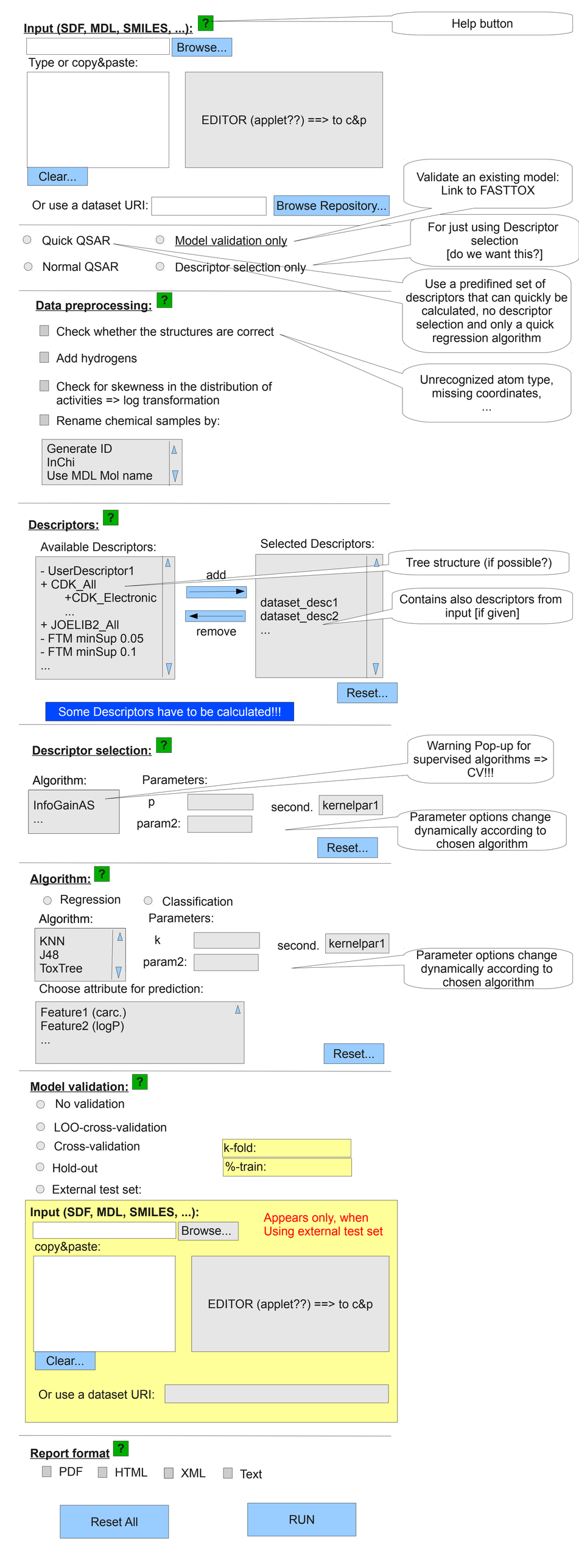
Input (SDF, MDL, SMILES, ...):
?
Help button
Browse...
Type or copy&paste:
EDITOR (applet??) ==> to c&p
Clear...
Validate an existing model: Link to FASTTOX
Or use a dataset URI:
Browse Repository...
Quick QSAR
Model validation only
For just using Descriptor selection [do we want this?]
Normal QSAR
Descriptor selection only
Use a predifined set of descriptors that can quickly be calculated, no descriptor selection and only a quick regression algorithm
Data preprocessing:
?
Check whether the structures are correct
Add hydrogens
Check for skewness in the distribution of activities => log transformation
Rename chemical samples by:
Unrecognized atom type, missing coordinates, ...
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:
?
Warning Pop-up for supervised algorithms => CV!!!
Algorithm:
Parameters:
InfoGainAS
...
p
param2:
second.
kernelpar1
Parameter options change dynamically according to chosen algorithm
Reset...
Algorithm:
?
Regression
Classification
Algorithm:
Parameters:
KNN
J48
ToxTree
k
param2:
second.
kernelpar1
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
k-fold:
Hold-out
%-train:
External test set:
Input (SDF, MDL, SMILES, ...):
Appears only, when Using external test set
Browse...
copy&paste:
EDITOR (applet??) ==> to c&p
Clear...
Or use a dataset URI:
Report format
?
PDF
HTML
XML
Text
Reset All
RUN