

Build and Validate QSAR models with ToxCreate

Description of Activity: Based on provided datasets build and examine a QSAR model. You can also try your own dataset.

Requirements: Browser with Java script activated, Java installed, Internet connection

Instructions:

1 Create

- Open your browser and go to <http://www.toxcreate.org/>
- You are logged in by default as “guest”, it is also possible to use your own OpenTox account.
- Follow the instructions on the webpage. Click on bold and purple topics to get further information.
- Upload training data in Excel or CSV format.
- After clicking on “Create Model” it will take a while until the dataset has been uploaded
- If you want to use your own data follow the “instructions for creating training datasets” at <http://www.toxcreate.org/help/>)

Create and evaluate models to predict toxicity

ToxCreate

Create **Inspect** **Predict** **Login** **Help**

User: guest

This service creates

- **lazar classification** models and
- **lazar regression** models (experimental)

from your uploaded datasets. Further modelling algorithms will be added in future versions.

Please read the **instructions for creating training datasets** before submitting.

Upload training data in **Excel** or **CSV** format:

You are currently logged in as **guest** and your models can be modified or deleted by other guests. Please **log in** with your OpenTox  account to control your model permissions.

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2 Inspect

- On this page you get a brief summary of all models with validation results
- Find your model by name and click on bold and purple links to get/download detailed information (e.g. the feature dataset as XML or a detailed validation report)

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User: **guest**

Get an overview about ToxCreate models. Parts of this page are refreshed every 5 seconds to update the model status.

ISSCAN_v3a_sal [\(edit\)](#)

Status: Completed([delete](#))
Started: 06/16/2011 - 08:05:39AM
Training compounds: 750
Warnings: [show](#)
Algorithm: lazar
Type: classification
Descriptors: [Fminer backbone refinement classes](#)
Training dataset: [Excel sheet](#) , [YAML](#) ([experts](#))
Feature dataset: [Excel sheet](#) , [YAML](#) ([experts](#))
Model: [QMRF Editor](#) , [YAML](#) ([experts](#), [models cannot be represented in Excel](#))

Validation:
Detailed report: [show](#)
Number of predictions: 706.0
Correct predictions: 71.46 %
Weighted area under ROC: 0.684
Specificity: 0.752
Sensitivity: 0.683

Confusion Matrix:

| | | Measured | |
|-----------|----------|----------|----------|
| | | active | inactive |
| Predicted | active | 236 | 89 |
| | inactive | 113 | 268 |

Fish_Toxicity_LC50_mmol_regression [\(edit\)](#)

Status: Completed([delete](#))
Started: 06/16/2011 - 07:30:08AM
Training compounds: 569
Algorithm: lazar
Type: regression
Descriptors: [Fminer backbone refinement classes](#)
Training dataset: [Excel sheet](#) , [YAML](#) ([experts](#))
Feature dataset: [Excel sheet](#) , [YAML](#) ([experts](#))
Model: [QMRF Editor](#) , [YAML](#) ([experts](#), [models cannot be represented in Excel](#))

Validation:
Detailed report: [show](#)
Number of predictions: 559.0
R-squared : 0.369
Root Mean Square Error : 28.7
Mean Absolute Error : 6.42

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3 Predict

- Draw a compound or enter a Smiles string
- Selected one or more prediction models and click on “Predict”

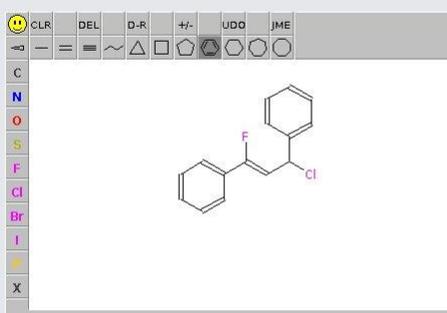
Create and evaluate models to predict toxicity

ToxCreate

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User: **guest**

Use this service to obtain predictions from OpenTox models.

Draw a compound



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or enter a Smiles string

Choose one or more prediction models

Fish-Toxicity-LC50-mmol-regression

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Prediction Result:

- Click on bold and purple topics to get further information.

Create and evaluate models to predict toxicity

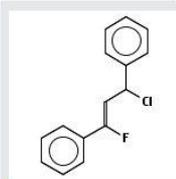
ToxCreate

Create Inspect Predict Login Help

User: **guest**

New prediction

FC(=CC(Cl)c1ccccc1)c2ccccc2



Fish_Toxicity_LC50_mmol_regression:
0.0144

(Confidence : 0.141)

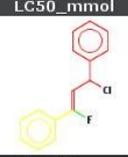
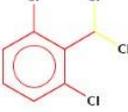
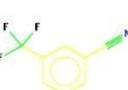
[Details](#)

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- Check on “Details” for prediction details (Neighbors, significant fragments, ...)

- activating fragments
- deactivating fragments
- **fragments** (Show activating and deactivating fragments overlap)
- inert parts

Please keep in mind that predictions are based on the measured activities of neighbors. **Significant fragments** are solely used to determine activity specific similarities of neighbors.

| LC50_mmol | Prediction | Confidence | Supporting information |
|-------------------------------------------------------------------------------------|-------------------|------------|---------------------------------------------|
|  | 0.0144 | 0.141 | Names and synonyms Significant fragments |
| Neighbors (1-5/22) next | Measured activity | Similarity | Supporting information |
|  | 0.002 | 0.591 | Names and synonyms Significant fragments |
|  | 0.0002 | 0.545 | Names and synonyms Significant fragments |
|  | 0.0042 | 0.522 | Names and synonyms Significant fragments |
|  | 0.247 | 0.5 | Names and synonyms Significant fragments |
|  | 0.279 | 0.48 | Names and synonyms Significant fragments |