

Knowledge Fair (E)

Predict the toxicity of a compound

OpenTox Workshop, Rhodes, 19th September 2010

ToxPredict

Objective

To demonstrate and evaluate a prototype OpenTox application (ToxPredict) that accepts chemical structures and names as input and automatically generates a toxicity report based on various pre-calibrated toxicity models.

Description of ToxPredict

ToxPredict is a web-based interface for predicting toxicity of individual chemicals. Users can either search for a compound in the OpenTox prototype database, which currently includes quality labeled data for 163122 chemicals (including all chemicals currently registered with REACH) grouped in 2409 datasets, or upload their own chemical structure in the SDF format. It runs the selected calculations automatically using a collection of distributed computational services. ToxPredict currently includes eighteen validated models addressing 15 different endpoints, and is extensible.

Exercise A. Predict the toxicity of a chemical in the database

ToxPredict searches its database for chemical structures entered as chemical names, SMILES strings, CAS number or via an integrated 2D chemical drawing editor. The steps below illustrate using the chemical name:

1. Open a Browser window (Internet Explorer or FireFox are recommended)
 2. Type in "toxpredict.org" (without the quotation marks)
 3. Click "NEXT"
 4. Type a chemical name in the text box, e.g. "benzene" (or CAS number, SMILES string...)
 5. Click "NEXT" (to see if the search was successful)
 6. Click "NEXT" again (to view the list of endpoints)
 7. Click to select each of the 18 boxes in the left column
 8. Click "NEXT"
 9. Click "NEXT" again (to view the results)
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Exercise B. Predict the toxicity of a new chemical (not in the database)

To predict the toxicity of a new chemical that is not in the current ToxPredict database, you will need to upload the structure file as an "SD" or "SDF" file as follows (please ask if you need some sample SD files to try):

1. Open a Browser window (Internet Explorer or FireFox are recommended)
2. Type in "toxpredict.org" (without the quotation marks), then "Enter"
3. Click "NEXT"
4. Click the "Upload" tab
5. Click "Browse..."
6. Navigate to and select your SDF file (example SD files are available)
7. Click "Open"
8. Click "NEXT"
9. Click "NEXT" again (to view the list of endpoints)
10. Click to select each of the 18 boxes in the left column
11. Click "NEXT"
12. Click "NEXT" again (to view the results)