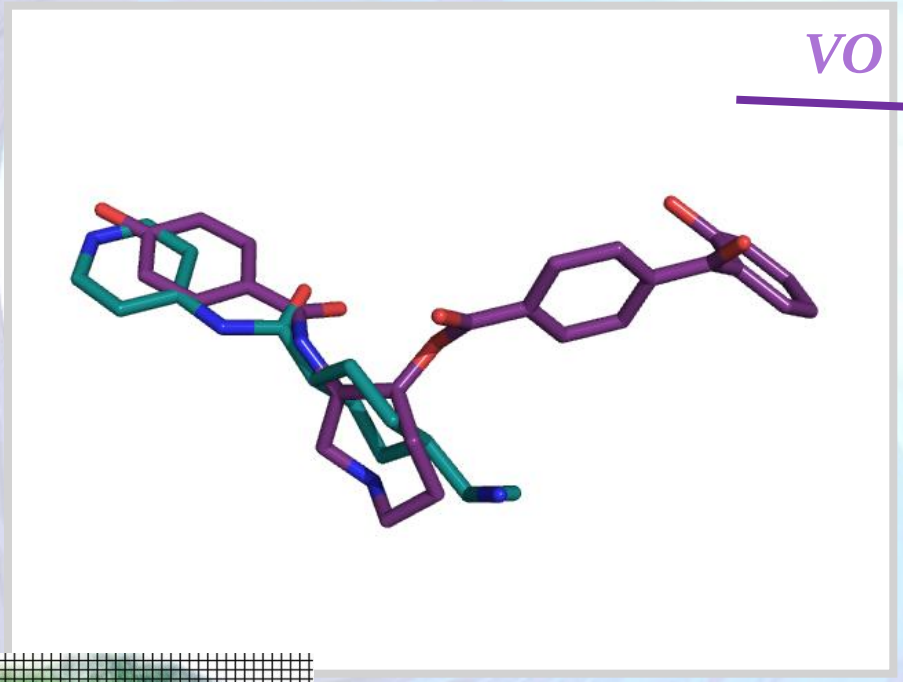
CAS RN	71-43-2
EINECS	200-753-7
IUPAC name	benzene
Synonym	(6)annulene; benzine; Benzol; Benzolene; bicarburet of hydrogen; carbon oil; Coal naphtha; cyclohexatriene; mineral naphtha; motor benzol; nitration benzene; Phene; Phenyl hydride; pyrobenzol.
Synonym	21742.0
Synonym	Benzene
Synonym	benzene
Quality label	OK

MolecularWeight MolecularWeight

MW	78.1112

Our Use Case

Input Structure



VO

Out – Toxic or Not?

- LD50
- Liver Toxicity
- Secondary Metabolites
- Interaction with the hERG Channel?
- Renal Clearance
- Bioavailability
- Mutagenicity
- Carcogenicity
- ReproductiveToxicology
- Skin Irritation
- Aqua Toxicity
- Combined predictions for arrays of mutiple end points

Business Driver

Increasing demands on industry to satisfy safety evaluation and risk assessment required by REACH legislation.

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Challenges to *in silico* Applications

- Lack of public standards, ontology
- Toxicity data collected in many different databases using different formats, frequently incompatible with computer programs
- Many databases lack important information for *in silico* modeling (e.g. chemical structures)
- Hard to integrate confidential in-house data with public data for model building and validation
- Models have been published in a variety of different formats (ranging from simple regression equations to complete computer programs)
- Need for New Business Cases
- There is no straightforward integration of predictions from various programs
- No commonly accepted framework for validation of *in silico* predictions, many tools provide limited support for reliable validation procedures
- Application, interpretation, and development of *in silico* models is still difficult for most toxicological experts
- It requires a considerable amount of statistical, cheminformatics and computer science expertise - procedures are labor intensive and prone to human errors

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Compelling Needs of Users

Multidisciplinary R&D

Good Support of Flexible Applications

Transparency – Not Black Box!

Mechanistic rationale

QSAR & Expert Systems

Workflows

Automated Integration

Applicability Domain

Categories

Systems Biology

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Communicated to OpenTox in 2009 by Stephanie Ringeissen (L'Oréal)

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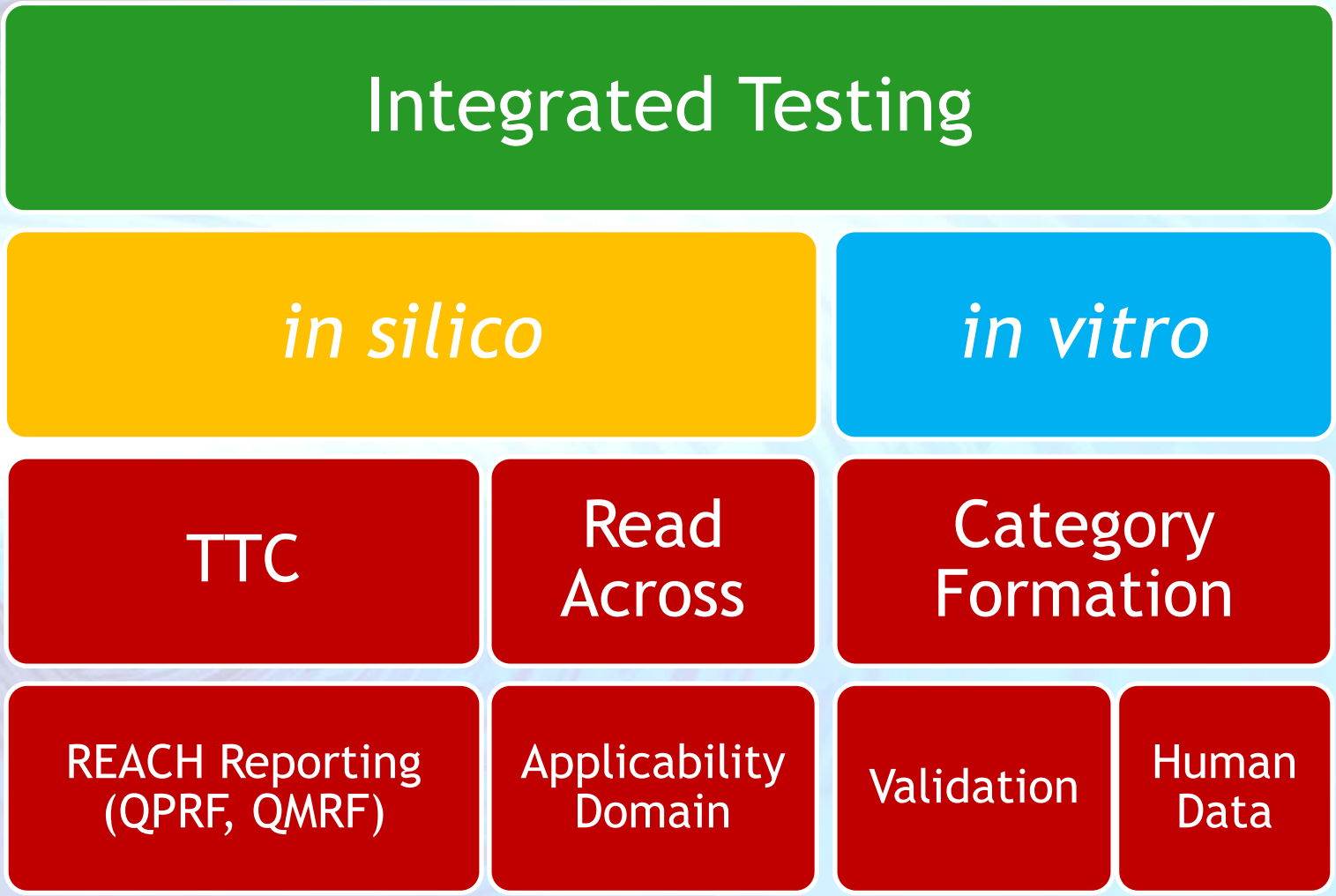
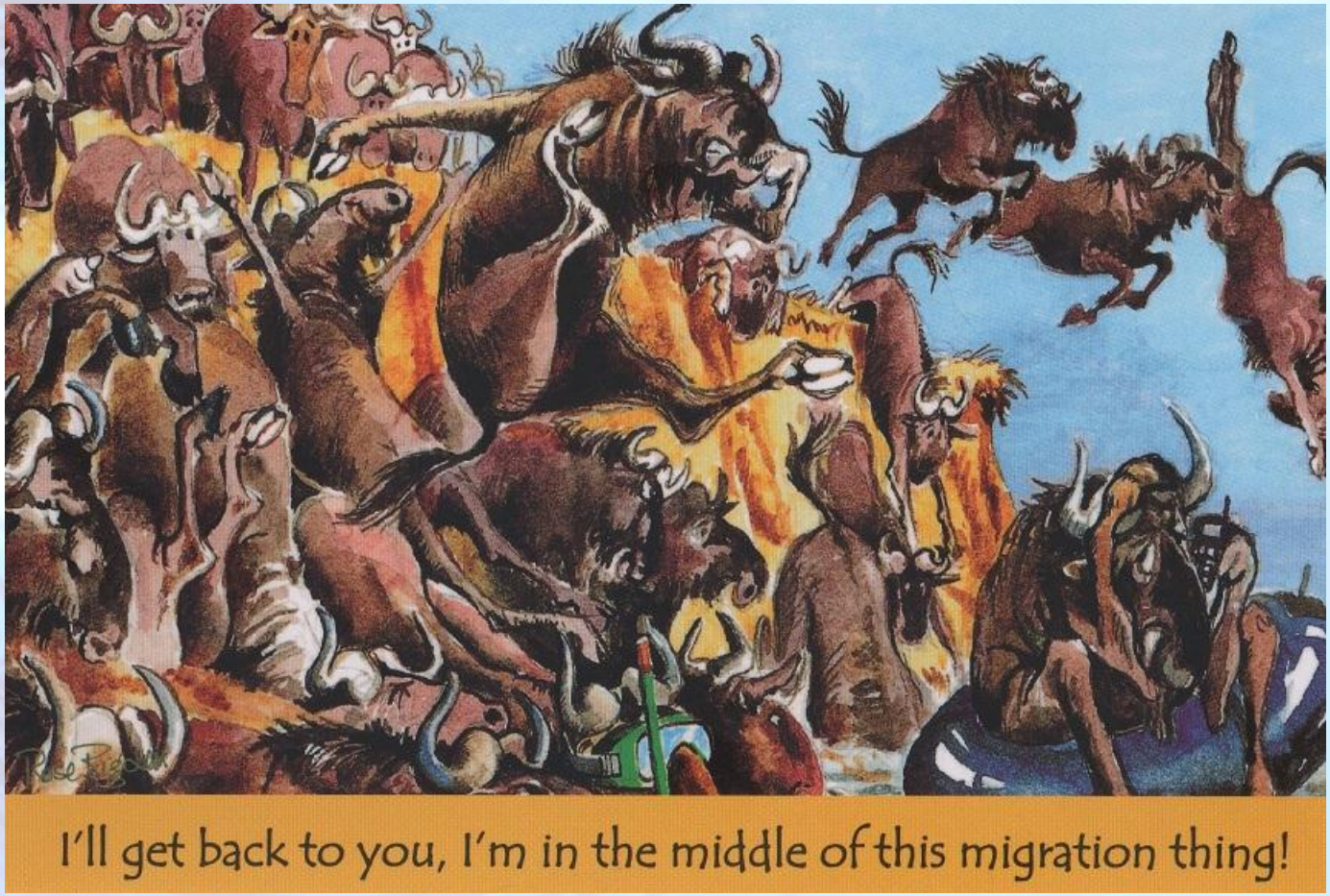
Compelling Needs of Users



Communicated to OpenTox 2009 by Grace Patlewicz (Du Pont)

Migration



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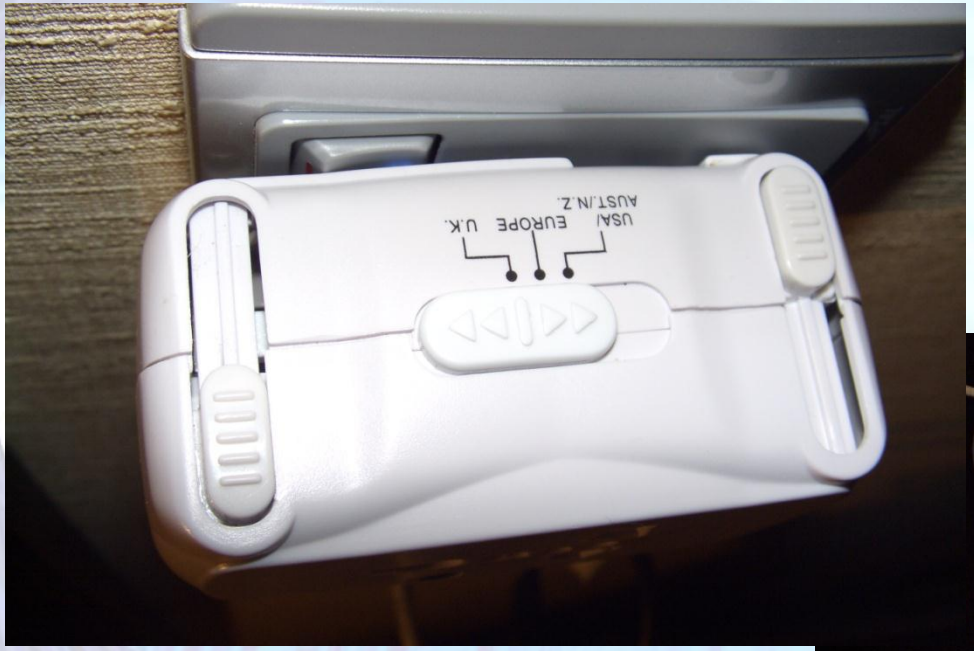
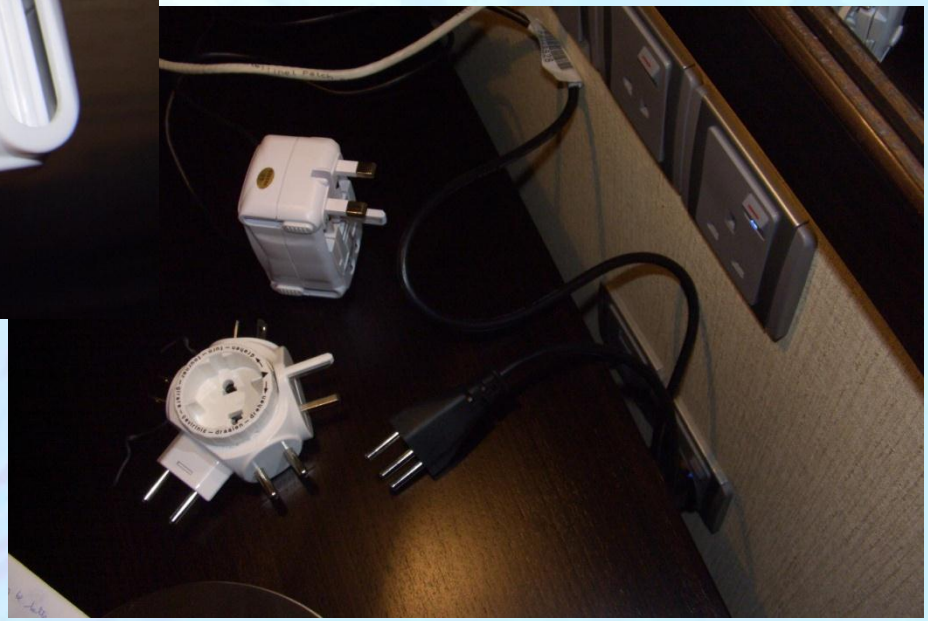
Ontology and Data - Interoperability





Adaptor Challenge in Jeddah, 2008

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Interacting Components create Solutions

Adaptor Solution in Jeddah, 2008

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OpenTox Components

Compounds: Structures, names, ...

Features: Chemical and biological (toxicological) properties, substructures, ...

Datasets: Relationships between compounds and features

Algorithms: Instructions for solving problems

Models: Algorithms applied to data yield models which can be used for predictions

Validation: Methods for estimating the accuracy of model predictions

Reports: Report predictions and models e.g. to regulatory authorities

Tasks: Handle long running calculations

Authentification and Authorisation: Protect confidential data

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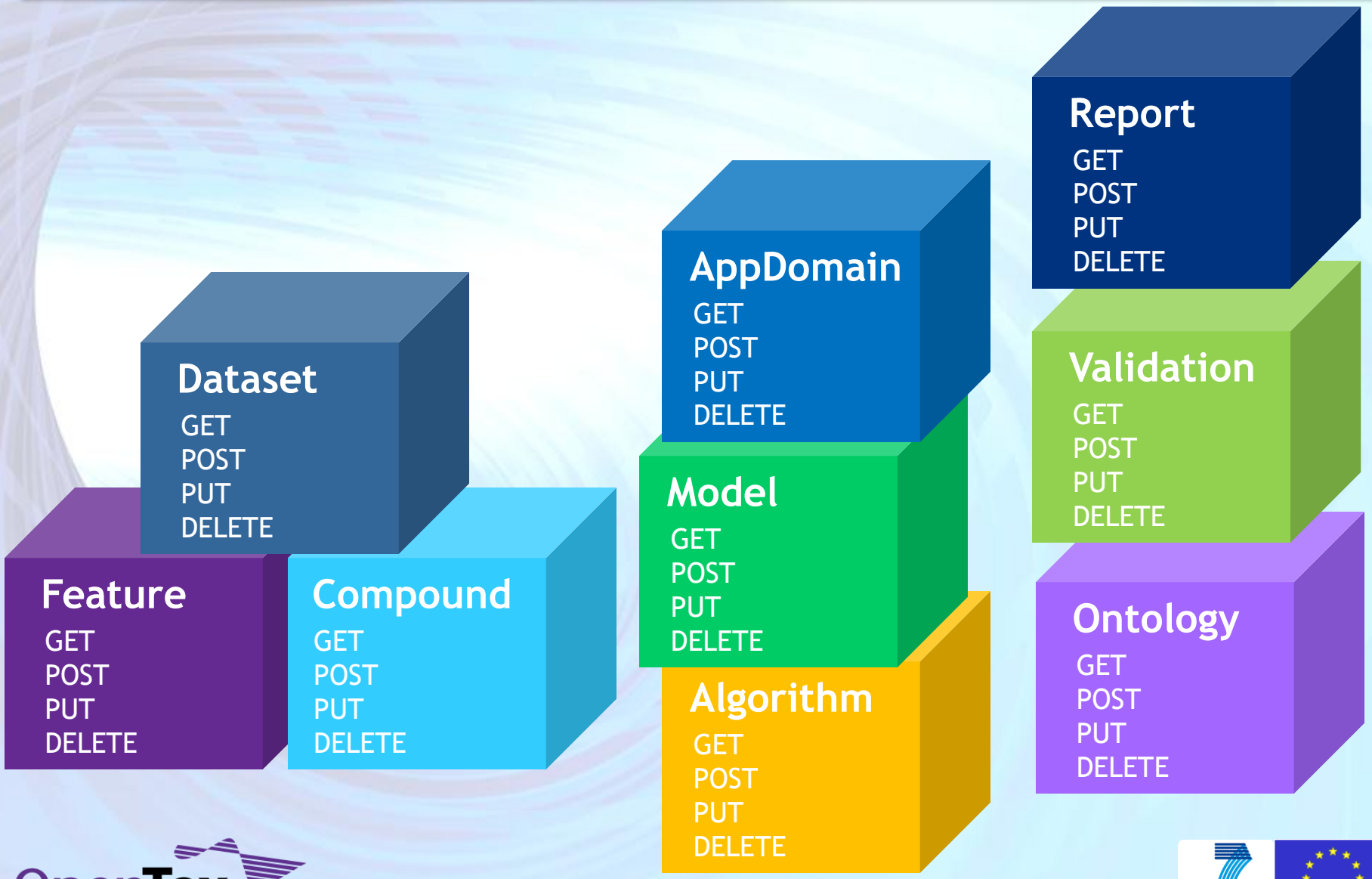
Overview of Application Programming Interfaces



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Representational State Transfer (REST)

What?

- Architectural style for distributed information systems on the Web
- Simple interfaces, data transfer via **hypertext transfer protocol (HTTP)**, stateless client/server protocol
  - GET, POST, PUT, DELETE
- Each **resource** is **addressed** by its own **web address**

Why?

- **Lightweight** approach to **web services**
- **Simplifies/enables** development of **distributed and local systems**
- Language independent

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Semantic Reflections

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

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Interoperability & Vocabulary

- Dogs
  - Collie
  - Labrador
- Cats
  - Siamese
  - Persian
- Birds
  - Sparrow
  - Owl

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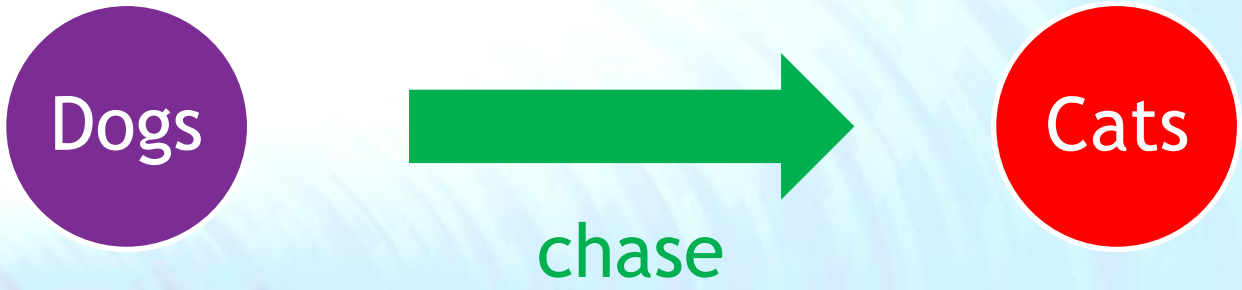
Interoperability & Vocabulary



Interoperability & Ontology

Org A

Collie

chase

Siamese

Org B

Collie

Siamese

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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

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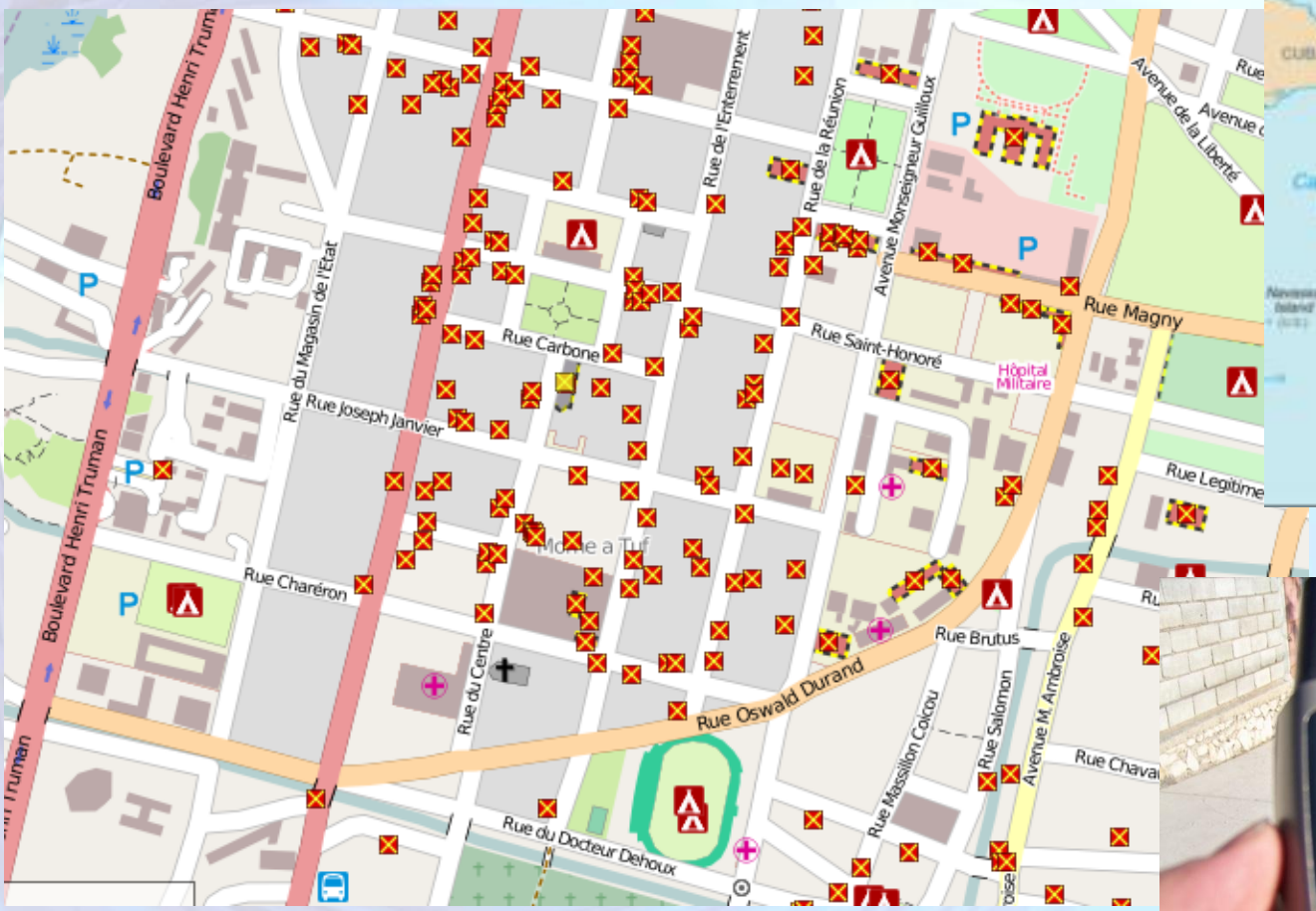
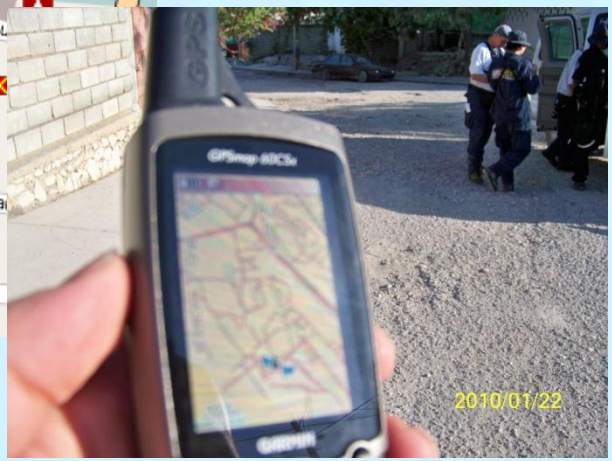
Solution created by Linked Open Data, Web Applications and Crowdsourcing





Haiti Earthquake Crisis Response (2010)

wiki.openstreetmap.org

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	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

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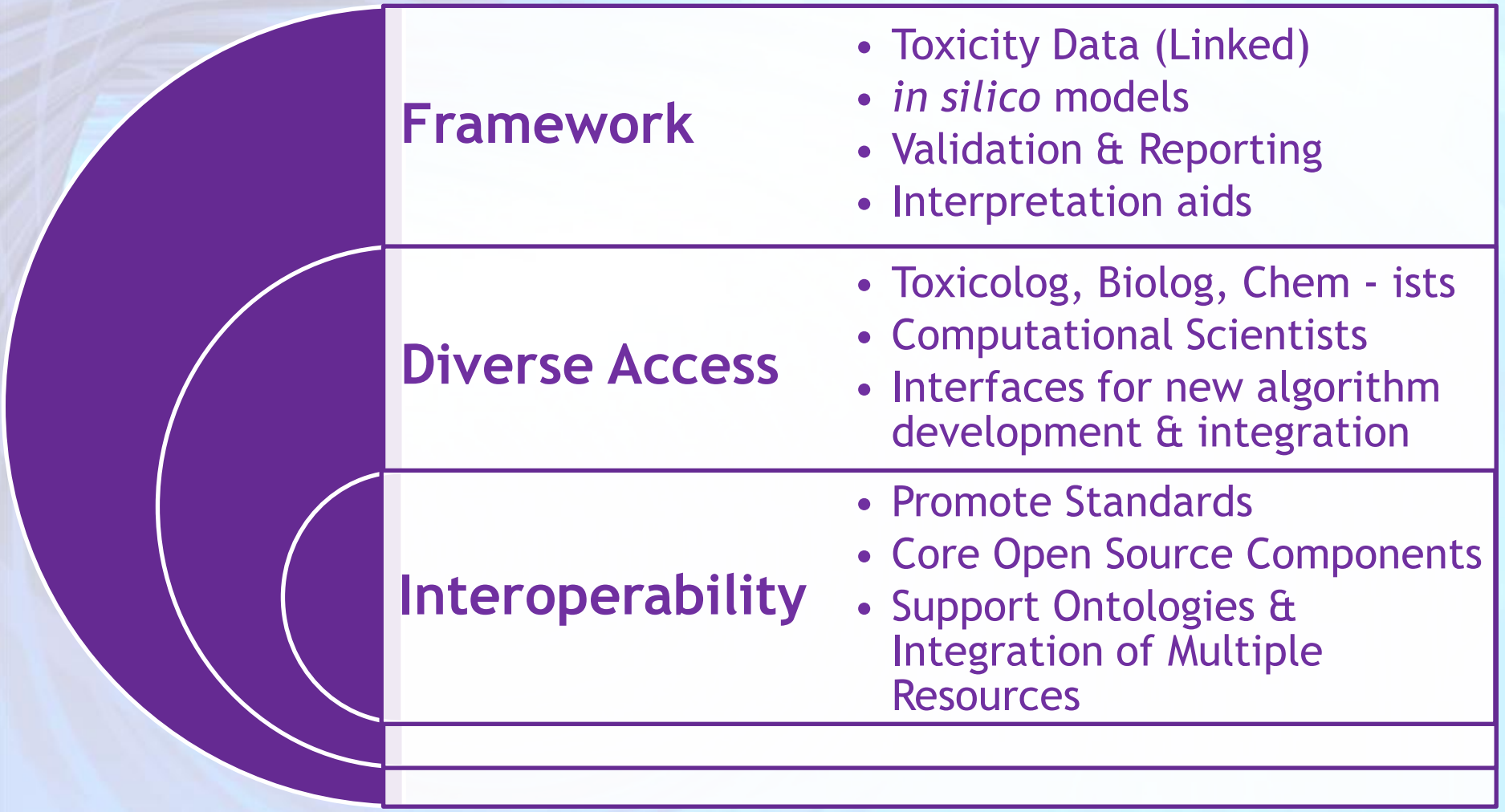
OpenTox is an Integrating Framework



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Journal of Cheminformatics Publication

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, JoergWicker, 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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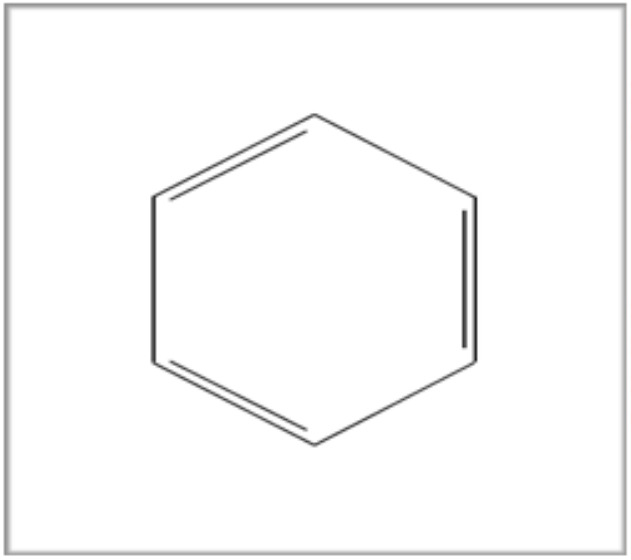

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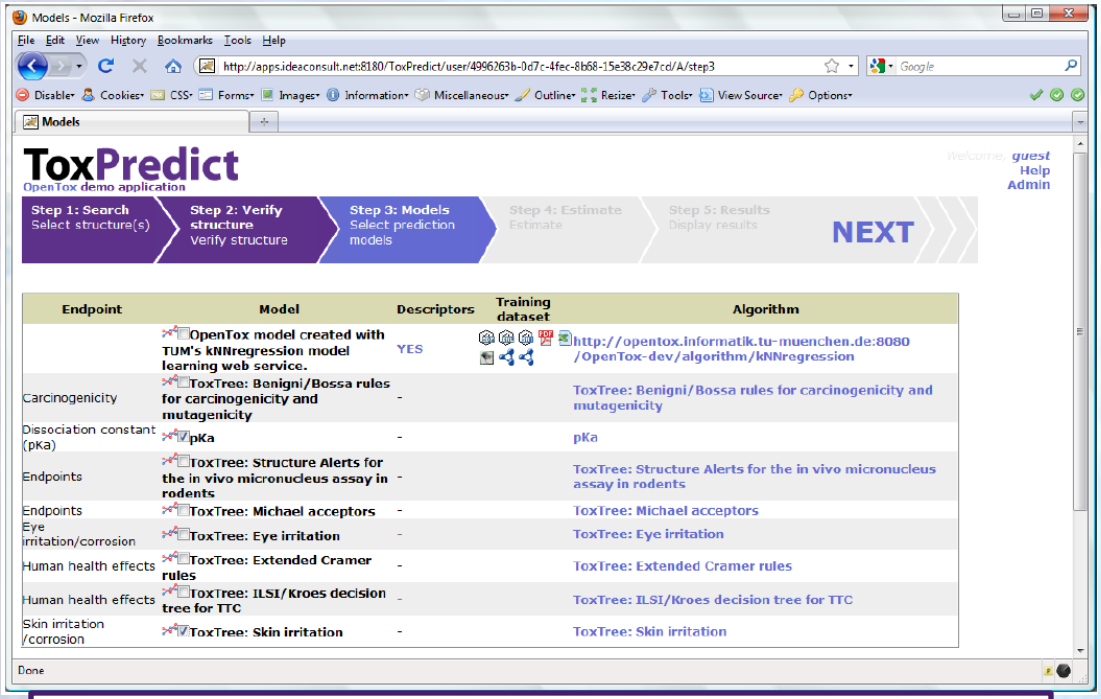
What you can do with it …



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

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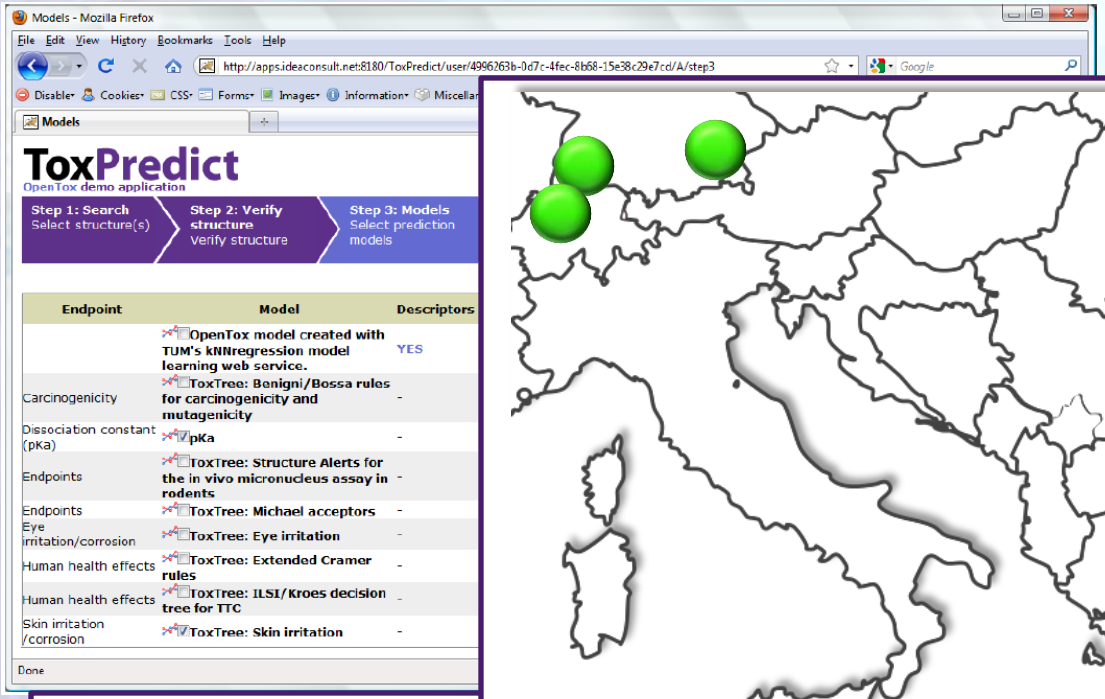
What you can do with it …



Simple building c

applications

methods and

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

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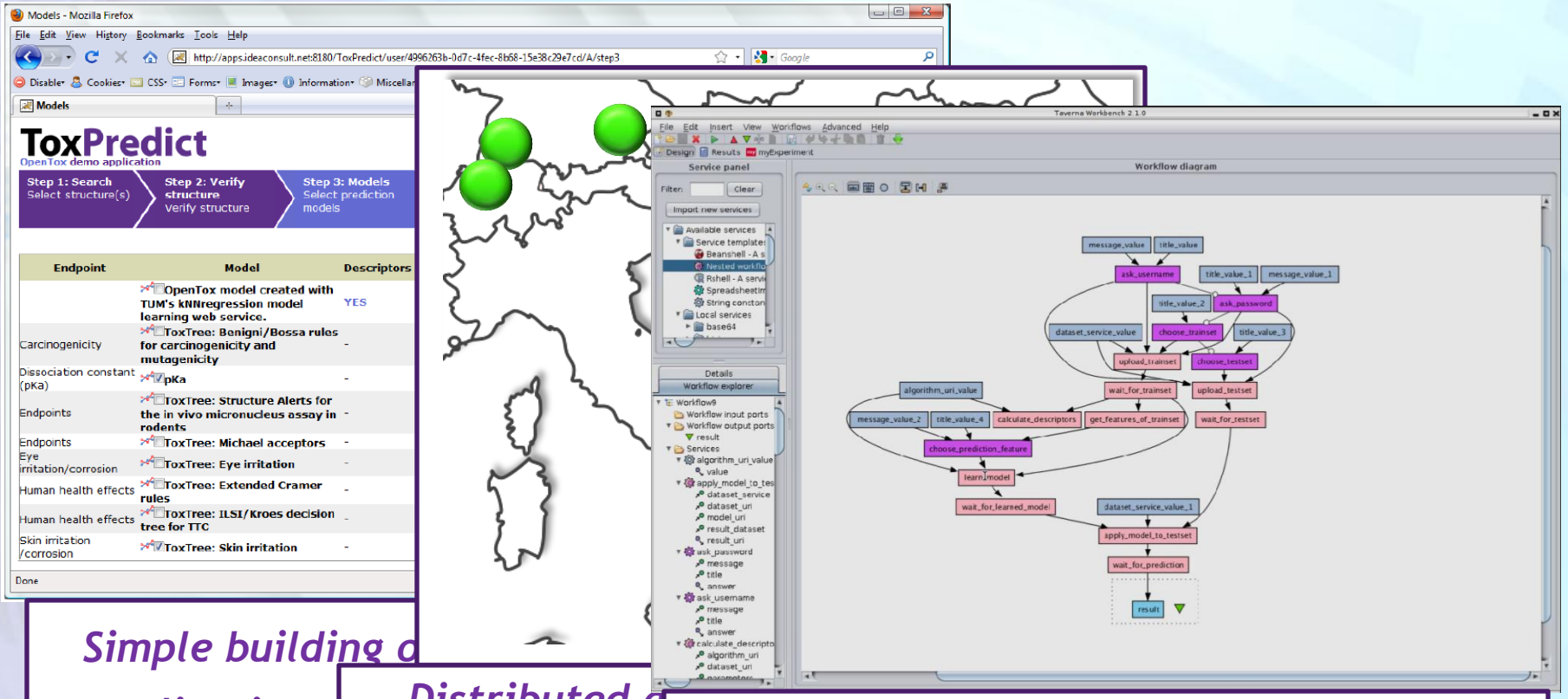
What you can do with it …



Simple building c
applications
methods and

Distributed c
wide range o
methods

Integration into workflow systems for computational biology

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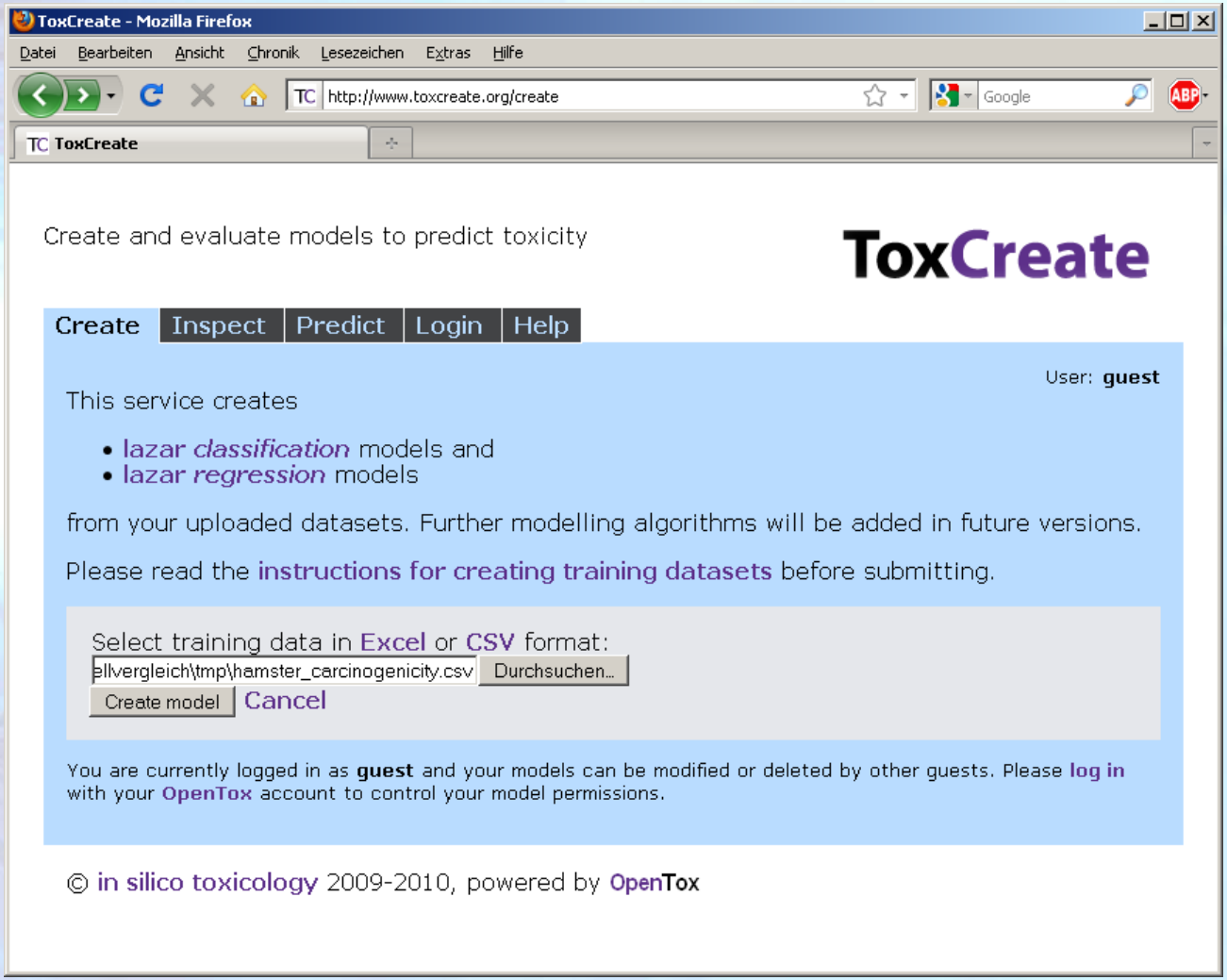
ToxCreate



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Developed by In Silico Toxicology

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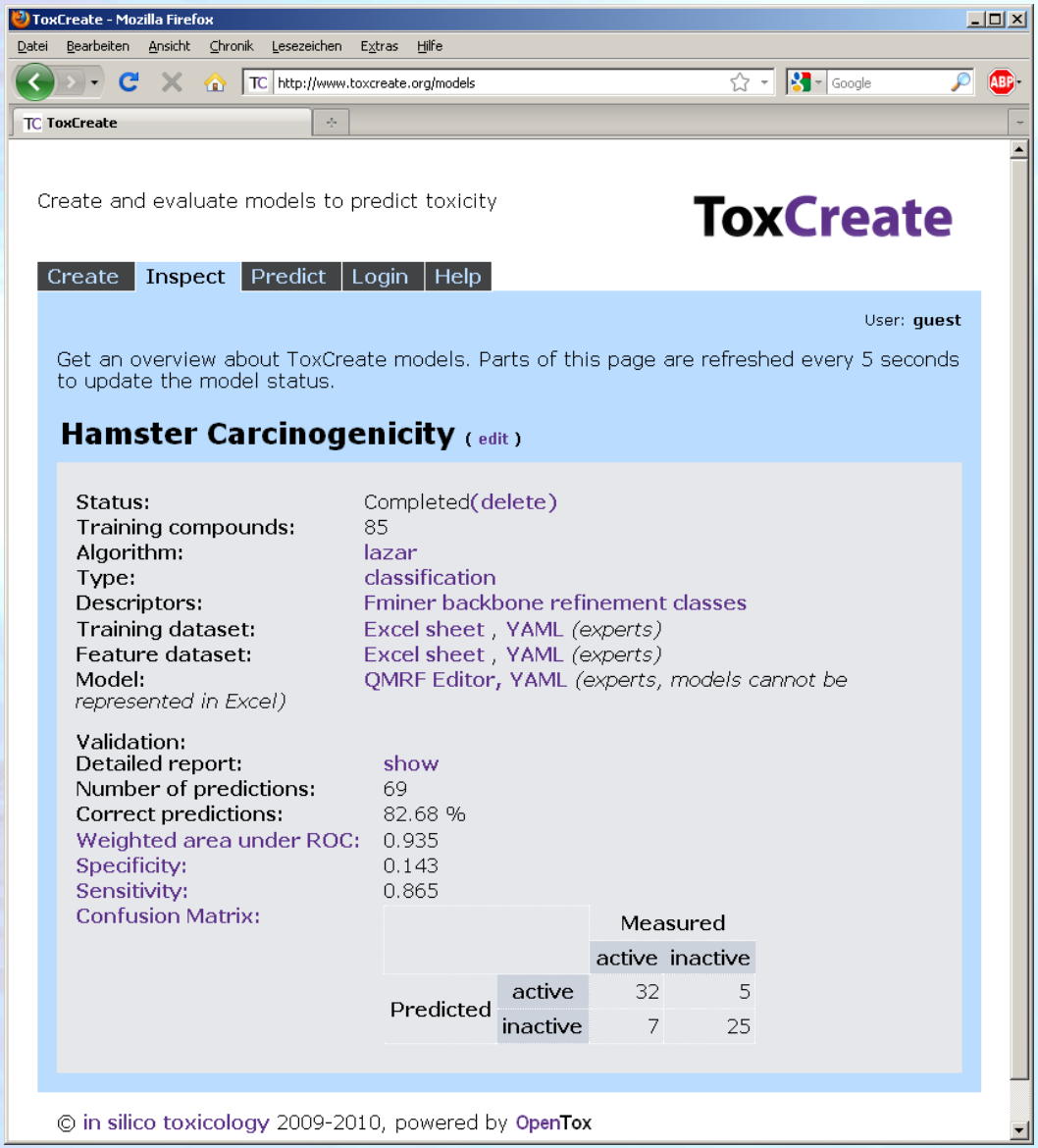
ToxCreate



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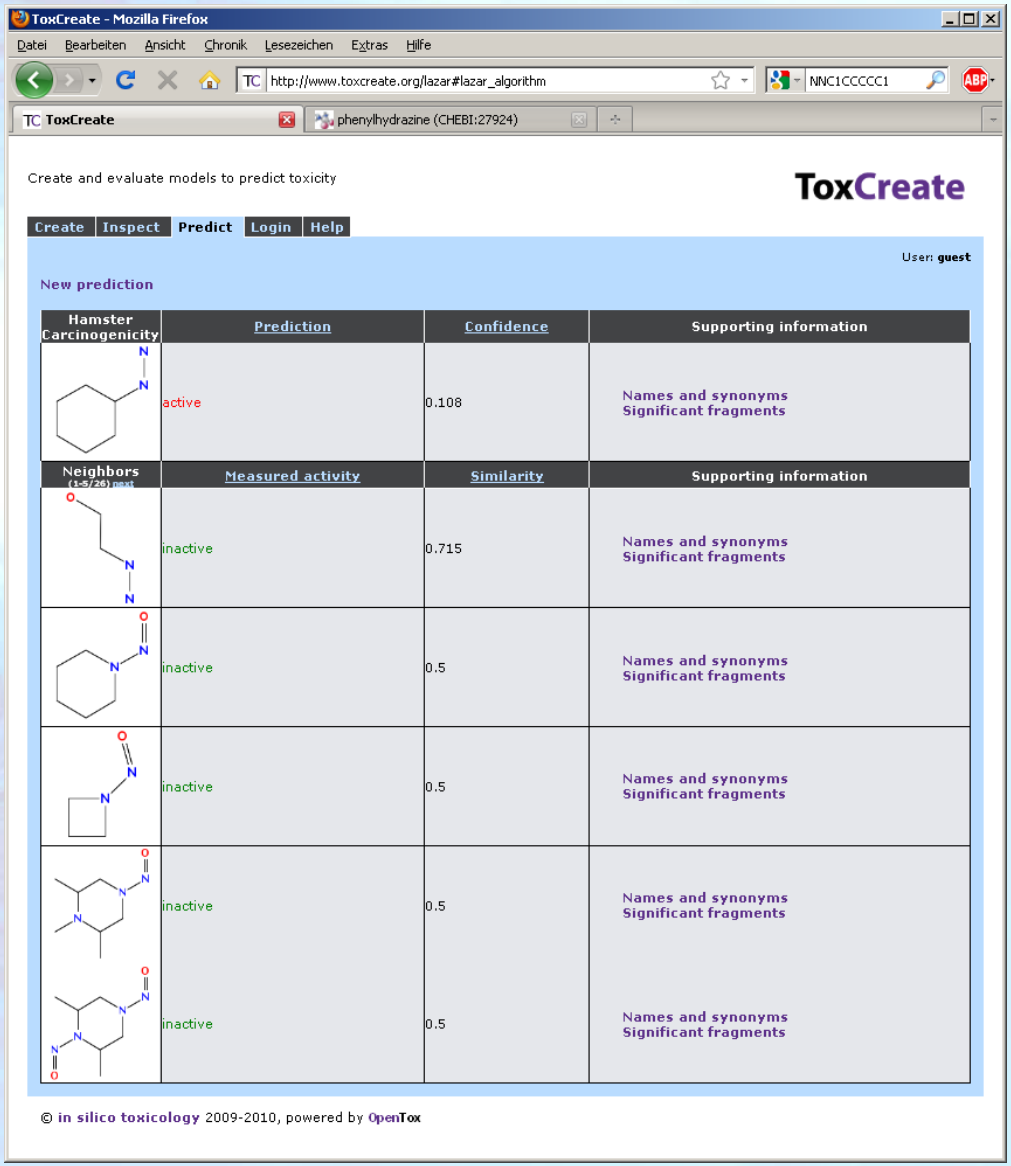

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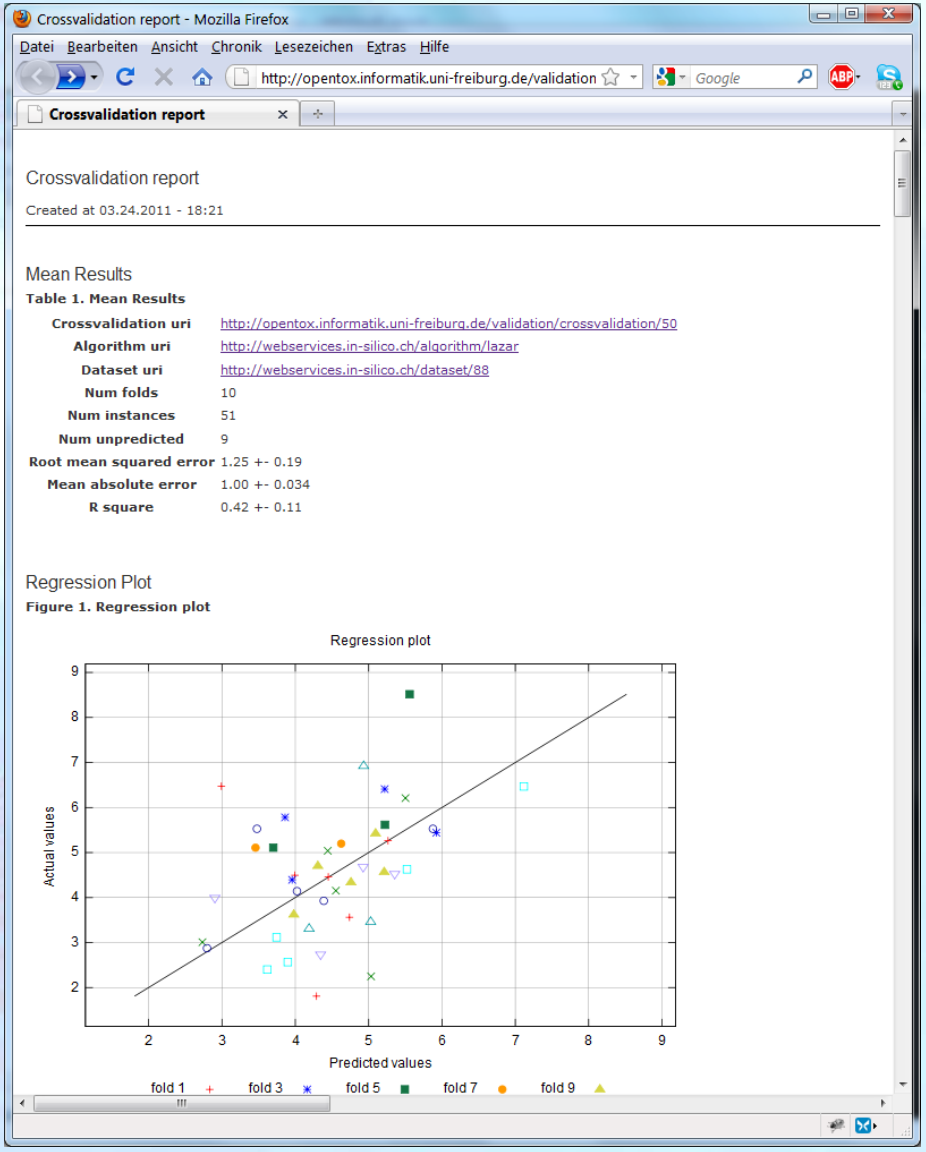

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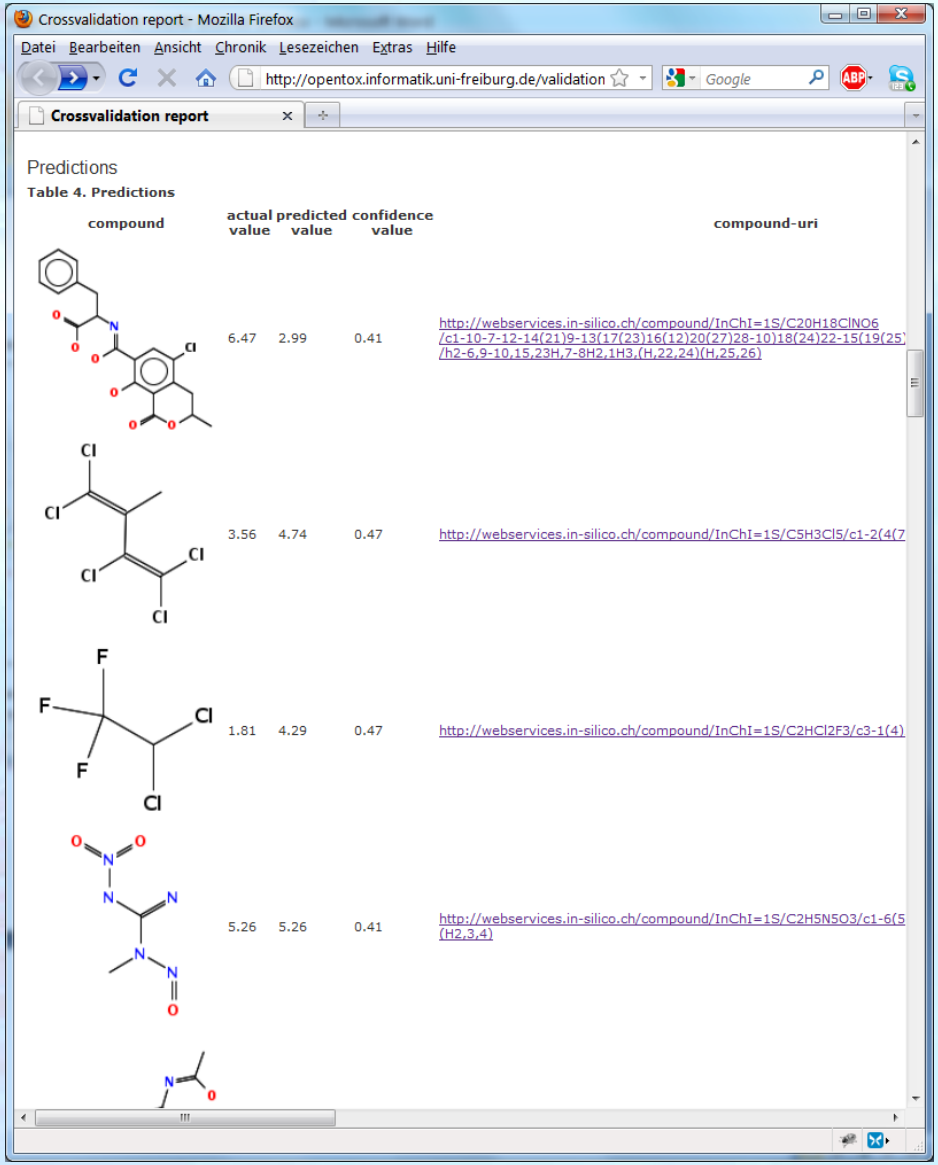

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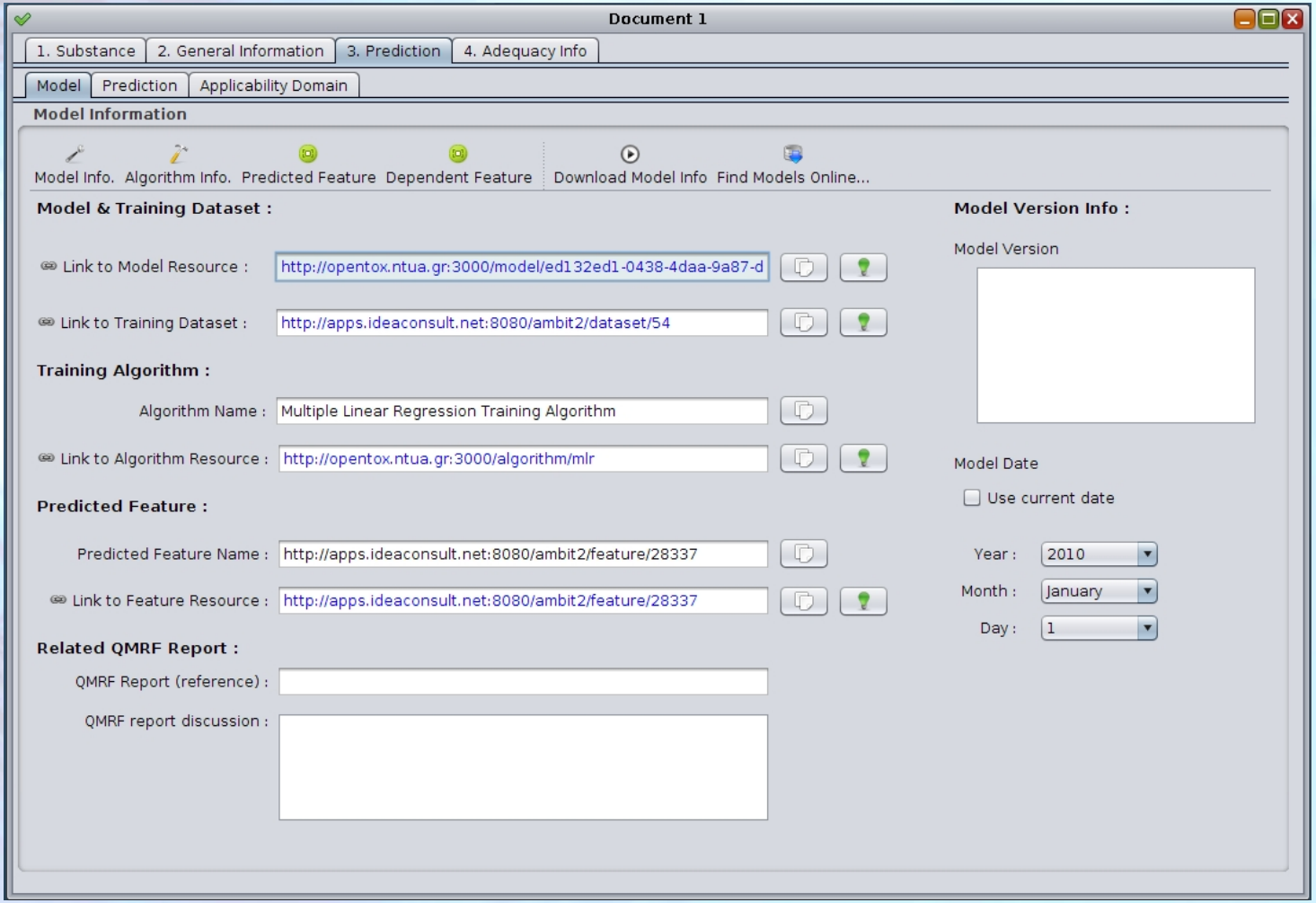
Reporting (Qedit)



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Application by Pantelis Sopasakis (NTUA)

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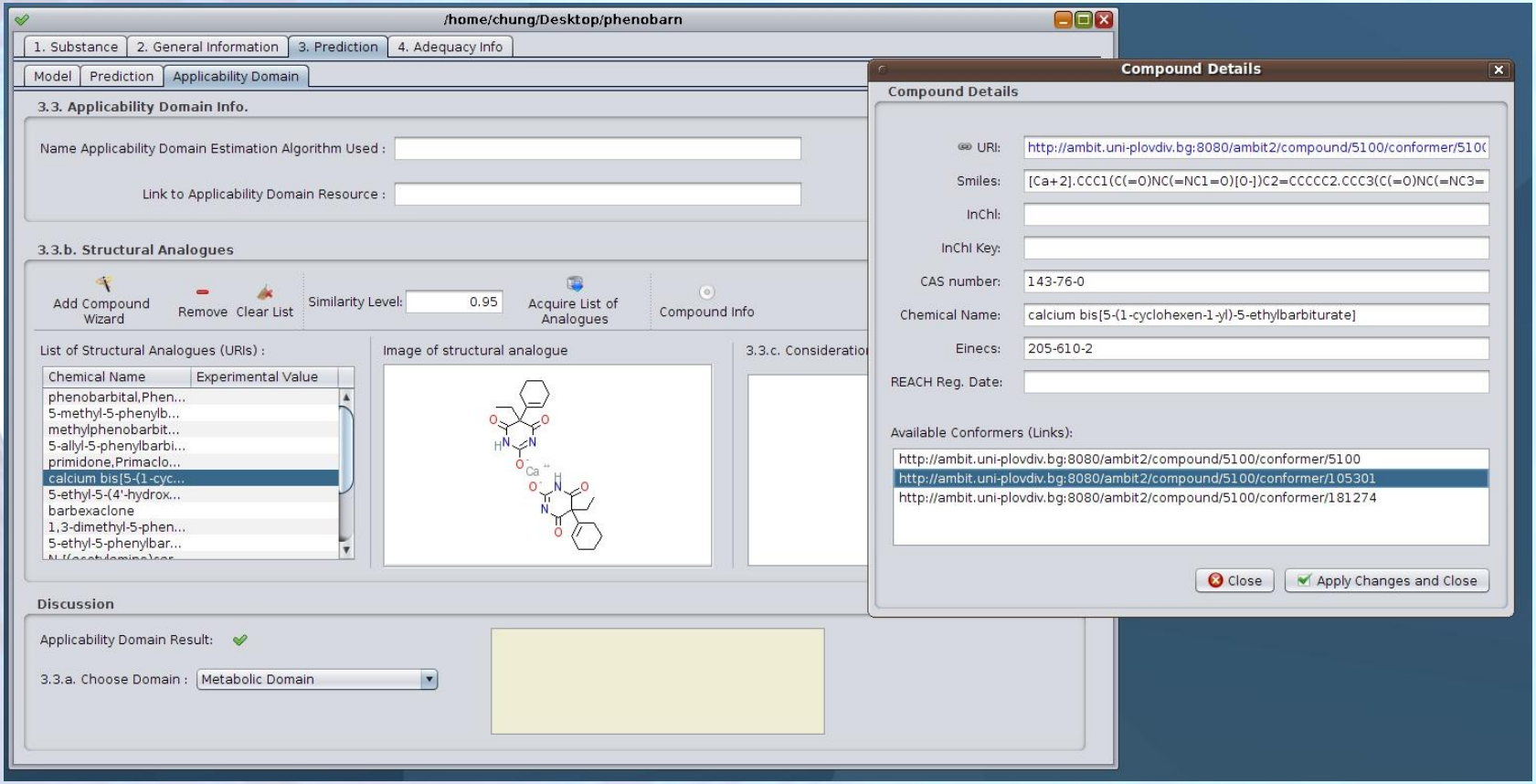

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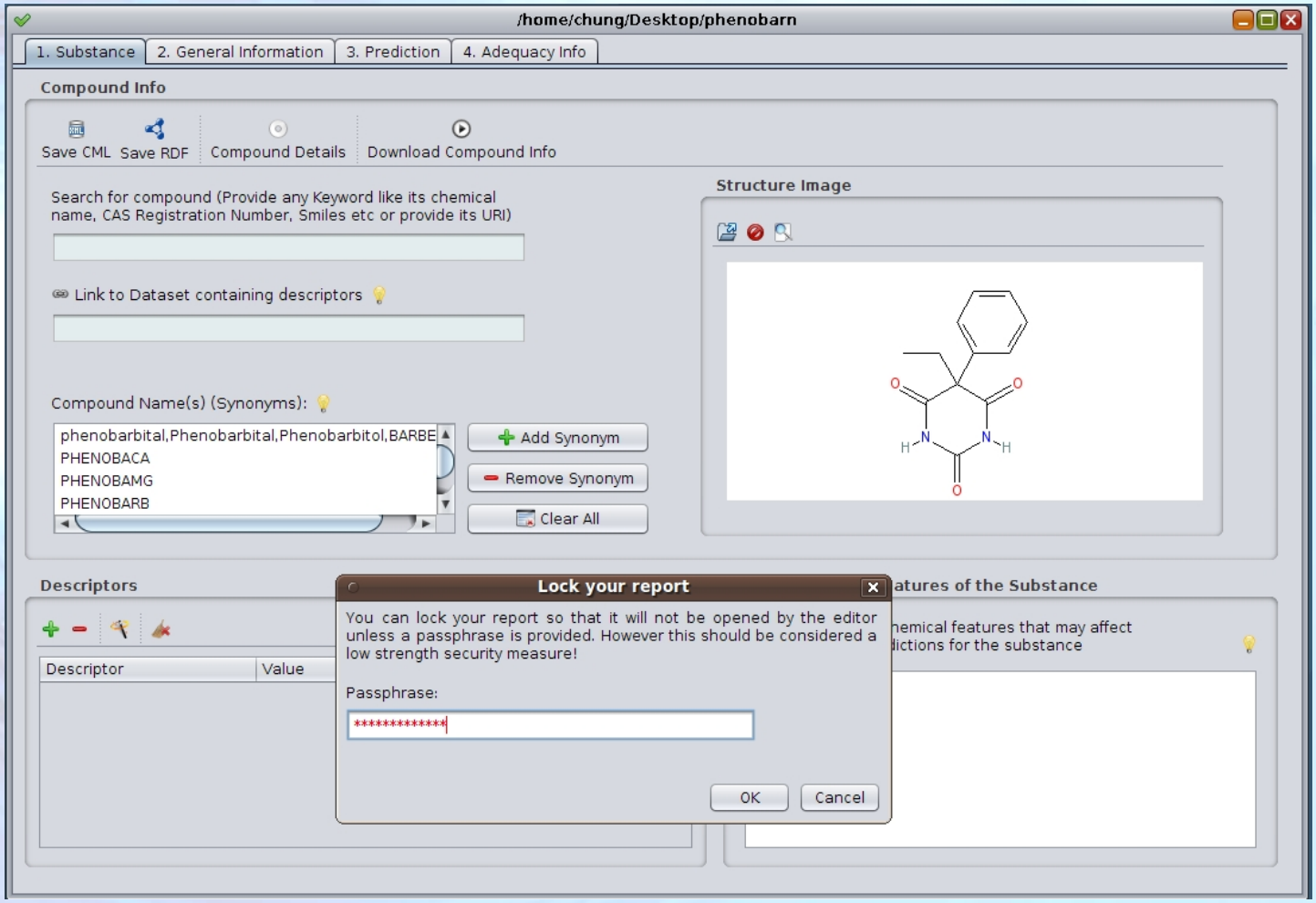

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Application by Pantelis Sopasakis (NTUA)

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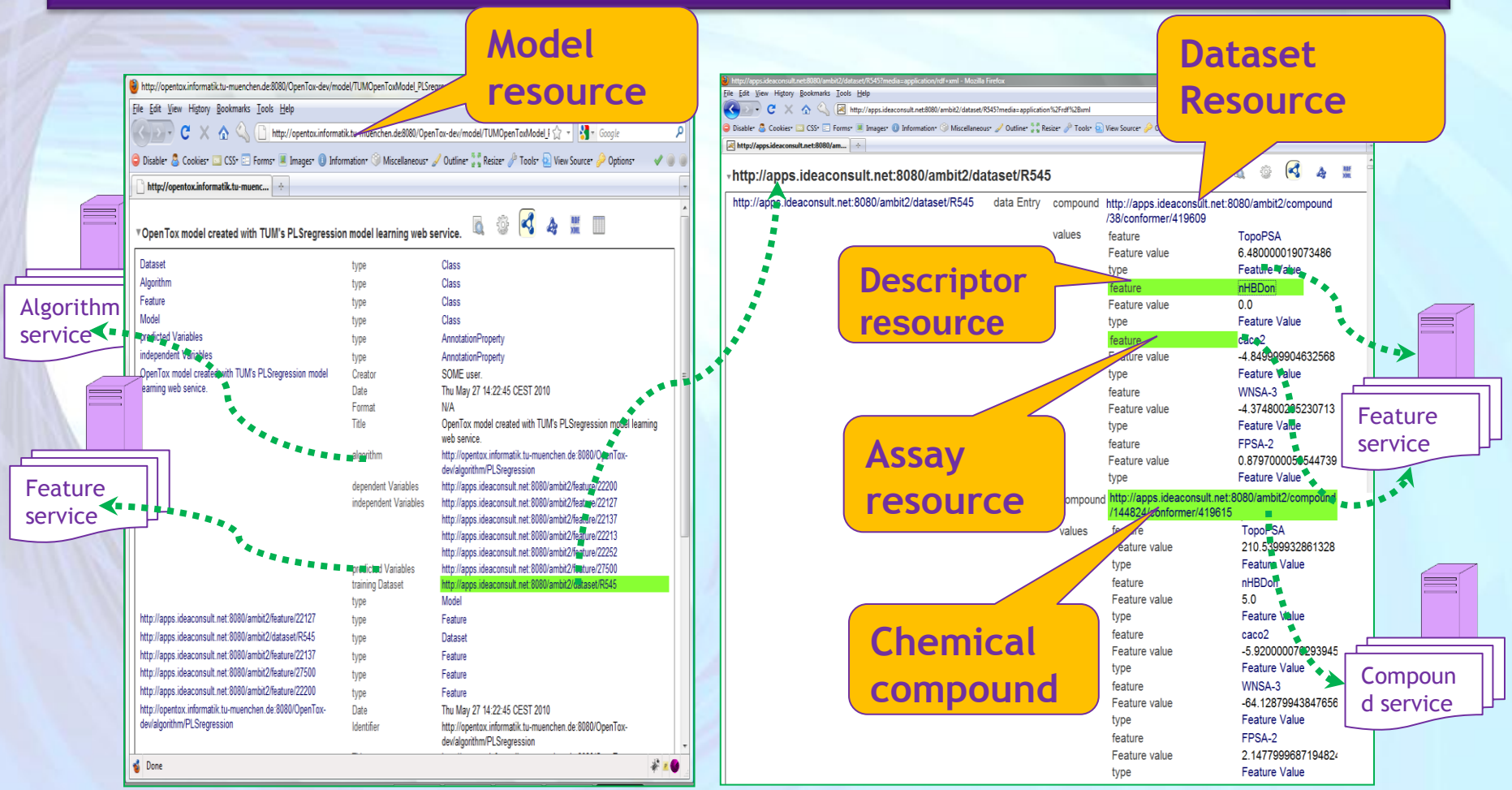
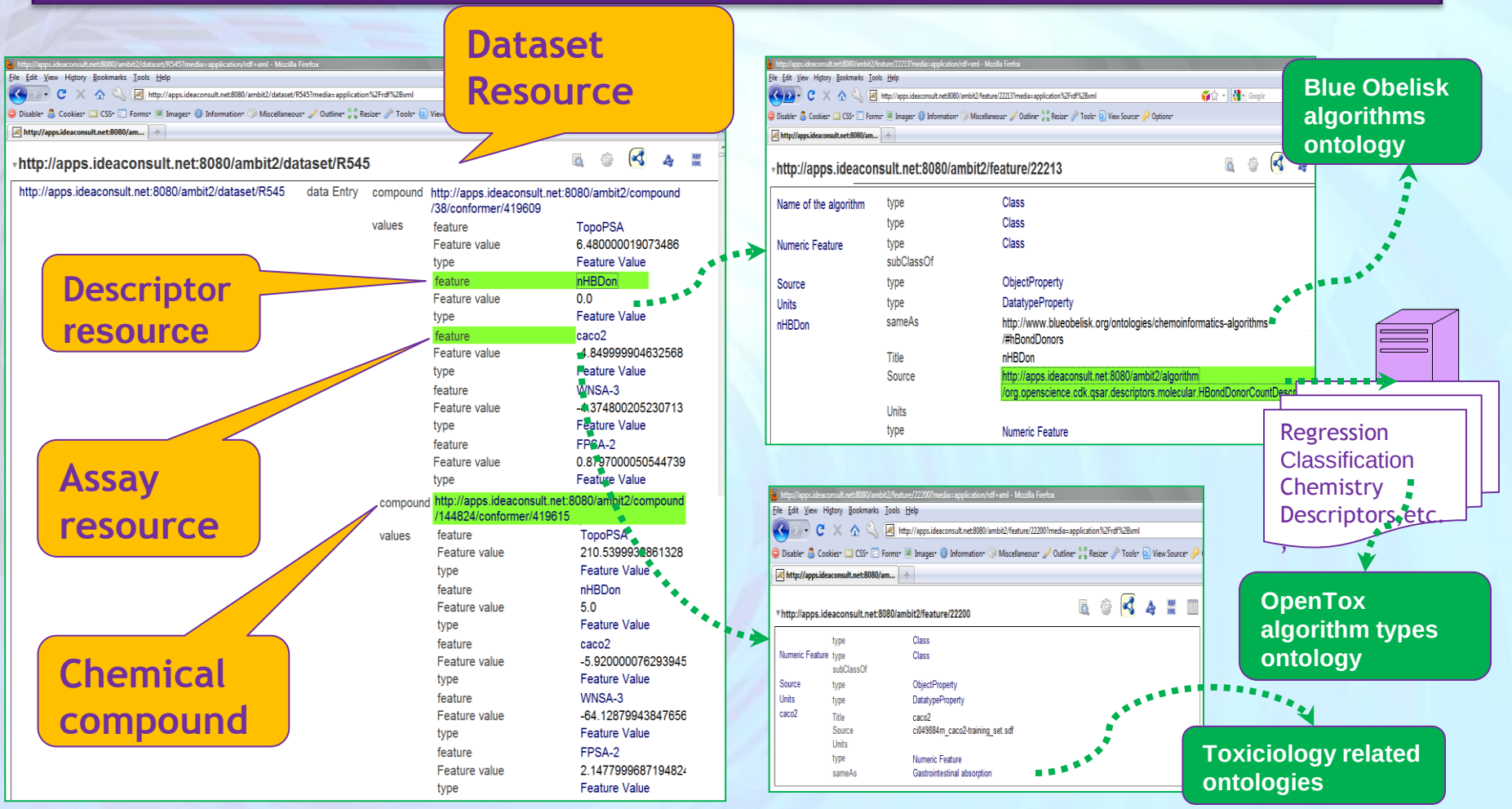
Linked resources: Compound, Algorithm, Model, Dataset, Features

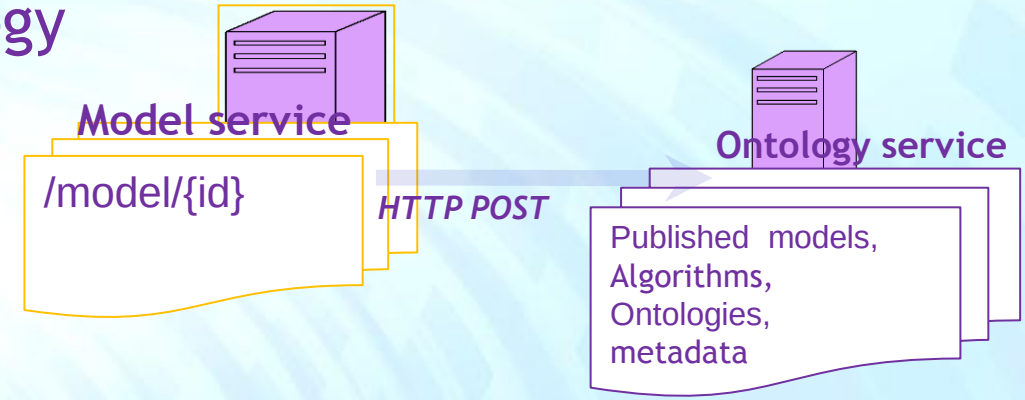


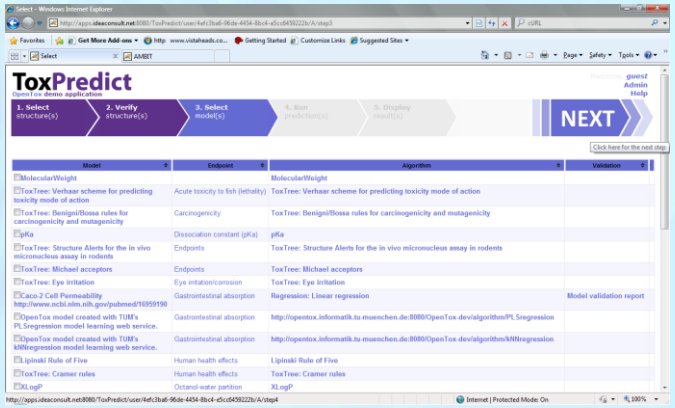
Linked resources:
Compound, Algorithm, Model, Dataset, Features



Make the model available

- Register at OpenTox ontology service
  - RDF triple storage
  - Accepts HTTP POST
  - SPARQL endpoint
- Curl –X POST –d ”uri=http://apps.ideaconsult.net:8080/ambit2/model/57” http://apps.ideaconsult.net:8080/ontology
- Becomes visible for applications





Need for communications in the community overcoming different languages and vocabularies

Explaining the rules of different games on a conservation project trip in the Caprivi, Namibia

From Conservation Project Trip in Caprivi Delta

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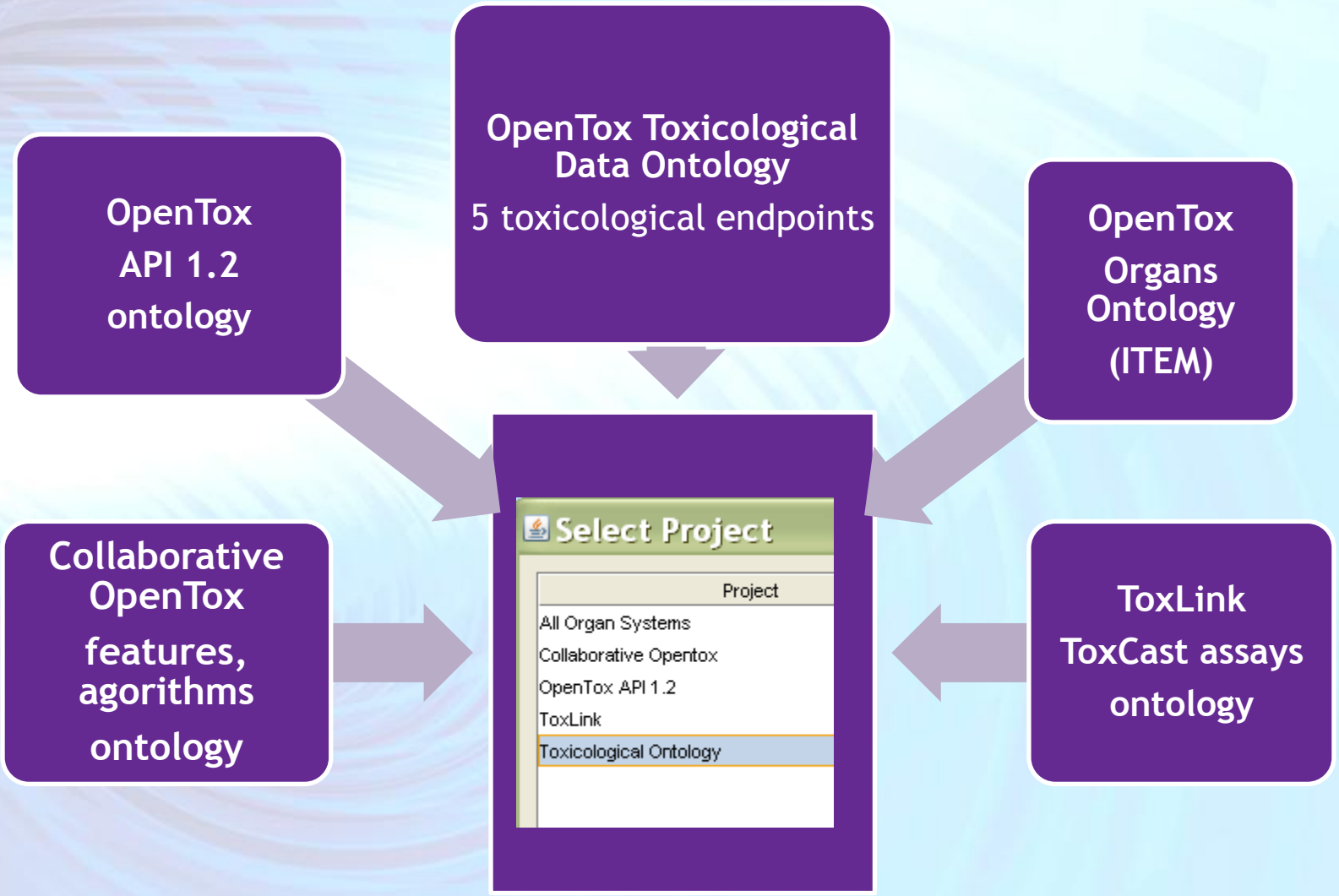
Collaborative Ontology Development: Collaborative Protege Server



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ToxML: conversion in OWL ontology

- Initial work to check out how costly would be to convert ToxML to an OWL ontology
- Why:
- -to integrate the Leadscope databases in the OpenTox service
- -to combine with data coming from different databases (e.g. for complex queries)

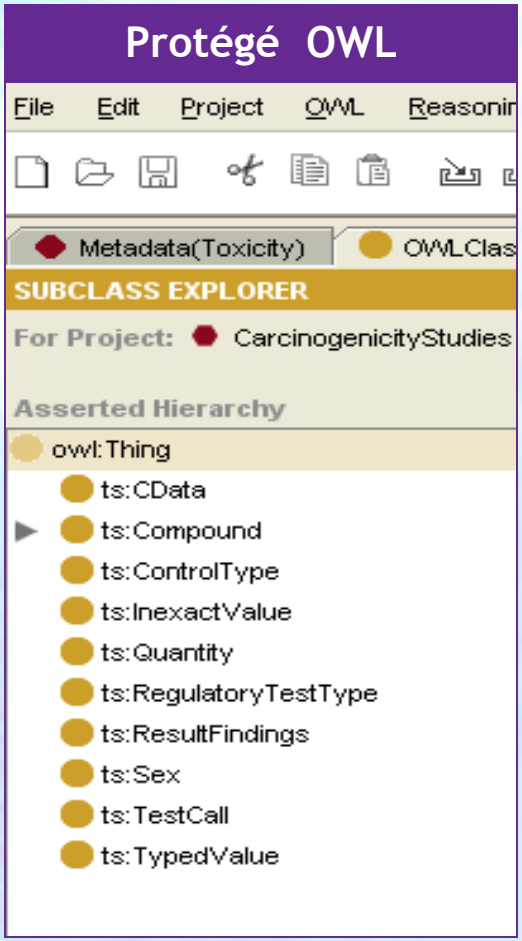
ToxML xsd schema

Procedures:

- each element which doesn't have a type in the schema is converted to an OWL class

each element which has a type in the summary file is considered as a property

the parent relationships are kept



Some parts of the taxonomy may need to be reorganized

Needs for extensions: e.g. target sites, target cells, species are free text fields. Solutions: development extension in OWL, e.g. Organs Ontology has been developed importing of parts of the neighboring ontologies

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www.opentox.org/dev/ontology/collaborative_protege

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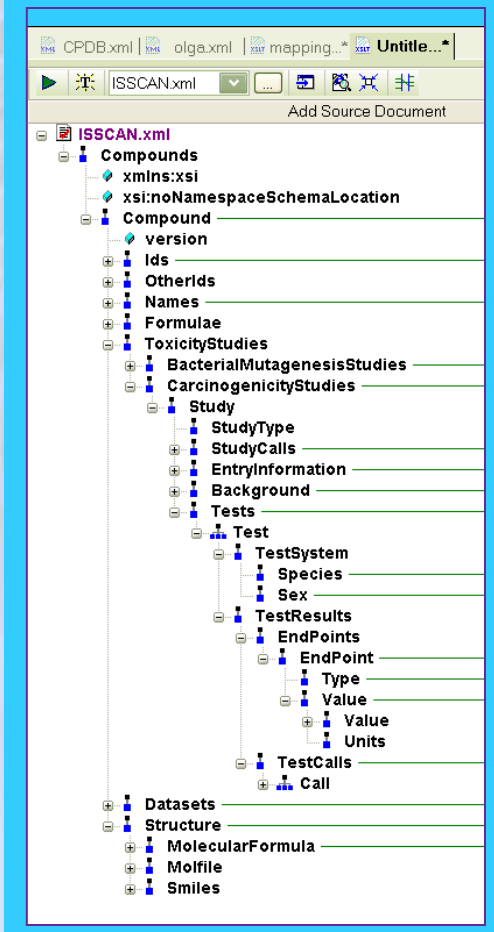
Toxicological Endpoint Ontology Development

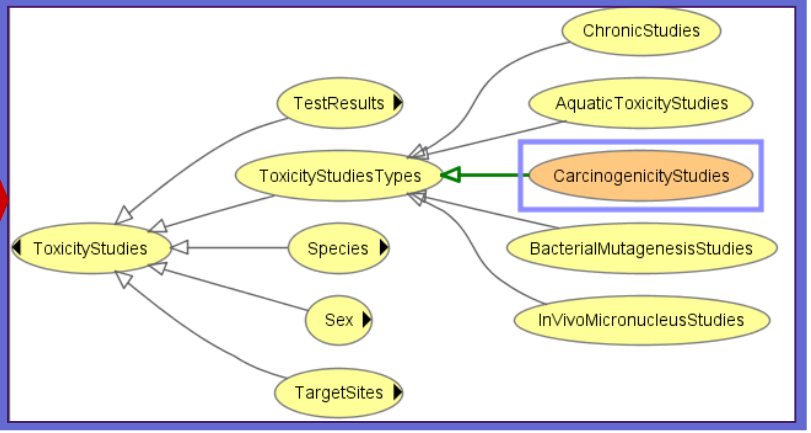
ToxML schema



Other publicly available resources:
DSSTox, GoReni (ITEM), ISSCAN ...

OpenTox Toxicological Endpoint Ontology

Ontology Development



Collaborative Protégé Environment

Re-use of terms defined in neighbouring ontologies (e.g. OBO)

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www.opentox.org/dev/ontology/collaborative_protege

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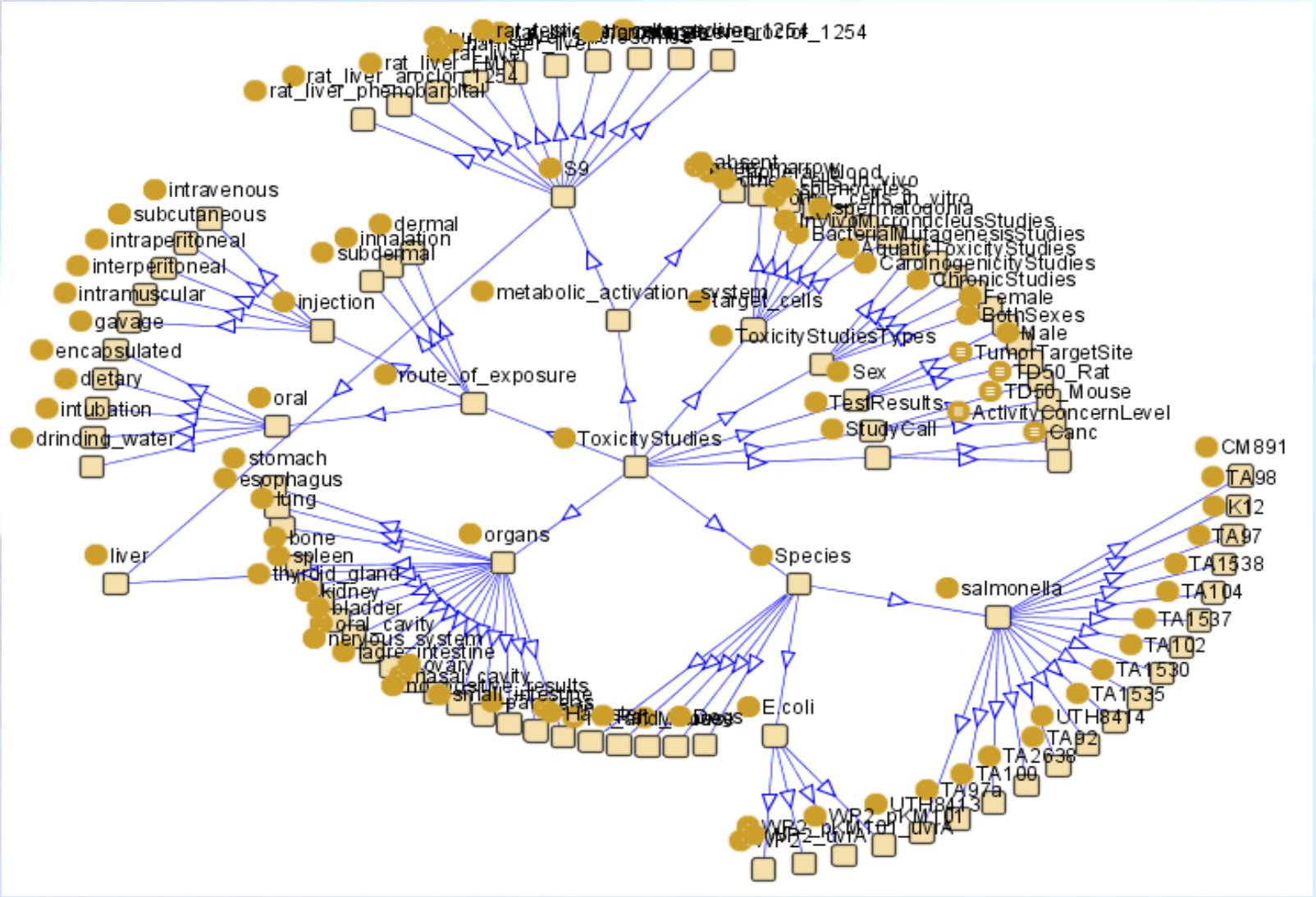
Toxicological Ontology: graphical representation



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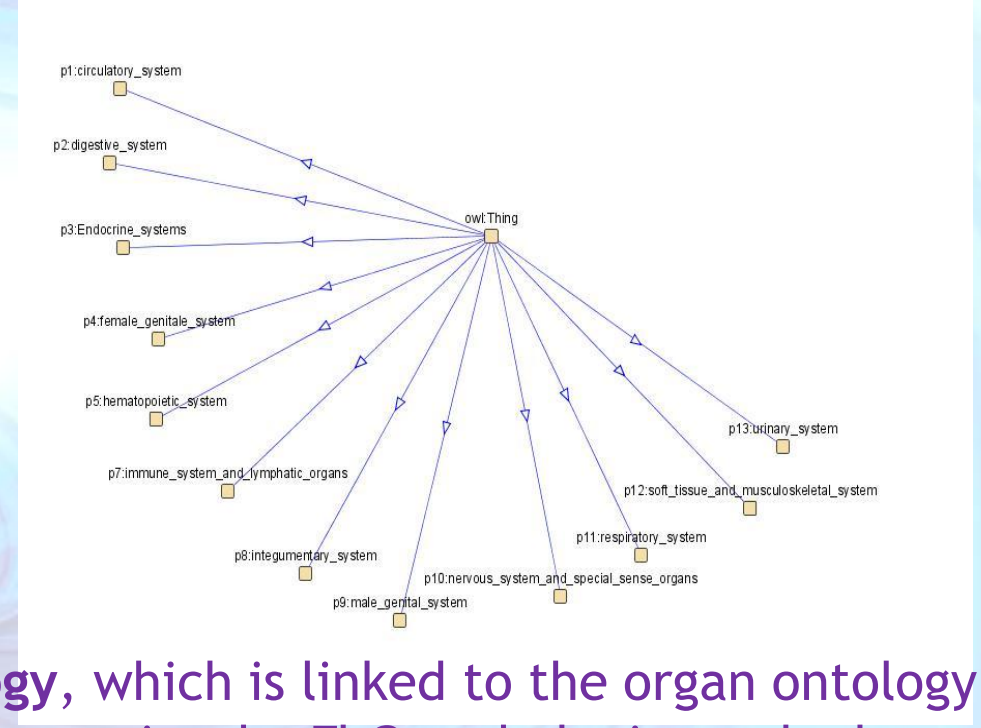
OpenTox Organ Ontology Development

- **organ ontology** consisting of 12 very detailed organ systems



- **effect ontology**, which is linked to the organ ontology
- comprehensive review by FhG pathologists, who have been involved in the INHAND process

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Fraunhofer

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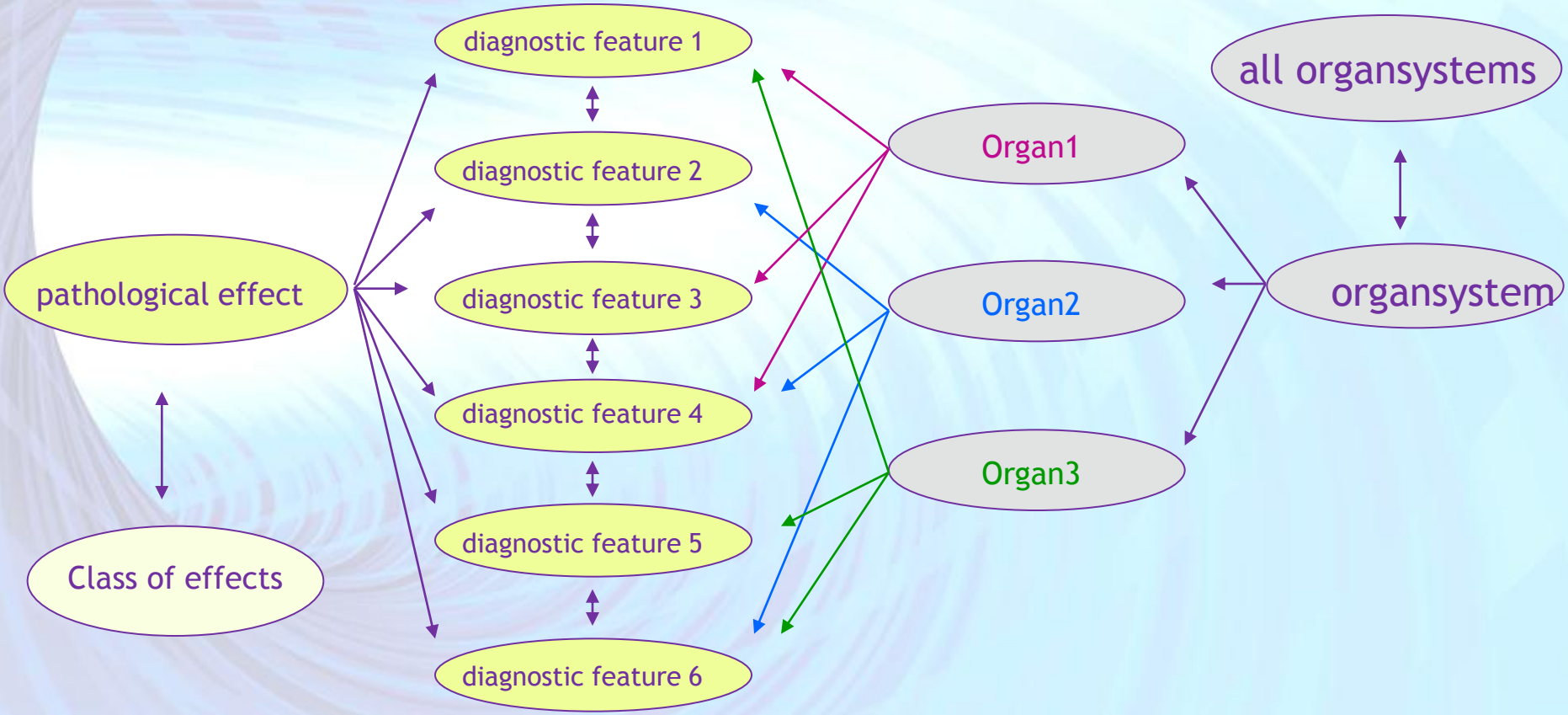


A Toxicology Ontology Roadmap

In Preparation by: Barry Hardy (Douglas Connect and OpenTox), Ian Dix (AstraZeneca & Pistoia Alliance), Sherri Matis-Mitchell (AstraZeneca), David Cook (AstraZeneca), David Heard (Novartis), Dominic Clark (EMBL-EBI), John Overington (EMBL-EBI), Philip Judson (Lhasa), David Watson (Lhasa), Anne Hersey (EMBL-EBI), Andrew White (Unilever), Loca Toldo (Merck KGaA), Gordana Apic (Cambridge Cell Networks), Imran Shah (US EPA), Chihae Yang (Altamira), Dave Bower (Leadscope), Ola Spjuth (Univ Uppsala), Janna Hastings (EMBL-EBI), Philip Carthew (Unilever), ----

Based on Proceedings from the **Toxicology Ontology Roadmap Workshop**

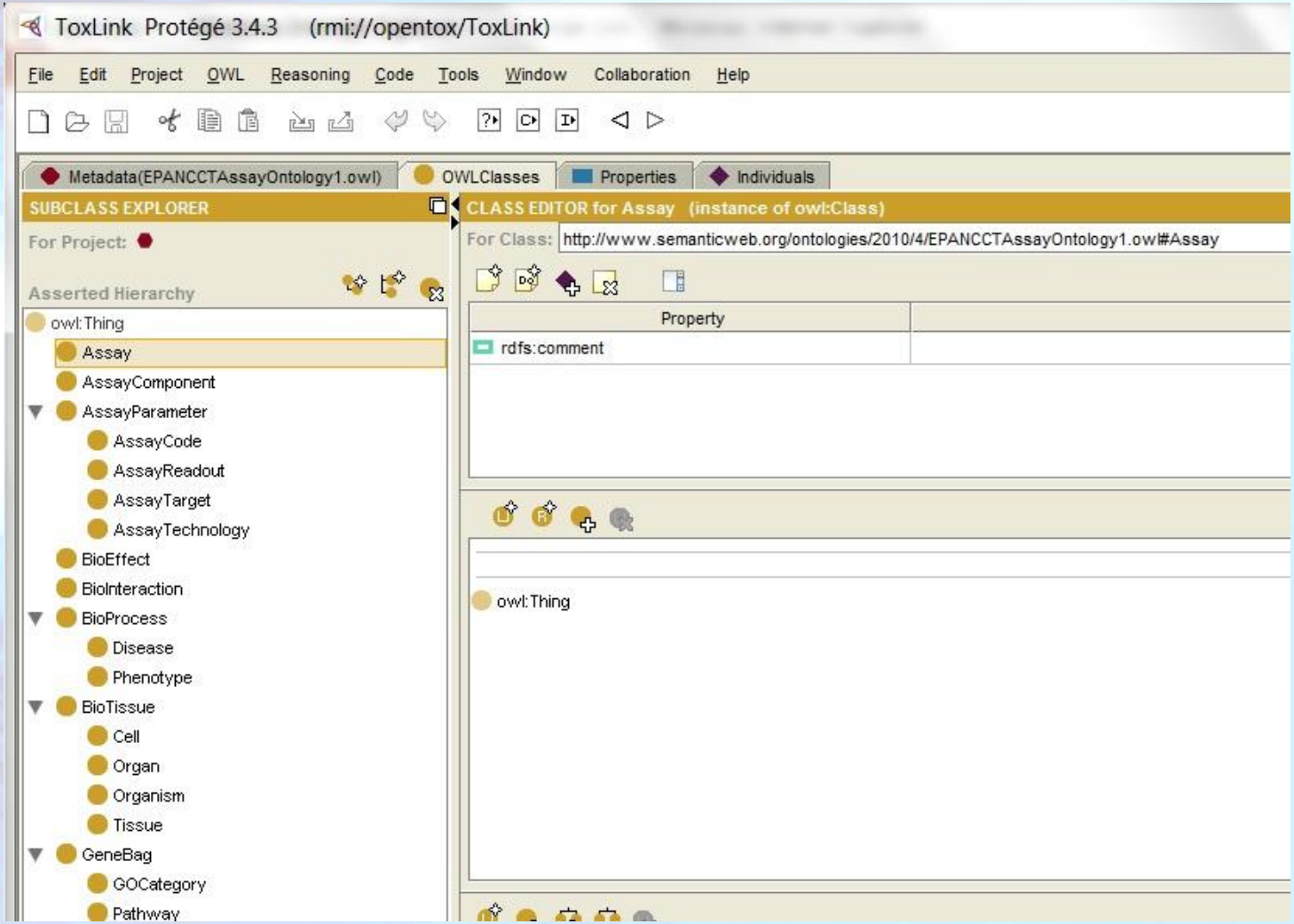
EMBL-EBI Industry Programme Workshop

16 -17th November 2010, Hinxton, UK

OpenTox

SEVENTH FRAMEWORK PROGRAMME

ToxLink: ToxCast Ontology



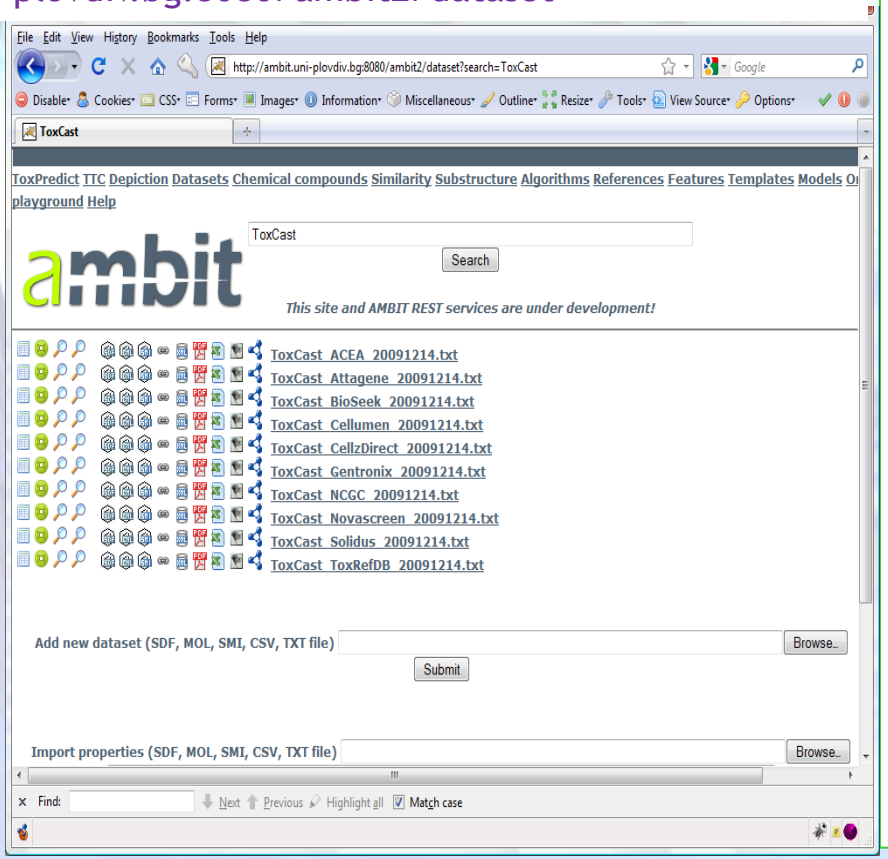
OpenTox

www.opentox.org/dev/ontology/collaborative_protege

SEVENTH FRAMEWORK PROGRAMME

Example: ToxCast

Dataset service at http://ambit.uni-plovdiv.bg:8080/ambit2/dataset



Query an OpenTox ontology service at http://ambit.uni-plovdiv.bg:8082/ontology

```
PREFIX ot:<http://www.opentox.org/api/1.1#>
PREFIX ota:<http://www.opentox.org/algorithms.owl#>
PREFIX owl:<http://www.w3.org/2002/07/owl#>
PREFIX dc:<http://purl.org/dc/elements/1.1/>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX rdf:<http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX otee:<http://www.opentox.org/echaEndpoints.owl#>
PREFIX toxcast:<http://www.opentox.org/toxcast#>
                select *
                where {
                ?Feature rdf:type ot:Feature.
  {?Feature dc:title ?title}.
  {?Feature owl:sameAs ?assay}.
  {?assay toxcast:gene ?geneid}.
  {?assay toxcast:hasProperty ?species}.
  {?species rdf:type toxcast:SPECIES}.
  {?assay toxcast:hasProperty ?target_source}.
  {?target_source rdf:type toxcast:ASSAY_TARGET_SOURCE}
  {?assay toxcast:hasProperty ?target_family}.
  {?target_family rdf:type toxcast:ASSAY_TARGET_FAMILY}.
  {?assay toxcast:hasProperty ?target}.
  {?target rdf:type toxcast:ASSAY_TARGET}.
   {?assay toxcast:hasProperty toxcast:Cytochrome_P450}.
                }
order by ?feature ?assay ?target
```

OpenTox

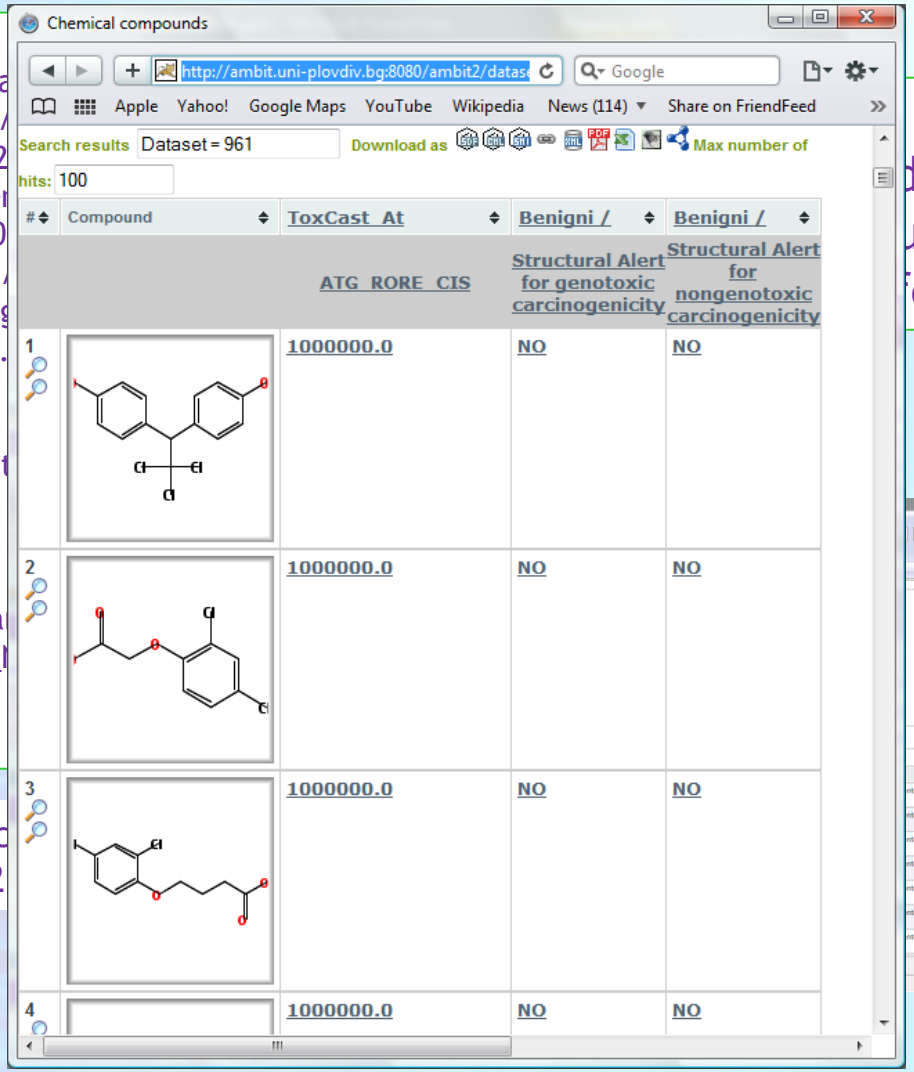
SEVENTH FRAMEWORK PROGRAMME

Example: ToxCast

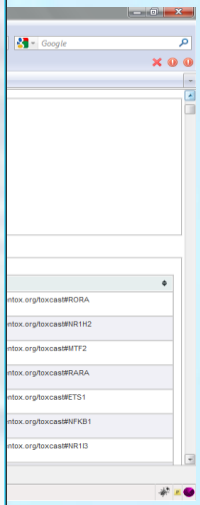
```
PREFIX ot:<http://www.opentox.org/a
PREFIX ota:<http://www.opentox.org/
PREFIX owl:<http://www.w3.org/2002
PREFIX dc:<http://purl.org/dc/elemer
PREFIX rdfs: <http://www.w3.org/200
PREFIX rdf:<http://www.w3.org/1999/
PREFIX otee:<http://www.opentox.org
PREFIX toxcast:<http://www.opentox.
                select ?Feature ?title ?id
                where {
                ?Feature rdf:type ot:Feat
  {?Feature dc:title ?title}.
  {?Feature owl:sameAs ?assay}.
  {?assay toxcast:gene ?geneid}.
  {?assay toxcast:hasProperty ?genena
  {?genename rdf:type toxcast:GENE_

                }
```

Query an OpenTox ontology servic
http://ambit.uni-plovdiv.bg:8082



dataset/961?feat
uni-
feature/335126



OpenTox

SEVENTH FRAMEWORK PROGRAMME

OpenToxipedia

OpenTox

Barry Hardy Log out Quicktools Site Setup Help

Site Map Accessibility Contact Data

Search Site

Home Toxicity Prediction OpenTox Blog People Partners Development OpenToxipedia

User Guidance Latest Entries A B C D E F G H I J K L M N O P Q R S T U V W X Y Z by Categories Entries OpenToxipedia

You are here: Home » OpenToxipedia

Contents View Edit Rules Sharing History

Actions ▾ Display ▾ Add new... ▾ State: Published ▾

OpenToxipedia

by **Barry Hardy** — last modified Sep 03, 2009 01:09 PM

OpenTox Community Resource for Toxicology Vocabulary and Ontology

OpenTox is supporting the creation and curation of OpenToxipedia, a community-based predictive toxicology knowledge resource. All members of the community are welcome to provide entries, suggested definiton edits or additional information to entries in the resource.

OpenTox is supporting the application and development of the **ToxML** standard for representation of toxicology data, the **OECD principles for (Q)SAR model validation**, and the use of the **OECD HT** standard for regulatory reporting purposes.

OpenToxipedia provides here a Vocabulary Resource of toxicology terminology. We hope you find the resource useful and consider contributing to terms and their content.

Guidance for Vocabulary Resource entries

www.opentox.org/opentoxipedia

OpenTox

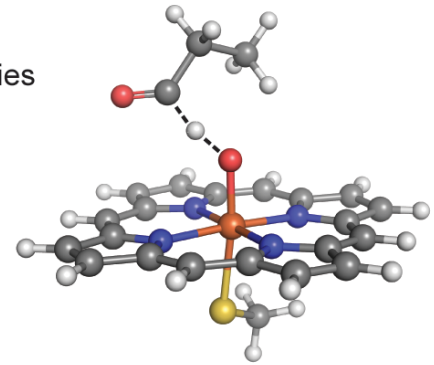
SEVENTH FRAMEWORK PROGRAMME

SMARTCyp Service for Predicting Metabolites

Atom Reactivity Library

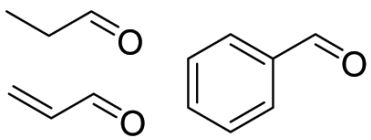
A. Calculate Quantum Chemical Reference Energies

Calculate transition state energies using density functional theory



B. Define SMARTS Rules

Group calculations by fragments and calculate average energies

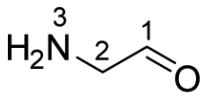


[CX3H1](=O)[#6]

40.2 kJ/mol

SMARTCyp

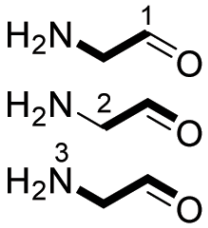
1. Assign Energies By SMARTS matching



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

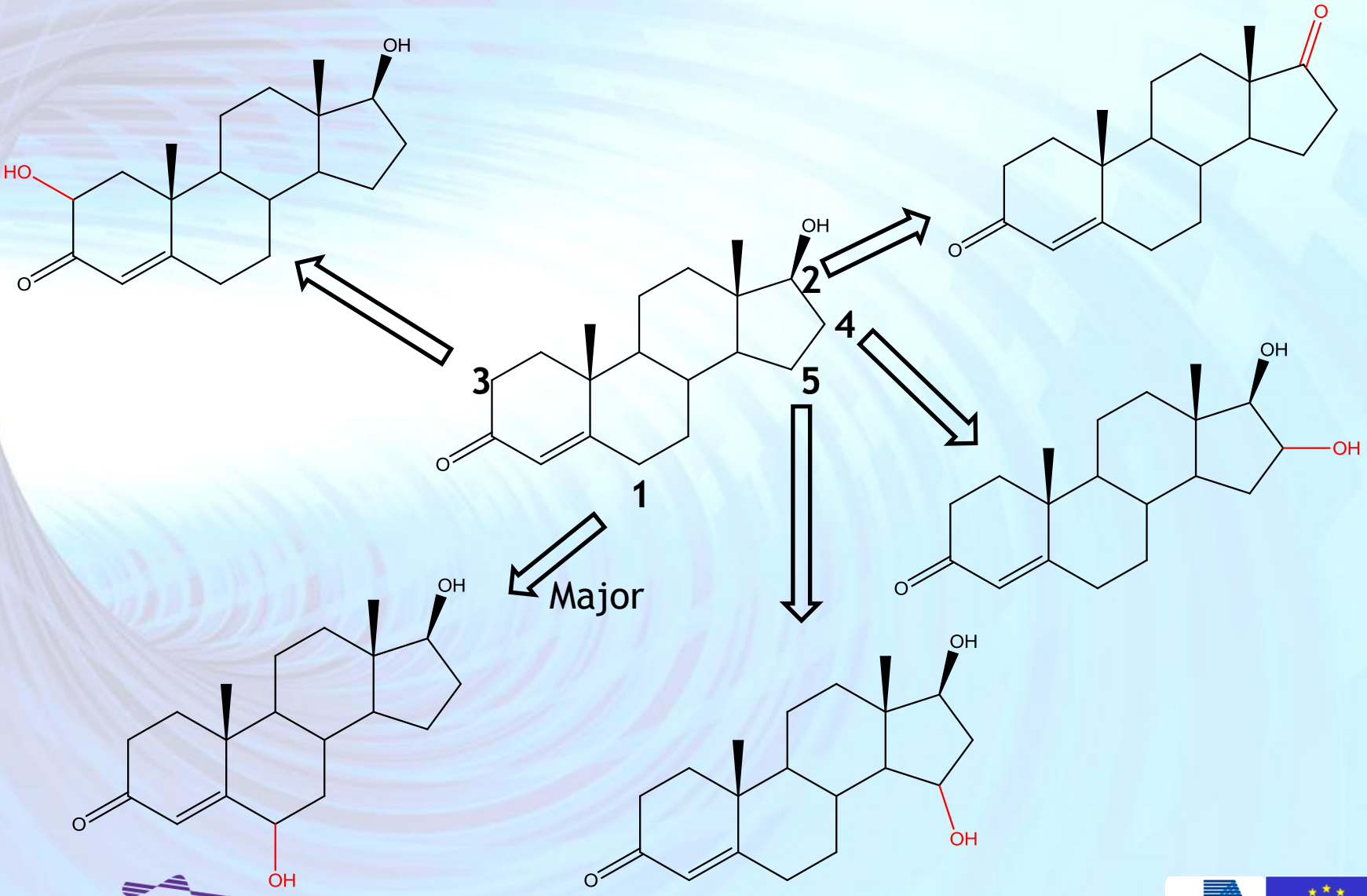
Atom 3 - Rank 3

SMARTCyp - developed by Patrik Rydberg, University of Copenhagen

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

OpenTox

SmartCYP Prediction of Testosterone Metabolites



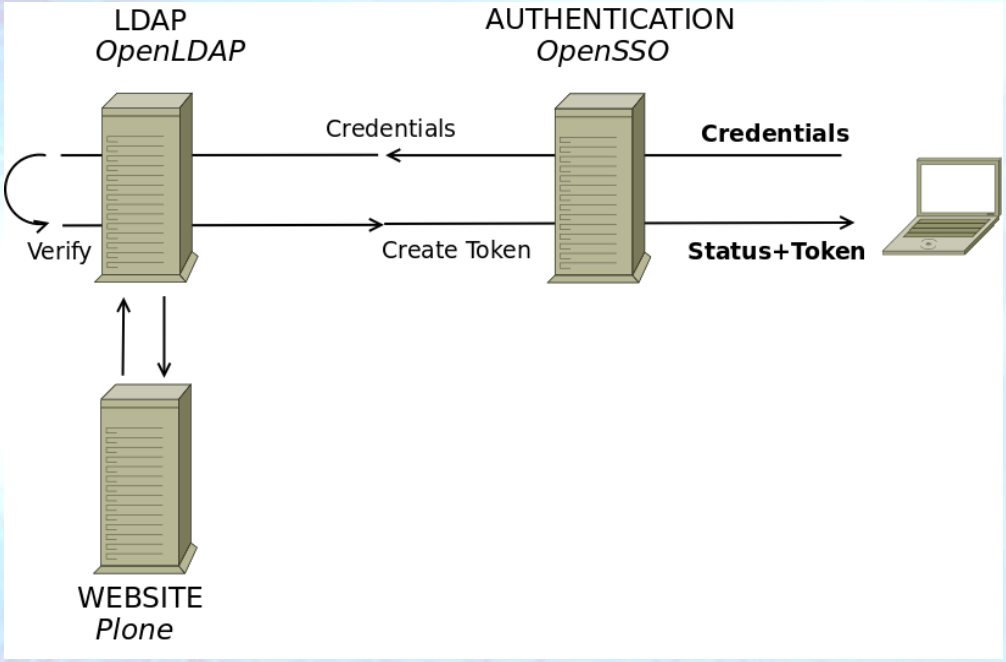
OpenTox

Controlling Access to Confidential Information

- OpenTox makes resources available through URIs
- OpenTox provides facilities to protect confidential information located at URIs. Two tasks are involved here:
  - Authentication: Confirming the identity of the user requesting access
  - Authorisation: Granting the confirmed identity access according to a set of restrictions described in policies

SEVENTH FRAMEWORK PROGRAMME

Authentication

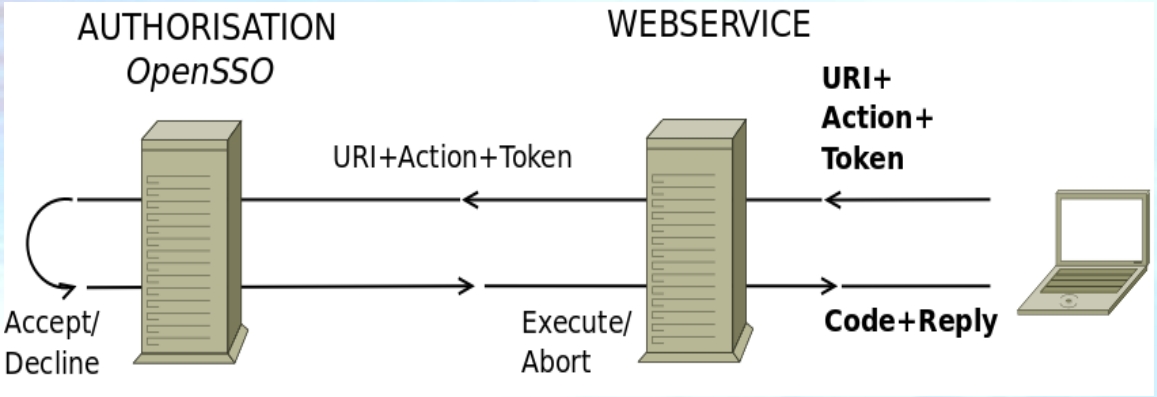


- Registered users are instantly available as potential users of OpenTox web services
- Users receive a token upon service request

OpenTox

SEVENTH FRAMEWORK PROGRAMME

Authorisation

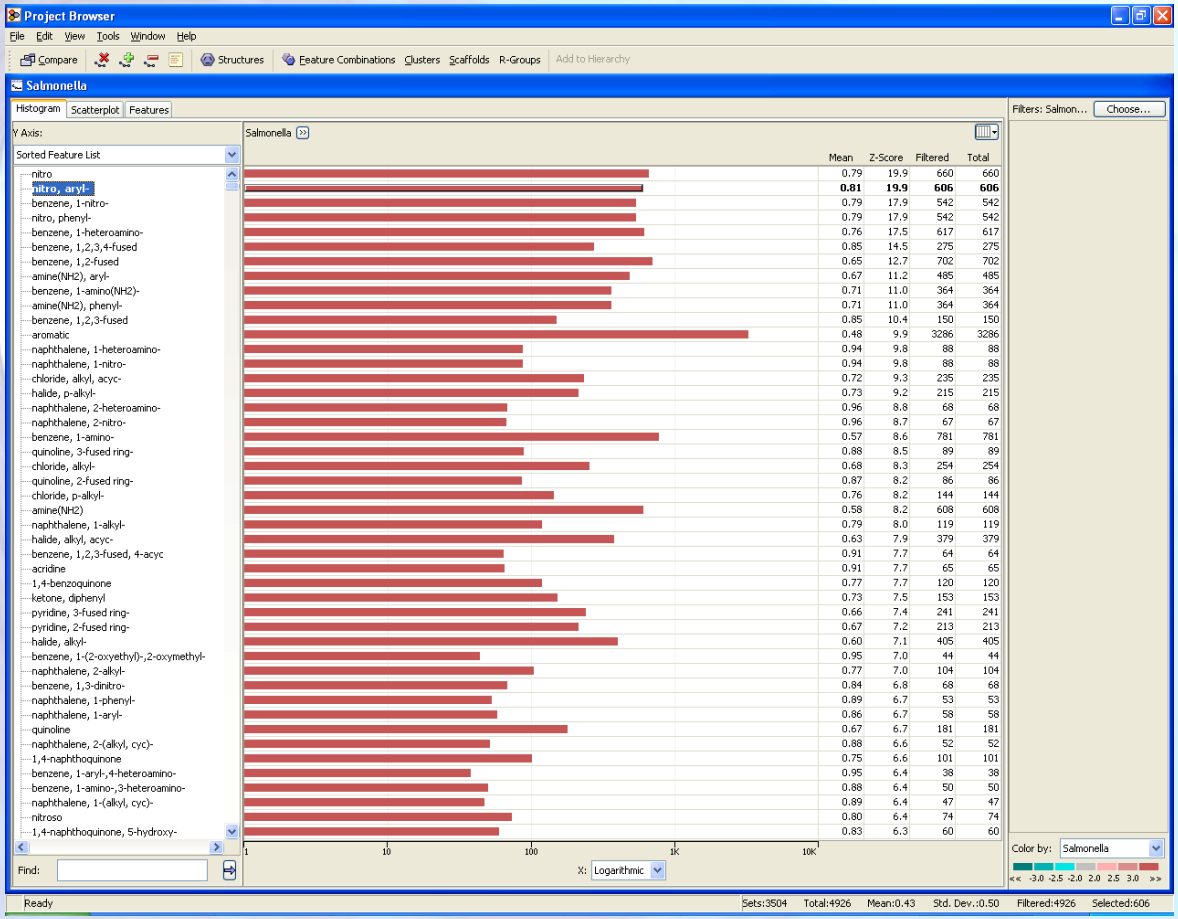


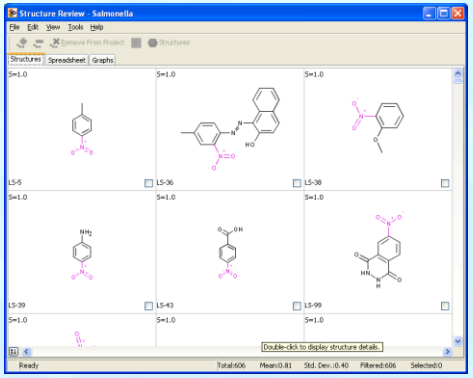
- Tokens encode user identity
- Tokens are valid for a certain time period only (customizable)
- The triplet URI+Action+Token makes up the call to be authorised
- All messages are encrypted (SSL)
- Resource Owners create and modify policies defining access rules

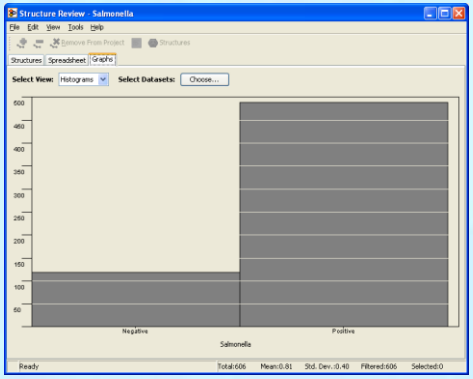
OpenTox

SEVENTH FRAMEWORK PROGRAMME

OpenTox - Leadscope



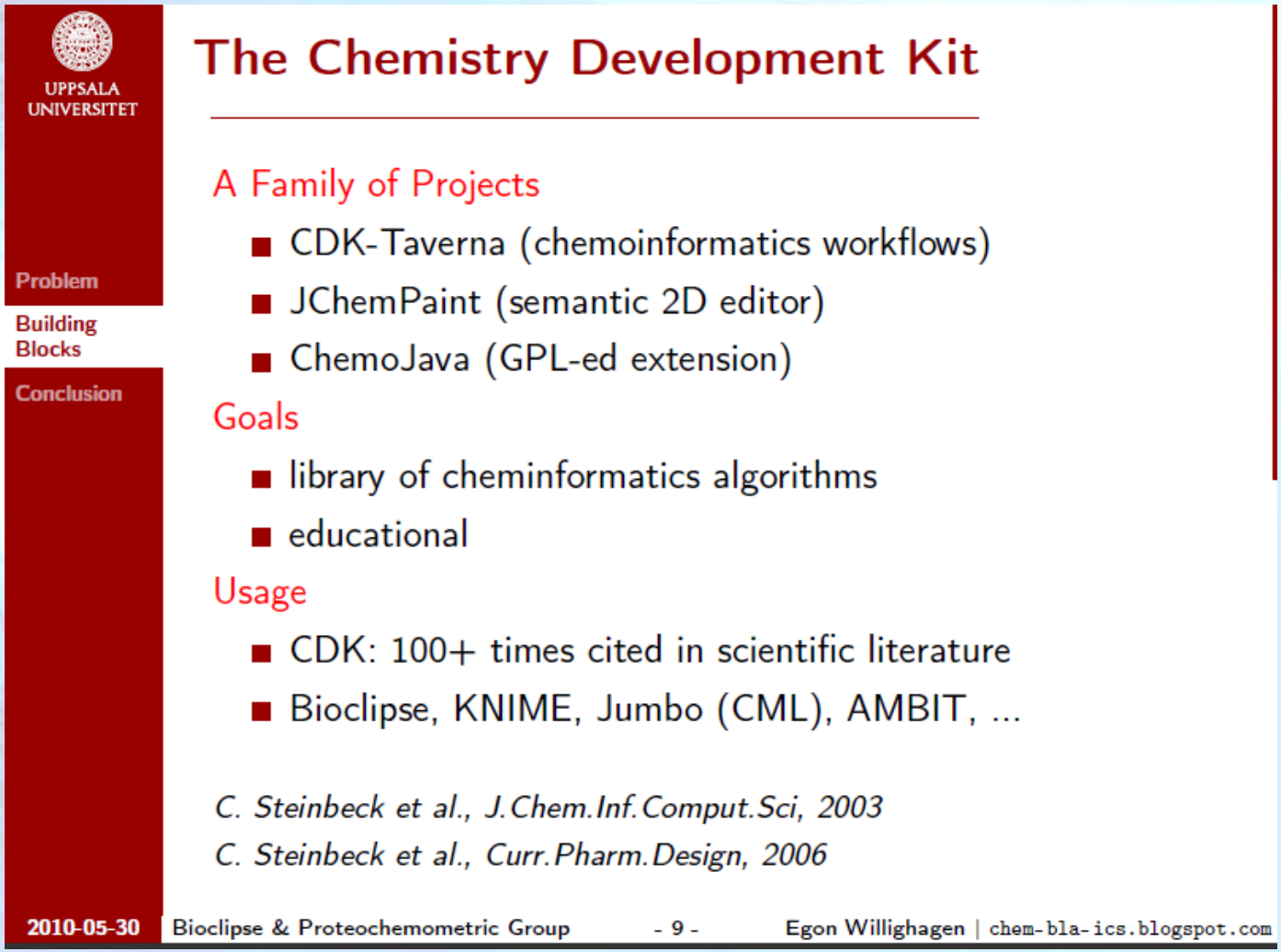




OpenTox

SEVENTH FRAMEWORK PROGRAMME

OpenTox - CDK



OpenTox

SEVENTH FRAMEWORK PROGRAMME

OpenTox - Bioclipse

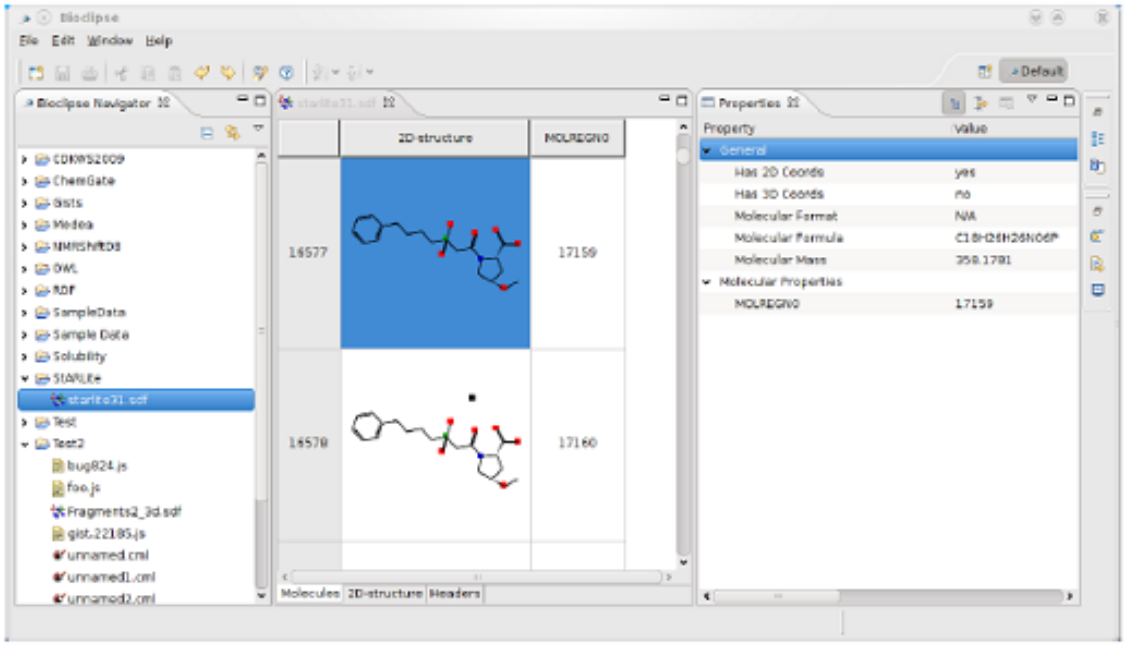
UPPSALA UNIVERSITET

Problem

Building Blocks

Conclusion

Bioclipse

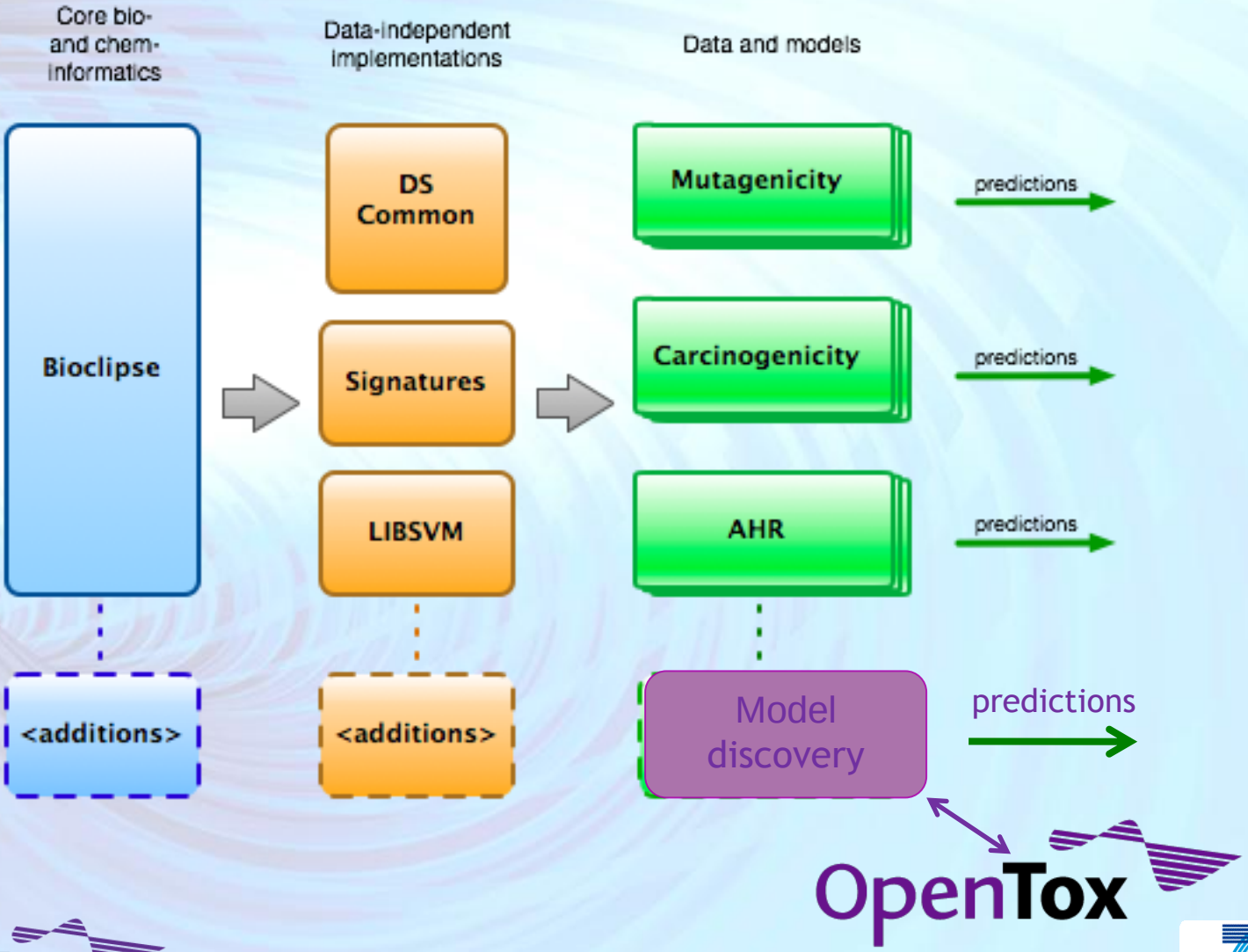


O. Spjuth et al., BMC Bioinformatics 2007, 8:59

OpenTox

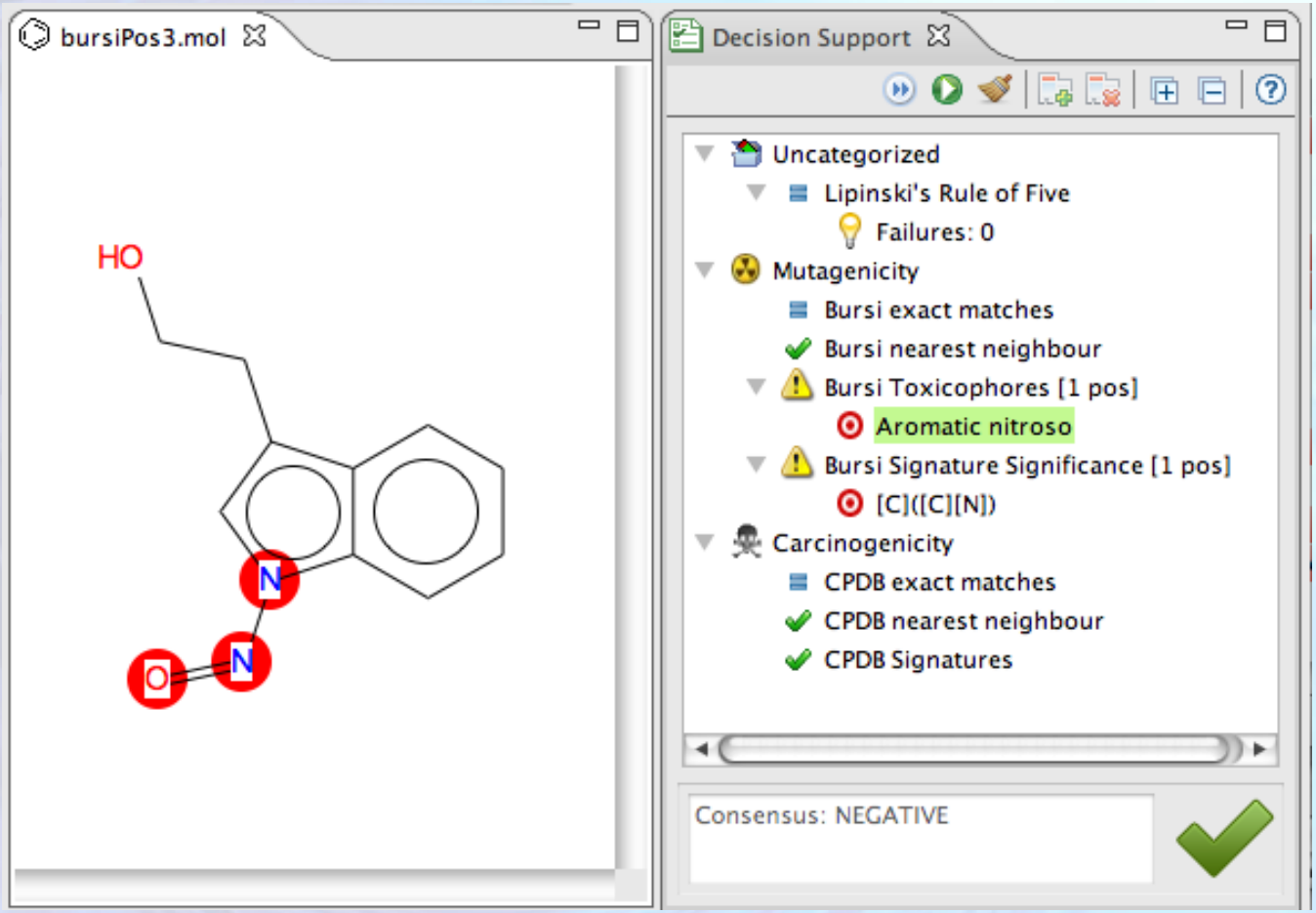
SEVENTH FRAMEWORK PROGRAMME

Bioclipse - OpenTox Interoperation



OpenTox

Bioclipse Visualisation Workbench

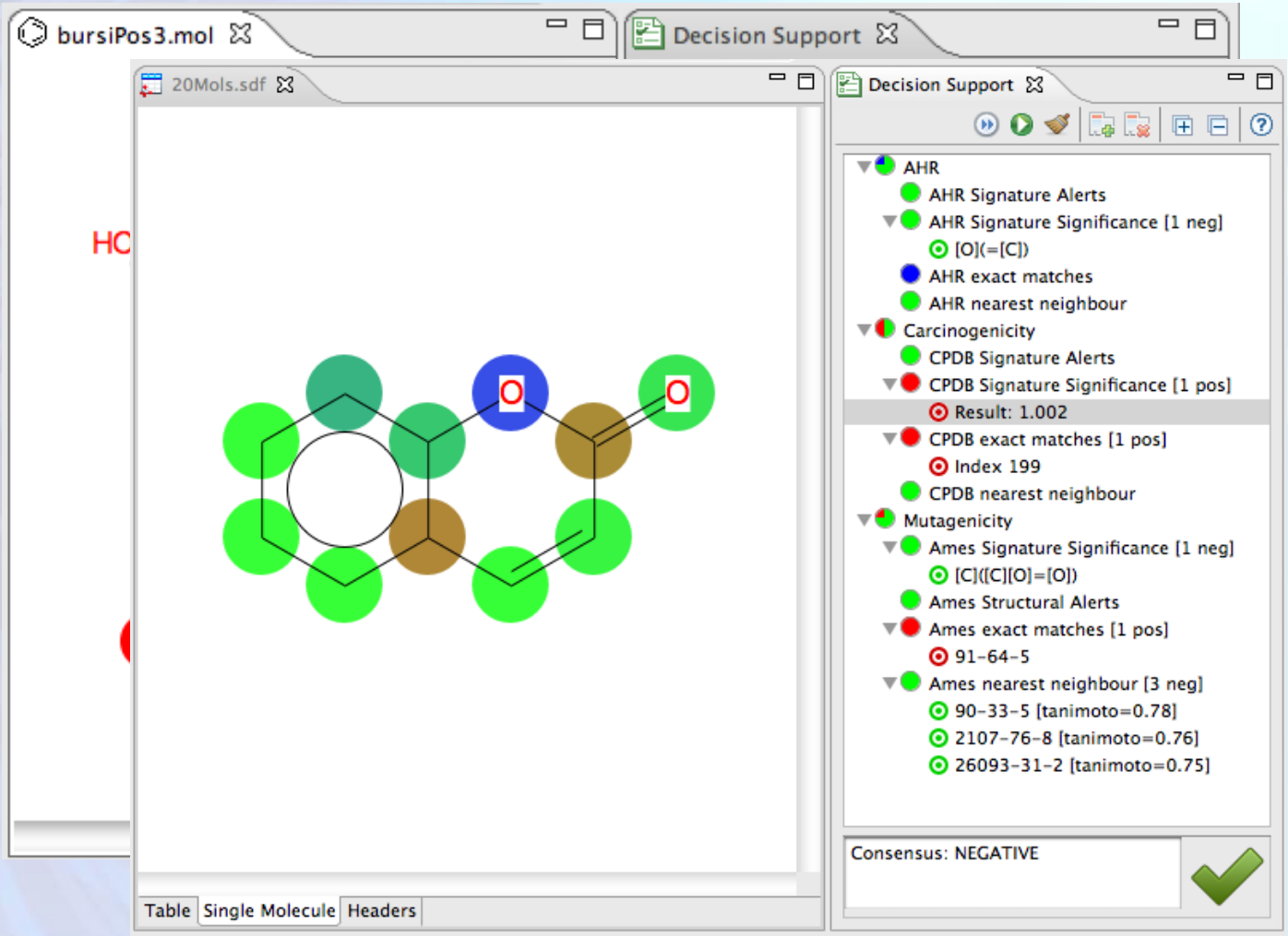


OpenTox

O. Spjuth, L. Carlsson, M. Eklund, E. Ahlberg Helgee, and Scott Boyer. *Integrated decision support for assessing chemical liabilities*. In preparation

SEVENTH FRAMEWORK PROGRAMME

Bioclipse Visualisation Workbench



OpenTox

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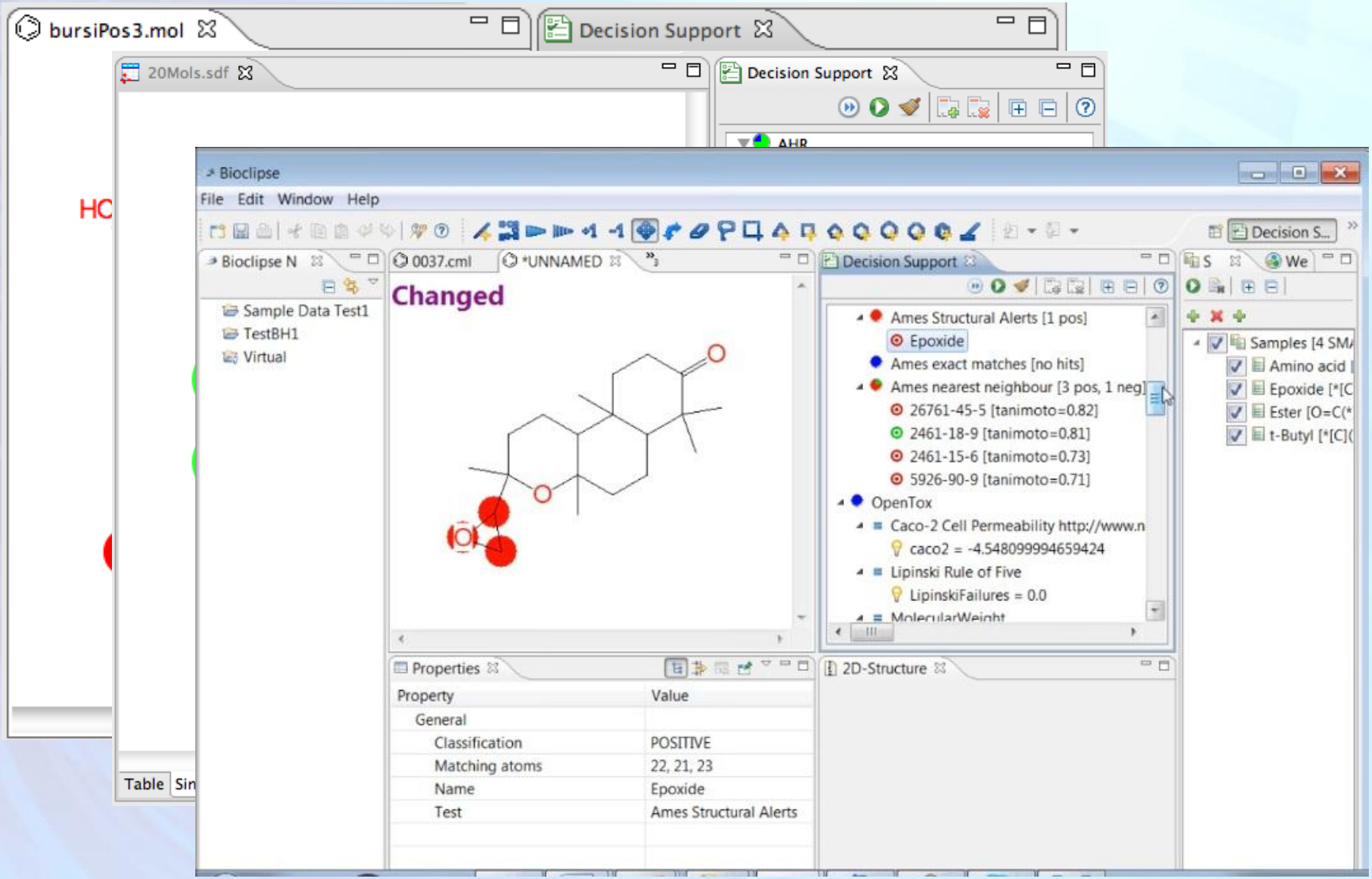
SEVENTH FRAMEWORK PROGRAMME

Bioclipse Visualisation Workbench - OpenTox

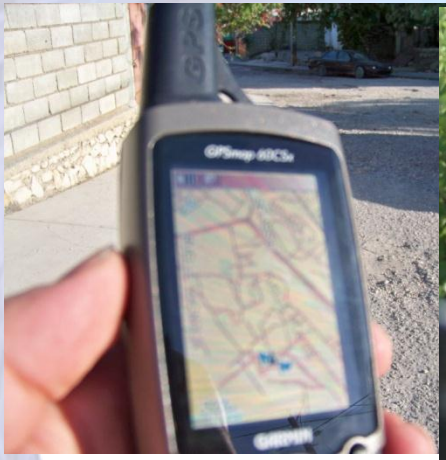


OpenTox

O. Spjuth, L. Carlsson, M. Eklund, E. Ahlberg Helgee, and Scott Boyer. *Integrated decision support for assessing chemical liabilities*. In preparation

SEVENTH FRAMEWORK PROGRAMME

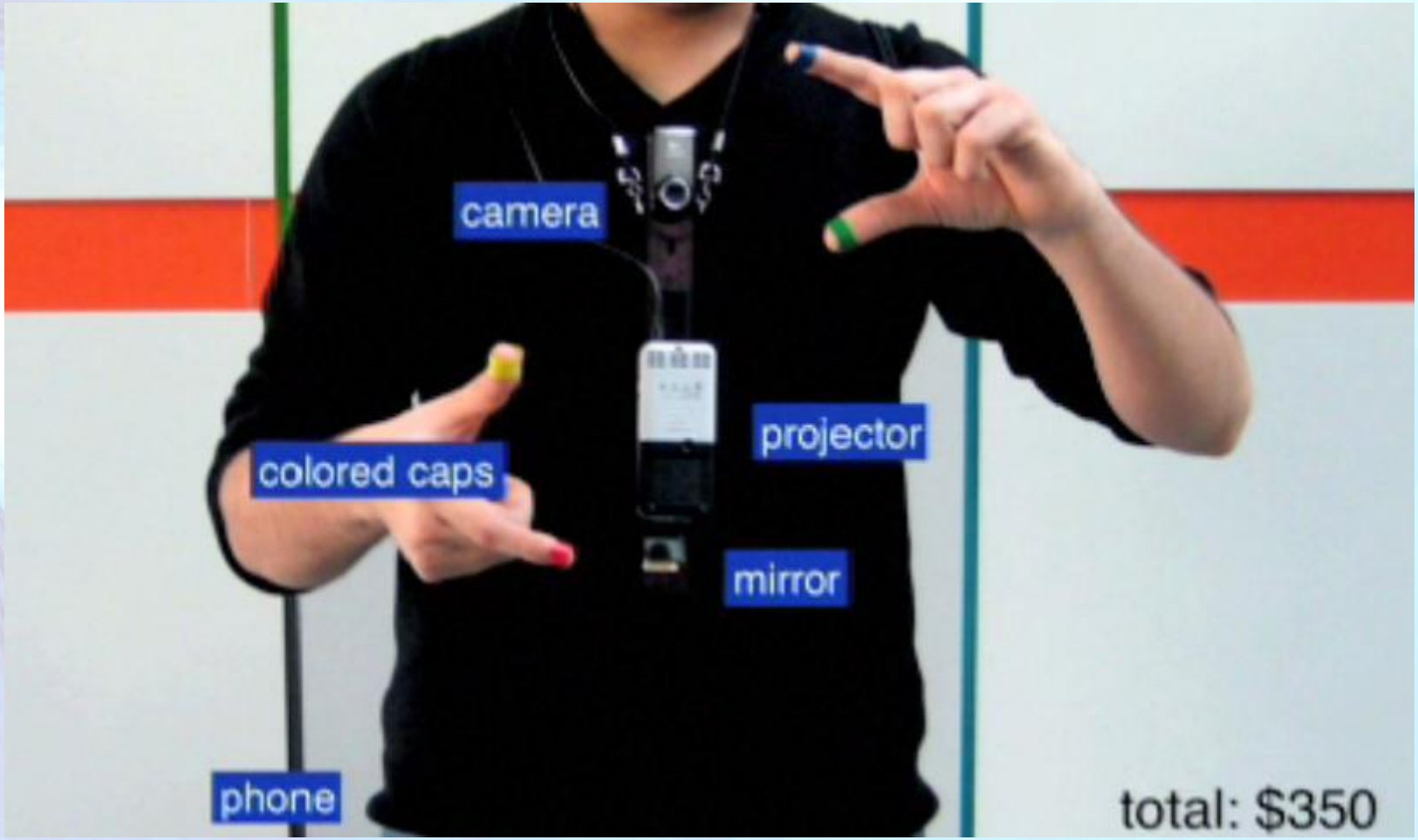
The “Tamboti Tree” Use case



OpenTox

SEVENTH FRAMEWORK PROGRAMME

Augmented Reality



MIT Media Lab

Processing Packaging Information

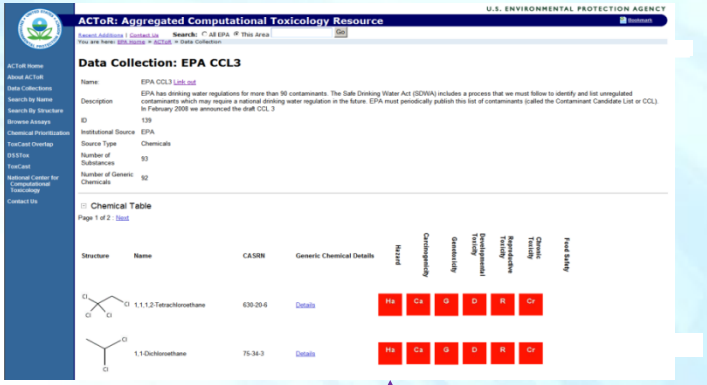
MIT Media Lab

Inspiration for *Saturday Shopping Do the right thing for Safety* Use Case

OpenTox

SEVENTH FRAMEWORK PROGRAMME

OpenTox - ToxCast



ACToR Web Browser

ACToR API

Chemical

Chemical ID, Structure

Targeted Testing

Assay

ToxRefDB

...

DevToxDB

Genomics

BioRefDB

ToxMiner

Internet Searches

Tabular Data, Links to Web Resources

Specialized Toxicology Databases

MicroArray Data

Biological Reference Data

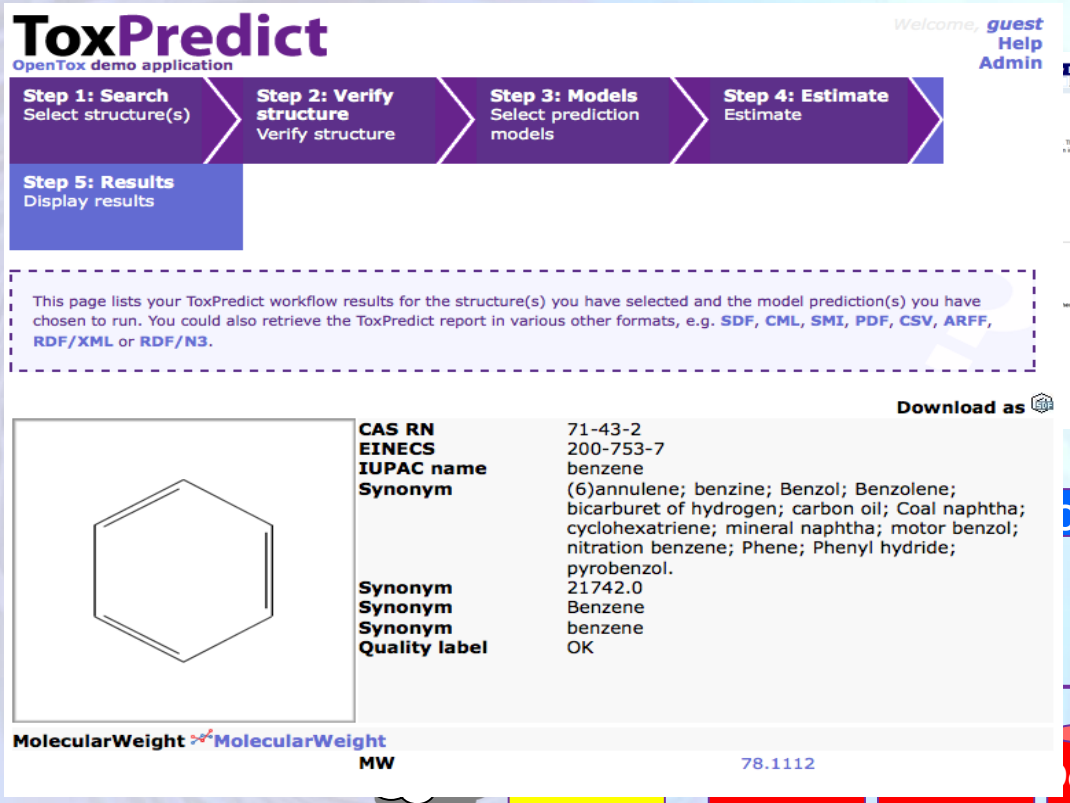
Data Mining

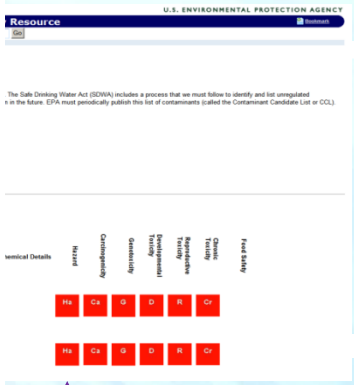
actor.epa.gov

OpenTox

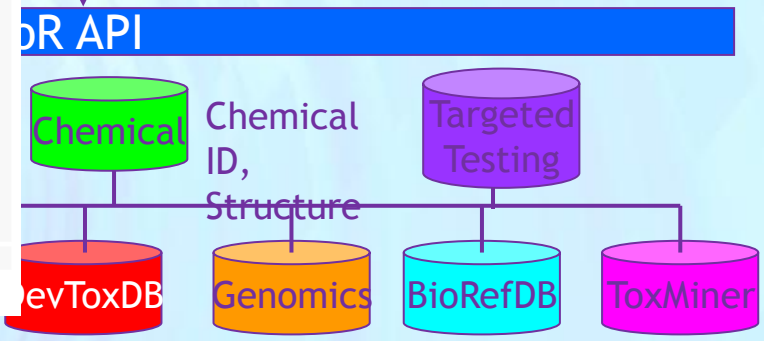
SEVENTH FRAMEWORK PROGRAMME

OpenTox - ToxCast





ACToR Web Browser



Internet Searches

Tabular Data, Links to Web Resources

Specialized Toxicology Databases

MicroArray Data

Biological Reference Data

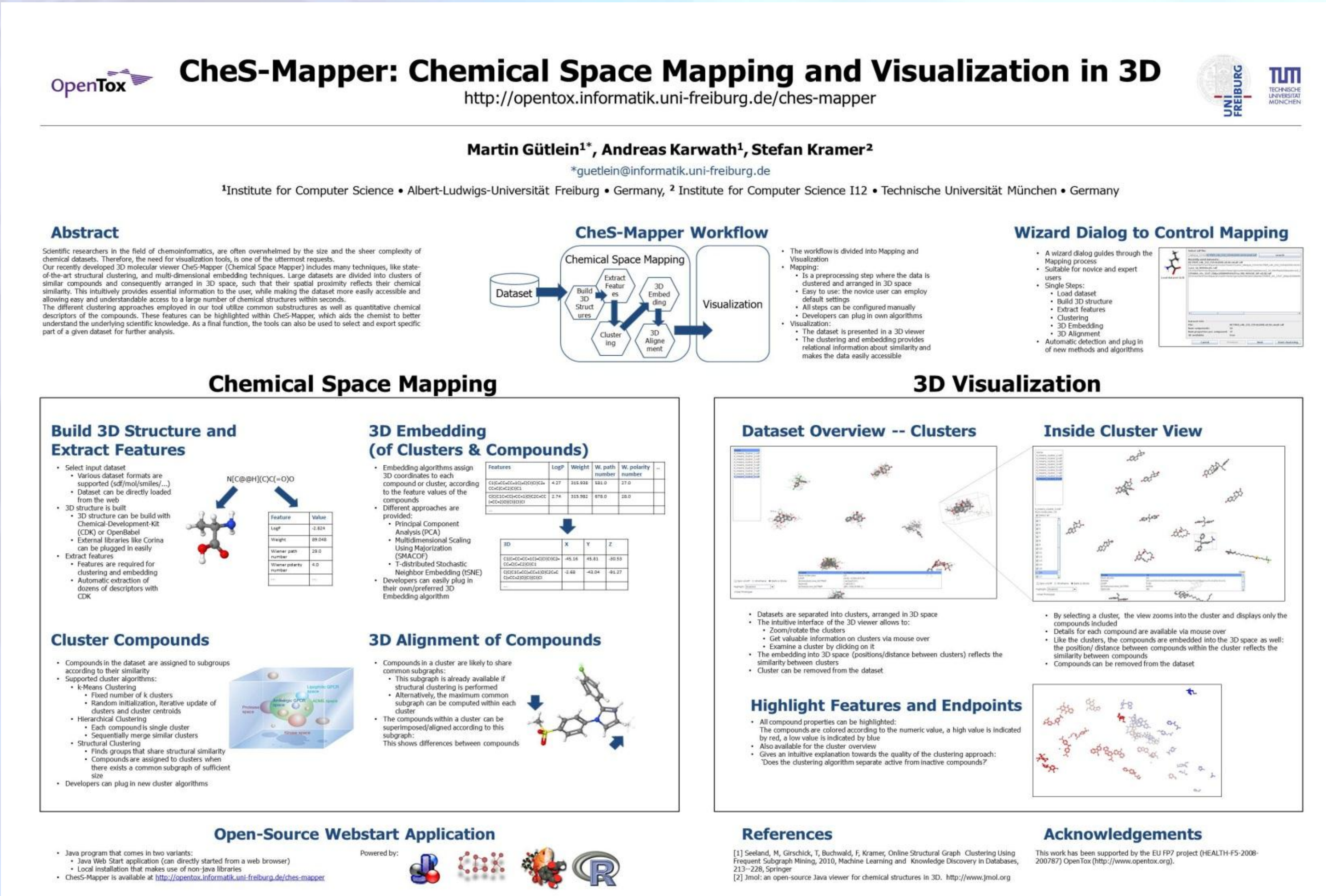
Data Mining

actor.epa.gov

OpenTox

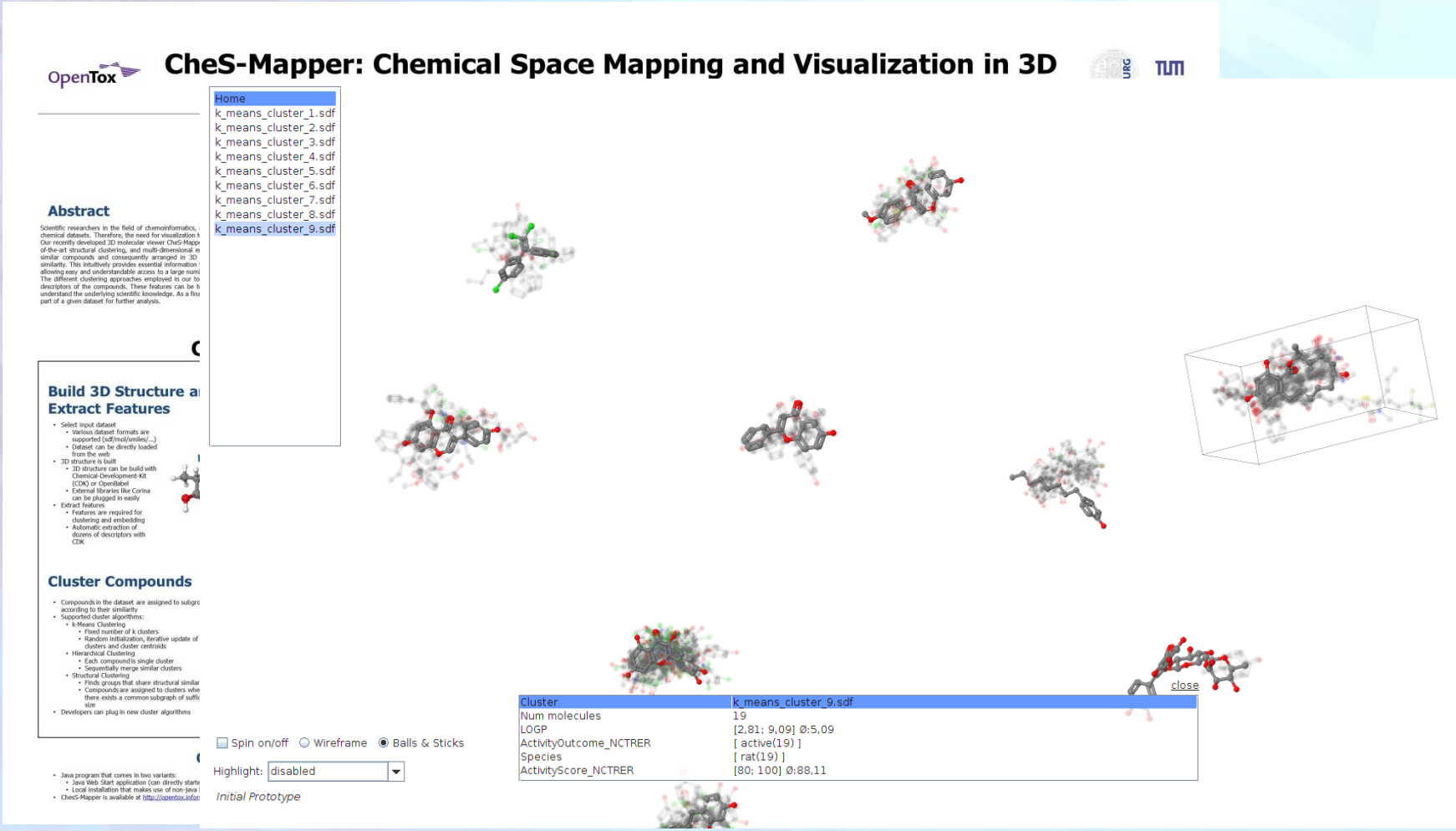
SEVENTH FRAMEWORK PROGRAMME

Chemical Space Visualisation (Ches-Mapper)



Martin Gütlein, Andreas Karwath, Stefan Kramer (ALU)

Chemical Space Visualisation (Ches-Mapper)

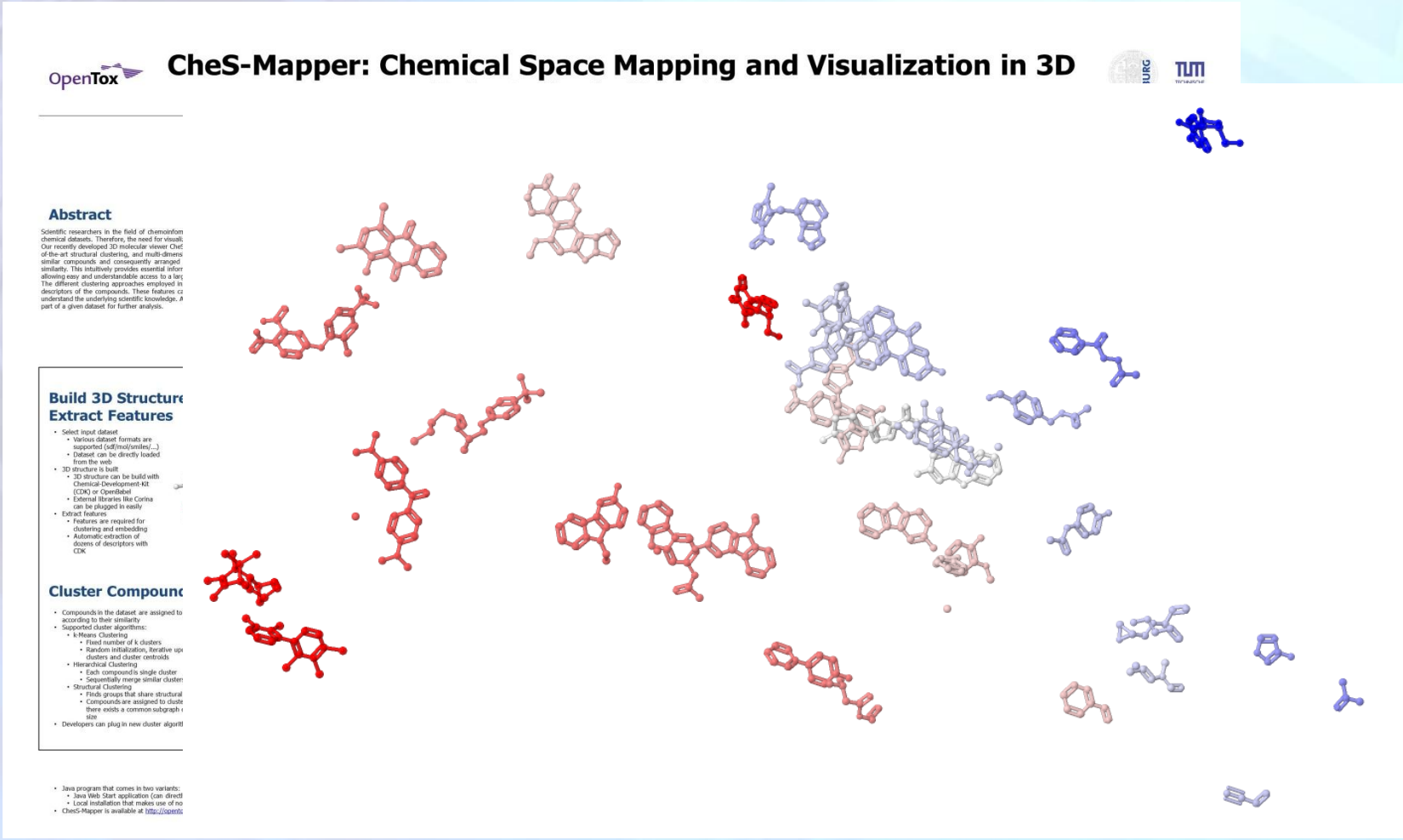


OpenTox

Martin Gütlein, Andreas Karwath, Stefan Kramer (ALU)

SEVENTH FRAMEWORK PROGRAMME

Chemical Space Visualisation (Ches-Mapper)



Martin Gütlein, Andreas Karwath, Stefan Kramer (ALU)

ToxBank Infrastructure Project
(started Jan 2011)

www.toxbank.net

Establishment of a …

… cell and tissue banking information resource

… repository for the selected test compounds

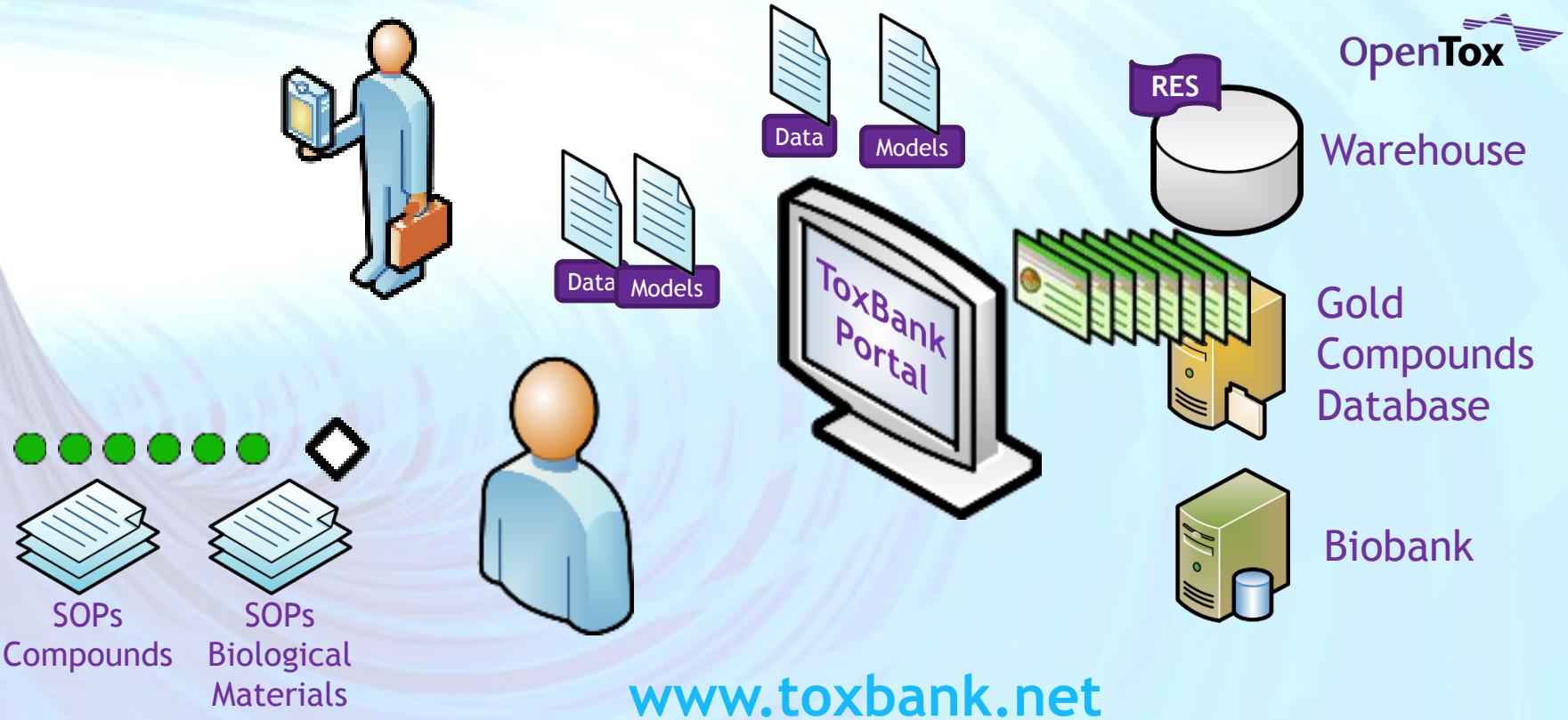
… database of reference test compounds

… dedicated web-based data warehouse

This project will be jointly funded by COLIPA and the EC. Any opinions expressed in this slide are those of the author. COLIPA is not liable for any use that may be made of the information contained therein.

Our Infrastructure Vision for ToxBank supporting all steps of Predictive Toxicology Research based on Alternative Testing methods

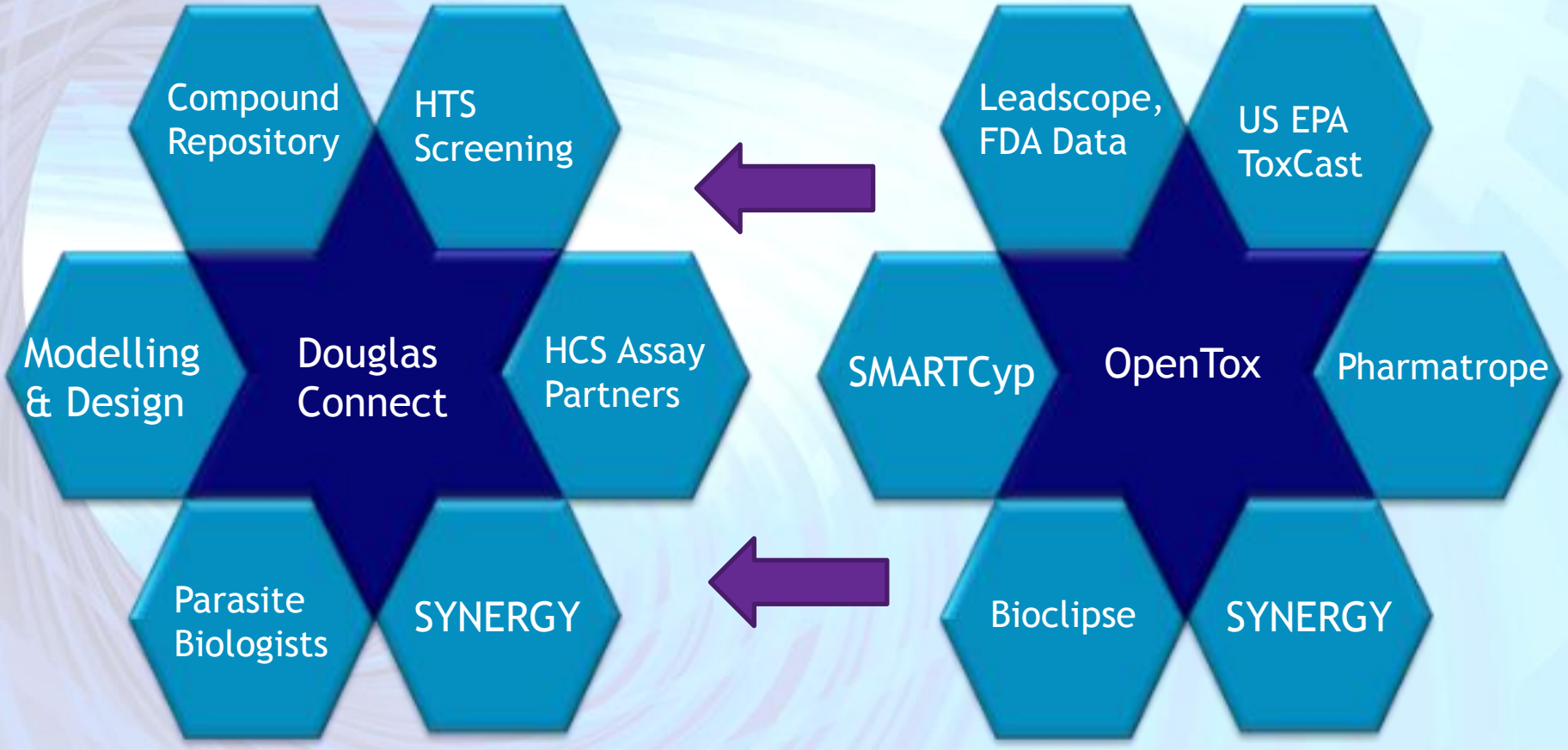
Users access compounds, biological materials, data and models for experimental planning and integrated analysis of experimental results



www.toxbank.net

This project will be jointly funded by COLIPA and the EC. Any opinions expressed in this slide are those of the author. COLIPA is not liable for any use that may be made of the information contained therein.

Virtual Organisation Pilots



Neglected Disease Drug Design VO

Predictive Toxicology VO

OpenTox

SEVENTH FRAMEWORK PROGRAMME

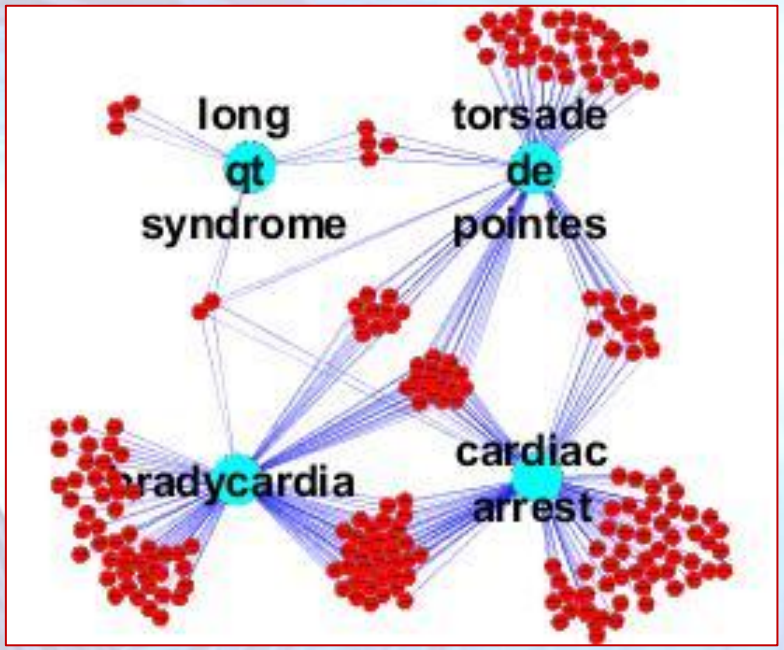
OpenTox - Synergy Predictive Toxicology VO Pilot Strategy Development & Case Study

1. Data Mining of Human Adverse Drug Events
   - Data Mining of Literature Knowledge
2. Creation of Mechanism-based Hypothesis
   - Selection of Biological Pathways & Targets
3. Selection of Compounds
   - Prediction of Metabolites of Compounds
4. Selection of *in vitro* assays relevant to Mechanism
   - Selection and integration of Toxicity Data
5. Creation of Predictive Toxicology Model including Model Validation and Applicability Domain
6. Selection of Low and High Content Assays for Testing in Cell Lines
   - Analysis of Results

OpenTox

SEVENTH FRAMEWORK PROGRAMME

Analysis of Adverse Events Based on Pharmacological Activity



- Cardiac adverse events
- Related to hERG ion channel?

cyan = adverse event, red = drug
lines define links

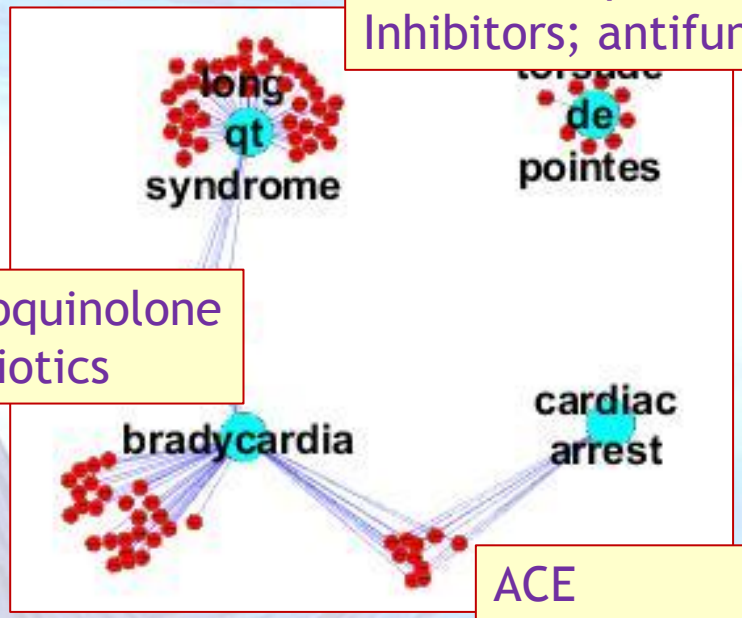
- Question addressed:
  - Are the adverse events a function of inhibiting the pharmacological target?
  - Or is the adverse event due to an off-target activity?

PHARMATROPE

OpenTox

SEVENTH FRAMEWORK PROGRAMME

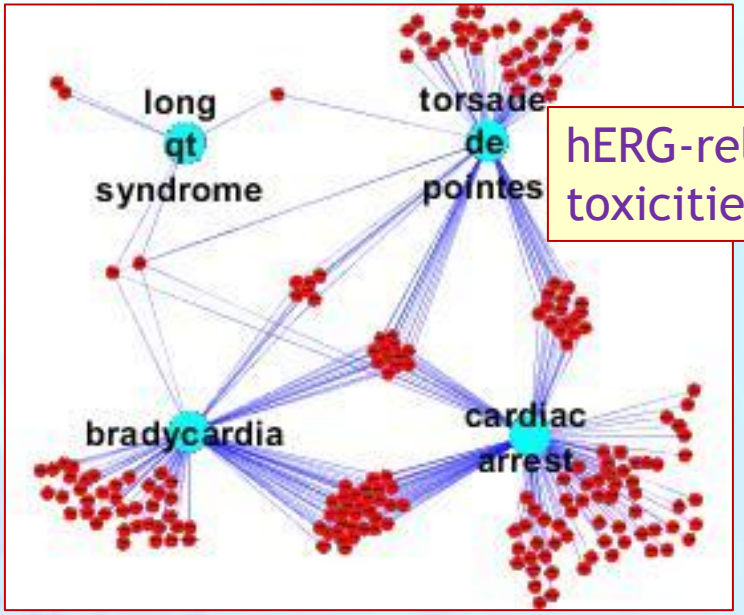
Example: Cardiac Adverse Events



serotonin uptake Inhibitors; antifungals

fluoroquinolone antibiotics

ACE Inhibitors



hERG-related toxicities?

On-target events

Off-target events

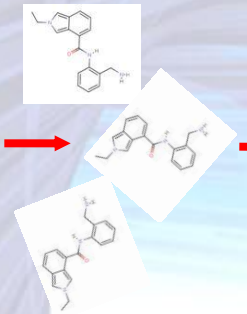
cyan = adverse event, red = drug lines define links

PHARMATROPE

OpenTox

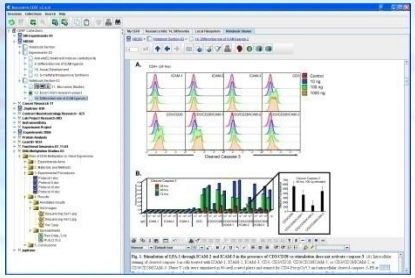
SEVENTH FRAMEWORK PROGRAMME

Synergy Drug Design Collaboration Pilot

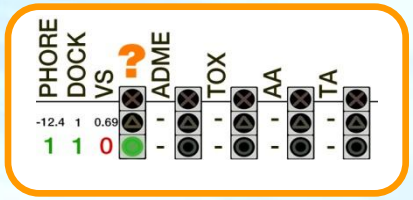


Screened Library

Data

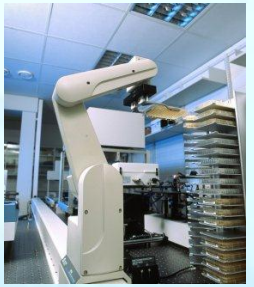


CERF



Refine Predictions

SYNERGY



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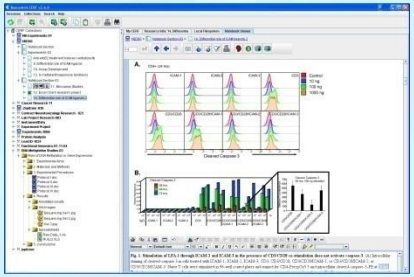

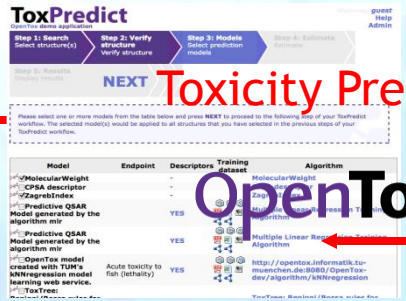

Toxicity Predictions

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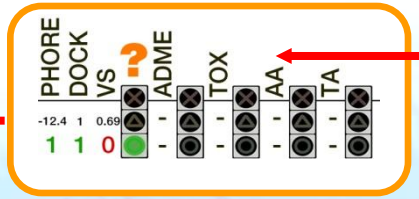
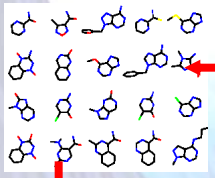
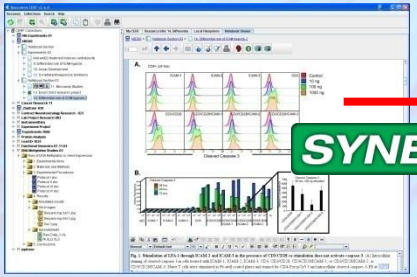


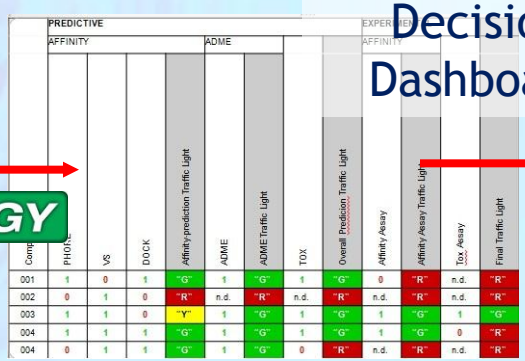
SYNERGY



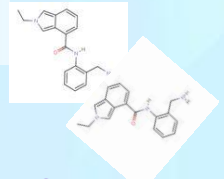
Toxicity Assays



SYNERGY



Decision Dashboard



(Safer) Drug Leads

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www.scientistsagainstmalaria.net

SEVENTH FRAMEWORK PROGRAMME

REACH

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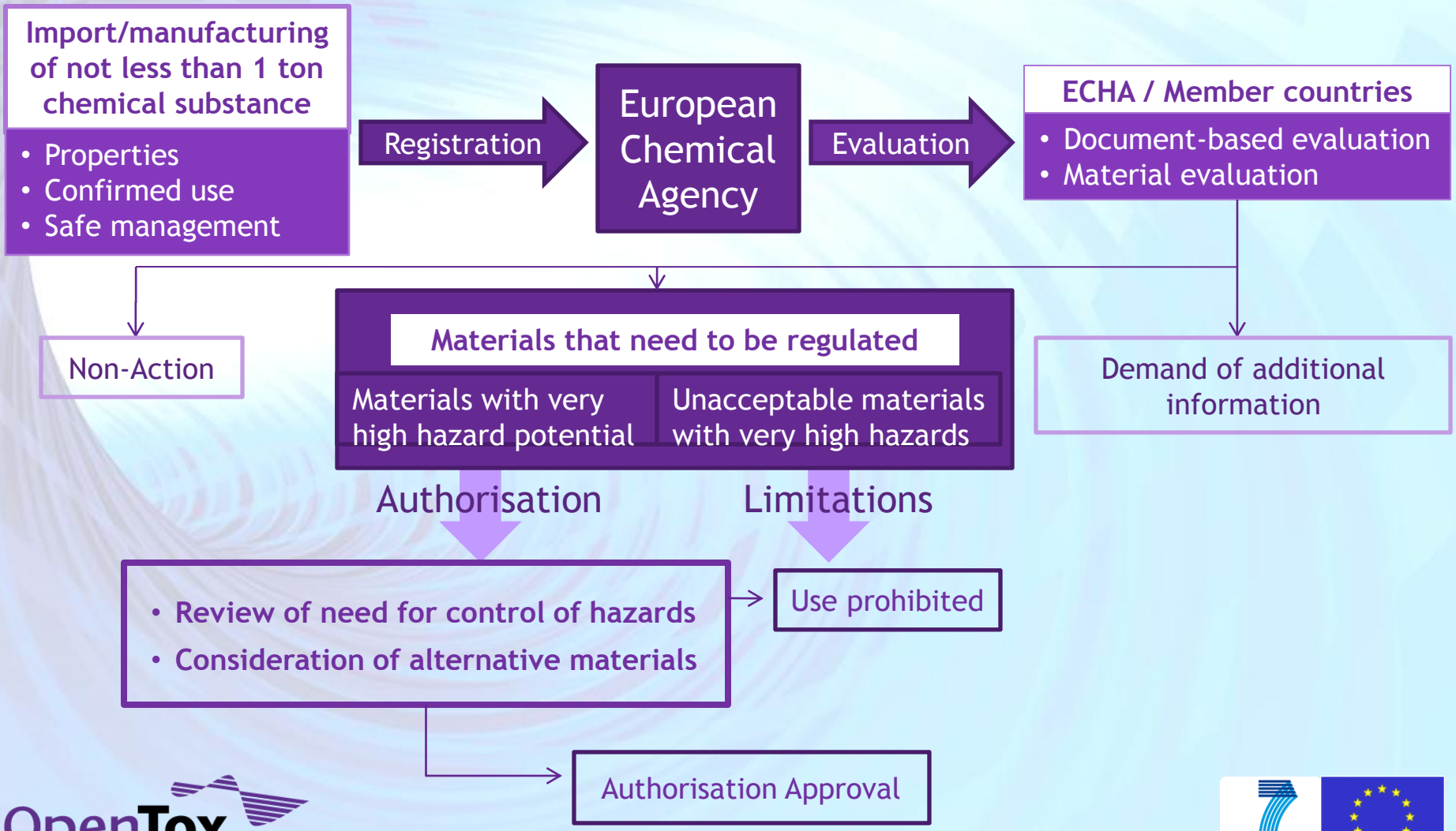
SEVENTH FRAMEWORK PROGRAMME

Introduction – REACH registration



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SEVENTH FRAMEWORK PROGRAMME

REACH

“Registration, Evaluation, Authorisation & Restriction of Chemicals”

European Union Legislation, 2007

All chemicals imported or manufactured in Europe must be registered

from 1st December 2010 (European Chemicals Agency - ECHA)

“…protecting human health and the environment…” Geert Dancet, ECHA

Responsibility:

Manufacturers and importers to

provide safety information & manage risks

Threshold:

Phased: **2010 > 1,000 tons p.a.**
2018 > 1 ton p.a.

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REACH

Registration per chemical: $2M to $14M[2]

IUCLID: International Uniform Chemical Information Database

Registration submitted by 22 Nov. 2010: 19,237[1]
Chemicals pre-registered by 1 Dec. 2008: **143,000[2]**

54M[3] - 9M[4] additional test animals

"...promote alternative methods for assessing hazards of substances.....animal testing as a last resort..." Geert Dancet, ECHA

1. C&EN, Nov 29, 2010, P. 15
2. en.wikipedia.org/wiki/Registration,_Evaluation,_Authorisation_and_Restriction_of_Chemicals
3. T. Hartung & C. Rovida: Chemical regulators have overreached. Opinion in Nature, vol. 460, 27 Aug '09.
4. ECHA - New study inaccurate on the number of test animals for REACH. Helsinki, 28 August 2009

REACH

OpenTox InterAction Meeting
Innovation in Predictive Toxicology

Modelling, Applications, REACH, Risk Assessment

9-12 August 2011
Technical University of Munich, Germany

Registration: Free but limited to 100 attendees
https://www.surveymonkey.com/s/opentox2011

Abstracts by: 30 April 2011, Posters: 30 June 2011

Bursary Award: three abstracts will be selected for travel & accommodation awards (by 30 April 2011)

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

Collaborating Partners

In Silico Toxicology, Switzerland

Douglas Connect, 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

OpenTox

Our Funding Support...

For more information, visit

www.opentox.org

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OpenTox - An Open Source Predictive Toxicology Framework, www.opentox.org, is funded under the EU Seventh Framework Program: HEALTH-2007-1.3-3 Promotion, development, validation, acceptance and implementation of QSARs (Quantitative Structure-Activity Relationships) for toxicology, Project Reference Number Health-F5-2008-200787 (2008-2011).

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SEVENTH FRAMEWORK PROGRAMME