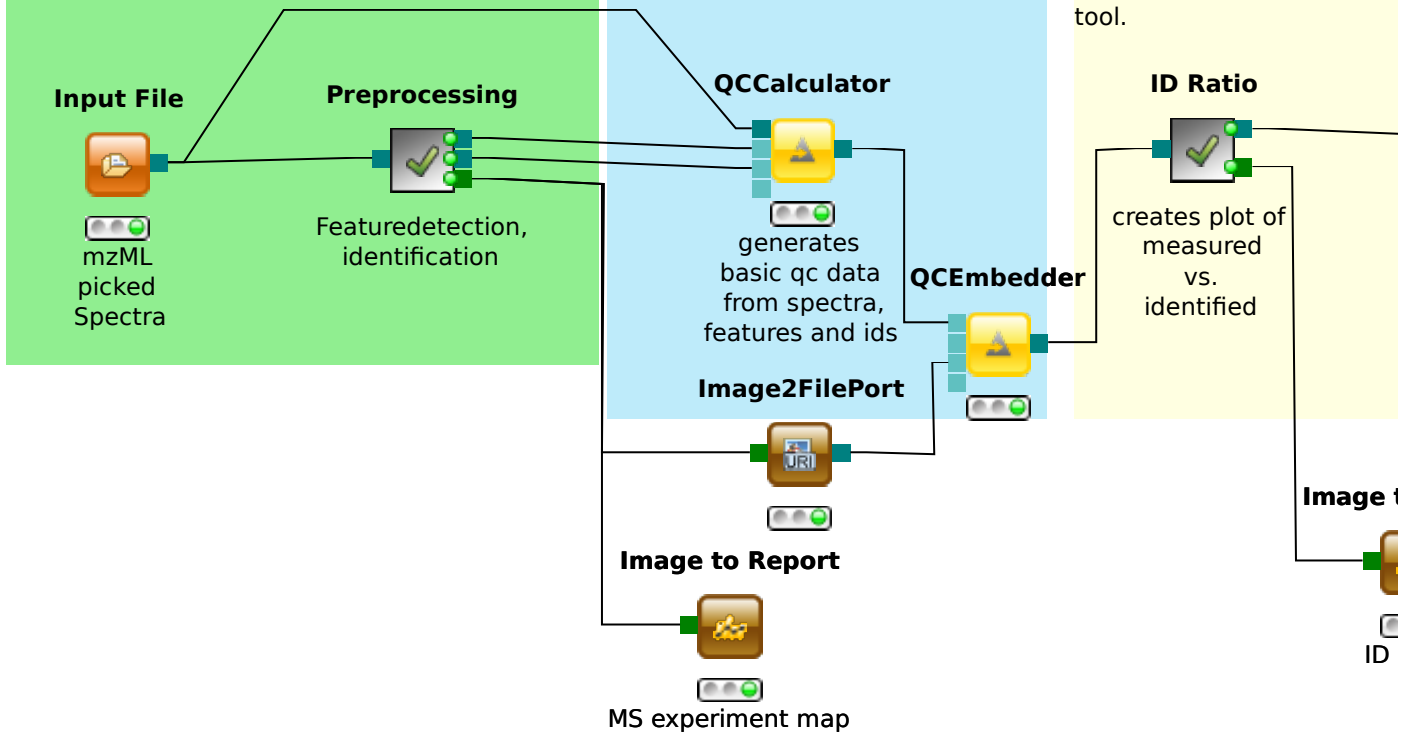This is the detailed qcML workflow example. It will create a qcML file like the simple example, but use more features generate a nice report for print or archiving.
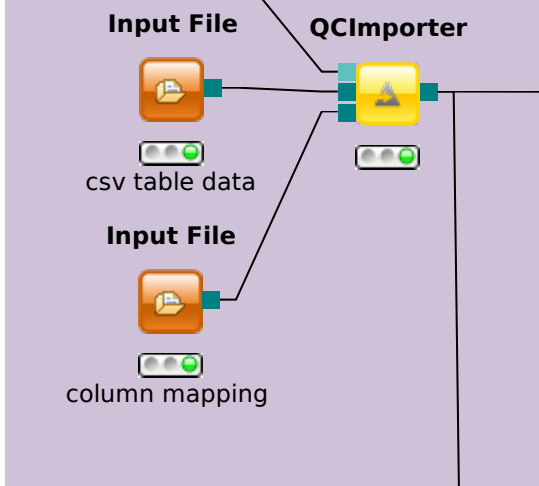
The preprocessing node is performing feature detection and identification, each resulting in a file we can use to have a look at the quality. Make sure the inputnode has the mzML file from the examle folder registered, and the database inputnode inside the preprocessing metanode has the supplied ecoli fasta file registered.

The QCCalculator will take the three files to calculate basic statistics and agglomerate quality data we need later to apply more advanced quality metrics. All will be stored in a qcML file, which will make it easy to access the data we need. We will add more data and hand the extended file over to the next step.
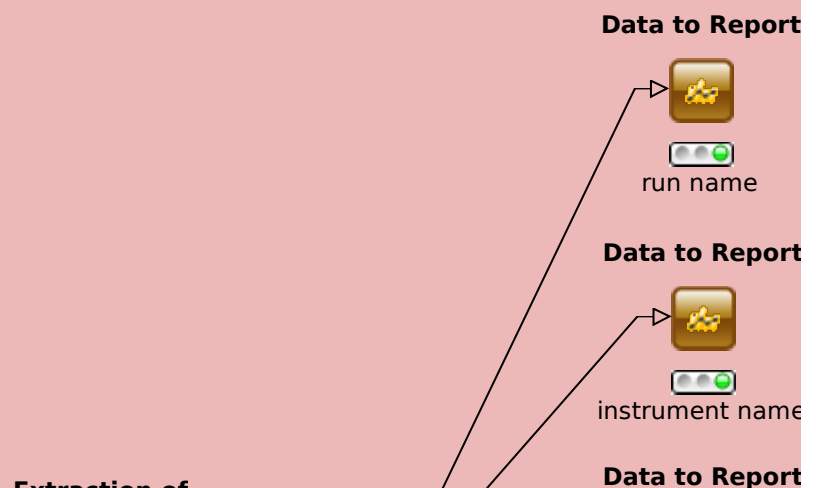
The ID Ratio metanode will a plot of the measured spe vs. the identified spectra in vs. RT map. The plot will be included in the qcML file ar addition sent to the reporti tool.

Input File

mzML
picked
Spectra

Preprocessing

Featuredetection,
identification

QCCalculator

generates
basic qc data
from spectra,
features and ids

QCEmbedder

Image2FilePort

ID Ratio

creates plot of
measured
vs.
identified

Image to Report

MS experiment map

Image

ID

If we have additional data available in tabular format, we can add these as well. In this case we can add the injection times of the machine to the qcML file.

Input File

csv table data

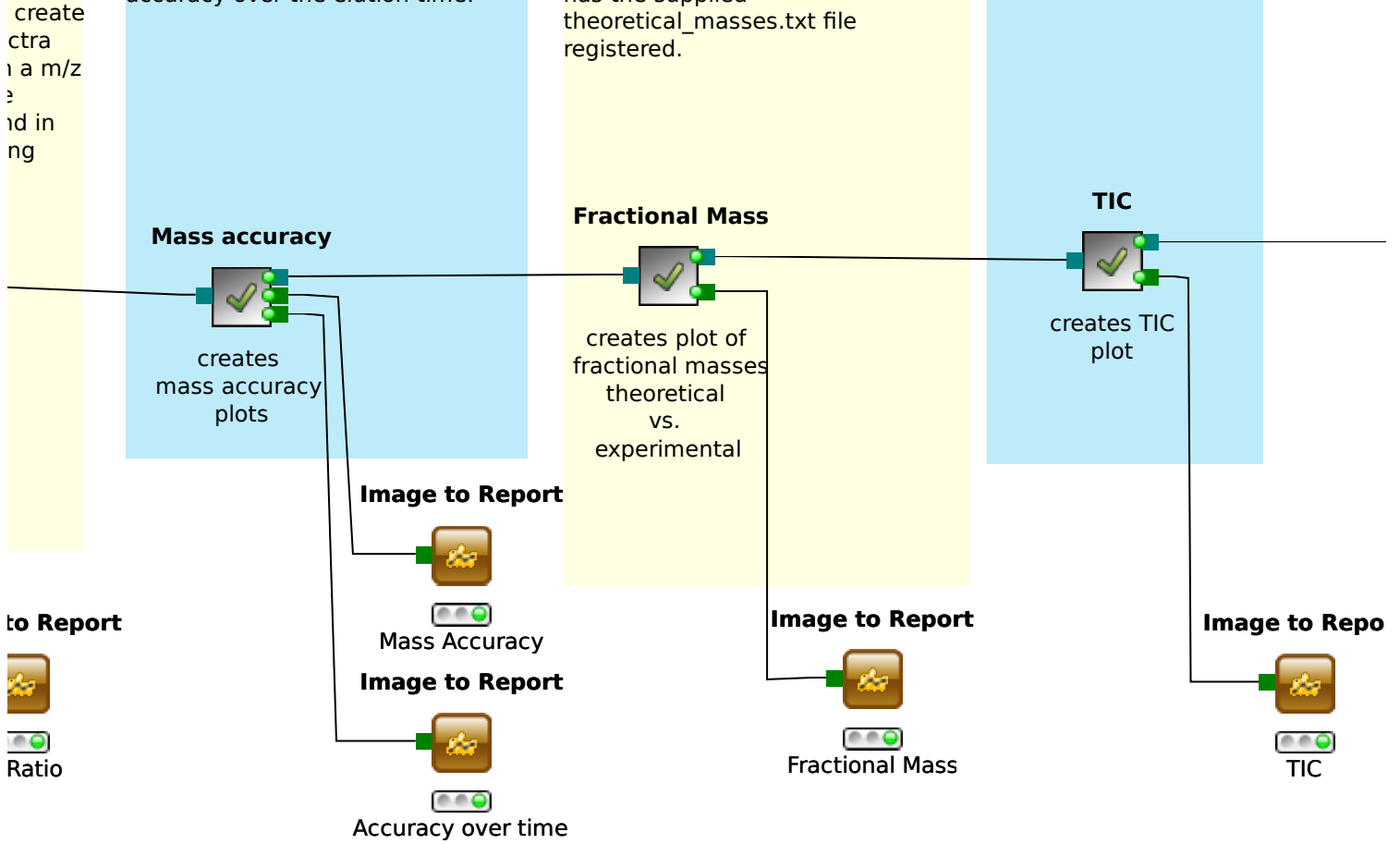**QCImporter**

Input File

column mapping

Pushing data into a qcML file is nice, but accessing the data is almost as easy. This metanode will do it by XPATH query. The accessed values will be made available to the reporting tool.

Data to Report

run name

Data to Report

instrument name

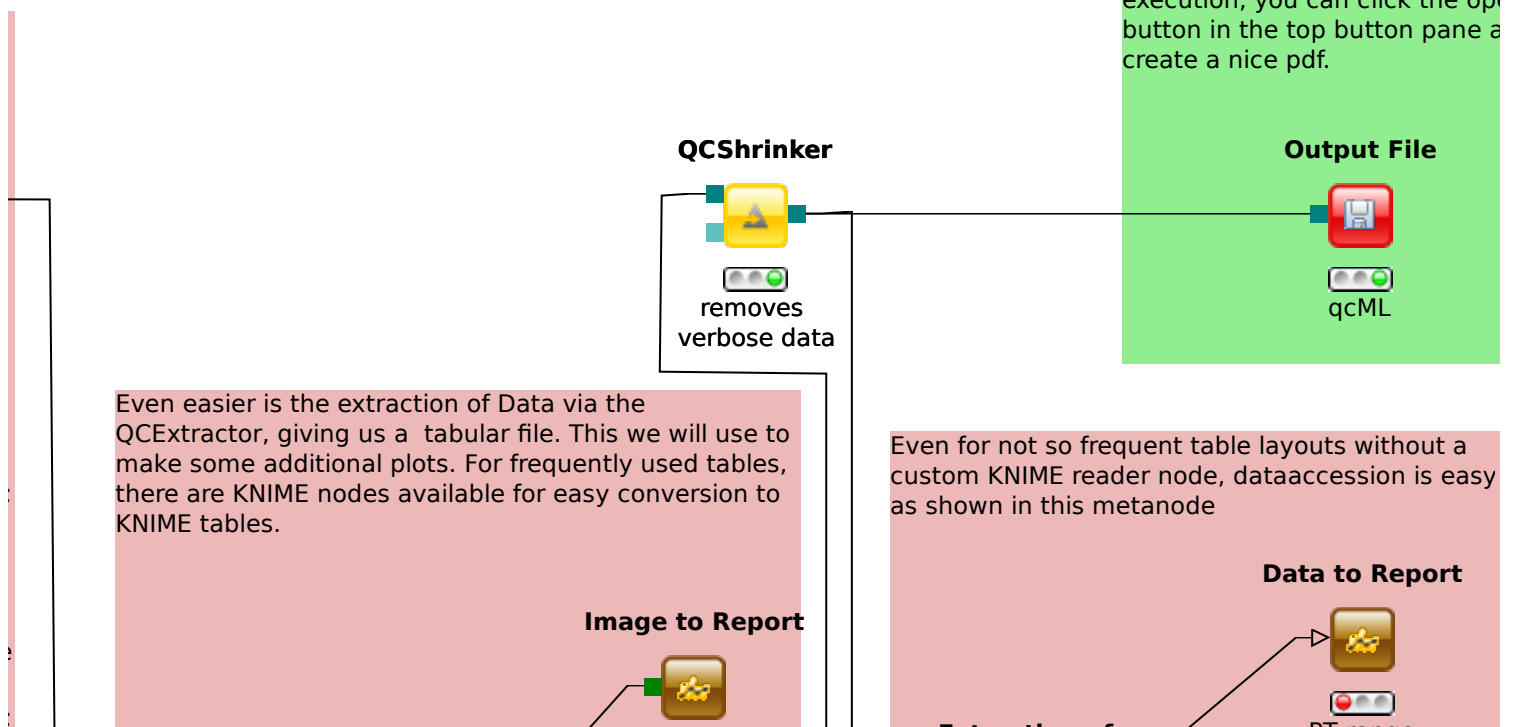**Data to Report**

Extraction of

In the Mass Accuracy metanode, the accuracy of the measurement will be analysed by reference to the identifications. The calculated median deviation and the corresponding plot will add to the qcML file. We will also plot the mass accuracy over the elution time.

In the following Fractional Mass metanode we will use a external reference file of theoretical masses to plot the experimentally aquired fractional masses on the theoretical possible. Make sure, the imputnode in the Theoretical Masses metanode has the supplied theoretical_masses.txt file registered.

The last metanode is plotting the total ion current of the experiment.

create
ctra
a m/z
e
d in
ng

Mass accuracy

creates
mass accuracy
plots

Fractional Mass

creates plot of
fractional masses
theoretical
vs.
experimental

TIC

creates TIC
plot

Image to Report

Mass Accuracy

Image to Report

Accuracy over time

to Report

Ratio

Image to Report

Fractional Mass

Image to Repo

TIC

When the workflow has comple
execution, you can click the op
button in the top button pane a
create a nice pdf.

QCShrinker

removes
verbose data

Output File

qcML

Even easier is the extraction of Data via the QCExtractor, giving us a tabular file. This we will use to make some additional plots. For frequently used tables, there are KNIME nodes available for easy conversion to KNIME tables.

Even for not so frequent table layouts without a custom KNIME reader node, dataaccession is easy as shown in this metanode

Image to Report

Data to Report

Extraction of

RT range

rt

ted
en report
nd

Extraction of QP details

completion time

Data to Report

aquisition details

Data to Report

identification details

Data to Report

feature details

**Extraction of
feature statistics**

FWHM to #ids

Image to Report

Node 109

quality to #ids

Image to Report

histo of #Ids

Image to Report

histo of q

**Extraction of
Aquisition details**

RT range

Data to Report

MZ range

Data to Report

id settings