

MaxTox Tutorial

Maxtox is a suite of models to predict toxicity of novel compounds based on their similarity to compounds with known toxicities. Compounds forming a model have the same Endpoint Toxicity.

For each model a set of compounds having the same toxicity endpoint are chosen. Substructures occurring (in more than 1 compound and which consist of more than 2 atoms) are extracted and dictionaries built. New compounds are compared to this dictionary and a fingerprint denoting the presence/absence (of dictionary fragments in the test molecule) is generated. This fingerprint is used in a statistical Random Forest Model (prebuilt and optimised) to generate a prediction of toxicity against the particular endpoint.

Maxtox is delivered as an open source application. It uses open source packages like CDK, Restlet, Jena & R to generate models and predict toxicities. It is part of the [OpenTox](#) initiative to create freely accessible resources to predict toxicity.

Maxtox can consume and respond in RDF datatypes and works with the [OpenTox](#) API specification. The Maxtox application can be used as a component of other prediction use-cases hosted from other servers, as long as the data transactions are performed according to the [OpenTox](#) API.

BUILDING MaxTox PREDICTION MODEL AND PREDICTING TOXICITY

The workflow for building a toxicity prediction model using MaxTox is described in fig 1. MaxTox provides the online service to fingerprint their dataset using Maximum Common Substructure Search . Also the toxicity can be predicted online using MaxTox prediction models (See below for the details). Presently MaxTox does not offer services to generate prediction model online so the user has to chose from one of the three stored Random Forest models to predict the toxicity (dashed out box in fig 1). This tutorial covers the instructions on how to fingerprint/predict toxic compounds using MaxTox online service and through cURL calls.

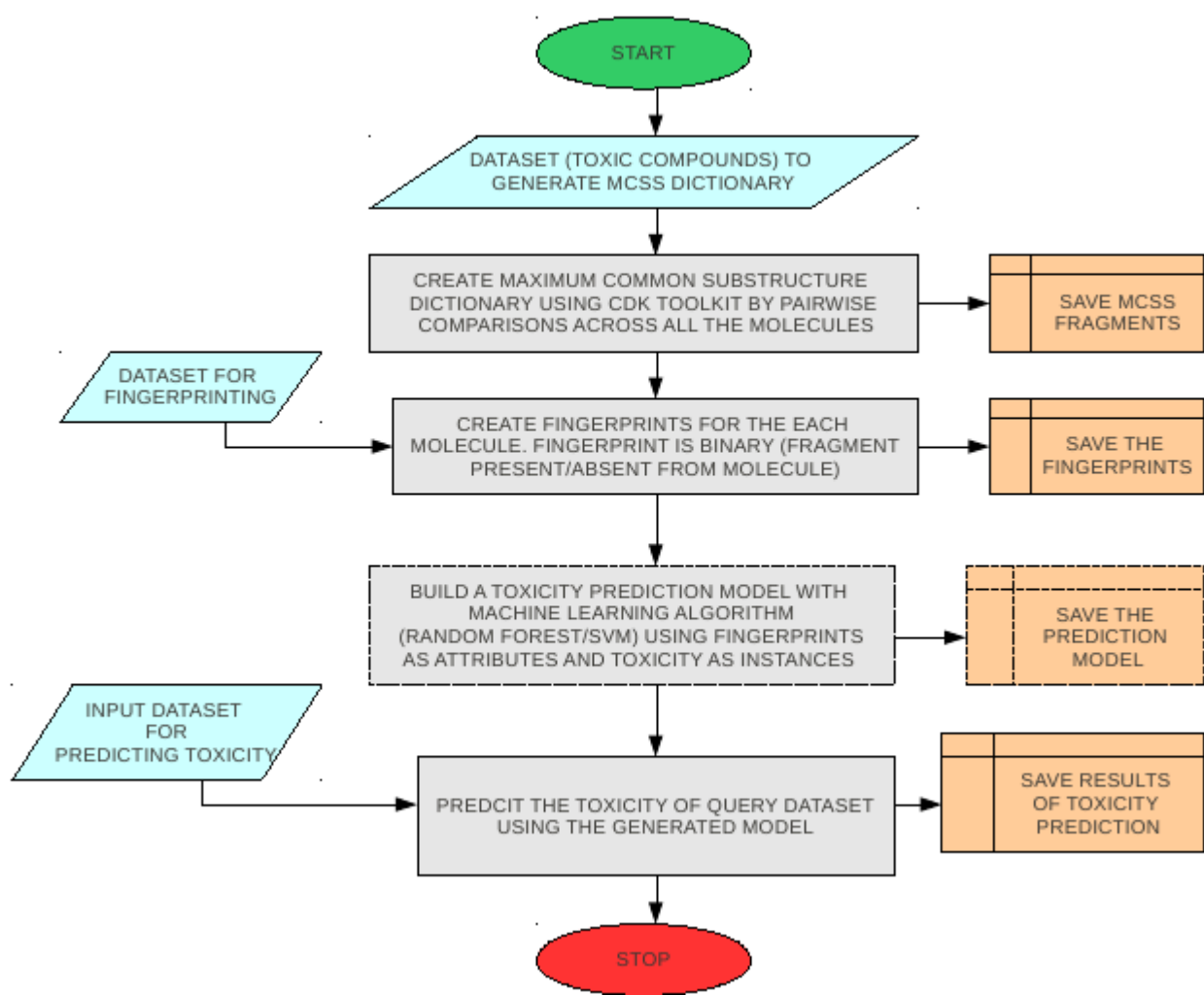


Fig 1. FlowChart for MaxTox Prediction Model building and Toxicity prediction

Create Fingerprints using MaxTox MCSS (Online service)

MaxTox MCSS utility can be used to generate MCSS (Maximum Common Substructure) dictionary for given set of compounds so that fingerprints for the query compound can be generated on the run using MaxTox algorithm and the generated MCSS dictionary. These fingerprints can then be fed to the models stored at MaxTox server to predict the toxicity of the query compound.

1. Submit the URI for the dataset whose MCSS dictionary has to be created using MaxTox at the MaxTox MCSS homepage at URL <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/findMCSS>

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OpenTox **MaxTox** MCSS

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- Find MCSS
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- Fingerprint/Predict
- View Datasets
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Find MCSS and common fragments between two compounds ...

Submit a dataset uri
example : <http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2>

Dataset URI :

Submit a dataset service uri
example : <http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2>

Dataset Service URI :

submit

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

running on Tomcat 6.0 bug-reports/feature-requests : support@maxtox.org

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Fig 2. MaxTox MCSS home page

2. Once the dictionary generation task is submitted, it takes a while to complete the task. On completion of task, the result URI for the MCSS model generated is given.

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Task name :
Task_ac9b584f_a28b_4931_8319_e31b8cb0e510

View Full Task History

taskName	Task_ac9b584f_a28b_4931_8319_e31b8cb0e510
type	0
title	MCSSFinder Run
description	A workflow to get MCSS and other common fragments between two compounds
status	Completed
percentageCompleted	100
dateStarted	27-Feb-2011 04:03:30
dateEnded	27-Feb-2011 04:03:32
requestingIP	202.41.10.242
result_uri	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model/Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4
source	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/MCSSFinder

RELATED LINKS

- [OpenTox](#)
- [ToxCreate](#)
- [ToxPredict](#)

OPENSOURCE

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- [Jena](#)
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- [R \(statistics\)](#)
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Fig 3. Task details after completion of MCSS dictionary generation

3. Model details, dataset and fragment set URIs can be seen at detail page for models when the user clicks on the model URI for example, http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model/Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4

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Model Number :
Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4

serial_number	4
date_created	2011-02-27 16:03:32
unique_id	Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4
description	Model created from the dataset uri : http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2 . The MCSS structures have been extracted from the source dataset using a series of pairwise comparisons. The structures were filtered for duplicates to yield a set of unique substructures. These were used to build a predictive model by fingerprinting the source molecules, and then using the fingerprint to create a predictive model for the feature to be predicted (from the source dataset).
type	0
predicted_endpoint	N/A. This model does not predict any endpoints. This model predicts the presence/absence of fragments within a structure. The fingerprints created may be used to build a predictive model.
R_model_path	N/A
source_dataset_uri	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2
source_dataset_table_id	Source_Compounds_of_Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4
fragment_set_table_id	Fragments_of_Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4

RELATED LINKS

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- [ToxCreate](#)
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OPENSOURCE

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Fig 4. MCSS Model details

To submit a set of compounds for fingerprint generation using the MCSS model built, click on the **“Fingerprint a dataset using this model”** tab.

4. If user wants to see the MCSS fragments generated from the given compounds, the SMILES for fragments are available on clicking the fragment set URI given on the model details page (Fig 4).

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OpenTox **MaxTox** MCSS

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Dataset :
Fragments_of_Model_c6ccd6d1_ef31_4f37_af

SINo	Smile
1	C1=CC=CC=C1C

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Fig 5. MCSS fragments generated using MCSS search (the given example contains only one MCSS fragment).

5. Submit the dataset URI whose fingerprints have to be generated and click **submit** button. The URL for fingerprinting : <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/predict>

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The screenshot shows the MaxTox MCSS web interface. At the top, it says "developed by JNU in collaboration with SL as a part of the OpenTox project". The logo for "OpenTox" and "MaxTox MCSS" is on the left, and the JNU logo is on the right. The main content area is titled "Submit a Prediction Task - Step 2" and contains a form to "Submit a dataset uri ...". An example URI is provided: "http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2". Below the example, it says "Submit a valid dataset" and "Dataset : " followed by an empty text input field. A "submit" button is located below the input field. On the left side, there are two navigation menus: "NAVIGATION" with links for Home, Find MCSS, View Models, Fingerprint/Predict, View Datasets, and Credits; and "SERVER STATS" with links for Full History, Task Histories, View Tasks, and Delete Tasks. On the right side, there are two more menus: "RELATED LINKS" with links for OpenTox, ToxCreate, and ToxPredict; and "OPENSOURCE" with links for Restlets, Jena, CDK, R (statistics), and Rserve. At the bottom, a footer contains the text "running on Tomcat 6.0 bug-reports/feature-requests : support@maxtox.org" and "OpenTox - An Open Source Predictive Toxicology Framework, www.opentox.org, is funded under the EU Seventh Framework Program: HEALTH-2007-1.3 Promotion, development, validation, acceptance and implementation of QSARs (Quantitative Structure-Activity Relationships) for toxicology, Project Reference Number Health-F5-2008-200787 (2008-2011)".

Fig 6. Submitting a dataset URI for fingerprinting task.

If user wants to select some other model to create fingerprints, all other fingerprinting models are available at <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model> .

6. Once the dataset is submitted to create fingerprints, MaxTox returns a task id stating the current status and other details like date of start, date of end, description, percentage completed etc for the fingerprinting task initiated. It takes a while to complete the job, so refresh the page after a while.

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Task name :
Task_494b6a2e_1b5d_4c89_9d0f_21b9045e50

[View Full Task History](#)

taskName	Task_494b6a2e_1b5d_4c89_9d0f_21b9045e5c07
type	0
title	Full Prediction Run with existing models
description	The full prediction workflow
status	Running
percentageCompleted	0
dateStarted	27-Feb-2011 06:25:43
dateEnded	n/a
requestingIP	202.41.10.242
result_uri	n/a
source	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model/Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4

RELATED LINKS

- [OpenTox](#)
- [ToxCreate](#)
- [ToxPredict](#)

OPENSOURCE

- [Restlets](#)
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- [R \(statistics\)](#)
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Fig 7. Running a fingerprinting task

7. When the task is completed the status is set 'completed' and a URI is returned which gives a link to the result dataset uploaded on the AMBIT server.

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Task name :
Task_494b6a2e_1b5d_4c89_9d0f_21b9045e5c07

[View Full Task History](#)

taskName	Task_494b6a2e_1b5d_4c89_9d0f_21b9045e5c07
type	0
title	Full Prediction Run with existing models
description	The full prediction workflow
status	Completed
percentageCompleted	100
dateStarted	27-Feb-2011 06:25:43
dateEnded	27-Feb-2011 06:25:48
requestingIP	202.41.10.242
result_uri	http://apps.ideaconsult.net:8080/ambit2/dataset/192975
source	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model/Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4

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Fig 8. Completed fingerprinting task

Create Fingerprints using MaxTox MCSS (using cURL)

Submit a dataset for creation of MCSS dictionary. The maximum Common Substructure fragments are extracted and a MCSS dictionary is created using CDK

```
curl -X POST -d "dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2"
http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/MCSSFinder
```

Get the task details. Retrieve the model id from the details.

```
curl -X GET http://opentox2.informatik.uni-
freiburg.de:8080/MaxtoxMCSS/task/Task_ac9b584f_a28b_4931_8319_e31b8cb0e510
```

Get the details about MCSS dictionary model

```
curl -X GET http://opentox2.informatik.uni-
freiburg.de:8080/MaxtoxMCSS/model/Model_c6ccd6d1_ef31_4f37_af18_7a57978f3bd4
```

Submit the dataset for creating fingerprints

Get the result dataset URI

Predict Toxicity Using MaxTox (Online service)

1. Go to <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/>

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OpenTox **MaxTox (beta!)**

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What is Maxtox ?

Maxtox is a suite of models to predict toxicity of novel compounds based on their similarity to compounds with known toxicities. Compounds forming a model have the same Endpoint Toxicity.

For each model a set of compounds having the same toxicity endpoint are chosen. Substructures occurring (in more than 1 compound and which consist of more than 2 atoms) are extracted and dictionaries built. New compounds are compared to this dictionary and a fingerprint denoting the presence/absence (of dictionary fragments in the test molecule) is generated. This fingerprint is used in a statistical Random Forest Model (prebuilt and optimised) to generate a prediction of toxicity against the particular endpoint.

Maxtox is delivered as an open source application. It uses open source packages like CDK, Restlet, Jena & R to generate models and predict toxicities. It is part of the [OpenTox](#) initiative to create freely accessible resources to predict toxicity.

Maxtox can consume and respond in RDF datatypes and works with the [OpenTox API](#) specification. The Maxtox application can be used as a component of other prediction use-cases hosted from other servers, as long as the data transactions are performed according to the [OpenTox API](#).

To run a test prediction task navigate to the "Predict Toxicity" page linked on the left.

Note : Maxtox is still in beta and needs many more development iterations before it is perfectly stable and usable. Please report bugs and suggestions to support@maxtox.org.

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RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve




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Fig 9. Homepage for MaxTox

2. To predict toxicity of a compound, navigate to Predict Toxicity link on the left. This link leads to page for “**Submit a Prediction Task – step 1**” which currently contains three different Random Forests models generated using MCSS (Maximum Common Substructure Search) extracted from three different datasets.

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NAVIGATION

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Submit a Prediction Task - Step 1

Select a model to use ...

Available models

Select	SI	No	Model_number	Description	Endpoint	Fragmentset	Dataset
<input type="radio"/>	1	1	See Details	Mutagenicity --> Aromatic amines for mutagenic activity in Salmonella typhimurium TA100 *** No of compounds in training set : 158 *** Toxic/Non-toxic = 93/65 *** No of Dictionary Scaffolds : 1585 *** Training Set Accuracy : 0.86-0.9 *** Training Set Sensitivity : 0.76-0.87 *** Training Set Specificity : 0.91-0.96 *** Test Set Accuracy : 0.53-0.71 *** Test Set Sensitivity : 0.47-0.63 *** Test Set Specificity : 0.6-1.0	Mutagenicity (0 = Active & 1 = NonActive) => Aromatic amines for mutagenic activity in Salmonella typhimurium TA100	FT_1 (See)	MT_1 (See)
				Carcinogenicity --> Aromatic amines for Carcinogenicity in rodents (mice/rats). *** No of compounds in training set : 91			

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Fig 10. Selecting a Model for toxicity prediction

Select one of the three models and click submit on the bottom of the page which follows to the page for “**Submit a Prediction Task – step 2**”.

Detailed description of models about dataset used, endpoint and fragmentset is available at following URI, for example for model 1 :

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/model/1>

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Model Number : 1

SINo	1
model_number	1
description	Mutagenicity --> Aromatic amines for mutagenic activity in Salmonella typhimurium TA100 *** No of compounds in training set : 158 *** Toxic/Non-toxic = 93/65 *** No of Dictionary Scaffolds : 1585 *** Training Set Accuracy : 0.86-0.9 *** Training Set Sensitivity : 0.76-0.87 *** Training Set Specificity : 0.91-0.96 *** Test Set Accuracy : 0.53-0.71 *** Test Set Sensitivity : 0.47-0.63 *** Test Set Specificity : 0.6-1.0
endpoint	Mutagenicity (0 = Active & 1 = NonActive) => Aromatic amines for mutagenic activity in Salmonella typhimurium TA100
fragmentset_uri	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/dataset/FT_1 Go
dataset_uri	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/dataset/MT_1 Go

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Fig 11. Details of Model 1 submitted on MaxTox

3. Submit the URI of the dataset whose toxicity is to be predicted by MaxTox. Note that dataset or the compound has to be first loaded on AMBIT server (<http://ambit.uni-plovdiv.bg:8080/ambit2>),

for example, <http://ambit.uni-plovdiv.bg:8080/ambit2/dataset/6?max=5>

Completion of this step may take a while.

NOTE : As presently MaxTox has not implemented A&A, the dataset URI's may be provided from ideaconsult server, example of dataset URI :

<http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2>

The screenshot displays the MaxTox (beta!) web interface. At the top, it states "developed by JNU in collaboration with SL as a part of the OpenTox project". The main header includes the "OpenTox" logo and "MaxTox (beta!)" with the JNU logo on the right. The interface is divided into several sections:

- NAVIGATION:** Home, Predict Toxicity, View Models, View Datasets, Credits.
- SERVER STATS:** Full History, Task Histories, View Tasks, Delete Tasks.
- HELP PAGES:** Error Codes.
- RELATED LINKS:** OpenTox, ToxCreate, ToxPredict.
- OPENSOURCE:** Restlets, Jena, CDK, R (statistics), Rserve.

The central area is titled "Submit a Prediction Task - Step 2" and contains the following instructions and form fields:

- Submit a compound uri or a smile. Select the appropriate option for your entry ...**
- Submit a dataset uri**
example : <http://ambit.uni-plovdiv.bg:8080/ambit2/dataset/6?max=5>
Dataset URI :
- Submit a result dataset uri**
example : <http://ambit.uni-plovdiv.bg:8080/ambit2/dataset/165>
Dataset URI :
- Submit a dataset service uri**
example : <http://ambit.uni-plovdiv.bg:8080/ambit2/dataset/165>
Dataset URI :

A "submit" button is located at the bottom of the form area. The footer contains the text: "running on Tomcat 6.0 bug-reports/feature-requests : support@maxtox.org" and "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)".

Fig 12. Enter the URI of the dataset whose toxicity is to be predicted

Once the prediction task is submitted, MaxTox returns a task id which contains full task details like date, status, percentage completed, result URI etc.

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RELATED LINKS

- OpenTox
- ToxCreate
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Task name : Task_20110225105236

View Full Task History

Task ID	Task_20110225105236
Date	2011:02:25
Creator	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/model/1
Title	Prediction Task :: Task_20110225105236
Description	Status code : 20 , Status Message : Compound URIs are being retrieved ...
Has Status	Running
Percentage Complete	20
Result URI	n/a
Requesting IP	202.41.10.242
Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2
Uploaded Dataset URI	n/a
Model No.	1

Fig 13. Task Id for a running prediction task.

5. When the user comes back after a while and refreshes the task page or clicks on the task id, the result URI is displayed if the task is completed successfully or if the task is interrupted, an error message is displayed explaining the reason for task failure.

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MaxTox (beta!)



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Task name : Task_20110225105236

[View Full Task History](#)

Task ID	Task_20110225105236
Date	2011:02:25
Creator	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/model/1
Title	Prediction Task :: Task_20110225105236
Description	Status code : 100 , Status Message : Task has been completed ... whew !
Has Status	Completed
Percentage Complete	100
Result URI	http://apps.ideaconsult.net:8080/ambit2/dataset/192745
Requesting IP	202.41.10.242
Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2
Uploaded Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/192745
Model No.	1

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Fig 14. Completed Prediction task

The Result URI links to the prediction results for the submitted dataset stating whether the compounds are predicted to be toxic or not according to the MaxTox model used.

Predict Toxicity Using MaxTox (using cURL commands)

To get the list of models available on MaxTox

In text form :

```
curl -X GET -H "Accept:text" http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/model
```

In rdf/xml form:

```
curl -X GET http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/model
```

To submit a dataset for prediction using model 1

```
curl -X POST -H "Content-Type:application/x-www-form-urlencoded" -d  
"dataset_uri=http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=2"  
http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/model/1
```

Above command returns the prediction task Id, which can be used to retrieve the task status as follows

```
curl http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxTest/task/Task\_20110225121806
```

On completion of task, result dataset URI is returned which can be retrieved using the following curl command

```
curl -X GET http://apps.ideaconsult.net:8080/am63t2/dataset/19276
```