

Compound property browser

The compound property browser is one of the main dialogs of OCHEM, which allows to search experimental data by a wide variety of criteria.

The main blocks of the compound property browser include:

- filters
- content area
- command panel

The screenshot displays the Compound Property Browser interface, divided into three main sections:

- FILTERS:** A sidebar on the left containing various filter categories:
 - SOURCE:** Article/Source [select], Page, Table.
 - PROPERTY:** Activity/Property [select], Boiling Point (highlighted).
 - CONDITIONS:** Pressure, Quality code.
 - MOLECULE:** Name / OCHEM ID [?] / Inchi-Key [search by fragment], Molecular mass [?] between [] and [].
 - MISCELLANEOUS:** Current set [?], Show all, Data origin and quality (Data introducers: All users, Data visibility: Public only, Data from other users: Only approved data), Discover issues with the data (Error records, Error in chies, Mismatching names, Include stereochem., Empty molecules).
- COMMANDS PANEL:** A top bar with icons for Basket, Records, Tags, and other actions. It shows "1 - 5 of 16984" items and "5 items on page" of 3397.
- CONTENT AREA:** A list of search results, each with a chemical structure, key properties (Boiling Point, Pressure, Quality code), and source information (The Pesticide Properties Database (PPDB) 2012...):
 - Record 1: Boiling Point = 370.5 (in °C), Pressure = 1.0 atm, Quality code = 5.0 %. Source: N: AUTO_173, 2012; AMES challenge (Training set). MoleculeID: M11220.
 - Record 2: Boiling Point = 527.0 (in °C), Pressure = 1.0 atm, Quality code = 3.0 %. Source: N: AUTO_318, 2012; AMES challenge (Training set). MoleculeID: M17194.
 - Record 3: Boiling Point = 230.0 (in °C), Pressure = 1.0 atm, Quality code = 5.0 %. Source: N: AUTO_317, 2012; AMES Challenge (Test set). MoleculeID: M3326.
 - Record 4: Boiling Point = 1537.0 (in °C), Pressure = 1.0 atm, Quality code = 3.0 %. Source: N: AUTO_316, 2012; MoleculeID: M3341880.

Filters

The filters in the compound property browser include filters by:

- data source (scientific publication, page, table)
- property (physicochemical property, biological activity); it can be selected from property browser
- conditions of experiments (for example, pressure for boiling point; S9 activation for Ames test)
- molecular structure (substructure search, filters by molecular mass range)
- data origin and quality (e.g., by data introducer, approval status, etc)

There is an additional block of filters used to discover problematic data records (invalid molecular structures, empty molecules, mismatching names and structures, etc.)

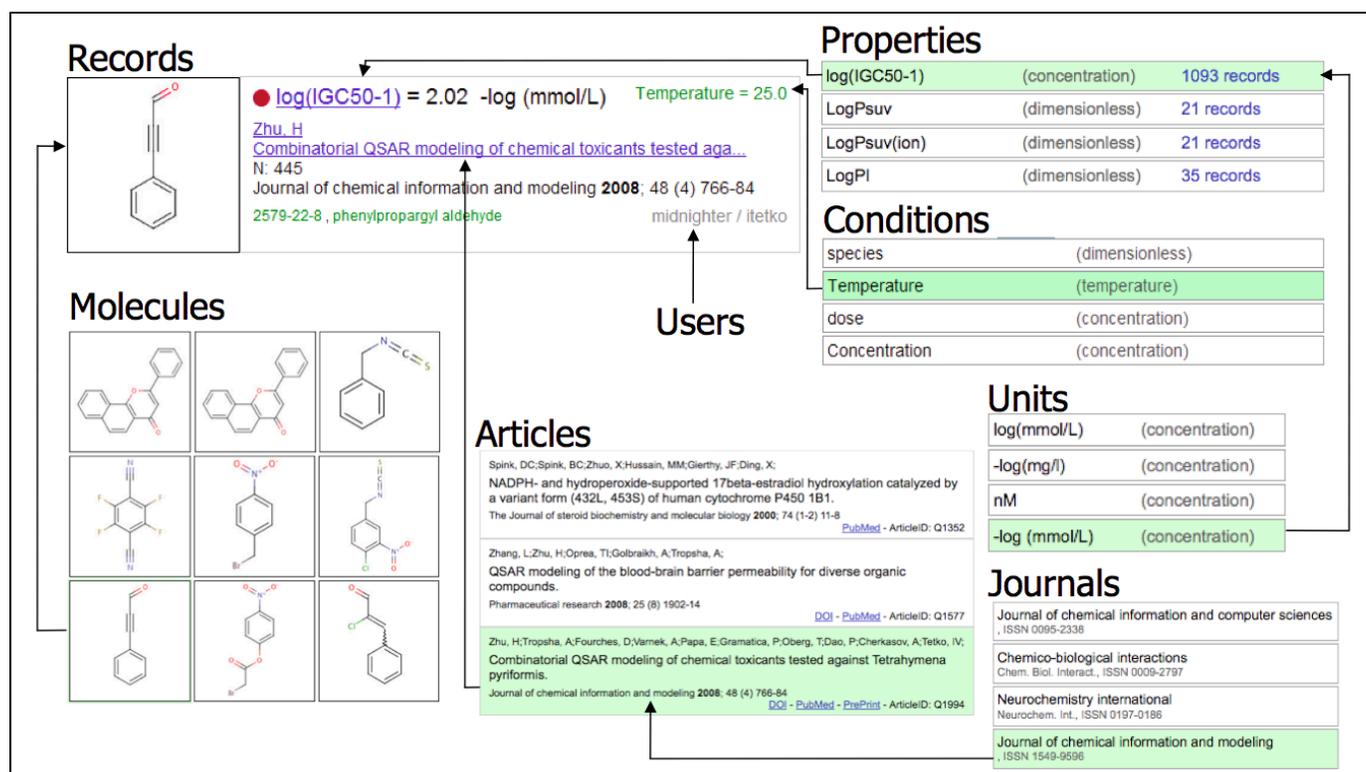
Content area

The content area displays the actual data records matching the specified filters. The content is can be browsed page by page.

The displayed information includes:

- the depiction of the compound
- the measured property, its value and unit of measurement
- the source of information
- the OCHEM identifiers of record, molecule, article
- the conditions of experiments, if available
- the users who introduced and modified a particular record

The image below summarizes the information from an individual record:

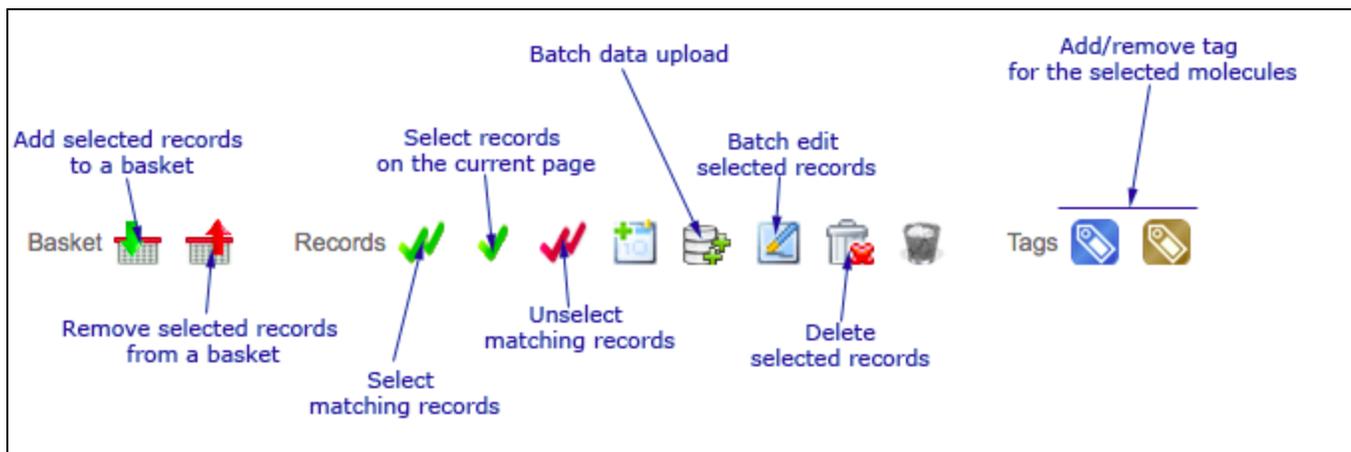


Command panel

The command panel allows to modify/delete/organize the experimental data records.

Some operations affect all the records matching the current filters ("**matching records**"), while other operations affect only explicitly **selected records**.

The figure below summarizes the available actions:



The records can be selected either individually (a checkbox on the right of each record) or with multiple selection (e.g., select all matching records, select records from the current page). The selection is *permanent*, it is not lost when user leaves the page or logs out. For more information about selecting records and organizing them into working sets ("baskets"), please refer to the section "[Working with datasets](#)".