

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) 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:

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



Impact of REACH



Registration per chemical: \$2M to \$14M²

IUCLID: International Uniform Chemical Information Database



Registration submitted by 22 Nov. 2010: 19,237¹
Chemicals pre-registered by 1 Dec. 2008: 143,000²



54M³ - 9M⁴ 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](http://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

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



QSAR: Quantitative Structure-Activity Relationships



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

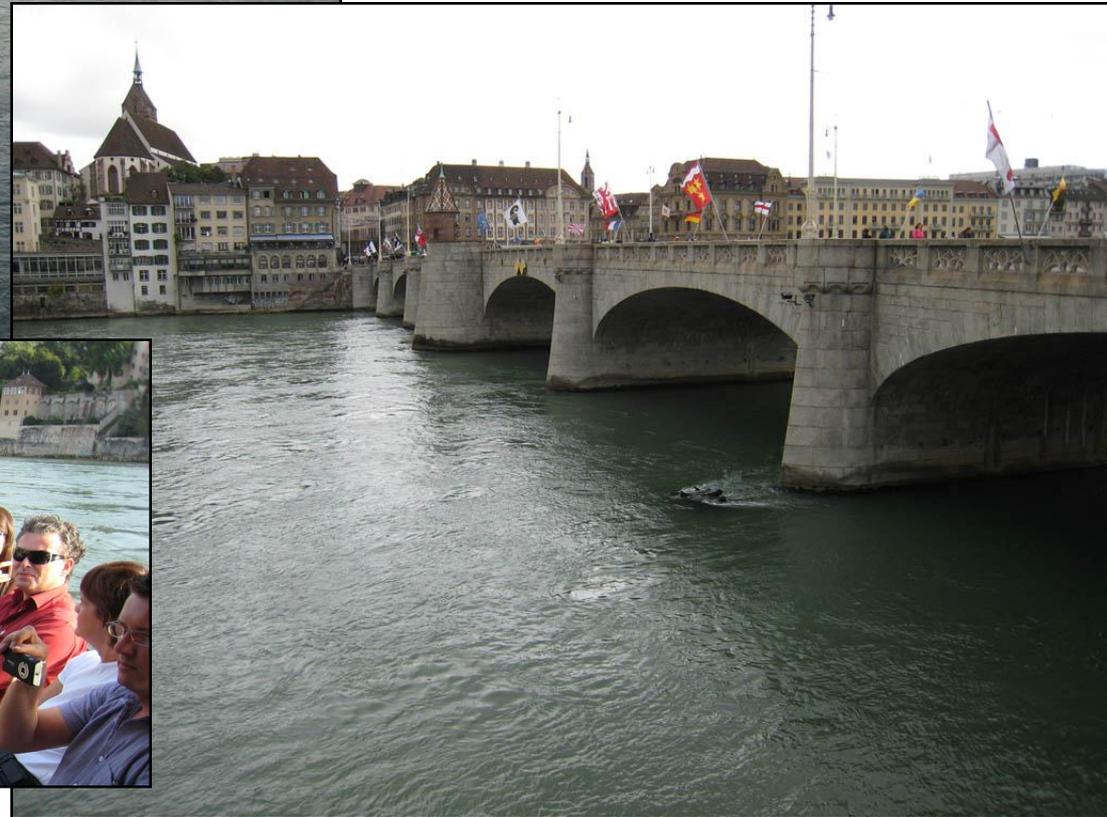
Communications between partners

- 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)

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 left, the logo 'ToxPredict' is shown in purple, with 'OpenTox demo application' underneath. In the top right corner, there is a 'Welcome' message for a 'guest' user, along with links for '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, and a large blue 'NEXT' button is positioned to the right of the progress bar. Below the progress bar, there are three buttons: 'Search' (highlighted in purple), 'Draw', and 'Upload'. A search bar is labeled 'Free text search' and contains the text '(Enter chemical name, registry identifier, SMILES, InChI, any keywords)'. The search input field contains 'benzoic acid'. To the right of the search bar, there is a dropdown menu set to 'Equals' and another dropdown menu labeled 'Number of hits' set to '1'. A second identical progress bar and 'NEXT' button are visible at the bottom of the interface.

ToxPredict (2)

Step 2: Verify structure and description

ToxPredict

OpenTox demo application

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

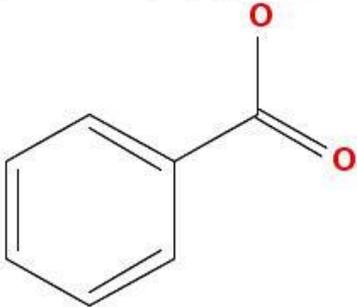
1. Select structure(s) 2. Verify structure(s) 3. Select model(s) 4. Run prediction(s) 5. Display result(s)

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; Diacylic acid; Carboxybenzene; Oracylic 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

The screenshot shows the ToxPredict web application interface. At the top, the logo 'ToxPredict' is displayed, along with the text 'OpenTox demo application' and a user greeting 'Welcome, guest' with links for 'Admin' and 'Help'. A progress bar indicates the current step: '3. Select model(s)', with previous steps '1. Select structure(s)', '2. Verify structure(s)', '4. Run prediction(s)', and '5. Display result(s)' shown as completed or next steps. A large 'NEXT' button is visible on the right side of the progress bar.

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

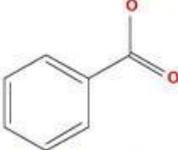
The screenshot displays the ToxPredict web application interface. At the top, a navigation bar shows five steps: 1. Select structure(s), 2. Verify structure(s), 3. Select model(s), 4. Run prediction(s), and 5. Display result(s). The current step is 5. Below the navigation bar, there is a search bar and a dropdown menu for 'Structure(s) & Model predictions & Experimental Data' with options for SDF, CSV, and PDF. The main content area shows the results for Benzoic acid (CASRN 65-85-0). A chemical structure of benzoic acid is displayed on the left. To the right of the structure, the following information is provided: CASRN 65-85-0, Synonym(s) including benzoic acid, Benzenecarboxylic Acid, benzeneformic acid, benzenemethonic acid, Diacrylic acid, Carboxybenzene, Gracrylic acid, phenyl carboxylic acid, phenylformic acid, retarded ba; retardax; tenplas., Benzoic acid / Benzoate, Benzoic acid, AMMONBENZ, BENZDIO LA, BENZOATE, BENZOATCA, JM-244, JM-2644, LITHIUMBZ, BENZOATEK, BENZOATNA, EINECS 200-618-2, IUPAC name benzoic acid, InChIKey_std WPMYKLBIDGXBTJ-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, and SMILES OC(=O)c1ccccc1,C1=CC=CC=C1C(=O)O,C(=O)C1=CC=CC=C1. Below the chemical information, there are sections for 'tree' (ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity), 'Acceptors' (Michael acceptors), and 'explanation' (Michael acceptors). A table of 'Alerts, Alerts' is also present, listing various alerts such as 'Q1.Ethynylene or acetylenic with a carbonyl' and 'Q2.Vinyl or vinylic with a carbonyl', all with a 'No' result.

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

1.  **CASRN 65-85-0**
Synonym(s) benzoic acid, Benzenecarboxylic Acid; benzeneformic acid; benzenemethonic acid; Diacrylic acid; Carboxybenzene; Gracrylic acid; phenyl carboxylic acid; phenylformic acid; retarded ba; retardax; tenplas., Benzoic acid / Benzoate, Benzoic acid, AMMONBENZ, BENZDIO LA, BENZOATE, BENZOATCA, JM-244, JM-2644, LITHIUMBZ, BENZOATEK, BENZOATNA
EINECS 200-618-2
IUPAC name benzoic acid
InChIKey_std WPMYKLBIDGXBTJ-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,C(=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

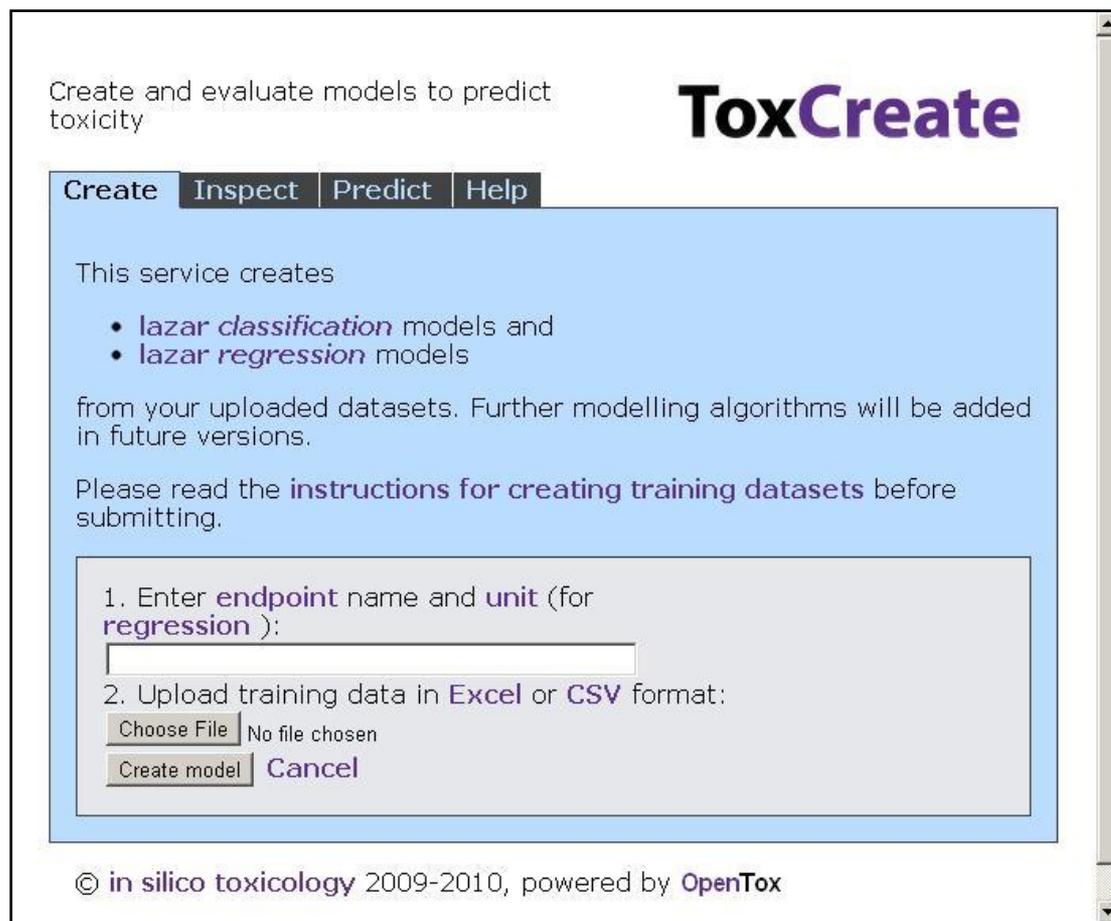
Alerts, Alerts Yes
Q1.Ethynylene or acetylenic with a carbonyl No
Q2.Vinyl or vinylic with a carbonyl No
Q3.1,4-C atom alkyl-substituted with a carbonyl No
Q4A.1,4-C atom substituted with a second carbonyl No
Q4B.1,4-C atom substituted with a second carbonyl No
Q5.Olefinic nitro No
Q6.Ethynylene or acetylenic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

www.ToxPredict.org

Prototype Application 2: ToxCreate

Creates a model from a training set (www.toxcreate.org)

Step 1, upload training set, and create model



Create and evaluate models to predict toxicity

ToxCreate

Create Inspect Predict Help

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

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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:
Detailed report: show
Number of predictions: 76
Correct predictions: 76.00 %
Weighted area under ROC: 0.904
Specificity: 0.771
Sensitivity: 0.756
Confusion Matrix:

	Mean
Predicted active	31
Predicted 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.

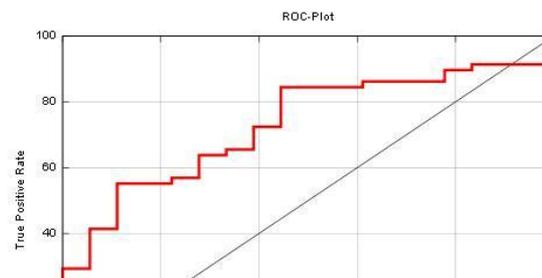
Table 1. Mean Results

Algorithm uri	http://webservices.in-silico.ch/algorithm/lazar
Dataset uri	http://webservices.in-silico.ch/dataset/1702
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

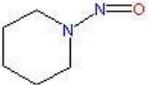
Create Inspect Predict Help

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



or enter a Name, InChI, Smiles

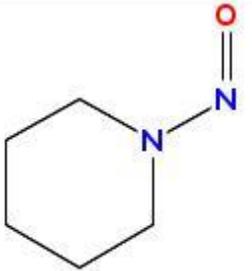
Choose one or more prediction models

- hamster test2
- Test BH 6
- hamster_carcinogenicity

Create Inspect Predict Help

New prediction

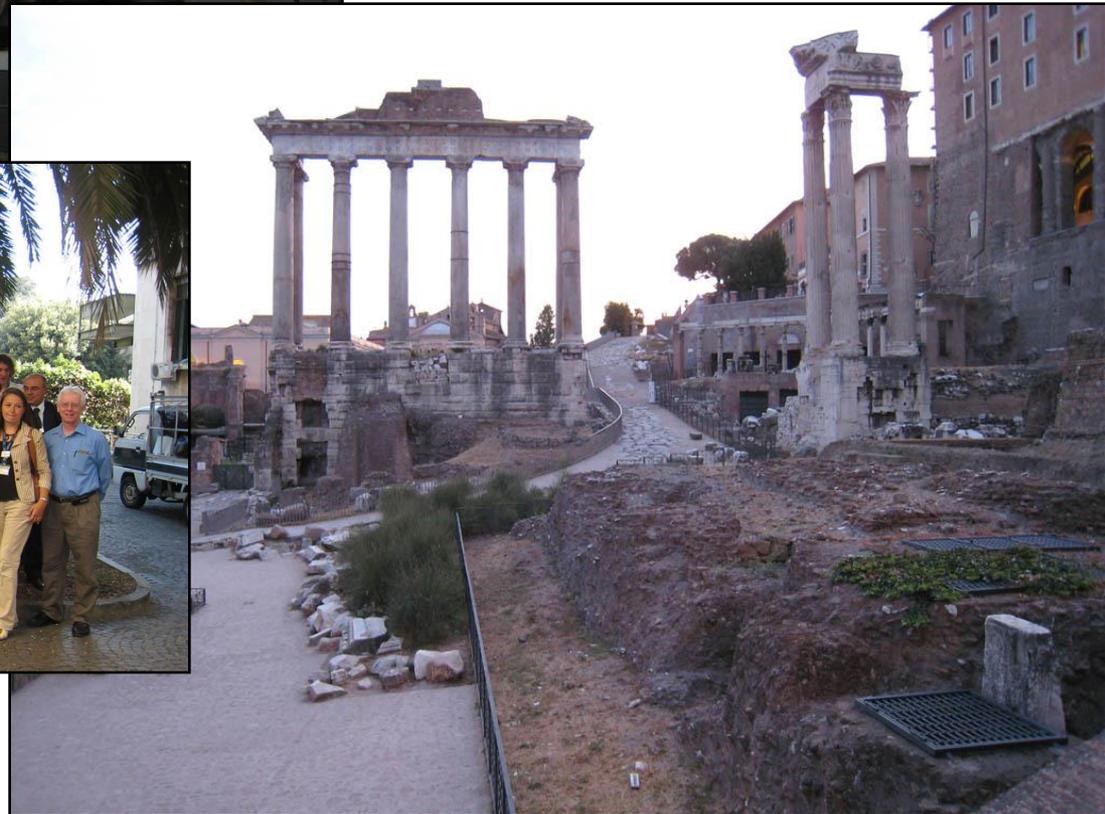
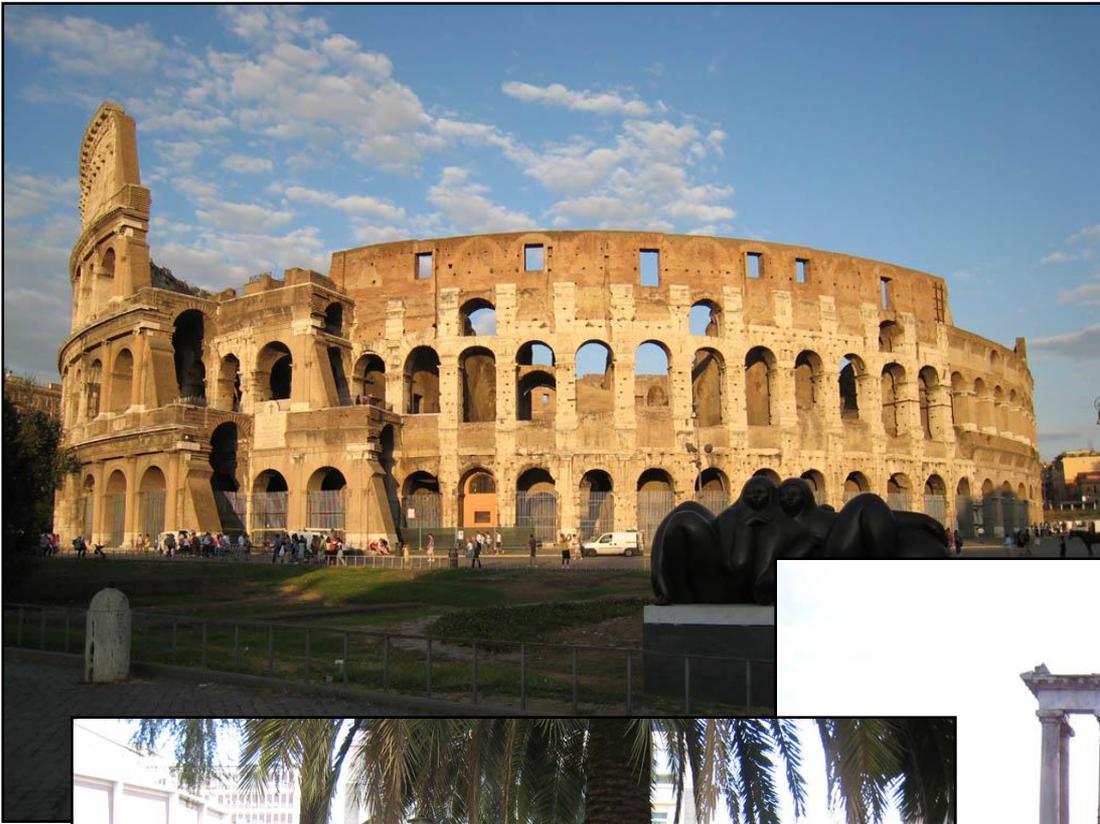
O=NN1CCCCC1



hamster test2:
active
(Measured activity)

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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

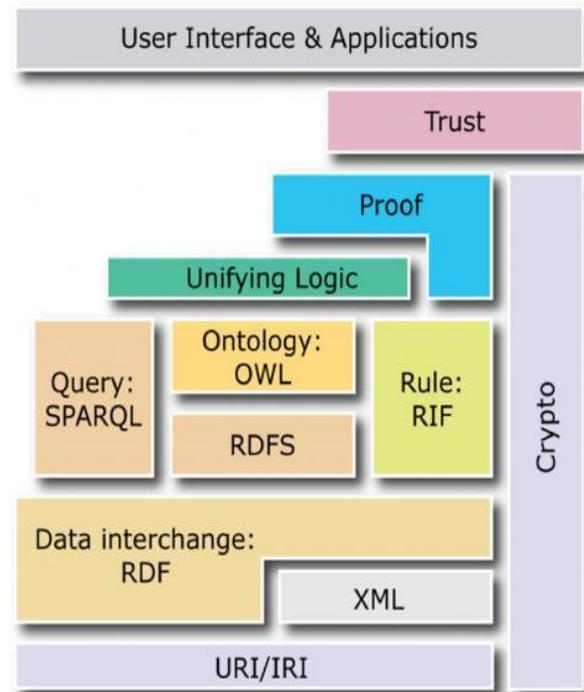
Communicated to OpenTox in 2009 by Stephanie Ringeissen (L'Oréal)

Semantic Web for Predictive Toxicology

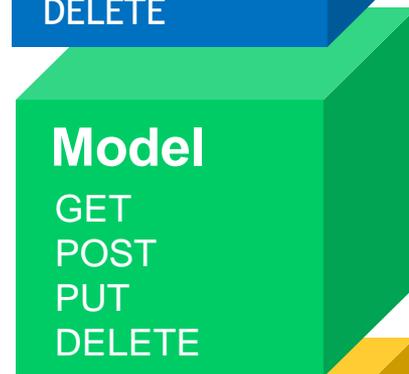
- **URIs:** Uniform Resource Identifier on the web with a name & location
- **RDF:** Resource Description Framework - Graph based Data interchange model to structure data and link resources
- **OWL:** Ontology (Web) Language to add vocabulary for describing properties and relationships



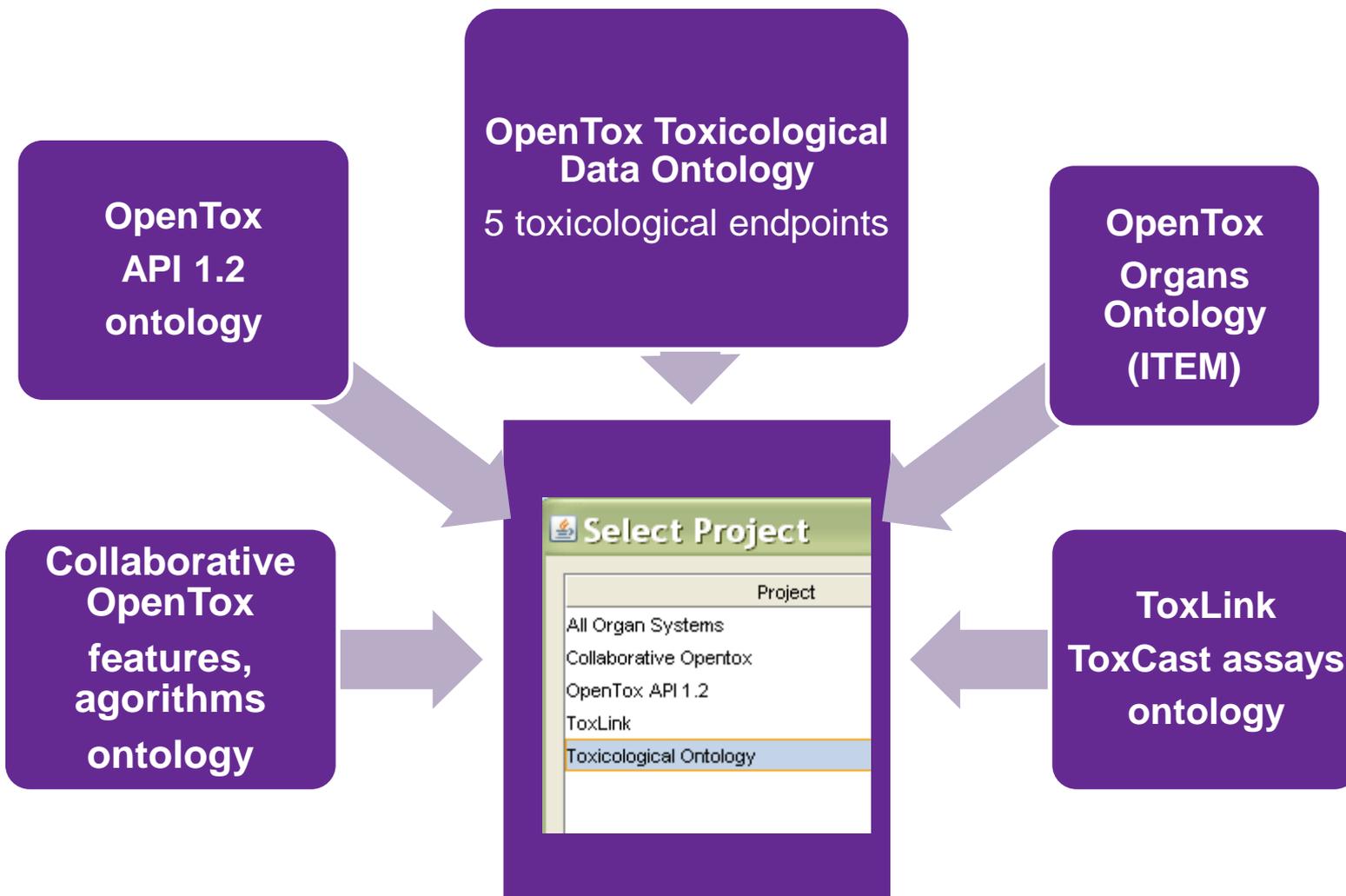
A www network of Linked Resources for Predictive Toxicology!



OpenTox Web Linked Resources



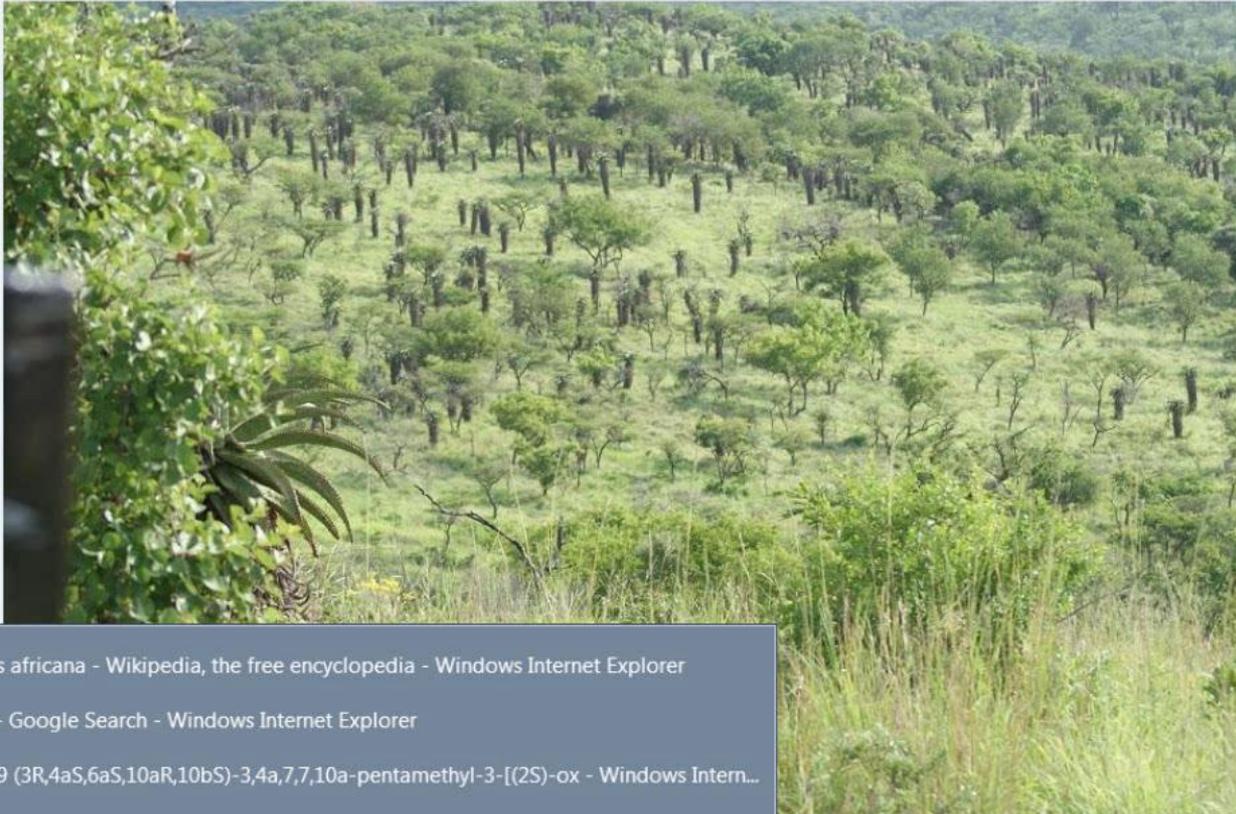
Collaborative Ontology Development: Collaborative Protege Server



Web service interoperability

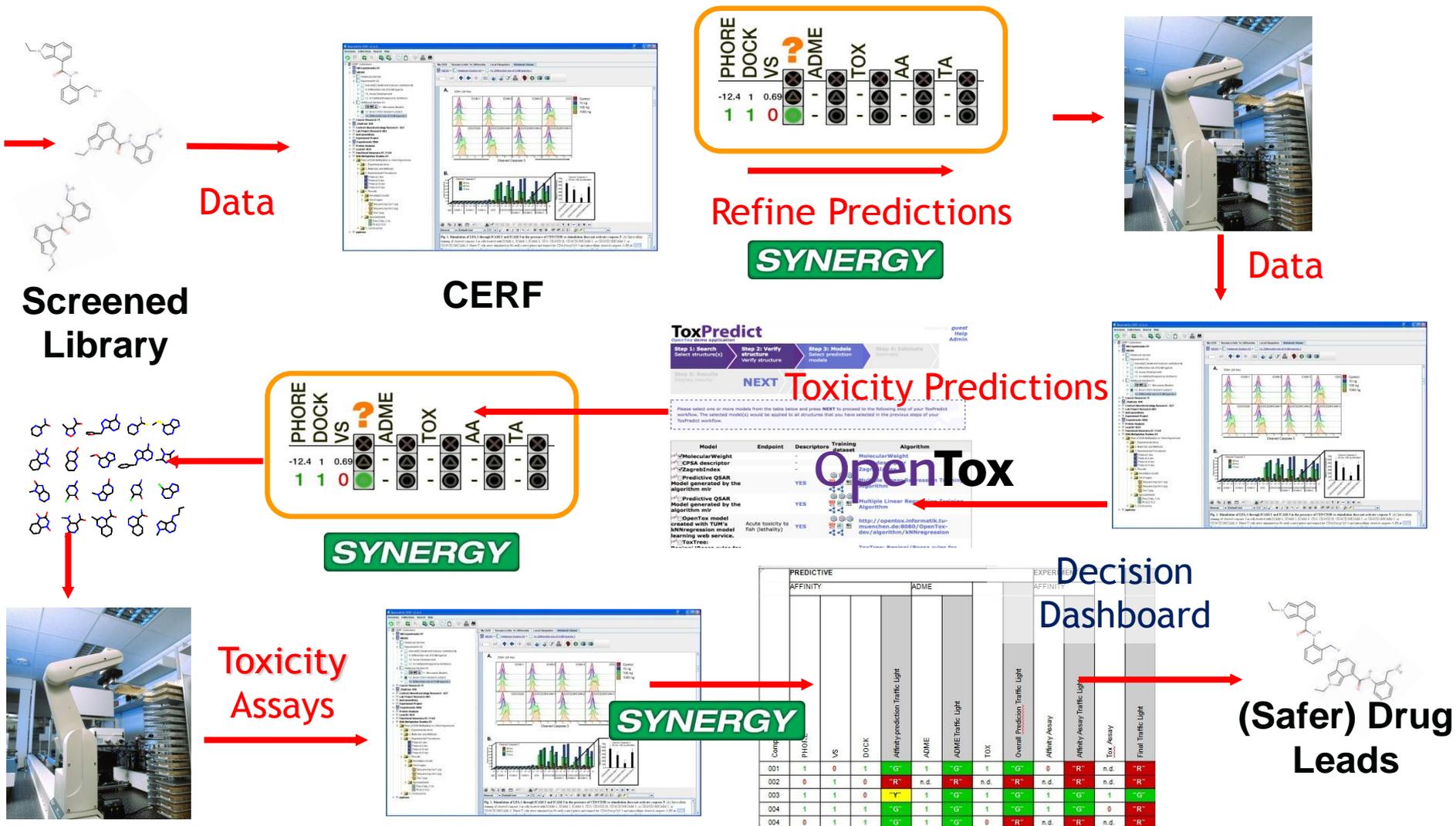
Bioclipse, CDK, Synergy

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

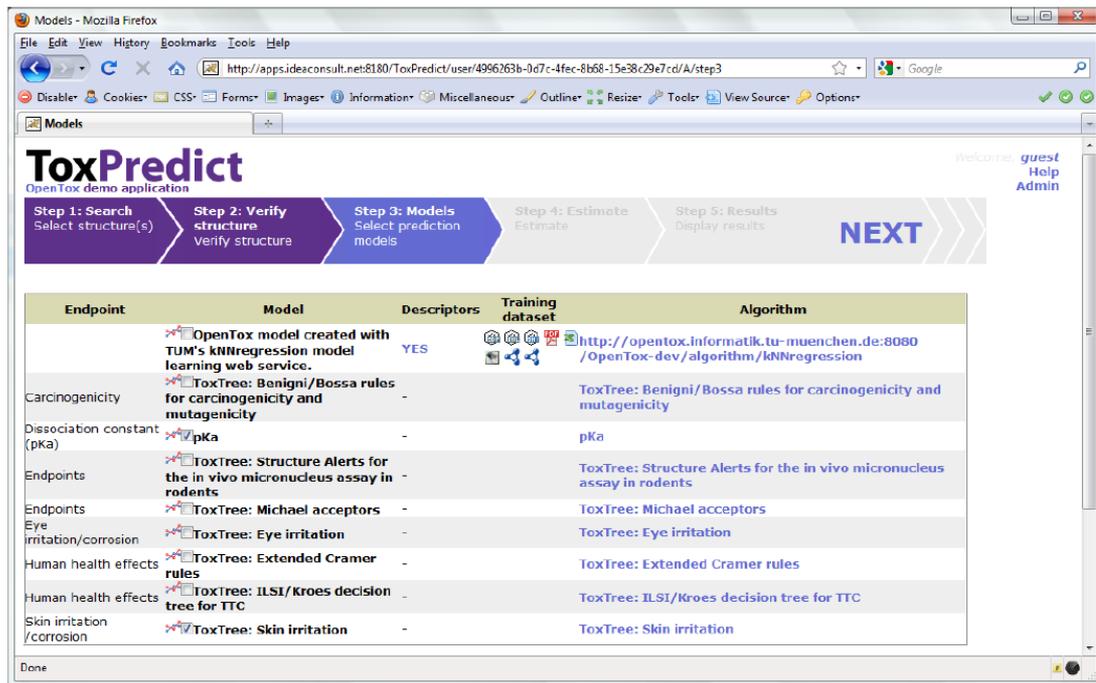


- W Spirostachys africana - Wikipedia, the free encyclopedia - Windows Internet Explorer
- excoecarin - Google Search - Windows Internet Explorer
- 183900-28-9 (3R,4aS,6aS,10aR,10bS)-3,4a,7,7,10a-pentamethyl-3-[(2S)-ox - Windows Intern...
- Download - Windows Internet Explorer
- GoToMeeting : My Meetings - Windows Internet Explorer

Synergy Drug Design Collaboration Pilot



Recap: What you can do with it ...



ToxPredict
OpenTox demo application

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

Step 1: Search
Select structure(s)

Step 2: Verify structure
Verify structure

Step 3: Models
Select prediction models

Step 4: Estimate
Estimate

Step 5: Results
Display results

NEXT

Endpoint	Model	Descriptors	Training dataset	Algorithm
	OpenTox model created with TUM's kNNregression model learning web service.	YES	http://opentox.informatik.tu-muenchen.de:8080/OpenTox-dev/algorithm/kNNregression	
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 interface in a Mozilla Firefox browser window. The URL is <http://apps.ideaconsult.net:8180/ToxPredict/user/4996263b-0d7c-4fec-8b58-15e38c29e7cd/A/step3>. The interface includes a navigation bar with three steps: Step 1: Search (Select structure(s)), Step 2: Verify structure (Verify structure), and Step 3: Models (Select prediction models). Below the navigation bar is a table with columns for Endpoint, Model, and Descriptors.

Endpoint	Model	Descriptors
	OpenTox model created with TUM's kNNregression model learning web service.	YES
Carcinogenicity	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	-
Dissociation constant (pKa)	pKa	-
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	-

Overlaid on the right side of the screenshot is a map of Europe with five green circular markers placed in various geographical locations: two in the north (Spain/France area), one in the east (Poland area), and two in the south (Italy/Greece 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 screenshot displays three main components:

- ToxPredict Web Application:** A browser window showing the ToxPredict interface with three steps: Step 1: Search (Select structure(s)), Step 2: Verify (Verify structure), and Step 3: Models (Select prediction models). Below the steps is a table of models and their descriptors.
- Map:** A map of Europe with three green circular markers indicating specific locations.
- Taverna Workbench:** A workflow diagram showing a sequence of tasks: ask_username, choose_trainset, upload_trainset, wait_for_trainset, calculate_descriptors, get_features_of_trainset, learn_model, wait_for_learned_model, apply_model_to_testset, and wait_for_prediction. The workflow is connected to various services and data sources.

Endpoint	Model	Descriptors
	OpenTox model created with TUM's kNN regression model learning web service.	YES
Carcinogenicity	ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity	-
Dissociation constant (pKa)	pKa	-
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	-

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, Olga Tcheremenskaia, 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 Glorizova, Sergey Novikov, Natalia Skvortsova, Dmitry Druzhilovsky, Sunil Chawla, Indira Ghosh, Surajit Ray, Hitesh Patel and Sylvia Escher

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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



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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

