

Explore OCHEM

Before starting with OCHEM, you have to login. Select [login page](#), click register a new user, provide required information and accept license agreement.

OCHEM operates as a site of browsers.

The main browsers are

- [experimental records](#) (experimental data uploaded by users)
- [properties](#) - any possible outcomes of experimental measurements
- [conditions](#) of properties, which are required to describe the properties (e.g., pressure for boiling point measurements)
- [units](#) of properties and conditions (OCHEM provides an automatic units conversion)
- [articles](#) (published and unpublished - the information is required to uniquely characterize origin of any experimental record)
- [published models](#), which can be used to predict data
- [baskets](#), which are required to create sets of records for analysis

It also provides following tools:

- [batch data upload](#)
- [ToxAlerts](#) to identify functional groups
- [descriptor calculations](#) (free export is available for many descriptors)
- [analysis of overrepresented scaffolds/groups](#)
- [modelling framework](#) for single model development
- [comprehensive modelling](#) (development and comparison of tens of models in one click)
- [Molecular Matched Pairs](#)
- [MolOptimiser](#)

A comprehensive description of OCHEM functionality [is also available](#).