

# Data access and manipulation

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All data records stored in the OCHEM database can be easily modified, filtered, searched and eventually grouped and organized for further convenient work.

## Batch editing

Data modification can be done in two ways: by either editing a single record separately or by using the batch editing tool to work with multiple records simultaneously. In the editor window, the user can change all fields of a record: measured property, article information, structure and conditions. Batch editing is useful to correct systematic errors that might have occurred during batch upload, e.g., wrong units or missing conditions of experiment.

## Filtering and search

Every browser of the OCHEM, e.g., molecules, articles, properties, etc., has a panel for data filtering. Filters are used to focus on a certain subset of the data, e.g., a set of certain properties, a set of specific organisms or conditions, etc. Records can be filtered by literature source (article or book where the data has been published), physicochemical property or experimental condition and structural information, e.g., molecule name or InChI key as well as by molecular sub-fragments. Comprehensive filter options to find duplicates, errors or non-validated entries are available.

The OCHEM supports relational filtering: for a given record, the user can find other records with the same structure (preserving or ignoring stereochemistry) or the records that have been modified at approximately the same time as this record.

Data can also be filtered by tags, i.e., labels assigned to molecules or properties. A desired set of tags, referred to as an “area of interest”, restricts all the displayed information (experimental measurements, publications, properties and compounds) to the selected tags.

## Data organization

By applying various filters, a user can specify and select records of interest that can be stored separately in sets called *baskets*. A typical use of a basket is to assign both training and validation sets for modeling. The content of a basket can be browsed and modified from the compound properties browser or from the basket browser.