

Q-edit: Documentation

Scope

Q-edit is a new QPRF editor developed under OpenTox which aims at exploiting implemented web services to provide functionalities that facilitate the creation of QPRF reports by an end user. In this article we provide instructions on how to use Q-edit: The OpenTox QPRF report editor/viewer. Online documentation can be found at <http://opentox.ntua.gr/blog/78-q-edit>.

Summary

The QSAR Prediction Reporting Format (QPRF) is a harmonised template for summarizing and reporting substance-specific predictions generated by (Q)SAR models (check the specification [here](#)). Q-edit is tool that **facilitates the whole procedure of prediction generation and reporting** combined with database lookups based on the OpenTox web services.

The [OpenTox](#) report on "Automated Validation Report Generation" available [here](#) contains the background and progress which has been achieved within [OpenTox](#) with respect to the creation of automated reporting facilities for validated (Q)SAR models of predictive toxicology data.

In this article, we will start by reviewing the key requirements of a QPRF report and then proceed with the necessary steps to generate a QPRF report using Q-edit - a new QPRF editor developed under [OpenTox](#) to facilitate the creation of QPRF reports by an end user.

Users can download the latest version of the OpenTox QPRF editor (Q-edit) from [here](#). Developers can access the source code at the CVS <https://github.com/alphaville/Q-edit>. Use the https git directory `https://github.com/alphaville/Q-edit.git` or the git read-only version : `git://github.com/alphaville/Q-edit.git`.

Users have to have installed some Java Runtime Environment and Virtual Machine on their operating systems. Until now we have tested Q-edit with Sun Java version 1.6.0.22 and 1.6.0.24. Normally users should not encounter any problems trying to run Q-edit on any other Sun JVMs of newer version or other JVMs.

Users that need to access protected resource in OpenTox (read the article posted at <http://opentox.ntua.gr/index.php/blog/5-authentication> on Access Control management in OpenTox) **should install the SSL certificate for opensso.in-silico.ch** on their machines. You will definitely find the information provided [here](#) useful.

You will find the latest version of Q-edit at <http://opentox.ntua.gr/files/Q-edit.jar>. Download it and run it locally. On Linux machines, using the terminal, use the command "java -jar ./Q-edit.jar". It is possible that Linux users need first to modify the permissions of the downloaded file to render it executable. In this case, the following warning message will pop up:



Figure 1 – Error message that sometimes pops up on Ubuntu due to restrictions related to execution of Java programs downloaded from the web.

In this case right click on the Q-edit.jar file and choose "Properties", once opened go to the "Permissions" tab and check "allow executing file as program":

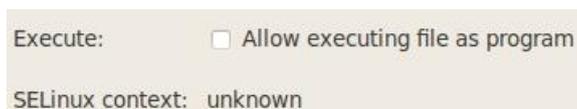


Figure 2 – Allow file to be executed as program (on Ubuntu)

Ubuntu users may use the following commands to download and run Q-edit :

```
wget http://opentox.ntua.gr/files/Q-edit.jar
chmod +x ./Q-edit.jar
java -jar Q-edit.jar
```

Q-edit features

Using Q-edit, users will be able to:

- Create new QPRF report objects: Q-edit provides detailed guidance throughout the whole procedure of the creation of a QPRF report with user-friendly visualization.
- Use OpenTox web-services (in the background) to offer to users access to the OpenTox web services. This way, users can
 - Search on-line for compounds
 - Download information for an OpenTox QSAR model
 - Access protected OpenTox resources (securely, over an encrypted SSL connection)
 - Retrieve experimental values for a compound and much more.
 - Run a model to get predictions for a given chemical compound. The whole procedure of generating molecular descriptors and submitting them to the QSAR model runs behind the scenes.
- Save/Open QPRF report objects using an in-house binary file format (.ro files).
- Export a report as PDF. The generated PDF is **compliant to the EC JRC standards**

Create a QPRF report and Load a Compound

Once you launch Q-edit, create a new report (File > New Project > Empty Report or just Ctrl+N). You should be able to see the new report in the desktop of Q-edit:

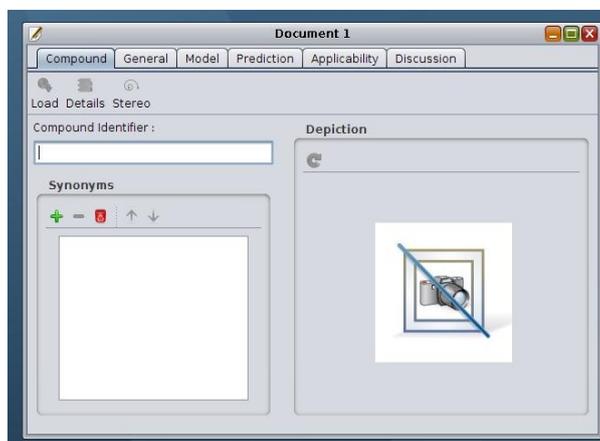


Figure 3 – A new empty QPRF report object – user interface.

Now enter the identifier of a compound in the text field as in the following figure:

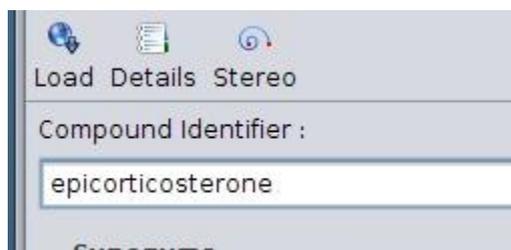


Figure 4 – Provide an identifier of a chemical compound

Strike the return key or click the Load button to retrieve all available information from the online OpenTox web services at <http://apps.ideaconsult.net:8080/ambit2>. The details are loaded on the same view and are presented as follows:

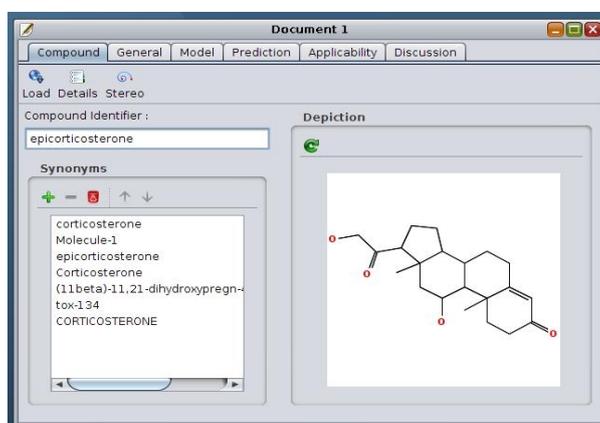


Figure 5 – Information loaded from OpenTox web services are presented to the user

The "Details" button gives you access to the various structural attributes of the compound like its SMILES string as well as to other identifiers like the CAS registration number and the INECS number as show in the next figure:

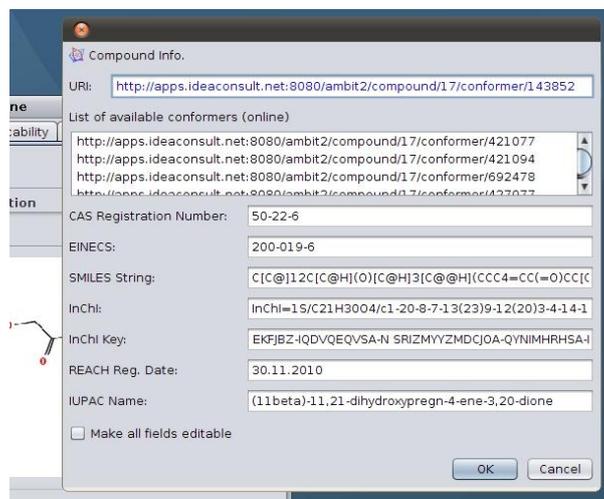


Figure 6 – Details about the chemical compound found online

The user is then expected to discuss on the stereochemical structural attributes of the compound that can possible affect the reliability of the prediction. The "Stereo" button in the toolbar of the same view will open a new dialog box in which this information should be provided:

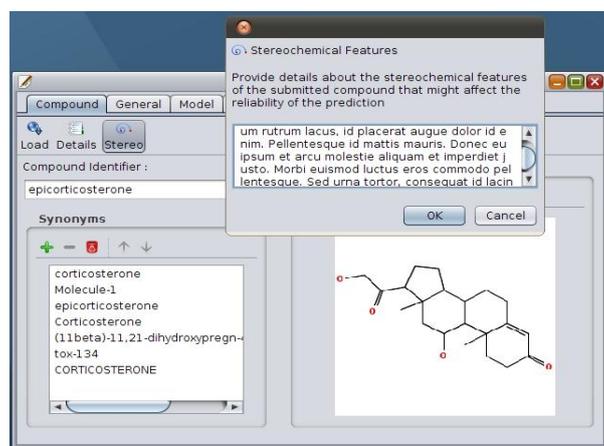


Figure 7 – Considerations on stereochemical features of the compound

A list of synonyms is also loaded but the user might need to add one or remove some synonym that is invalid according to their opinion. For example in this example, the synonym "Molecule-1" needs to be removed:

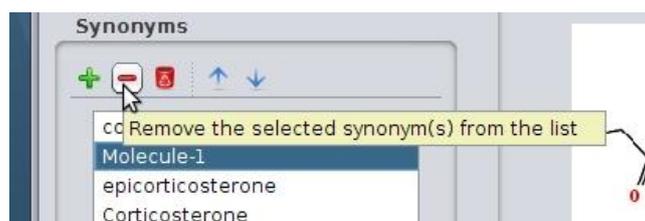


Figure 8 – Remove a synonym from the list

You can add a synonym of your own using the green + button:

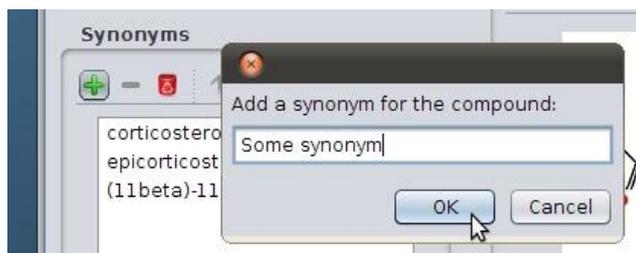


Figure 9 – Add a synonym

Finally, note that one can look up for a compound using directly its OpenTox URI, for example try <http://apps.ideaconsult.net:8080/ambit2/compound/24793/conformer/372927> instead of "carbasalate calcium".

Authors of the QPRF report

The authors of the reports are included using the wizard you'll find under the second tab:

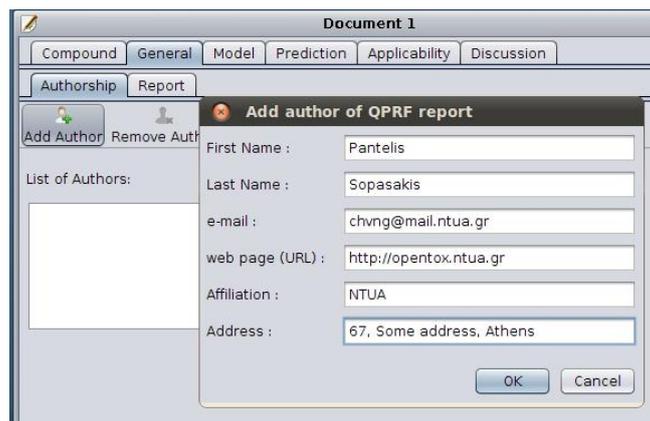


Figure 10 – Add an author for the QPRF report

Fill in your name, email and other information as requested and click OK. The first two fields are mandatory. Also note that you cannot add the same author (i.e. an author with the same name) more than once. Select any author from the list on the left to see their data:

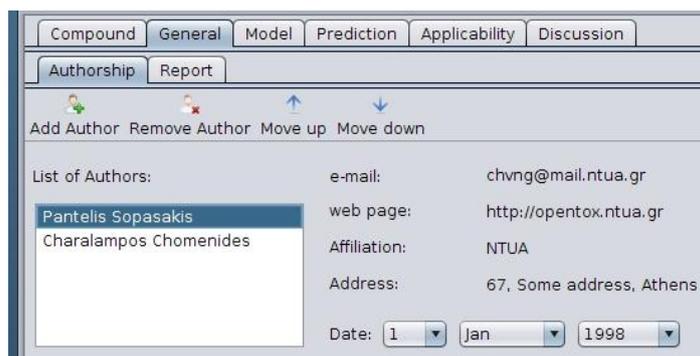


Figure 11 – Authors of the QPRF report

You can also update/edit the information you previously submitted for an author using the "Edit Author" button:

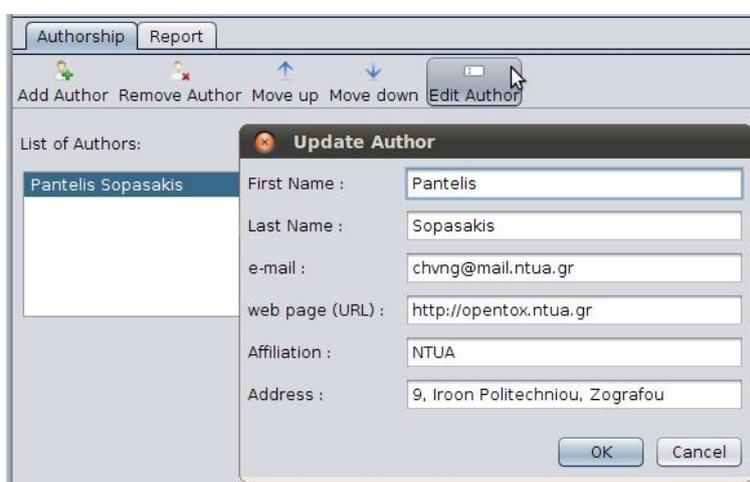


Figure 12 – Edit or Update the information for an author

Set the date when the report was created before proceeding to the next step.

Load an OpenTox Model

If you have a URI of an OpenTox model resource, you may enter it directly to the corresponding field in Q-edit:

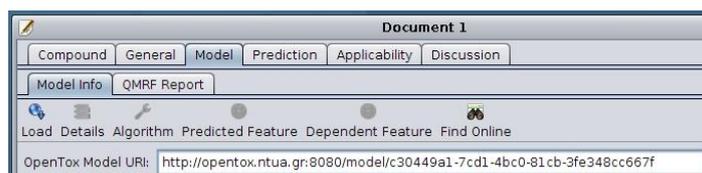


Figure 13 – Load a model given its URI

OpenTox services list the URIs of all available models under /model. For instance check out <http://opentox.ntua.gr:8080/model> and <http://apps.ideaconsult.net:8080/ambit2/model>. You can also

search for approved models that are also included in ToxPredict at <http://apps.ideaconsult.net:8080/ontology>. Copy a URI and paste in Q-edit as shown in the figure above. Then click the "Load" button or strike enter to load all information available for it. In case the model you chose is password-protected you will need to provide your credentials. The following dialog box will appear:



Figure 14 – Unauthorized user is prompted to provide its credentials

In case you don't have an account, you may just "Login as Guest" clicking on the corresponding button. Afterwards, you can inspect details about the loaded model - just click on the "Details" button that appears in the Model tab toolbar:

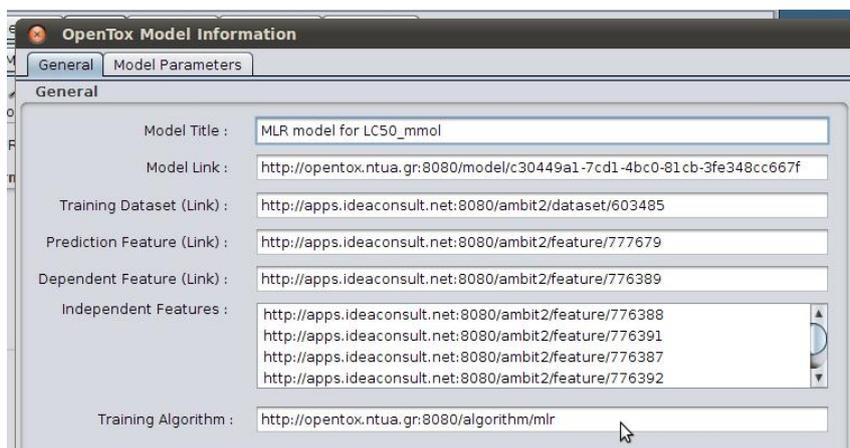


Figure 15 – Model Details

Therein one may find the Model's title (e.g. here it is "MLR model for LC50_mmol"), the prediction, dependent and independent features of the model, a link to its training dataset, all identified by their URIs. Later we'll show how to access more human-readable information about all these. If the model has a certain parametrization, this can be found in the second tab, namely "Model parameters":

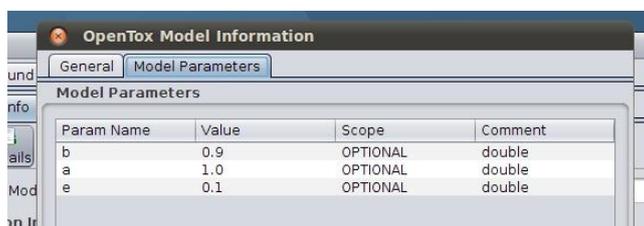


Figure 16 – Parameters of the model

Information regarding the training algorithm that was used to create the model can be retrieved by clicking on the "Algorithm" Button:

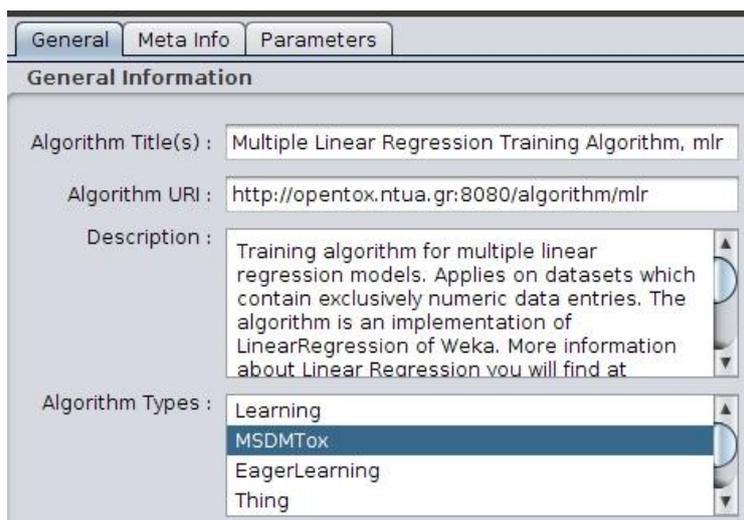


Figure 17 – Algorithm details

and the same way one can inspect all available information for the predicted and dependent features of the model:

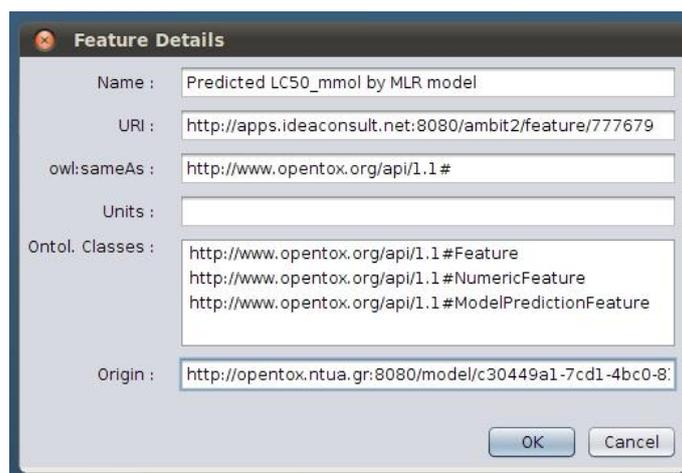


Figure 18 – Predicted feature information

Using the compound and the QSAR model provided by the user in the previous sections, Q-edit can invoke the necessary OpenTox web services to return the predicted value as well as (if available) the experimental value for the compound. This functionality is available under the fourth tab - namely Prediction - where the user is required to report the predicted value and comment on the uncertainty of the prediction and the possible chemical and/or biological mechanisms that might affect its reliability - for example a particular compound might appear to be active according to a QSAR model but in practice it is not well absorbed.

π
 Predict Download Exp. Value

3.2. Prediction (output of the model) :

Experimental value - if available :

Figure 19 – Predicted value obtained using an OpenTox model on-line resource and experimental value retrieved from OpenTox services.

Retrieve structural analogues

A list of structural analogues can be retrieved on the basis of some similarity index provided by the user. Under the tab "Applicability" find the tab "Structural Analogues" where one can provide a similarity threshold in the range 0.5 - 1.0 and click on the button "Acquire List" to get a list of compounds that are similar to the one submitted in the beginning. This is illustrated in the following screenshot where the analogues of sucrose (up to 95% similarity) are listed.

Document 1

Compound General Model Prediction Applicability Discussion

Reliability Structural Analogues Domains Discussion

Similarity : Acquire List Exp. Values Compound Info Remove

Compound	Experimental Value
alpha-D-glucopyranosyl alp...	
beta-D-fructofuranosyl alp...	
alpha-D-Glucopyranoside, beta-D-f...	
Oxirane, 2-methyl-, polyme...	
alpha-D-Glucopyranoside, beta-d-f...	
http://apps.ideaconsult.ne...	
sucrose	
beta-D-fructofuranosyl alp...	

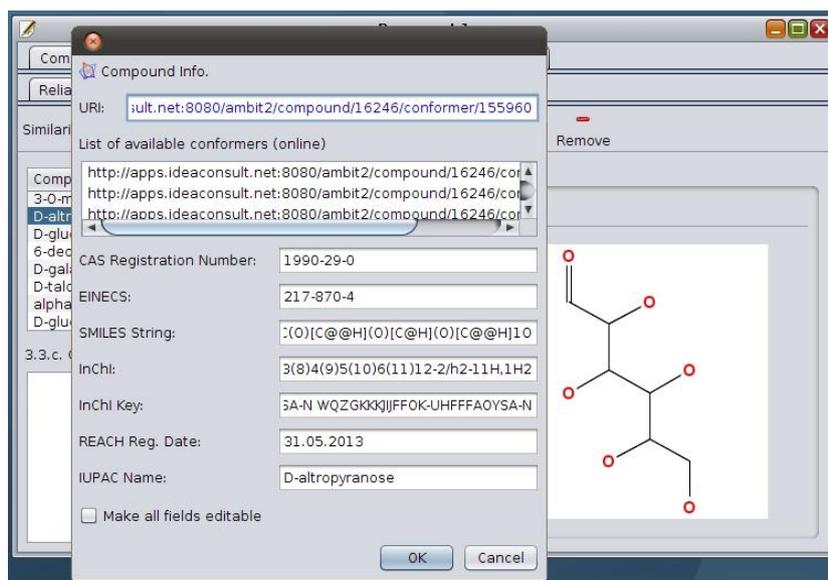
3.3.c. Considerations on structural analogues

Depiction

OC[C@H]1O[C@H](OC[C@H]2O[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O

Figure 20 – Structural analogues

If a model is loaded, then one can download all experimental values for each one of the structural analogues. Finally, after the list of structural analogues is loaded and one of them is selected, one can inspect its structural information available by clicking on the button "Compound Info" which is found in the toolbar.



Report an issue

We're pretty fast in fixing issues with Q-edit, so if you notice any bugs or have some improvement in mind please file an issue at <https://github.com/alphaville/Q-edit/issues> - for that you need a github account which you can create [here](#). Github will automatically notify you by email once there is an update on your issue.