

# **OpenTox:** **An open source web service platform for toxicity prediction**

**ACS, Anaheim, 30th March 2011**

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**\*Co-Presenters**

# Abstract

The new European Union (EU) REACH chemical legislation will require over 9 million additional test animals, if no alternative methods for toxicity prediction are accepted. However, the number of test animals could be significantly reduced by utilizing existing experimental data in conjunction with (Quantitative) Structure Activity Relationship ((Q)SAR) models.

To address the challenge, the European Commission has funded the OpenTox ([www.OpenTox.org](http://www.OpenTox.org)) project to develop an open source web-service-based framework, that provides unified access to experimental toxicity data, *in Silico* models (including (Q)SAR), and validation/reporting procedures.

Now, in the final year of the initial three-year project, the current state of architecture, Open API, algorithms, ontologies, and approach to web services are presented. Our experiences on current collaborative approaches aiming to combine OpenTox with other systems such as CERF, Bioclipse, CDK, and SYNERGY to create “superinteroperable K-infrastructure” are discussed both in terms of conceptual promise and implementation reality.

# Topics

- New EU legislation “REACH”

*David Gallagher*

- The chemistry challenges

- Prototype applications (Tox prediction)

- User Needs

*Sunil Chawla*

- Semantic Web for Predictive Toxicology

- Key Components

- Web Service Interoperability

- Achievements

*Barry Hardy (P.I.)*

# Background - 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:

<b>Phased:</b>	<b>2010</b>	<b>&gt; 1,000 tons p.a.</b>
	<b>2018</b>	<b>&gt; 1 ton p.a.</b>



# Impact of REACH



**Registration per chemical: \$2M to \$14M<sup>2</sup>**

*IUCLID: International Uniform Chemical Information Database*



**Registration submitted by 22 Nov. 2010: 19,237<sup>1</sup>**  
**Chemicals pre-registered by 1 Dec. 2008: 143,000<sup>2</sup>**



**54M<sup>3</sup> - 9M<sup>4</sup> additional test animals**

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

# Funding



## European Union Seventh Framework Programme



Program: HEALTH-2007-1.3-3

**Promotion, development, validation, acceptance  
and implementation of QSARs for toxicology**

Project Reference Number Health-F5-2008-200787.

**ca. \$4M (2008 - 2011)**

Awarded to: **OpenTox Consortium**  
**Proposal:** “An Open Source Predictive Toxicology Framework”  
**[www.opentox.org](http://www.opentox.org)**

# OpenTox Partners

Douglas Connect, Switzerland (P.I.)

In Silico Toxicology, Switzerland

Ideaconsult, Bulgaria

David Gallagher, UK

Seascope Learning & JNU, India

Superior Health Institute (ISS), Italy

Technical University of Munich, Germany

Albert Ludwigs University Freiburg, Germany

Fraunhofer Institute for Toxicology & Experimental Medicine, Germany

Institute of Biomedical Chem. of the Russian Acad. of Medical Sci., Russia

National Technical University of Athens, Greece



# OpenTox Goals



Development of:

- an interoperable, extensible predictive toxicology framework

Containing state-of-the-art:

- QSARs & SARs
- cheminformatics, bioinformatics
- statistical and data mining tools
- computational chemistry & biology algorithms & models
- *in vitro* and *in vivo* data resources
- ontologies
- user interfaces...



# OpenTox & “The Internet & Chemistry”



## **Seamless integration of services distributed over the internet**

- toxicity databases
- prediction algorithms
- computation servers
- user interfaces

## **Communications between partners**

- Email
- Collaboration web site (OpenTox.org)
- ‘GoToMeeting’ for regular group meetings
- Skype for smaller meetings



# Basel, Switzerland

Sept. 2008

## OpenTox kick-off meeting



# The Challenges

- **QSARs for predicting toxicity**

(Q)SAR algorithms & descriptors  
consensus predictions  
validation of models  
applicability domains  
transparency



- **Toxicity data**

standards, quality, licensing, confidentiality

- **Metabolite predictors**

e.g. *SMARTcyp*, *CypScore*

- **Retrieval of supporting information**

database mining, text mining

- **Integrated across the internet**





# *in Silico* Methods Considered

**(Q)SAR**

Quantitative Structure-Activity Relationships

**Structural Alerts**

(de)activating fragments or functional groups

**Read Across**

Expert knowledge, compare related chemicals

**Database mining**

for same or similar chemicals

**Text mining**

for reports on same or similar chemicals

**Third-party packages....**



# Reporting: Validation of Predictions

## OECD Guidelines:

### 1. Defined endpoint

well defined 'homogeneous' training data

### 2. Unambiguous prediction algorithm

fully documented prediction models

### 3. Defined applicability domain

documented algorithms for chemical space of model

### 4. Appropriate measures of goodness-of-fit, robustness, & predictivity

scientifically sound:  $r^2$ ,  $CVR^2$ , RMSE, skew, confusion matrix, etc.

### 5. Mechanistic interpretation, if possible

key descriptors, human evaluation, can improve confidence

# Prototype Application 1: ToxPredict

## ToxPredict ([www.toxpredict.org](http://www.toxpredict.org))

Browser-based GUI enables non-computational experts to enter a single structure and get a toxicity report back based on available end-points (currently 18)

### Step 1, Enter the compound

The screenshot displays the ToxPredict web application interface. At the top, the logo 'ToxPredict' is shown, with 'OpenTox demo application' underneath. In the top right corner, there is a 'Welcome' message and links for 'guest', 'Admin', and 'Help'. A horizontal progress bar contains five steps: '1. Select structure(s)', '2. Verify structure(s)', '3. Select model(s)', '4. Run prediction(s)', and '5. Display result(s)'. The first step is highlighted in blue. To the right of the progress bar is a large blue 'NEXT' button. Below the progress bar are three buttons: 'Search' (highlighted in purple), 'Draw', and 'Upload'. A 'Free text search' section follows, with a prompt '(Enter chemical name, registry identifier, SMILES, InChI, any keywords)' and a star icon. A text input field contains 'benzoic acid'. To the right of the input field is a dropdown menu set to 'Equals' and another dropdown menu labeled 'Number of hits' set to '1'. At the bottom, there is a second identical progress bar and 'NEXT' button.

# ToxPredict (2)

## Step 2: Verify structure and description

**ToxPredict**  
OpenTox demo application

Welcome [guest](#)  
[Admin](#)  
[Help](#)

1. Select structure(s)

2. Verify structure(s)

3. Select model(s)

4. Run prediction(s)

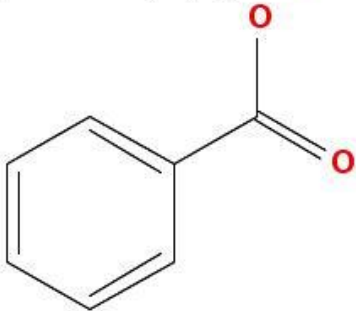
5. Display result(s)

NEXT

« Page 1 Records per page 1 »

Structure(s) & Experimental Data [SDF](#) [CSV](#) [PDF](#)

1.



**CASRN** 65-85-0  
**Synonym(s)** benzoic acid,Benzenecarboxylic Acid; benzeneformic acid; benzenemethonic acid; Diacrylic acid; Carboxybenzene; Oracrylic acid; phenyl carboxylic acid; phenylformic acid; retarded ba; retardex; tennplas.,Benzoic acid / Benzoate,Benzoic acid,AMMONBENZ; BENZDIOLA; BENZOATE; BENZOATCA; JM-244; JM-2644; LITHIUMBZ; BENZOATEK; BENZOATNA  
**EINECS** 200-618-2  
**IUPAC name** benzoic acid  
**InChIKey\_std** WPYMKLBDIGXBTP-UHFFFAOYSA-N  
**InChI\_std** InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)  
**REACHRegistrationDate** 30.11.2010  
**SMILES** OC(=O)c1ccccc1,C1(=CC=CC=C1)C(=O)O,OC(=O)C1=CC=CC=C1

# ToxPredict (3)

## Step 3: Select toxicity models Run calculations

**ToxPredict**  
OpenTox demo application

Welcome, *guest*  
[Admin](#)  
[Help](#)

1. Select structure(s)   2. Verify structure(s)   **3. Select model(s)**   4. Run prediction(s)   5. Display result(s)   **NEXT**

Model	Endpoint	Algorithm
<input checked="" type="checkbox"/> MolecularWeight		MolecularWeight
<input checked="" type="checkbox"/> ToxTree: Michael acceptors		ToxTree: Michael acceptors
<input checked="" type="checkbox"/> ToxTree: Verhaar scheme for predicting toxicity mode of action	Acute toxicity to fish (lethality)	ToxTree: Verhaar scheme for predicting toxicity mode of action
<input checked="" type="checkbox"/> ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	Carcinogenicity	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity



# ToxPredict (4)

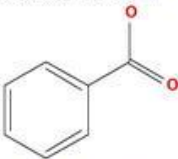
## Step 4: View predictions & validation reports

**ToxPredict**  
OpenTox demo application


1. Select structure(s) 2. Verify structure(s) 3. Select model(s) 4. Run prediction(s) 5. Display result(s)


Page 1 Records per page 1


Structure(s) & Model predictions & Experimental Data SDF CSV PDF



**CASRN 65-85-0**  
**Synonym(s)** benzoic acid, Benzenecarboxylic Acid; benzenecarboxylic acid; benzenemethanoic acid; Diacrylic acid; Carboxybenzene; Gracrylic acid; phenyl carboxylic acid; phenylformic acid; retarded ba; retardex; tennplas; Benzoic acid / Benzoate, Benzoic acid, AMMONBENZ, BENZDIOLA, BENZOATE, BENZOATCA, JM-244, JM-2644, LITHIUMBZ, BENZOATEK, BENZOATNA  
**EINECS** 200-618-2  
**IUPAC name** benzoic acid  
**InChIKey\_std** WPMYKLBODGXBTU-UHFFFAOYSA-N  
**InChI\_std** InChI=1S/C7H6O2/C8-7/9/6-4-2-1-3-5-6/h1-5H,(H,8,9)  
**REACHRegistrationDate** 30.11.2010  
**SMILES** OC(=O)c1ccccc1, C1=CC=CC=C1C(=O)O, OC(=O)C1=CC=CC=C1

**tree**  ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity  
**Error when applying the decision tree** NO

**Acceptors**  ToxTree: Michael acceptors  
**Michael Acceptors** Not reactive via Michael addition

**explanation**  ToxTree: Michael acceptors  
**Michael Acceptors#explanation**

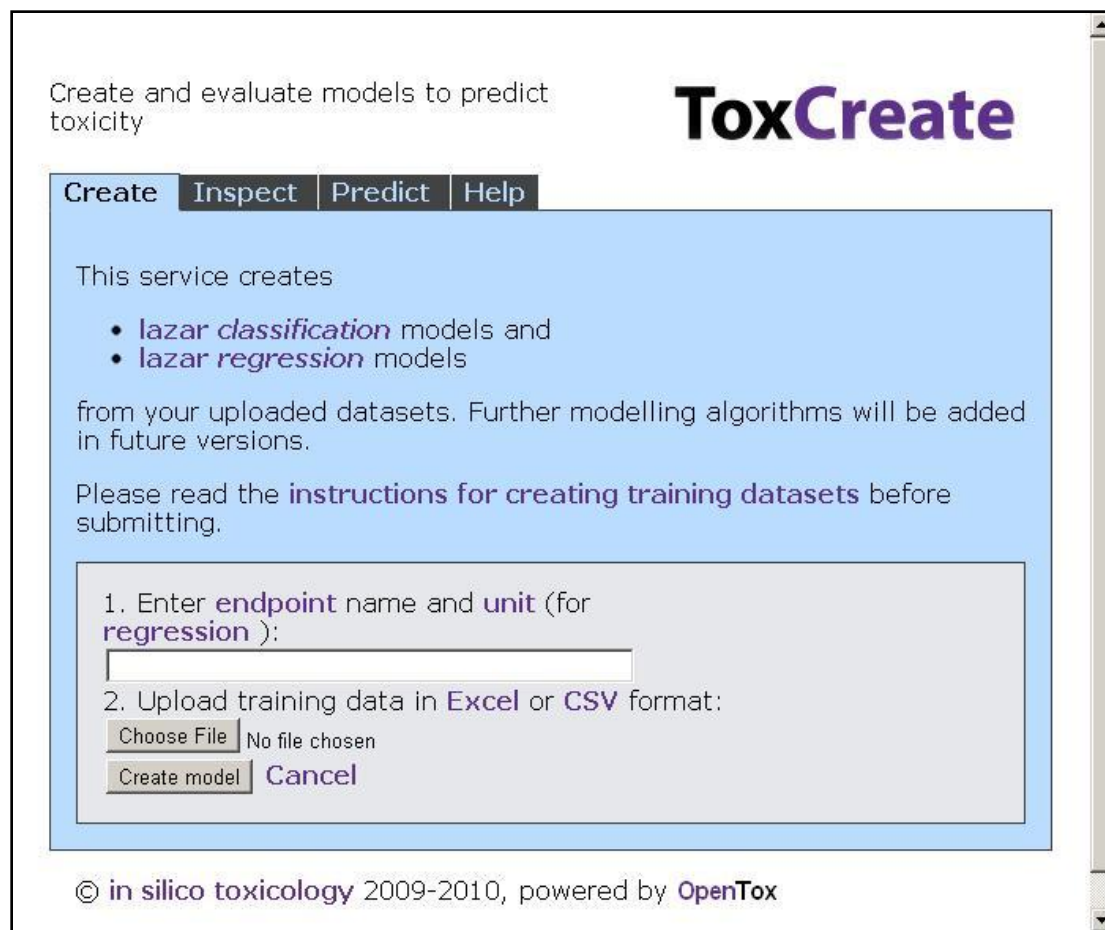
**Alerts, Alerts Yes**  
Q1. Ethynylene or acetylenic with a carbonyl No  
Q2. Vinylidene or vinylenic with a carbonyl No  
Q3. 1,4-C atom alkyl-substituted with a carbonyl No  
Q4A. 1,4-C atom substituted with a second carbonyl No  
Q4B. 1,4-C atom substituted with a second carbonyl No  
Q5. Olefinic nitro No  
Q6. Ethynylene or acetylenic with a S=O group No  
Q7. Vinylidene or vinylenic with a S=O group No  
Q8. Olefinic cyano No  
Q9A. Ortho-ethynylene azarone No  
Q9B. Ortho-vinyl azarone No  
Q10A. Para-ethynylene azarone No  
Q10B. Para-vinyl azarone No  
Q11. Vinylene carboxylic acid No  
Q12A. Ortho-quinone No  
Q12B. Ortho-quinone No  
Q13A. Para-quinone No  
Q13B. Para-quinone No  
Q14. Azarone No

[www.ToxPredict.org](http://www.ToxPredict.org)

# Prototype Application 2: ToxCreate

Creates a model from a training set ([www.toxcreate.org](http://www.toxcreate.org))

Step 1, upload training set, and create model



The screenshot shows the ToxCreate web application interface. At the top, it says "Create and evaluate models to predict toxicity" and "ToxCreate". Below this is a navigation bar with "Create", "Inspect", "Predict", and "Help" tabs. The "Create" tab is active. The main content area has a light blue background and contains the following text:

This service creates

- *lazar classification* models and
- *lazar regression* models

from your uploaded datasets. Further modelling algorithms will be added in future versions.

Please read the [instructions for creating training datasets](#) before submitting.

1. Enter **endpoint** name and **unit** (for **regression**):

2. Upload training data in **Excel** or **CSV** format:

No file chosen

At the bottom, it says "© in silico toxicology 2009-2010, powered by OpenTox".

# ToxCreate (2)

## Step 2, View prediction model & validation report

### hamster test2

Status: Completed  
Started: 03/02/2011 - 03:00:18AM  
Training compounds: 85  
Warnings: -  
Algorithm: lazar  
Type: classification  
Descriptors: Fminer backbone refinement  
Training dataset: Excel sheet , RDF/XML (experts, d  
Feature dataset: RDF/XML , YAML (experts, d  
Model: RDF/XML , YAML (experts, m  
Validation: show  
Detailed report: 76  
Number of predictions: 76.00 %  
Correct predictions: 0.904  
Weighted area under ROC: 0.771  
Specificity: 0.756  
Sensitivity:  
Confusion Matrix:

		Mean
		active
Predicted	active	31
	inactive	10

### Crossvalidation report

Created at 03.02.2011 - 03:01

#### Table of Contents

[Mean Results](#)  
[Roc Plot](#)  
[Confusion Matrix](#)  
[Results](#)  
[All Results](#)  
[Predictions](#)

#### Mean Results

This section contains results.

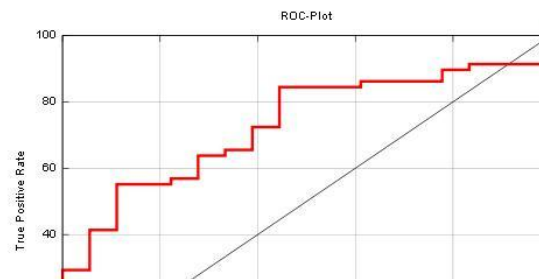
Table 1. Mean Results

Algorithm uri	<a href="http://webservices.in-silico.ch/algorithm/lazar">http://webservices.in-silico.ch/algorithm/lazar</a>
Dataset uri	<a href="http://webservices.in-silico.ch/dataset/1702">http://webservices.in-silico.ch/dataset/1702</a>
Num folds	10
Percent correct	69.17 +- 475.31
Weighted area under roc	0.90
Area under roc	true: 0.94, false: 0.89 +- true: 0.03, false: 0.05
F measure	true: 0.78, false: 0.73
True positive rate	0.77
True negative rate	0.77

#### Roc Plot

This section contains the roc plot.

Figure 1. Roc plot



# ToxCreate (3)

## Step 3: enter new structure to predict...

Create and evaluate models to predict toxicity

## ToxCreate

Create | Inspect | Predict | Help

Use this service to obtain predictions from OpenTox models

Draw a compound

☺ CLR DEL D-R +/- UDO

C N O S F Cl Br I X

O=N1CCCCC1


or enter a Name, InChI, Smiles

Choose one or more prediction models

hamster test2 ☒  
Test BH 6 ☐  
hamster carcinogenicity ☐

### New prediction

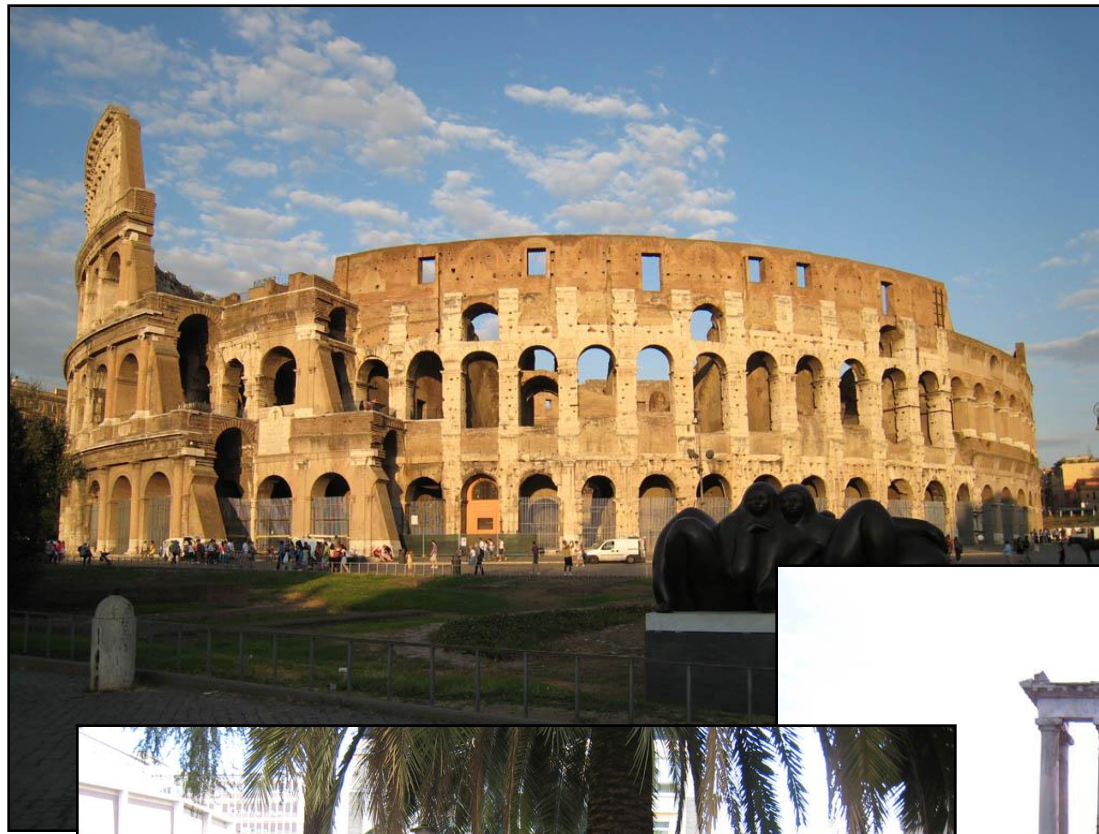
O=NN1CCCCC1



hamster test2:  
active  
( Measured activity )

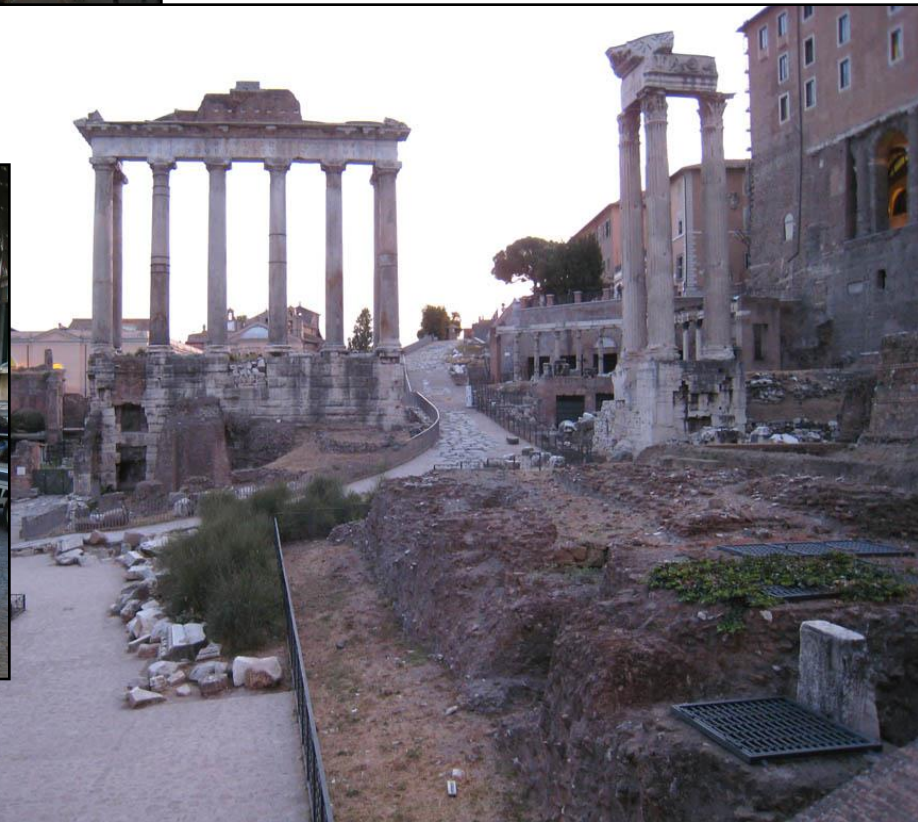
© in silico toxicology 2009-2010, powered by OpenTox





# Rome, Italy

Sept. 2009  
OpenTox 2nd meeting



# OpenTox Implementation Outline

- **User Needs**
- **Semantic Web for Predictive Toxicology**
- **Key Components**
- **Web Service Interoperability**
  - Bioclipse, CDK
  - Synergy Pilots

# Compelling User Needs, 1

## Integrated Testing

*in silico*

*in vitro*

TTC

Read  
Across

Category  
Formation

REACH  
Reporting (QPRF,  
QMRF)

Applicability  
Domain

Validation

Human  
Data

Communicated to OpenTox in 2009 by Grace Patlewicz (Du Pont)

# Compelling Users Needs, 2

## 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

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

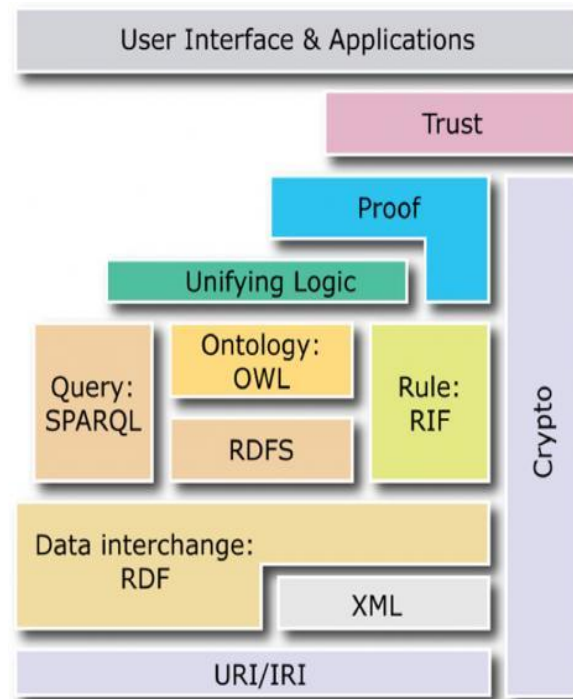


# Semantic Web for Predictive Toxicology

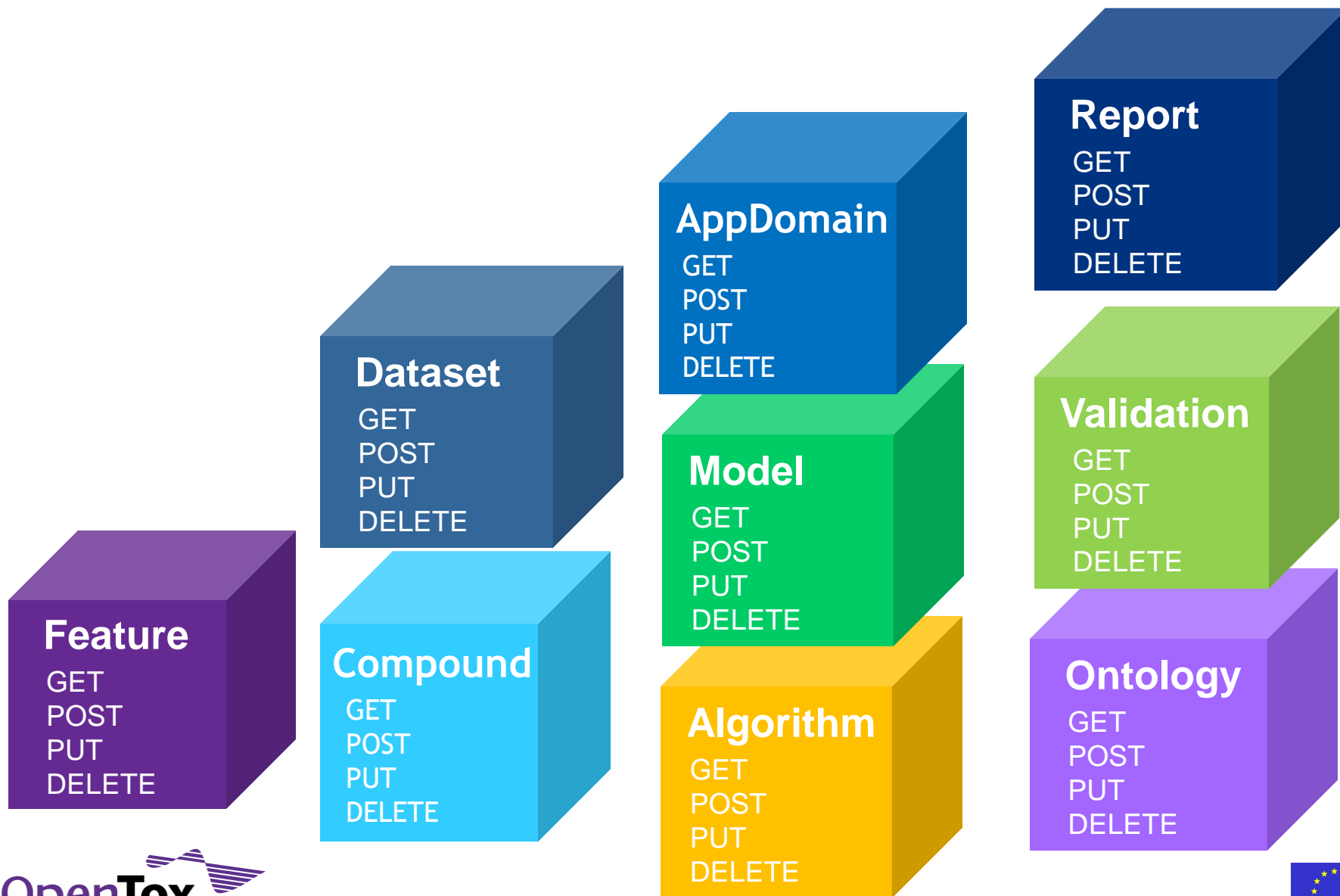
- **URIs:** Uniform Resource Identifier on the web with a name & location
- **RDF:** Resource Description Framework - Graph based Data interchange model to structure data and link resources
- **OWL:** Ontology (Web) Language to add vocabulary for describing properties and relationships



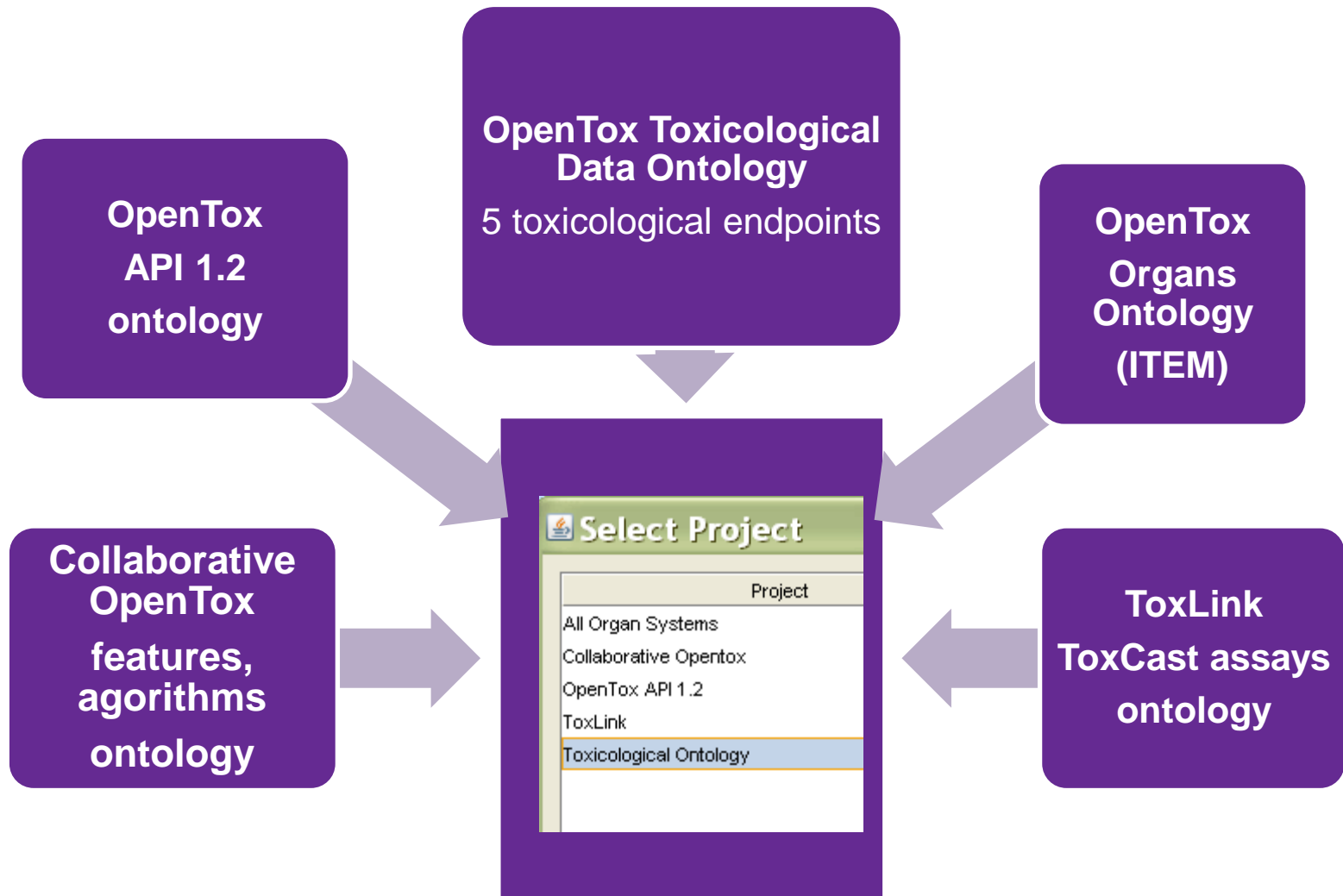
**A www network of Linked Resources for Predictive Toxicology!**



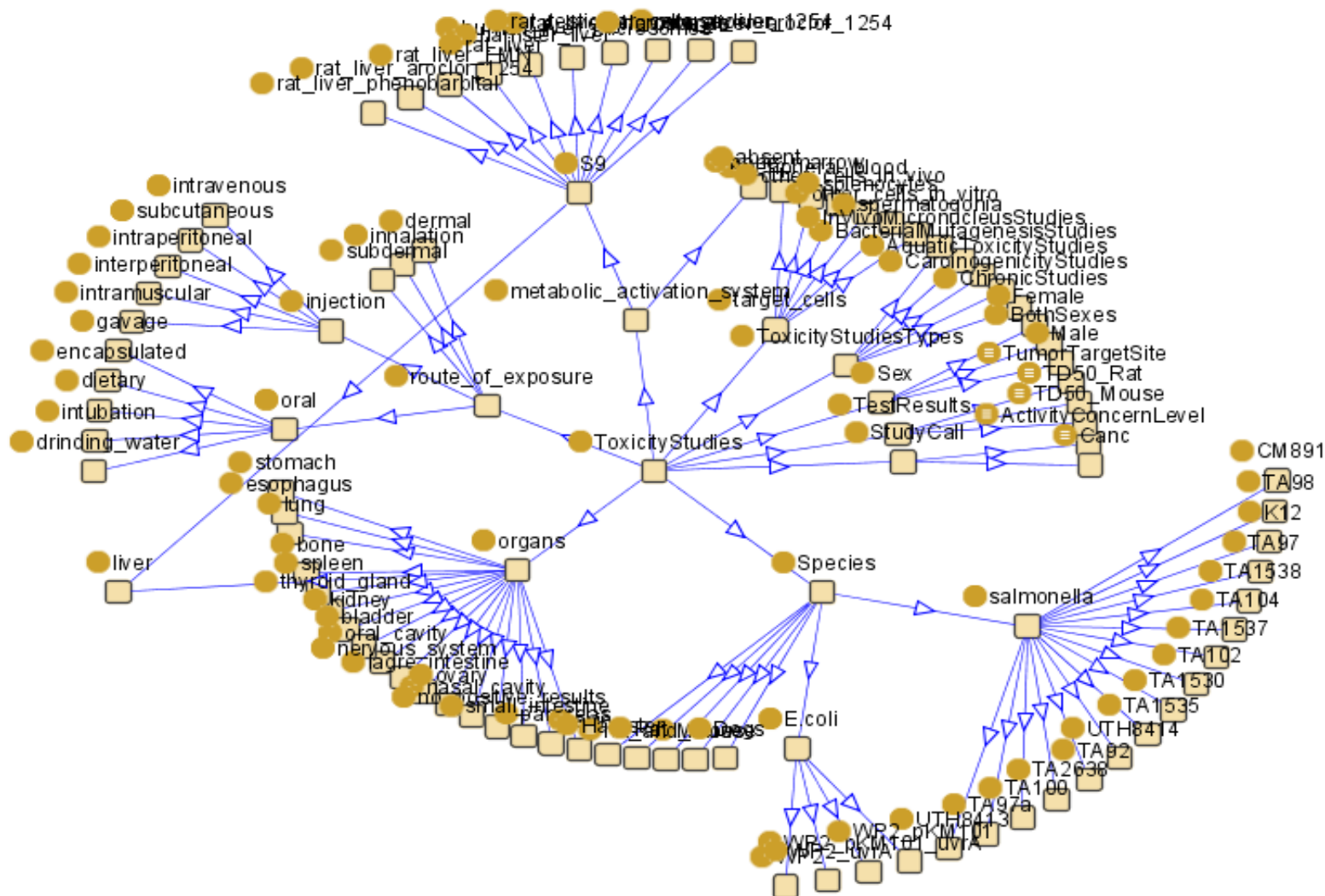
# OpenTox Web Linked Resources



# Collaborative Ontology Development: Collaborative Protege Server



# Toxicological Ontology: Graphical Representation

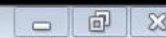


# Web service interoperability

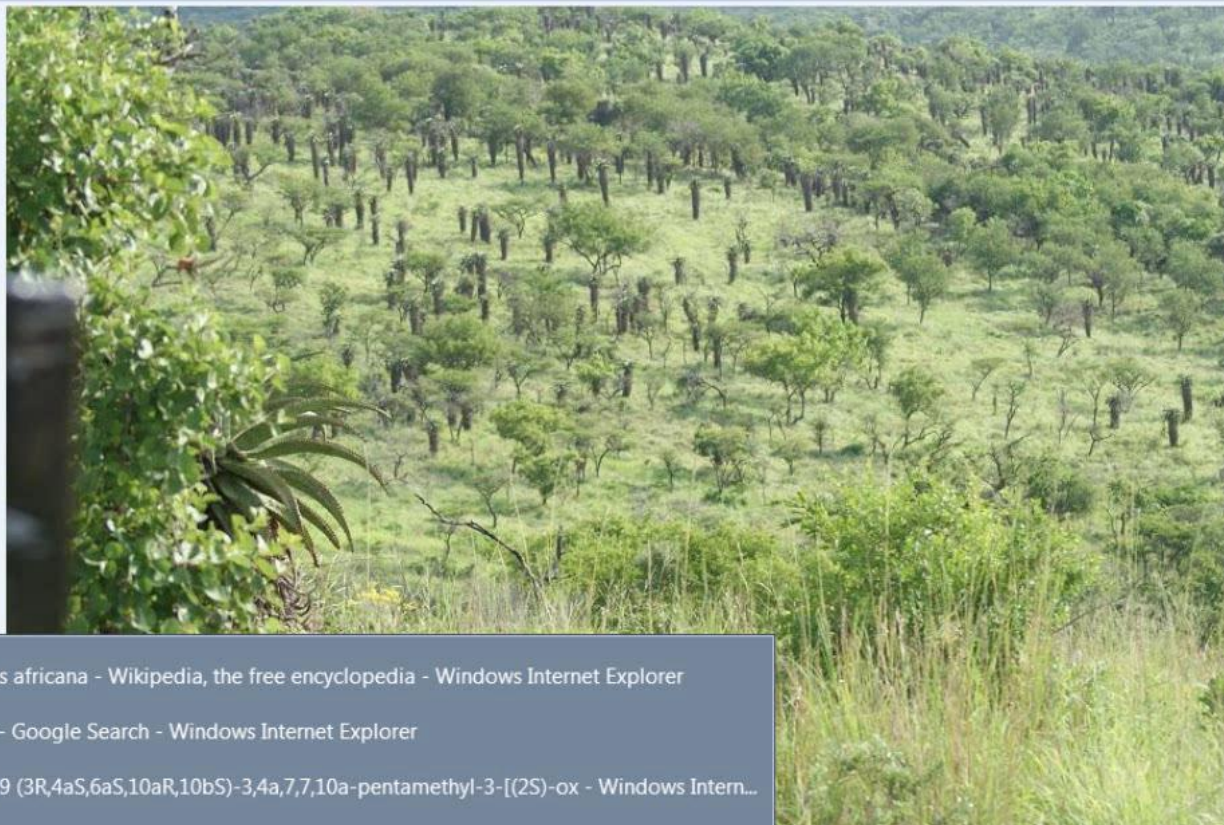
**Bioclipse, CDK, Synergy**

***“Tamboti Tree Use Case” & Bioclipse-  
OpenTox Demo follows***

13 Thanda Bush 101211 1.JPG - Windows Photo Viewer



File Print E-mail Burn Open



Spirostachys africana - Wikipedia, the free encyclopedia - Windows Internet Explorer

excoecarin - Google Search - Windows Internet Explorer

183900-28-9 (3R,4aS,6aS,10aR,10bS)-3,4a,7,7,10a-pentamethyl-3-[(2S)-ox - Windows Intern...

Download - Windows Internet Explorer

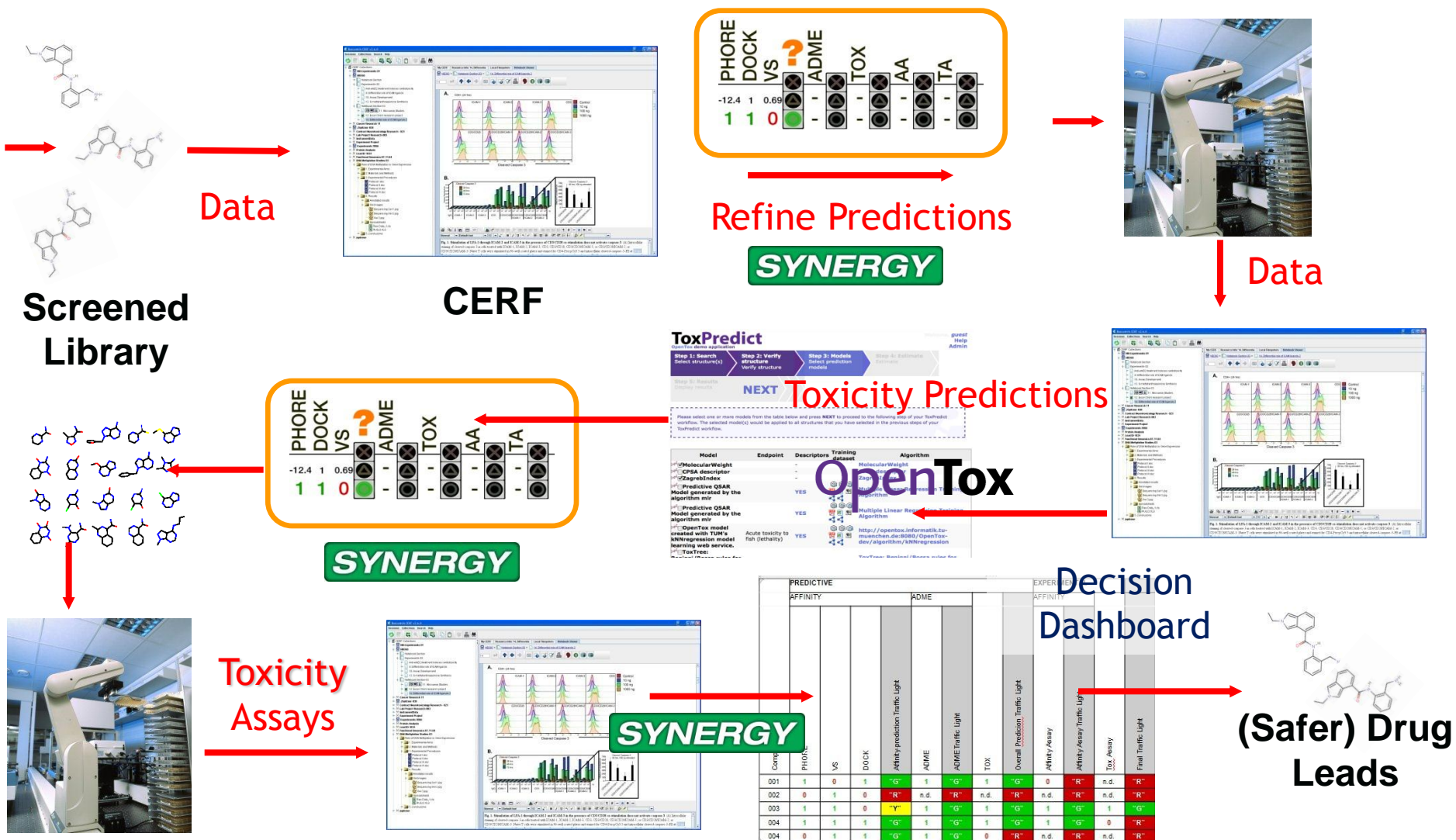
GoToMeeting : My Meetings - Windows Internet Explorer



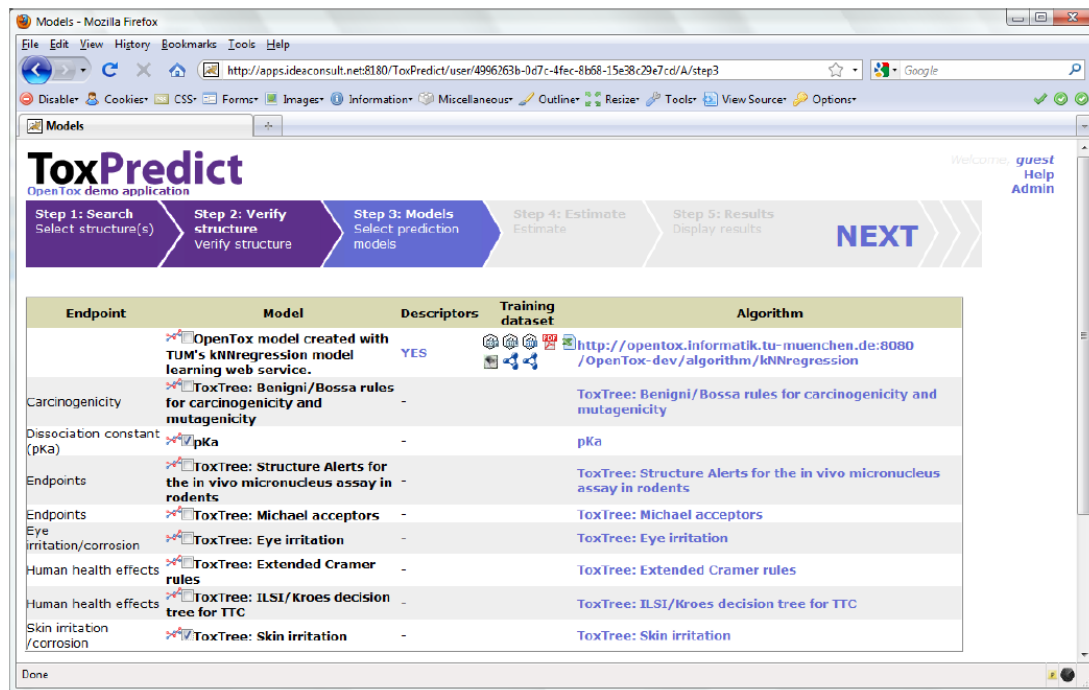
DE 03:42  
31.01.2011



# Synergy Drug Design Collaboration Pilot



# Recap: What you can do with it ...



Endpoint	Model	Descriptors	Training dataset	Algorithm
	OpenTox model created with TUM's kNNregression model learning web service.	YES	<a href="http://opentox.informatik.tu-muenchen.de:8080/OpenTox-dev/algorithm/kNNregression">http://opentox.informatik.tu-muenchen.de:8080/OpenTox-dev/algorithm/kNNregression</a>	
Carcinogenicity	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	-		ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity
Dissociation constant (pKa)	pKa	-		pKa
Endpoints	ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents	-		ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents
Endpoints	ToxTree: Michael acceptors	-		ToxTree: Michael acceptors
Eye irritation/corrosion	ToxTree: Eye irritation	-		ToxTree: Eye irritation
Human health effects	ToxTree: Extended Cramer rules	-		ToxTree: Extended Cramer rules
Human health effects	ToxTree: ILSI/Kroes decision tree for TTC	-		ToxTree: ILSI/Kroes decision tree for TTC
Skin irritation/corrosion	ToxTree: Skin irritation	-		ToxTree: Skin irritation

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



# Recap: What you can do with it ...



The screenshot shows the ToxPredict web application in a Mozilla Firefox browser. The URL is <http://apps.ideaconsult.net:8180/ToxPredict/user/4996263b-0d7c-4fec-8b58-15e38c29e7cd/A/step3>. The interface includes a navigation bar with 'Step 1: Search', 'Step 2: Verify', and 'Step 3: Models'. A table lists various endpoints and models, with a 'Descriptors' column showing 'YES' for Carcinogenicity.

Endpoint	Model	Descriptors
Carcinogenicity	OpenTox model created with TUM's kNN regression model learning web service.	YES
Dissociation constant (pKa)	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	-
Endpoints	ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents	-
Endpoints	ToxTree: Michael acceptors	-
Eye irritation/corrosion	ToxTree: Eye irritation	-
Human health effects	ToxTree: Extended Cramer rules	-
Human health effects	ToxTree: ILSI/Kroes decision tree for TTC	-
Skin irritation/corrosion	ToxTree: Skin irritation	-

Below the screenshot is a map of Europe with five green circular markers placed in various locations: two in the north (Spain/France area), one in the east (Russia/Ukraine area), one in the south (Italy/Greece area), and one in the southeast (Greece/Turkey area).

**Simple building of applications methods and**

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

# Recap: What you can do with it ...

The top-left screenshot shows the ToxPredict web interface. It has three steps: Step 1: Search, Step 2: Verify, and Step 3: Models. Below the steps is a table with columns: Endpoint, Model, and Descriptors.

Endpoint	Model	Descriptors
Carcinogenicity	OpenTox model created with TUM's kNN regression model learning web service.	YES
Dissociation constant (pKa)	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	-
Endpoints	ToxTree: Structure Alerts for the in vivo micronucleus assay in rodents	-
Endpoints	ToxTree: Michael acceptors	-
Eye irritation/corrosion	ToxTree: Eye irritation	-
Human health effects	ToxTree: Extended Cramer rules	-
Human health effects	ToxTree: ILSI/Kroes decision tree for TTC	-
Skin irritation/corrosion	ToxTree: Skin irritation	-

The top-right screenshot shows a workflow diagram in Taverna Workbench. The workflow includes steps like: ask\_username, title\_value, message\_value, dataset\_service\_value, choose\_trainset, upload\_trainset, wait\_for\_trainset, calculate\_descriptors, get\_features\_of\_trainset, choose\_prediction\_feature, learn\_model, wait\_for\_learned\_model, dataset\_service\_value\_1, apply\_model\_to\_testset, wait\_for\_prediction, and results.

The bottom-center screenshot shows a map of Europe with three green circles indicating distributed locations.

**Simple building of applications methods and**

**Distributed and wide range of methods**

**Integration into workflow systems for computational chemistry & biology**

## **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 Jeliaskova, Vedrin Jeliaskov, 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: [www.jcheminf.com/content/2/1/7](http://www.jcheminf.com/content/2/1/7)

# OpenTox Achievements to Date:



- ✓ **Integrated services:** prediction models & creation, descriptors, validation
- ✓ **Integrated databases:** ToxCast, ISS, Fraunhofer Inst., Leadscope
- ✓ **Ontologies:** Organs, Toxicological end-points
- ✓ **OpenToxipedia:** terminology related to the study of toxicity
- ✓ **Prototype applications published:** ToxPredict, ToxCreate
- ✓ **API & framework design:** freely available from open source repository
- ✓ **Integration and interoperability:** e.g. OpenTox with Bioclipse & CDK



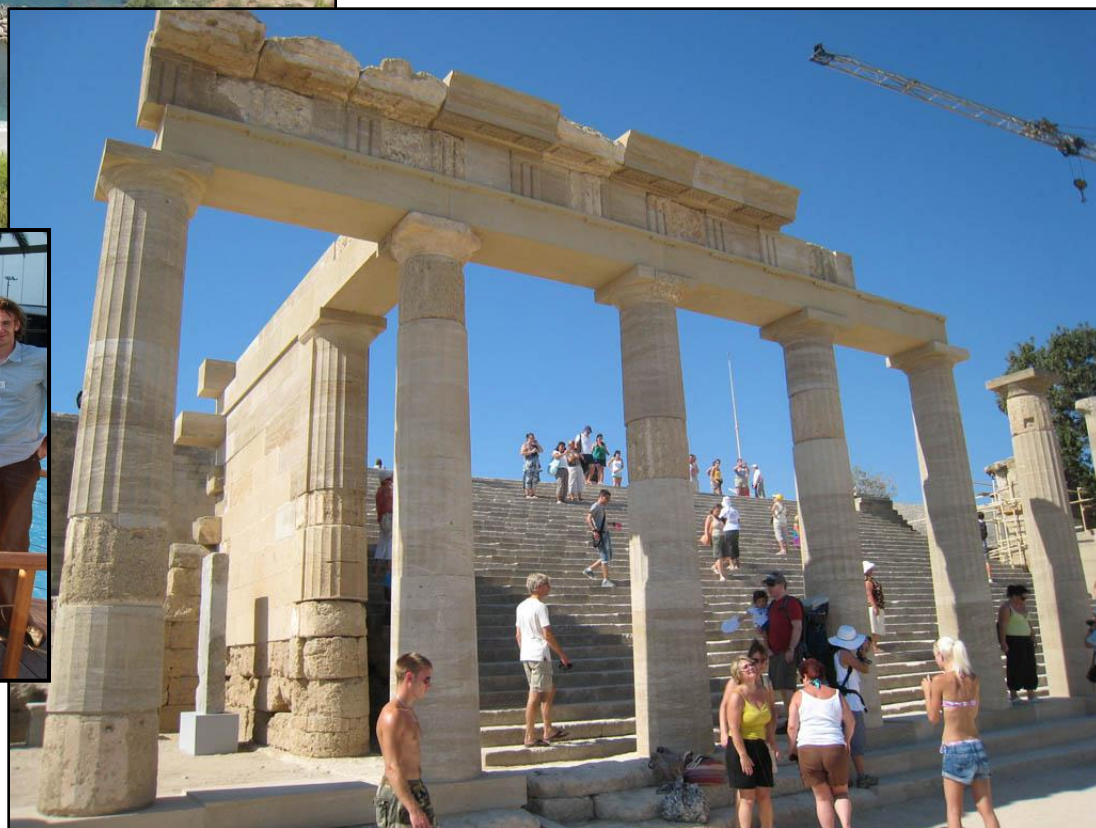


# Rhodos, Greece

Sept. 2010

OpenTox 3rd meeting

**EuroQSAR 2010**



# Acknowledgements

**FUNDING:** European Union, 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).

**Douglas Connect, Switzerland (P.I.)**

**In Silico Toxicology, Switzerland**

**Ideaconsult, Bulgaria**

**David Gallagher, UK**

**Seascape Learning & JNU, India**

**Superior Health Institute (ISS), Italy**

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**Albert Ludwigs University Freiburg, Germany**

**Fraunhofer Institute for Toxicology & Experimental Medicine, Germany**

**Institute of Biomedical Chem. of the Russian Acad. of Medical Sci., Russia**

**National Technical University of Athens, Greece**





# Invitation to OpenTox in Munich, Aug. 2011

## 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](http://www.opentox.org/meet/opentox2011)

