

Input (SDF, MDL, SMILES, ...): ?

Help button

Browse...

Type or copy&paste:

EDITOR (applet??) ==> to c&p

Clear...

Or use a dataset URI:

Browse Repository...

- Quick QSAR Model validation only
 Normal QSAR Descriptor selection only

Validate an existing model:
Link to FASTTOX

For just using Descriptor selection
[do we want this?]

Use a predefined set of descriptors that can quickly be calculated, no descriptor selection and only a quick regression algorithm

Unrecognized atom type,
missing coordinates,
...

Data preprocessing: ?

- Check whether the structures are correct
 Add hydrogens
 Check for skewness in the distribution of activities => log transformation
 Rename chemical samples by:

Generate ID
InChi
Use MDL Mol name

Descriptors: ?

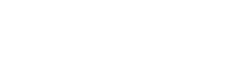
Available Descriptors:

- UserDescriptor1
+ CDK_All
 +CDK_Electronic
...
+ JOELIB2_All
- FTM minSup 0.05
- FTM minSup 0.1
...

add



remove



Selected Descriptors:

dataset_desc1
dataset_desc2
...

Tree structure (if possible?)

Contains also descriptors from input [if given]

Reset...

Some Descriptors have to be calculated!!!

Descriptor selection: ?

Algorithm:

InfoGainAS
...

Parameters:

p

second. kernelpar1

param2:

Reset...

Warning Pop-up for supervised algorithms => CV!!!

Parameter options change dynamically according to chosen algorithm

Algorithm: ?

- Regression Classification

Algorithm:

KNN
J48
ToxTree

Parameters:

k

second. kernelpar1

param2:

Reset...

Parameter options change dynamically according to chosen algorithm

Choose attribute for prediction:

Feature1 (carc.)
Feature2 (logP)
...

Reset...

Model validation: ?

- No validation
 LOO-cross-validation
 Cross-validation
 Hold-out
 External test set:

k-fold:

%-train:

Input (SDF, MDL, SMILES, ...):

Appears only, when Using external test set

Browse...

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Or use a dataset URI:

Report format ?

- PDF HTML XML Text

Reset All

RUN