OCHEM glossary

- Basket
- Feature nets
- Obligatory condition
- Primary record
- Record

Basket

OCHEM allows to combine experimental records into reusable sets. Such sets of records are referred to as **baskets**. Baskets have names and user can virtually have as many baskets as required. Baskets are typically used as training or validation sets for the development of QSAR models.

Feature nets

OCHEM supports training models that use other models' outputs as inputs (along with other molecular descriptors). Such models are referred to as *feature nets*.

Obligatory condition

An obligatory condition is a condition of an experiment that is required to be provided for a particular property.

For example:

- *Pressure* is an obligatory condition for *Boiling point.*
- *S9 activation* type is an obligatory condition for *Ames test.*

OCHEM users themselves define which conditions are obligatory for the properties they have created.

Primary record

In a series of records with the same molecular structure, property and value but from different publications, the primary record is a record from the earliest publication. If a record corresponds to a unique measurement, then it is always primary.

Record

A record in the OCHEM database is the experimental measurement, defined by

- a molecule,
- the measured property and its value in the original nits of measurements,
- the source of the information,

Optionally, a record can include:

- the conditions of the experiment
- chemical names