ToxPredict Beta Testing Report Template

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Purpose of Document:	To document beta testing results for the ToxPredict prototype use case implementation

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General Instructions

Please complete the ToxPredict Beta Test Tasks described below. To run the ToxPredict software you would need a web browser (a recent version of Firefox or Internet Explorer) and a network connection to Internet. Please answer the questions on the attached form, either by hard copy, or by editing an electronic copy of this document. Please return your feedback to Vedrin Jeliazkov vedrin.jeliazkov@gmail.com. With your permission, we may contact you occasionally during the course of the beta testing to solicit interim feedback. You might also want to register at the OpenTox site[1] and provide further feedback through the test case development issue tracker[2].

The ToxPredict software implements a prototype use case of the OpenTox framework, which enables end users to run existing endpoint-specific models on a given compound (or dataset) and get model predictions. The main steps of the workflow are as follows:

1. Select input compound (enter chemical name, registry identifier (e.g. CAS, EINECS), SMILES, InChI, arbitrary keyword, SMARTS or draw molecule in molecular editor);
2. Select specific endpoint (e.g. Human Health Effects / Carcinogenicity);
3. Select one or more models, available for this particular endpoint (e.g. ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity);
4. Apply selected model(s);
5. View and/or retrieve the resulting report, available in various formats, e.g. HTML, SDF, CML, SMI, PDF, XLS, ARFF or RDF.

Beta Testing Objectives

The main objectives of this beta testing exercise are:

- To evaluate ToxPredict' technical capabilities and scientific value;
- To evaluate ToxPredict' ease of use and interactivity;
- To evaluate the end user documentation;
- To identify errors/bugs;
- To compile and prioritise a wish list of missing features, to be implemented in subsequent versions of the OpenTox framework.

Beta Testing Tasks

1. Complete **Part-A: Identification** (provide your name and contact details, web browser type/version and time period when the testing has been performed).
2. Open the following URL in your web browser http://toxpredict.org
3. Proceed with functional evaluation of ToxPredict by following as many variants of the provided workflow as possible. These activities aim to evaluate the software's basic ability to generate the expected results, in the way you need them. Report your findings in **Part-B: Functional Evaluation**.

[1] www.opentox.org/join_form

[2] www.opentox.org/dev/testing/testcasedevelopment/testcasedevelopmentissuetracker

4. Complete **Part-C: Overall Comments and Usability Evaluation**. This section asks you to rate various aspects of the software using a 5-point scale.
5. List any bugs or problems in **Part-D: Specific Bugs and Problems Noted** as you proceed.
6. Please answer any other relevant questions listed in **Part-E: Other Generic Topics**.

Known ToxPredict Problems

1. Bugs/usability problems:
    a. Workflow navigation doesn't work always as expected and is subject to improvement;
    b. The overall GUI design is subject to improvement.
2. Missing features:
    a. The integrated online help doesn't provide sufficiently detailed guidance;
    b. Support for batch processing of datasets is under development;
    c. Support for file upload is under development;
    d. Support for molecular structure drawing is under development;
    e. Support for SMARTS searching is under development;
    f. Integrated descriptor calculation is under development;
    g. Model integration is under development (only ToxTree and pKa models are fully supported at the time of this writing);
    h. Models are available only for a subset of endpoints.

Part-A: Identification

Your Name	
Your Organisation	
Your Phone number	
Your E-mail address	
Used web browser (type/version)	
Time period when the testing has been performed	

Part-B: Functional Evaluation

Test Case ID	Function	Tested? (yes/no)	Comments, Ideas and Issues
ToxPredict -01	Input chemical structure as SMILES		
ToxPredict -02	Input chemical structure as MOL		
ToxPredict -03	Input chemical structure as SDF		
ToxPredict -04	Input chemical structure as InChI		
ToxPredict -05	Input chemical structure as compound name		
ToxPredict -06	Input chemical structure as CAS number		
ToxPredict -07	Input chemical structure as EINECS number		
ToxPredict -08	Input chemical structure as SMARTS		
ToxPredict -09	Input chemical structure as arbitrary string		
ToxPredict -10	Input chemical structure through the integrated molecular structure editor		
ToxPredict -11	Select an endpoint from a list of available endpoints		
ToxPredict -12	Select a relevant model from a list of available models for a given endpoint		
ToxPredict -13	Apply model(s) (make a prediction(s))		
ToxPredict -14	Follow the progress of a prediction task		
ToxPredict -15	View predictions and experimental data (HTML format)		
ToxPredict -16	Retrieve resulting report in SDF format		
ToxPredict -17	Retrieve resulting report in CML format		
ToxPredict -18	Retrieve resulting report in SMI format		
ToxPredict -19	Retrieve resulting report in PDF format		
ToxPredict -20	Retrieve resulting report in CSV format		

Test Case ID	Function	Tested? (yes/no)	Comments, Ideas and Issues
ToxPredict -21	Retrieve resulting report in ARFF format		
ToxPredict -22	Retrieve resulting report in RDF format		

Part-C: Overall Comments and Usability Evaluation

Usability Question	Rating Scale 1 – Strongly Disagree 2 – Somewhat Disagree 3 – Neither Agree, Nor Disagree (No Opinion) 4 – Somewhat Agree 5 – Strongly Agree	Specific Comments on Rating
Overall		
This software is useful to me now, or it will be in the near future		
System output and visualization are useful and meet my needs		
Software has the capabilities I need (note any exceptions)		
General impression is good (why?)		
Software was easy to apply to my specific situation		
Data entry effort is manageable		
Technical Content		
Appropriate technical and scientific basis is used		
Uses proper terminology		
Performs calculations correctly		
Toolbars, menus, commands and options are appropriate		
Labels and terms are accurate and easy to understand (if not, what would you prefer?)		
Data formats are useful (if not, what would you prefer?)		
I entered my own data and received the expected results		
Boundary values (largest and smallest chemical samples) were handled correctly		

Usability Question	Rating Scale 1 – Strongly Disagree 2 – Somewhat Disagree 3 – Neither Agree, Nor Disagree (No Opinion) 4 – Somewhat Agree 5 – Strongly Agree	Specific Comments on Rating
Software Operation		
Trouble-free operation		
Easy to navigate within the software		
Consistent and logical flow in using the software		
Easy to find what you are looking for		
Software works as expected (uses standard user interface features)		
Software works well within its family of software applications (if known)		
Files import and export to other needed applications		
Prints properly to a printer		
Documentation		
Clearly describes software purpose		
Organization is clear and logical		
Examples show how to use the main features (please list any features needing more explanation or examples)		
Tables, graphs & figures provide sufficient guidance through major software options		
Do error messages clearly direct the user to a solution?		
On-line help: was it easy to find what you wanted?		
Included necessary technical support information		
Appearance		
Colours, symbols, and graphics are legible and pleasing		
Looks professional		
Correct spelling & grammar		
Application windows have consistent look and feel		

Part-D: Specific Bugs and Problems Noted

Test Case ID (e.g. ToxPredict-01, ToxPredict-02, …, ToxPredict-xy)	Nature of Problem	Full List of Steps to Reproduce the Problem

Part-E: Other Generic Topics

Please comment on the following (if relevant):

- scientific value of algorithms included
- speed of user interface interactivity and of calculations
- order of screens and steps, and number of steps to complete an action
- compatibility of the software with existing workflows
- organization of menu items
- quality of written explanations
- terms or abbreviations used
- annoying or frustrating experiences