



Deliverable D2.1

Project Repository and Website

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| Name | An Open Source Predictive Toxicology Framework |
| Coordinator | Douglas Connect |



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| Purpose of Document: | The OpenTox Deliverable Report WP2-D2.1 introduces OpenTox's repository and website (www.opentox.org) and describes the features offered by the site. |
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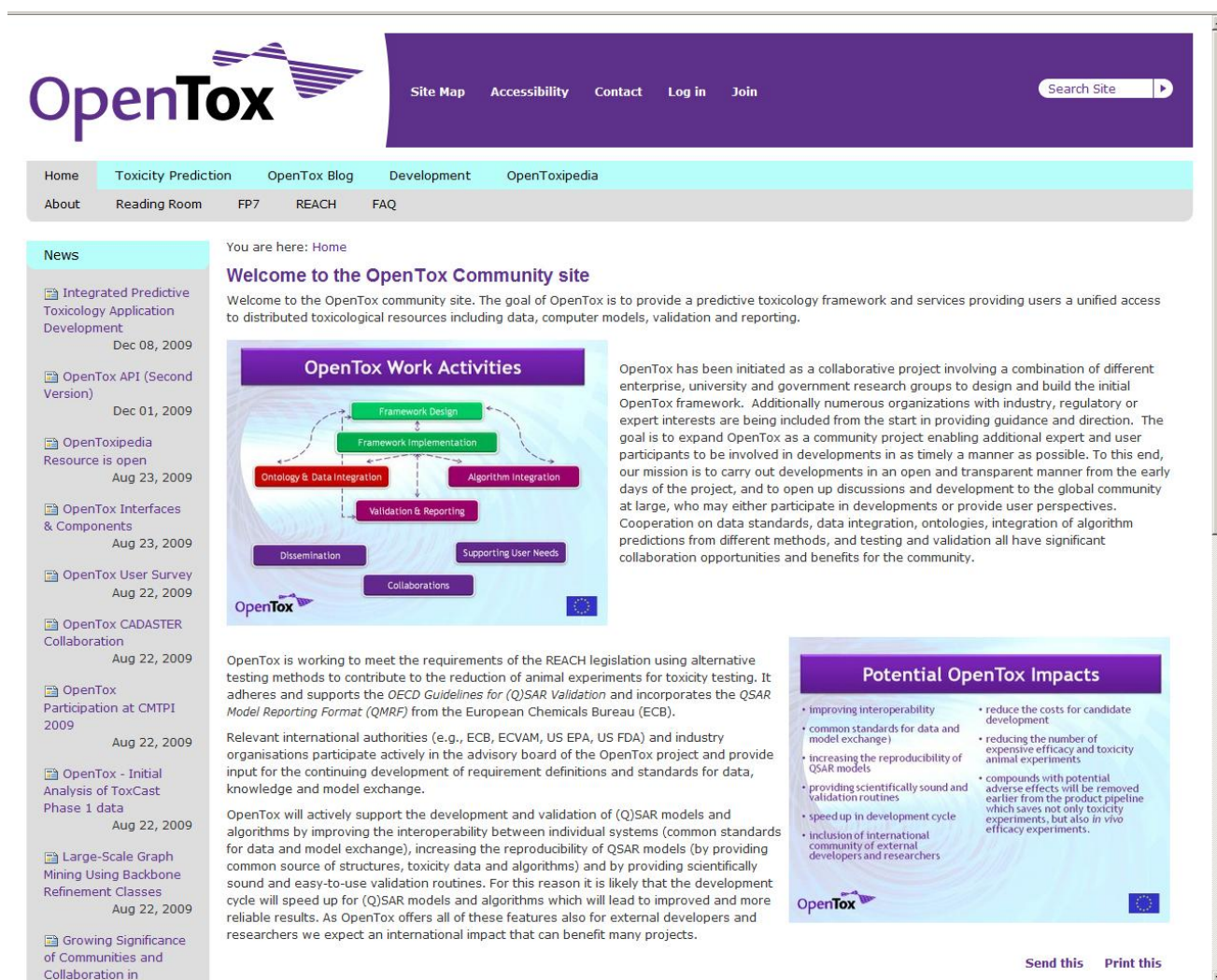
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Summary

The OpenTox Deliverable Report WP2–D2.1 introduces OpenTox’s repository and website (www.opentox.org) and describes the features offered by these services. The top level public areas of the OpenTox website are used to raise public awareness of the project activities and to provide news on OpenTox developments and applications. The “OpenTox Development” area of the OpenTox website is used to involve users, advisors and other developers in the OpenTox Community approach to development, and to disseminate the project’s technical results. The OpenTox website is part of the overall communications system setup for supporting project activities and it is updated regularly. The website together with the mailing lists, document templates and agreed communication rules, as documented in the OpenTox Project Handbook, constitute the overall communication infrastructure of OpenTox.

1. Introduction

The OpenTox website has public sections that are read accessible by anyone with a web browser. The OpenTox Development area is also read and write accessible with a user name/password registration and registration approval. Various levels of access rights have been implemented. All services are accessed from www.opentox.org, the official website of the project. The following is a screenshot of the www.opentox.org home page:



The screenshot shows the OpenTox website home page. At the top left is the OpenTox logo. To its right is a navigation bar with links for Site Map, Accessibility, Contact, Log in, and Join, along with a search box. Below this is a secondary navigation bar with links for Home, Toxicity Prediction, OpenTox Blog, Development, and OpenToxipedia, and another row with About, Reading Room, FP7, REACH, and FAQ. The main content area is divided into several sections:

- News:** A list of recent news items with dates, such as "Integrated Predictive Toxicology Application Development" (Dec 08, 2009) and "OpenTox API (Second Version)" (Dec 01, 2009).
- Welcome to the OpenTox Community site:** A central message stating the goal of OpenTox is to provide a predictive toxicology framework and services.
- OpenTox Work Activities:** A flowchart diagram showing the process from Framework Design and Implementation to Validation & Reporting, Dissemination, and Collaborations.
- Potential OpenTox Impacts:** A list of benefits including improved interoperability, common standards, increased reproducibility, and faster development cycles.

At the bottom right of the page, there are links for "Send this" and "Print this".

Figure 1: OpenTox Home Page

2. OpenTox portal

The public sections of the OpenTox website are used to involve users, advisors and other developers in the OpenTox Community approach to development, and to disseminate the project's results.

A top level set of information, accessibility and dissemination-oriented pages provide a number of sections, e.g., Site Map (www.opentox.org/sitemap), Accessibility (www.opentox.org/accessibility-info), Contact (www.opentox.org/contact-info), Log in (www.opentox.org/login_form), Join (www.opentox.org/join_form), and News (www.opentox.org/news). Besides News, links to these pages are located in the title bar of the page and are accessible from any page under www.opentox.org.

The main content areas of the web site Toxicity Prediction (www.opentox.org/toxicity-prediction), OpenTox Blog (www.opentox.org/blog), Development (www.opentox.org/dev), and OpenToxipedia (www.opentox.org/opentoxipedia) are also on the site's top level. Links to these areas are placed in a menu bar below the title bar, and are directly accessible from any page under www.opentox.org.

2.1 Site Map

This area provides an overview of the structure of the available content on the website.

2.2 Accessibility

Accessibility options such as text size can be adjusted in this area.

2.3 Contact

Users can contact the site owners through a feedback form.

2.4 Log in

Account owners' log in area.

2.5 Join

This area provides a registration form for requesting an OpenTox account, including options for joining the OpenTox general interest and development mailing lists.

2.6 News

Latest news messages on OpenTox are displayed in this area.

2.7 Home

The Home area contains the additional information-oriented subsections About (www.opentox.org/home/about), Reading Room (www.opentox.org/home/documents), FP7 (www.opentox.org/home/fp7), REACH (www.opentox.org/home/reachlegislation), Mailinglist (www.opentox.org/home/maillinglist, for registered users only) and FAQ (www.opentox.org/home/faq).

2.7.1 About

Under About, the mission of the OpenTox framework is briefly described (with a link to an extended description at www.opentox.org/home/about/more).

2.7.2 Reading Room

The Reading Room provides access to OpenTox-related presentation materials, reports, and guidance documents.

2.7.3 FP7

The OpenTox framework FP7 research project is described on this page. Further, there are subsections listing the profiles of the OpenTox partners, the project collaborations, and the advisory board.

2.7.4 REACH

This area provides information on the REACH legislation.

2.7.5 Mailing List

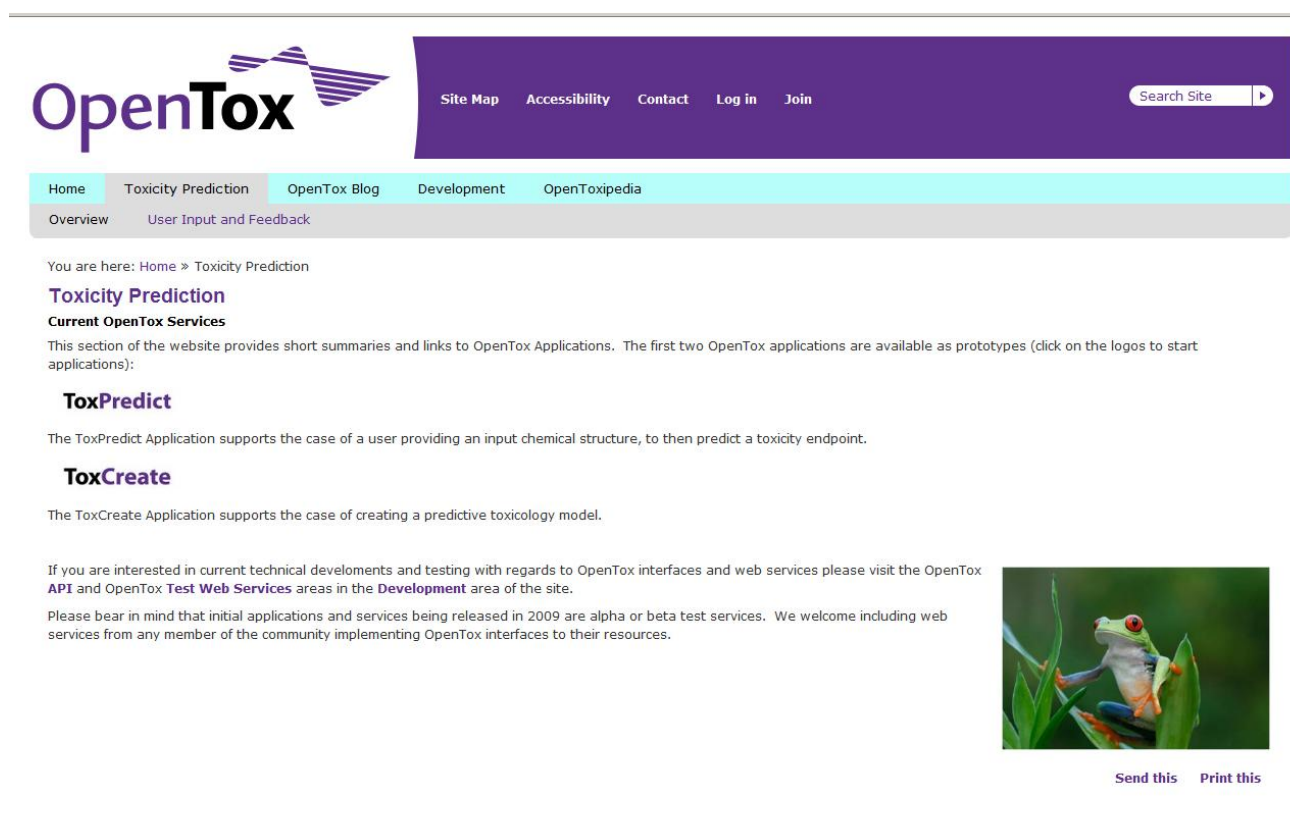
This page hosts the OpenTox General Interest mailing list and its searchable web archives (www.opentox.org/home/maillinglist)

2.7.6 FAQ

The FAQ page contains frequently asked questions on OpenTox and on using its website.

2.8 Toxicity Prediction

This section of the OpenTox website provides short summaries and links to OpenTox Applications, and a possibility for user input and feedback through a web survey. See Figure 2.



The screenshot shows the OpenTox website interface. At the top left is the OpenTox logo. To its right is a purple navigation bar containing links for Site Map, Accessibility, Contact, Log in, and Join, along with a search box. Below this is a light blue navigation bar with links for Home, Toxicity Prediction, OpenTox Blog, Development, and OpenToxipedia. The main content area starts with a breadcrumb trail: 'You are here: Home » Toxicity Prediction'. This is followed by the heading 'Toxicity Prediction' and a sub-heading 'Current OpenTox Services'. A paragraph explains that this section provides short summaries and links to OpenTox Applications, with the first two available as prototypes. Two applications are listed: 'ToxPredict' and 'ToxCreate', each with a brief description of their function. On the right side of the page, there is a photograph of a tree frog. At the bottom right of the page, there are links for 'Send this' and 'Print this'.

Figure 2: Toxicity Prediction Page

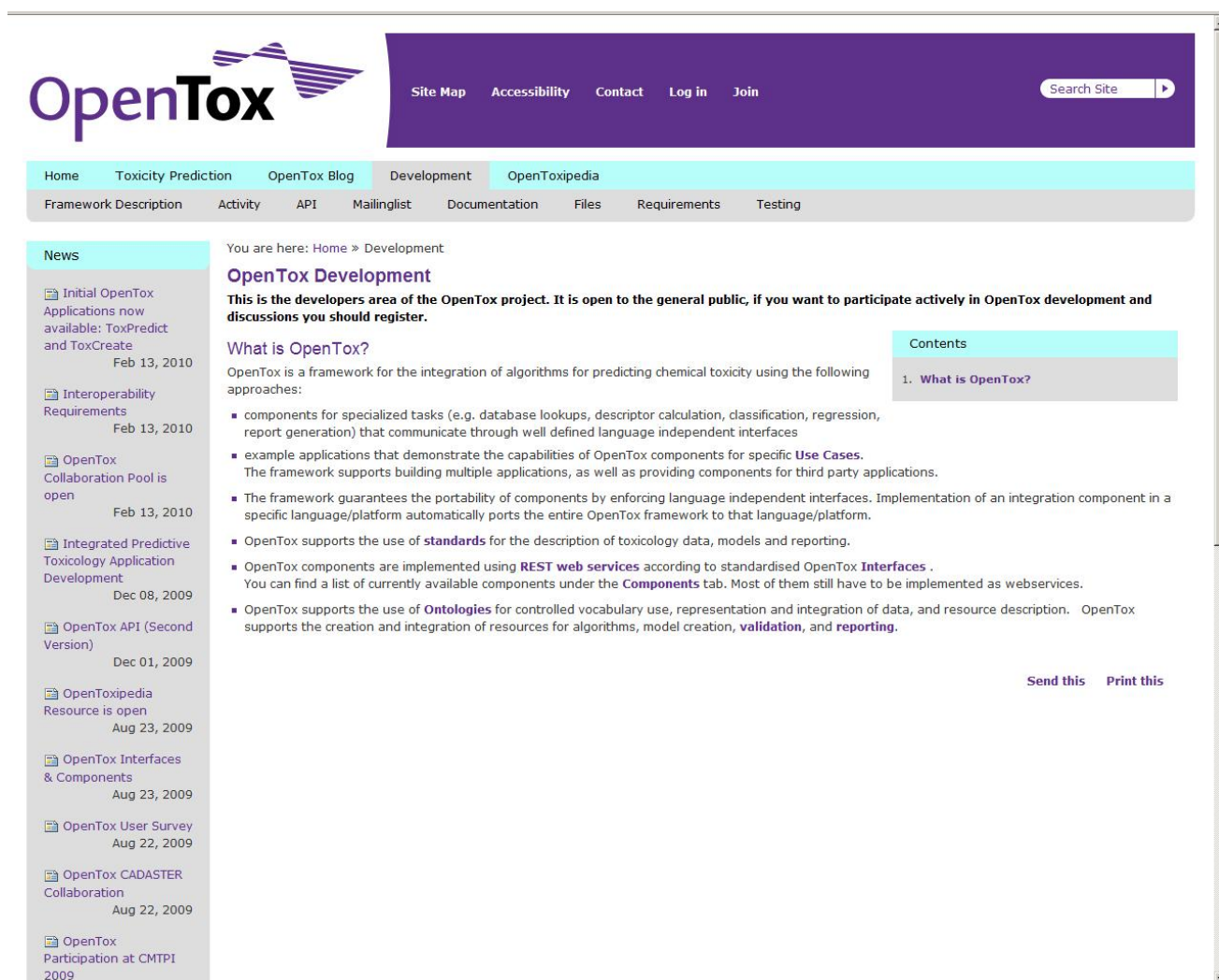
2.9 OpenTox Blog

The OpenTox Blog is a collective open blog for the community to post news, scientific developments and results, comments, opinions, insights, links and discussions related to computer-based predictive toxicology.

2.10 OpenTox Development

This area of the website is used by the OpenTox Development community for knowledge exchange, discussion, documentation of development, and development issues management. The portal entry page to the OpenTox Development community (www.opentox.org/dev, see Figure 3) provides a short description of OpenTox development activities, with internal links to different constituent OpenTox development areas.

The Development area contains the following subsections: Framework Description (www.opentox.org/dev/framework), Activity (www.opentox.org/dev/activity), API (www.opentox.org/dev/apis), Development Mailinglist (www.opentox.org/dev/maillinglist), Documentation (www.opentox.org/dev/documentation), Files (www.opentox.org/dev/documents), Requirements (www.opentox.org/dev/requirements), and Testing (www.opentox.org/dev/testing).



The screenshot shows the OpenTox website's 'Development' section. At the top, there is a navigation bar with the OpenTox logo, a search box, and links for Site Map, Accessibility, Contact, Log in, and Join. Below this is a secondary navigation bar with links for Home, Toxicity Prediction, OpenTox Blog, Development (selected), and OpenToxipedia. A third bar contains links for Framework Description, Activity, API, Mailinglist, Documentation, Files, Requirements, and Testing.

The main content area is titled 'OpenTox Development' and includes a breadcrumb trail: 'You are here: Home » Development'. A key message states: 'This is the developers area of the OpenTox project. It is open to the general public, if you want to participate actively in OpenTox development and discussions you should register.' Below this, a section titled 'What is OpenTox?' describes the framework as a tool for integrating algorithms for predicting chemical toxicity. It lists several key features and goals:

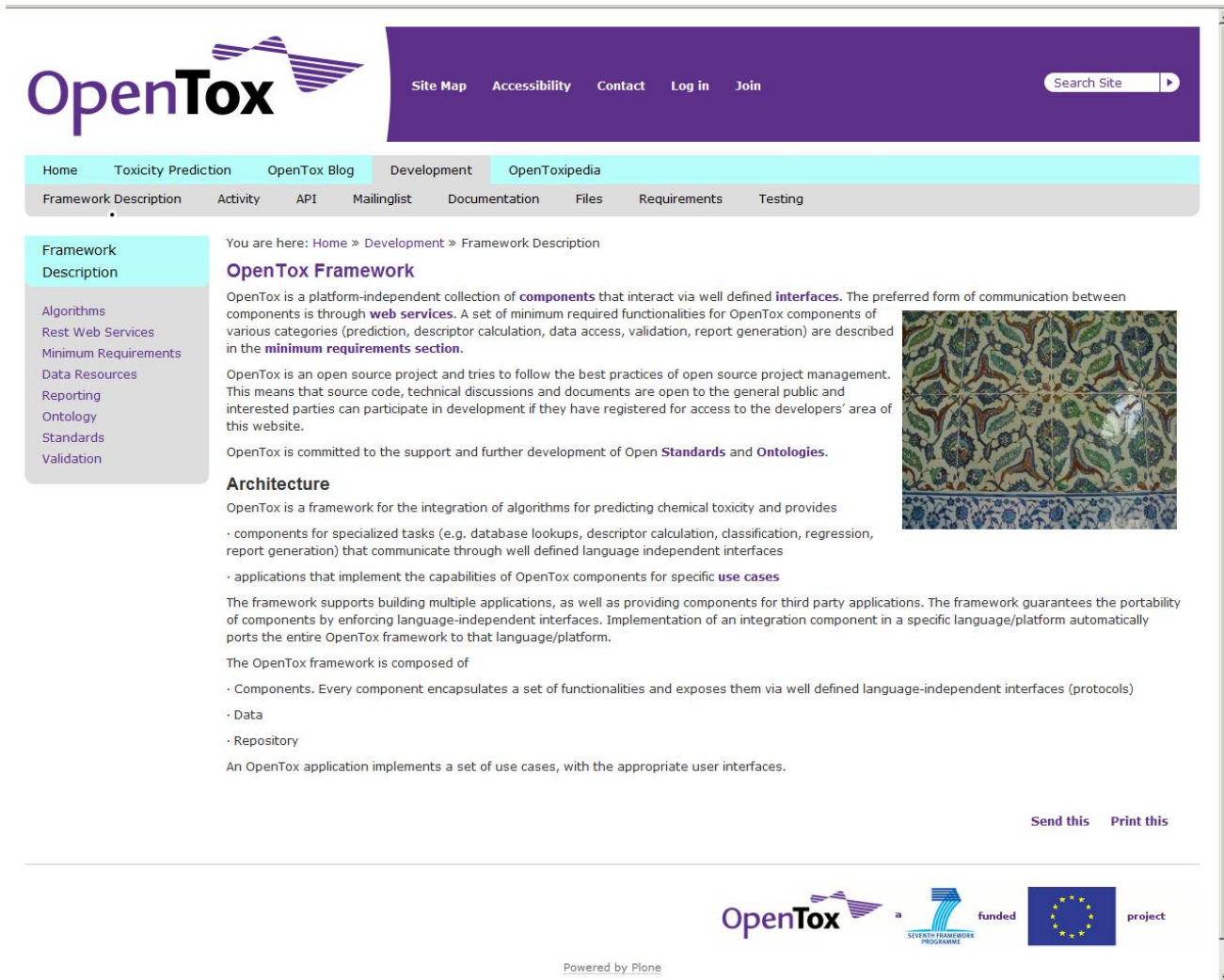
- components for specialized tasks (e.g. database lookups, descriptor calculation, classification, regression, report generation) that communicate through well defined language independent interfaces
- example applications that demonstrate the capabilities of OpenTox components for specific **Use Cases**. The framework supports building multiple applications, as well as providing components for third party applications.
- The framework guarantees the portability of components by enforcing language independent interfaces. Implementation of an integration component in a specific language/platform automatically ports the entire OpenTox framework to that language/platform.
- OpenTox supports the use of **standards** for the description of toxicology data, models and reporting.
- OpenTox components are implemented using **REST web services** according to standardised OpenTox **Interfaces**. You can find a list of currently available components under the **Components** tab. Most of them still have to be implemented as webservice.
- OpenTox supports the use of **Ontologies** for controlled vocabulary use, representation and integration of data, and resource description. OpenTox supports the creation and integration of resources for algorithms, model creation, **validation**, and **reporting**.

On the left side, there is a 'News' sidebar with several recent articles, including 'Initial OpenTox Applications now available: ToxPredict and ToxCreate' (Feb 13, 2010) and 'OpenTox API (Second Version)' (Dec 01, 2009). On the right side, there is a 'Contents' table of contents with '1. What is OpenTox?' as the first item. At the bottom right of the main content area, there are links for 'Send this' and 'Print this'.

Figure 3: Portal of the OpenTox Developers' Area

2.10.1 Framework Description

This page (see Figure 4) describes in detail the OpenTox framework, with links to constituents (components, interfaces, and use cases), and with subsections for Algorithms, REST web services, Minimum Requirements, Data Resources, Reporting, Ontology, Standards, and Validation.



OpenTox

Site Map Accessibility Contact Log in Join Search Site

Home Toxicity Prediction OpenTox Blog Development OpenToxipedia

Framework Description Activity API Mailinglist Documentation Files Requirements Testing

Framework Description

Algorithms Rest Web Services Minimum Requirements Data Resources Reporting Ontology Standards Validation

You are here: Home » Development » Framework Description

OpenTox Framework

OpenTox is a platform-independent collection of **components** that interact via well defined **interfaces**. The preferred form of communication between components is through **web services**. A set of minimum required functionalities for OpenTox components of various categories (prediction, descriptor calculation, data access, validation, report generation) are described in the **minimum requirements section**.

OpenTox is an open source project and tries to follow the best practices of open source project management. This means that source code, technical discussions and documents are open to the general public and interested parties can participate in development if they have registered for access to the developers' area of this website.

OpenTox is committed to the support and further development of Open **Standards** and **Ontologies**.

Architecture

OpenTox is a framework for the integration of algorithms for predicting chemical toxicity and provides

- components for specialized tasks (e.g. database lookups, descriptor calculation, classification, regression, report generation) that communicate through well defined language independent interfaces
- applications that implement the capabilities of OpenTox components for specific **use cases**

The framework supports building multiple applications, as well as providing components for third party applications. The framework guarantees the portability of components by enforcing language-independent interfaces. Implementation of an integration component in a specific language/platform automatically ports the entire OpenTox framework to that language/platform.

The OpenTox framework is composed of

- Components. Every component encapsulates a set of functionalities and exposes them via well defined language-independent interfaces (protocols)
- Data
- Repository

An OpenTox application implements a set of use cases, with the appropriate user interfaces.

Send this Print this

Powered by Plone

OpenTox SEVENTH FRAMEWORK PROGRAMME funded project

Figure 4: Framework Design page in the OpenTox Developers' Area

2.10.2 Activity

This area displays all recent changes made on OpenTox development pages including author, date and time of change or addition.

2.10.3 API

This area provides current specifications of OpenTox Application Programming Interfaces (APIs) and discussion and commenting mechanisms.

2.10.4 Mailinglist

Here, the developer's area provides access to an OpenTox Development specific mailing list, including a searchable web archive.

2.10.5 Documentation

This area provides documentation for the individual constituents of the OpenTox framework. As of now, descriptions of current OpenTox components are described.

2.10.6 Files

In the Files area, documents relating to development (e.g., framework design, validation and XML schema) are provided.

2.10.7 Requirements

This section provides information about the different requirements of OpenTox users. Once finalised and peer-reviewed, OpenTox Use Cases are published in this area.

2.10.8 Testing

This section describes the procedures followed in the testing of OpenTox services and provides details on application cases currently undergoing development and testing, as well as summaries on current test cases.

2.11 OpenToxipedia

The OpenToxipedia area (see Figure 5) provides a community-based Vocabulary Resource of toxicology terminology. Registered users can provide entries, suggested definitions edits or add information to entries in the resource. The entries in OpenToxipedia can be browsed alphabetically or by categories. The latest entries are directly accessible through the “Latest Entries” page.

User guidance for adding or editing terms as well as for existing and proposed categories is provided in the OpenToxipedia area (www.opentox.org/opentoxipedia/guidance), together with useful reference resources (www.opentox.org/opentoxipedia/guidance/referenceresources).

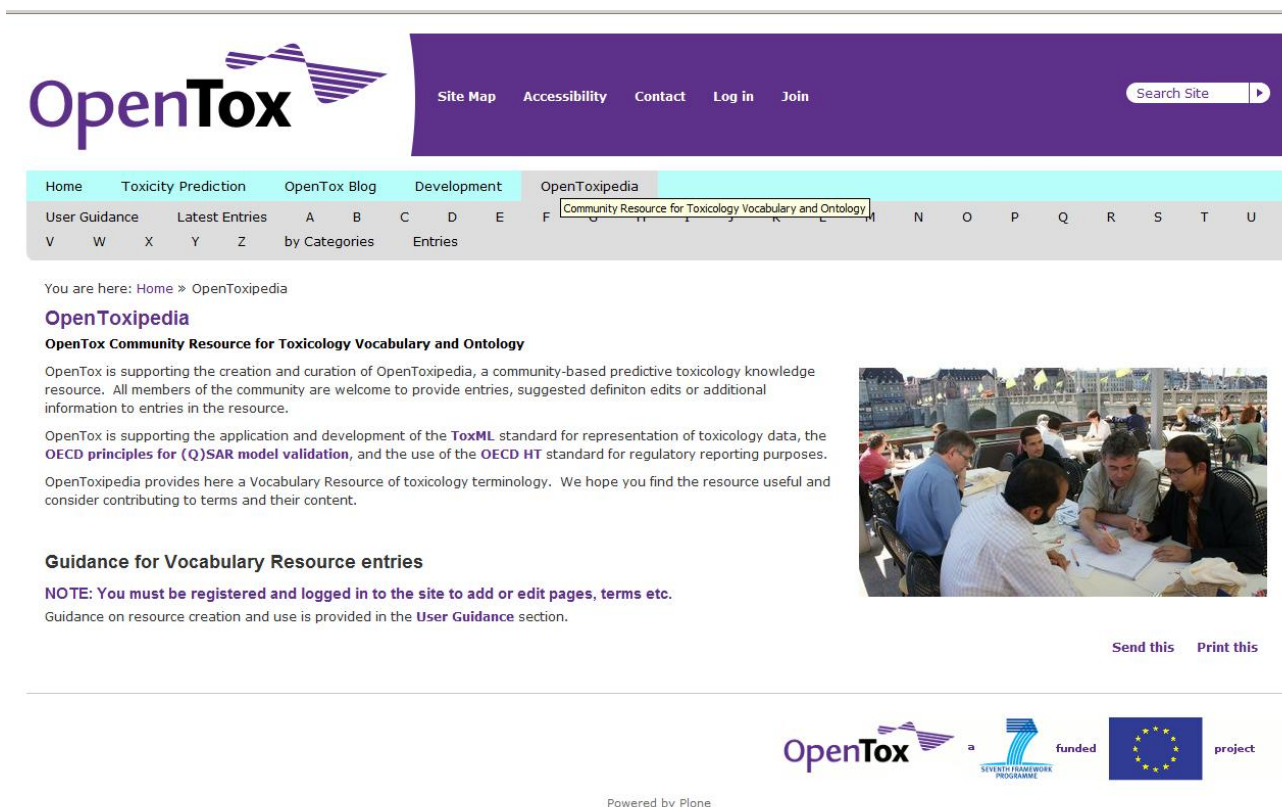


Figure 5: OpenTox OpenToxipedia page.

3. Domains

The DNS domains opentox.org and opentox.net were secured for the OpenTox project, and are currently used to serve the web pages.

4. Server

A DS 3000 CE server has been setup with hosting centre Hetzner Online AG with an IP address used for serving opentox.org and opentox.net of 88.198.47.76 The Linux operating system chosen was Debian 4.0 minimal 32.

5. Mailing Lists

The following public OpenTox mailing lists serving as news and discussion forums are established:

1) Development@OpenTox.org. This list is for communications on technical development aspects of OpenTox, and includes all members of the OpenTox Developer community including partners and external developers. The subject heading of emails to this list commences with [OTDev].

2) Interest@OpenTox.org is a general mailing list providing a signup mechanism for people interested in receiving news and announcements with regards to OpenTox and other developments in the area of predictive toxicology. List members may submit content for consideration for inclusion in a periodic newsletter digest.

Mailing lists have a searchable web archive accessible through the equivalent areas of the website.

6. Conclusions

The first stage of establishing web resources for support of the OpenTox project has been completed with the setup of a server, website, project management infrastructure and mailing lists.