KNIME integration

> ⓘ Please note, that the functionality described in this section is under development. The release of KNIME nodes for OCHEM integration is planned for March-April 2014

KNIME (www.knime.org) is a popular workflow engine that facilitates the combination of different kind of analytical and data manipulation nodes into workflows.
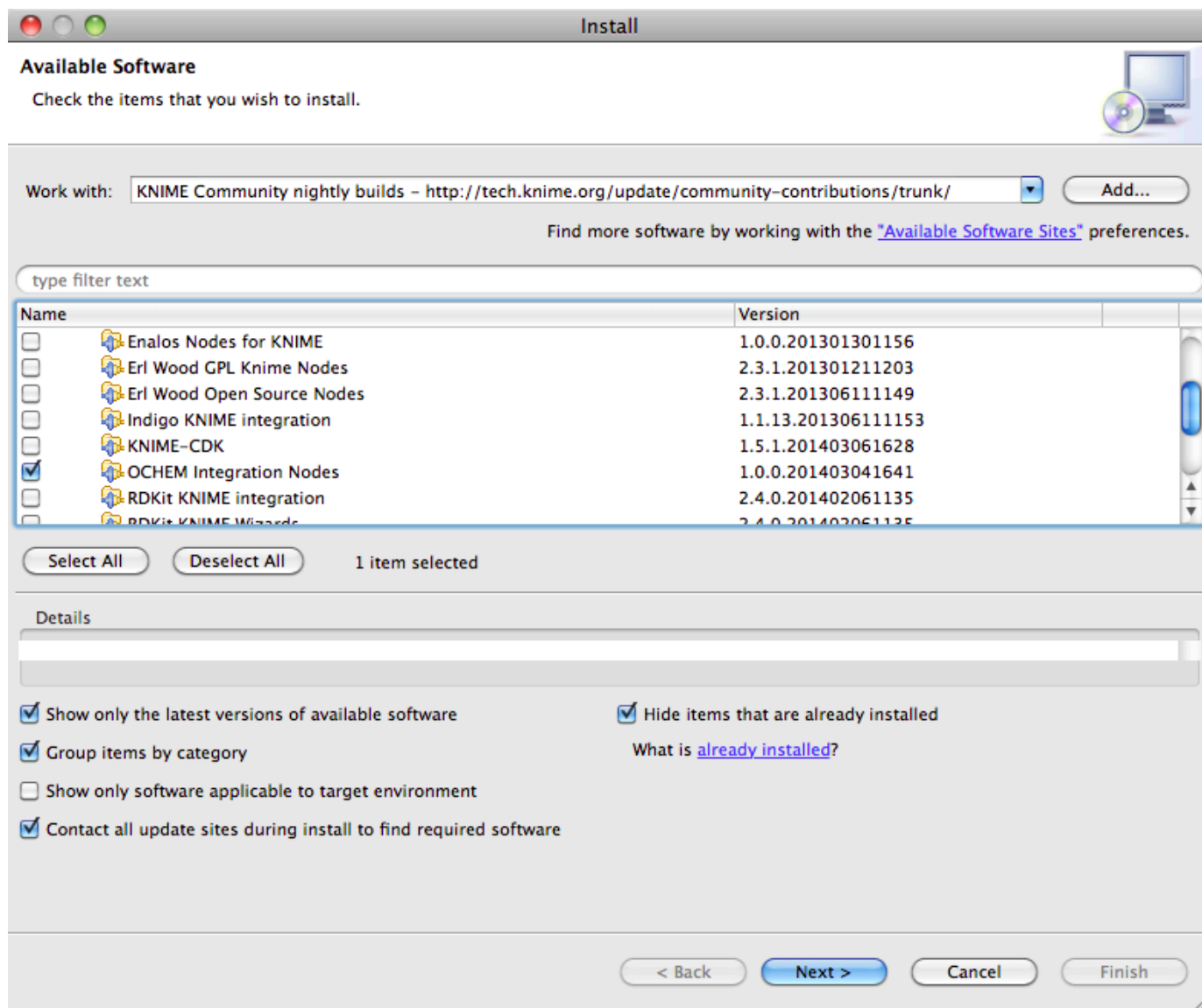
OCHEM provides a set of KNIME nodes (www.knime.org) that exposes a basic set of OCHEM features:

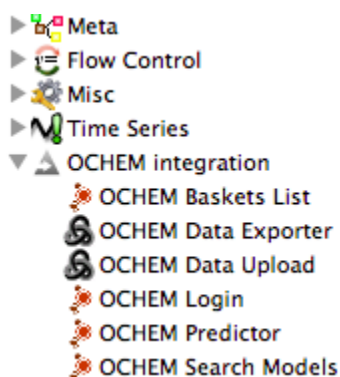- running predictions
- data export
- data import

Installing the nodes

> ⓘ Please note, that OCHEM nodes are currently supported for KNIME 2.9.x

To add OCHEM nodes to your KNIME installation, use the community nodes update site: http://tech.knime.org/update/community-contributions/trunk/ and install the "OCHEM Integration nodes" feature:
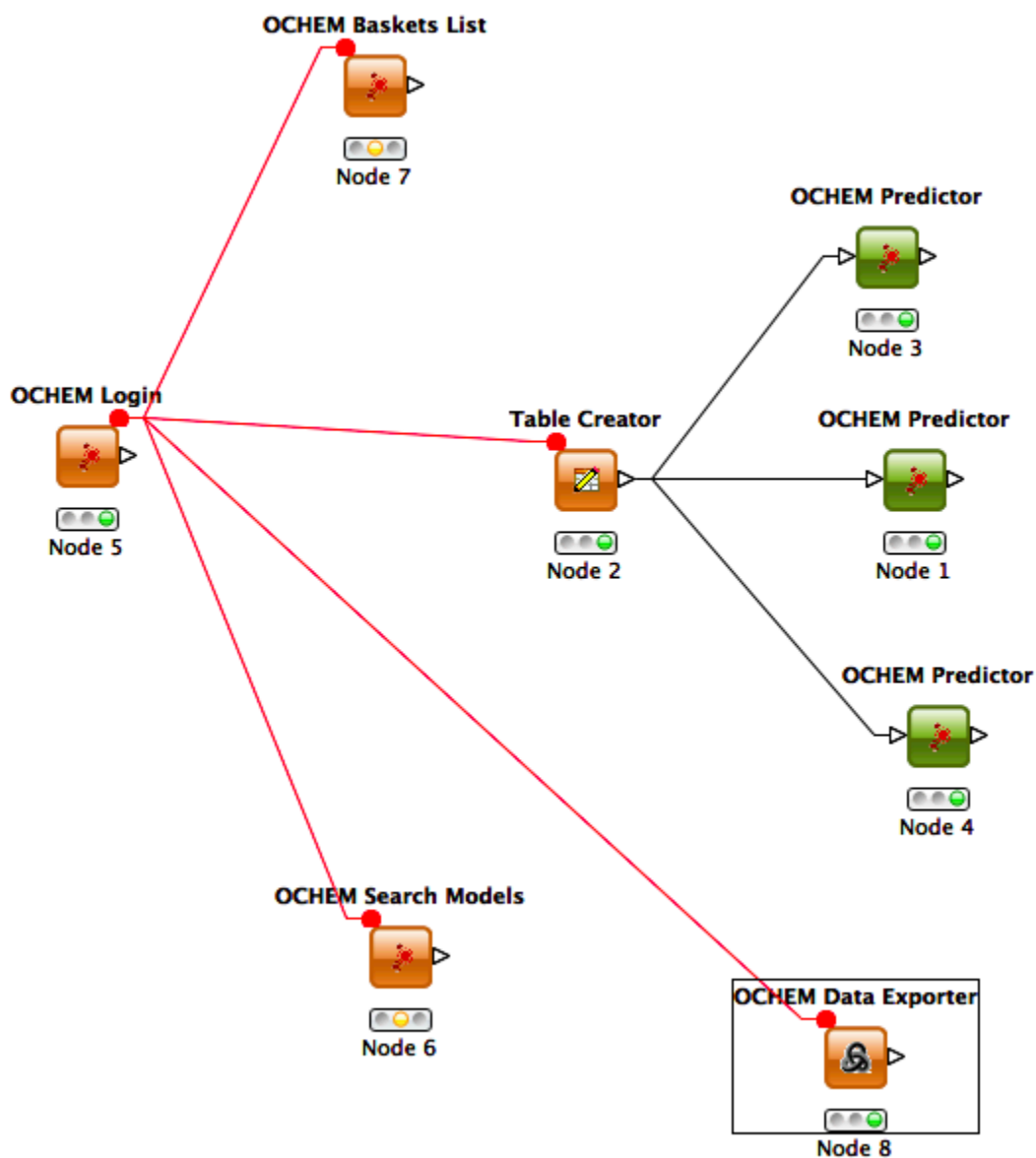
After copying the plugin and restaring your KNIME, you should see an extra category of OCHEM nodes in the node repository:

Authentication and the login node

Most OCHEM functionality require a user to login into the system using his account and password. Therefore, most of the KNIME-OCHEM nodes require authentication.

OCHEM provides a special **login node**, which allows the user to enter his login data. The flow variables generated by the login node should be passed to every other node in the workflow:

OCHEM Baskets List

Node 7

OCHEM Predictor

Node 3

OCHEM Login

Table Creator

OCHEM Predictor

Node 5

Node 2

Node 1

OCHEM Predictor

Node 4

OCHEM Search Models

Node 6

OCHEM Data Exporter

Node 8

Predictor node

The predictor node allows to run the models available on OCHEM (publicly available models or your private models).

To configuration includes the model selection. You can filter the models by name and select the model from a dialog or enter the model ID manually:

Dialog – 0:4 – OCHEM Predictor

Options Flow Variables Memory Policy

Filter the models by entering a partial name or an endpoint: [   ] (Update list)

ID	Model name	Endpoint
70	Ames levenberg	AMES
43	BCF tutorial	BCF
1013467	PhysProp v3.01 Boiling Point	Boiling Point
52	ONS Melting Point 008a	Melting Point
54	ONS Melting Point 008b	Melting Point
59	k-Medoid logBCF, DRAGON	BCF
1013468	Melting Point_CDK_ASNN_Bagging_D...	Melting Point
67	Melting Point – 3D (Dragon 6 + Cori...	Melting Point
68	Melting Point – 2D (ALOGPS 2.01 +...	Melting Point
2	CYP450 modulation e-state	CYP450 modulation
27	CYP450 Inhibition (Full Set, J48, Bag...	CYP450 modulation
28	CYP450 Inhibition (Full Set, ASNN, B...	CYP450 modulation
26	CYP450 Inhibition (Dragon, J48, Bag...	CYP450 modulation
25	CYP450 Inhibition (SMF, J48, Bagging)	CYP450 modulation
1	Ames levenberg	AMES
3	Toxicity against T. Pyriformis	log(IGC50-1)
14350545	BCF_ASNN_[EState, ALogPS], 122275	BCF
5698388	BCF_ASNN_[ALogPS], 122722	BCF
32470866	Merck 10_PLS_[PureCache]	MProperty 10
11666862	BCF_ASNN_[CDK]	BCF
4474473	BCF_PLS_[CDK]	BCF
35397996	Consensus BCF, 131548	BCF
21878213	AMES_ASNN_[EState, ALogPS], 132013	AMES
31241189	Copy of AMES_ASNN_[EState, ALogPS...	AMES
10855429	AMES_ASNN_[EState, ALogPS], 132242	AMES

Alternatively, enter the model ID manually: [68]

(OK) (Apply) (Cancel) ⑦