

Using SOAP web-services

Web-services allow advanced users to use part of the OCHEM functionality in their automated workflows, such as KNIME or Pipeline pilot.

Basic info

OCHEM provides a SOAP web-service that allows to create and apply predictive models as well as to upload data. WSDL descriptor for the service can be found at

<http://ochem.eu/services/ModelService?wsdl> for work with model (calculation of models, download of statistics)

<http://ochem.eu/services/DataService?wsdl> for work with data (creation of baskets, upload,download of records, etc.)

Based on this WSDL, you can assemble your own clients or invoke the web-service via, e.g., KNIME.

Please note, that web-service API can change and you will have to recompile your client.

The functionality exposed via web-services include:

- application of a model for obtaining predictions
- upload of experimental data
- download of model statistics
- creation of a new QSAR model
- deletion of QSAR models
- export of a [basket](#)

Authentication

Some methods exposed via web-service require user authentication (session GUID).

The session GUID can be obtained from OCHEM web site. For this, login to your OCHEM account, go to your account page ("My Account") in the top right corner and copy the session GUID as shown below:

Session information

Session ID: 72012

Session GUID: 2c4440dc-ed58-4106-b2fa-1fb7507f5789

Java client example

[Download an exemplary JAVA client](#)

The client's code was automatically generated with Axis WSDL2Java Utility.

Workflow example (using Knime)

Another example of using OCHEM through webservices is via workflow applications such as [Knime](#), [Pipeline Pilot](#) and others.

KNIME [naim] is a user-friendly graphical workbench for the entire analysis process. You can download a free copy of Knime through its websire (<http://www.knime.org/>).