InstantJChem

General information

IJC object	DB object	Comment
Schema	Database	Or more correctly, a connection to a database.
Entity	Database table	Contains data is a row and column paradigm, just like a database table. Usually a single database table, but potentially multiple tables.
Field	Column from a database table	Represents data from one of more columns in a database table.
Relationship	Foreign key constraint	An association between two entities as reflected by a foreign key constraint in the database.

In addition Instant JChem provides these additional types of objects:

IJC object	Description
Project	Allows you to separate different bits of work into discrete units. You can have one of more projects open at a time. They are displayed in the projects window. A project usually contains one or more IJC Schemas and any other files you may have added to your project.
DataTree	A hierarchical arrangement of Entities that define an arrangement of master-detail data. For each row in a master entity there might be one or more corresponding rows in its detail entities.
ResultSet	Data from a particular DataTree that reflects the current query and sort instructions.
View	A display of data from a single ResultSet. Currently there are 2 types of view, the Grid View which provides a tabular (spreadsheet) representation of data and the Form View that allows you to define a form with which to display your data. Multiple views can use the same result set, in which case the query, sorting and selection is coordinated between the views.
Query	A set of query criteria that can be applied to a ResultSet. Queries can be stored and re-executed at a later stage.
List	A set of IDs that can be restored to a ResultSet (and hence view) at a later stage. e.g. "Active compounds". Lists can be edited and combined.

Full structure search, substructure search (extracted from ChemAxon Manual)

Chemists are most often interested in *substructure search*, that is, whether one molecular structure contains the other one as a substructure or not. By definition, the examined molecule is called a target, the structure we are looking for is called a query, and a target molecule matching the query structure is called a *hit* (Table 1).

If special molecular features are present on the query (eg. stereochemistry, charge, etc.), only those targets match which also contain the feature. However, if a feature is missing from the query, it is not checked by default.

A *full structure search* finds molecules that are equal (in size) to the query structure. (No additional fragments or heavy atoms are allowed.) Molecular features (by default) are evaluated the same way as described above for substructure search.

Other search types

Besides the above, InstantJChem supports *similarity*, *duplicate*, *superstructure* and *full fragment* type searches.

Similarity is only used in database searches, and its similarity concept is based on hashed binary chemical fingerprints with Tanimoto metrics. (For a more detailed description, see the Developers Guide.) For a more sophisticated approach of similarity, we provide the Screen package.

Duplicate search is mainly used before database inserts to check whether the given molecule is already contained in the database or not. All molecular features need to be equal here, eg. non-stereo query will only match non-stereo target, etc.

Superstructure search is the opposite of substructure search: It searches for those target molecules which can be found in the given superstructure query. (In this case the roles of the query and target molecules are simply exchanged, so query properties should be specified on the target!)

Full fragment search is between substructure and full search: the query must fully match to a fragment of the target. Other fragments may be present in the target, they are ignored. This search type is useful to perform a "Full search" that ignores salts or solvents beside the main structure in the target.

Table 1. Full structure search, substructure search

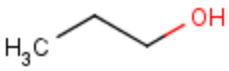
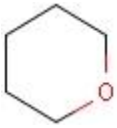
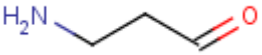
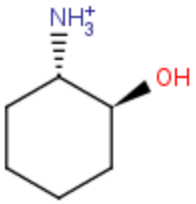
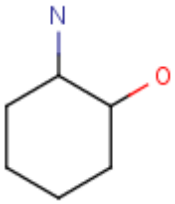
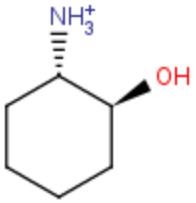
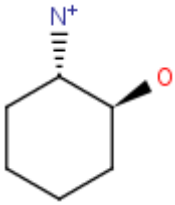
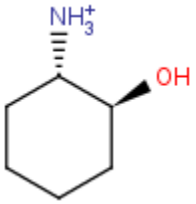
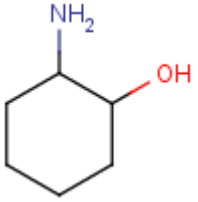
query	target	hit	
		full structure search	*substructure search*
		✓	✓
		✗	✓
		✗	✗
		✗	✓
		✓	✓
		✓	✓
		✗	✗

Table 2. details the main differences amongst these search types.

Table 2. Search type differences

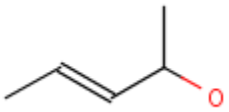
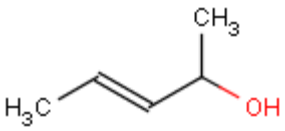
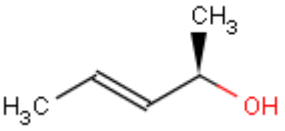
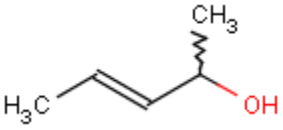
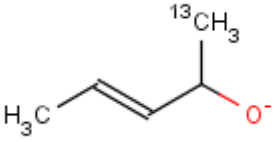
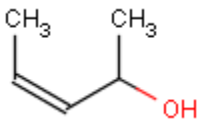
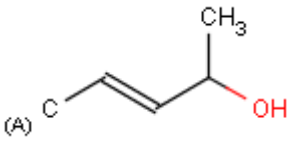
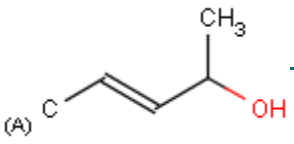
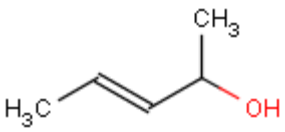
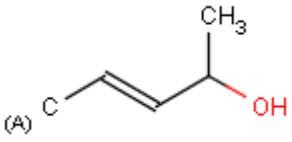
Search type	Search feature							
	Similarity	Tests if target contains query	Tests if query contains target	Full fragment coverage	Exact topology matching	Exact stereo matching	Exact atom features matching	Exact bond matching
SUBSTRUCTURE	n/a	✓	✗	✗	✗	✗	✗	✗
SUPERSTRUCTURE	n/a	✗	✓	✗	✗	✗	✗	✗
FULL_FRAGMENT	n/a	✓	✗	✓	✗	✗	✗	✗
FULL	n/a	✓	✓	✓	✓	✗	✗	✗
DUPLICATE	n/a	✓	✓	✓	✓	✓	✓	✓
SIMILARITY	✓	n/a	n/a	n/a	n/a	n/a	n/a	n/a

The definition of the search features are:

- Similarity: similarity search using chemical hashed binary fingerprint and Tanimoto metrics.
- Full fragment coverage: the query must cover a whole fragment of the target, but the target may contain other fragments. (Implicit and explicit hydrogens are treated equal.)
- Exact topology matching: the whole molecular graph must match (Implicit and explicit hydrogens are treated equal.)
- Exact stereo matching: equality is needed in stereochemistry, eg. non-stereo query only matches non-stereo target.
- Exact atom features matching: whether matching of certain atom properties should be switched to "exact". This requires equality of the properties (eg. uncharged query only matches uncharged target), and includes the following switches:
  - chargeMatching : exact
  - isotopeMatching : exact
  - exactQueryAtomMatching : true
  - radicalMatching : exact
  - valenceMatching : exact
- Exact bond matching: generic bonds are not evaluated, equality is needed.

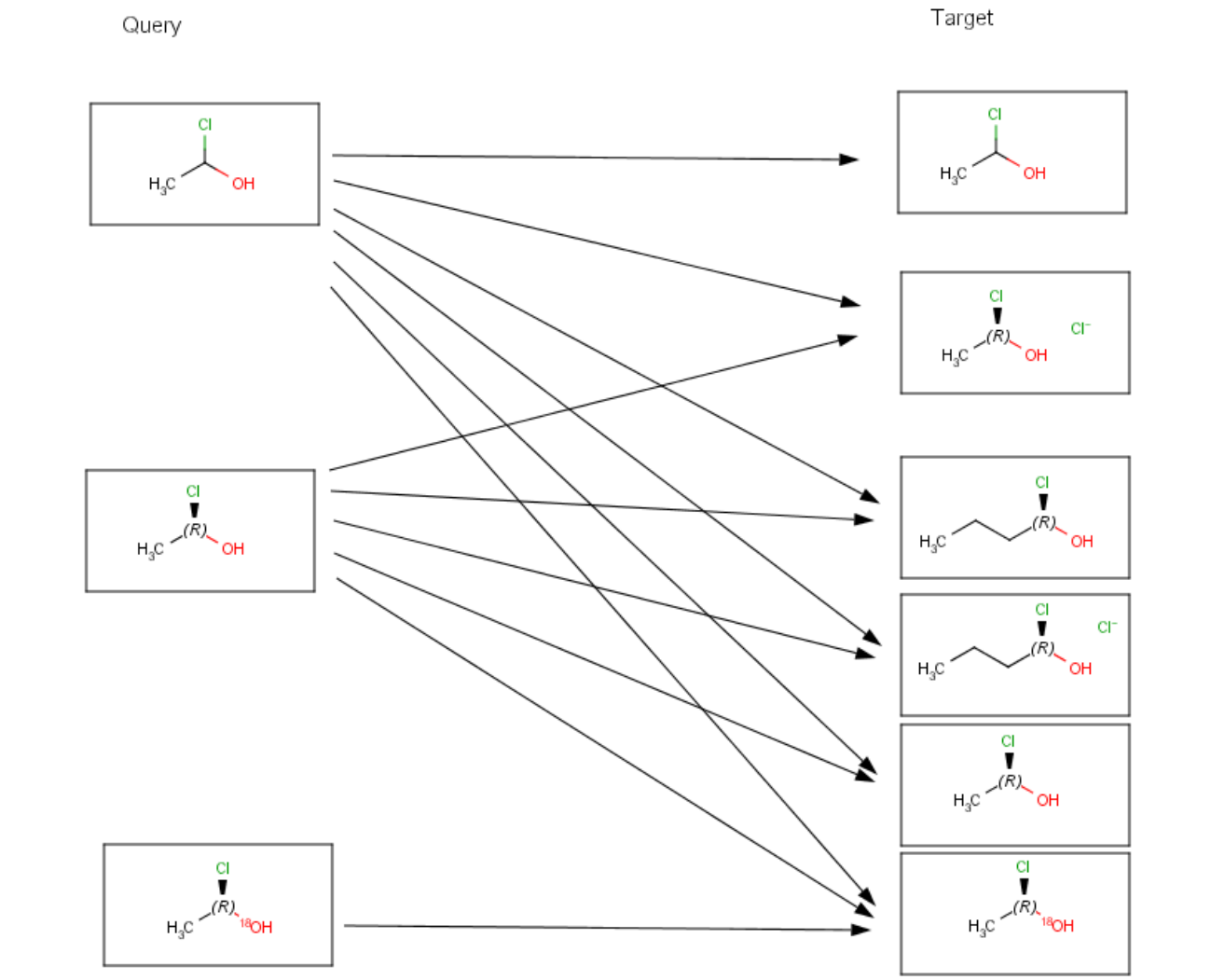
Table 3. illustrates the most important differences between FULL and DUPLICATE searches.

Table 3. FULL and DUPLICATE search differences

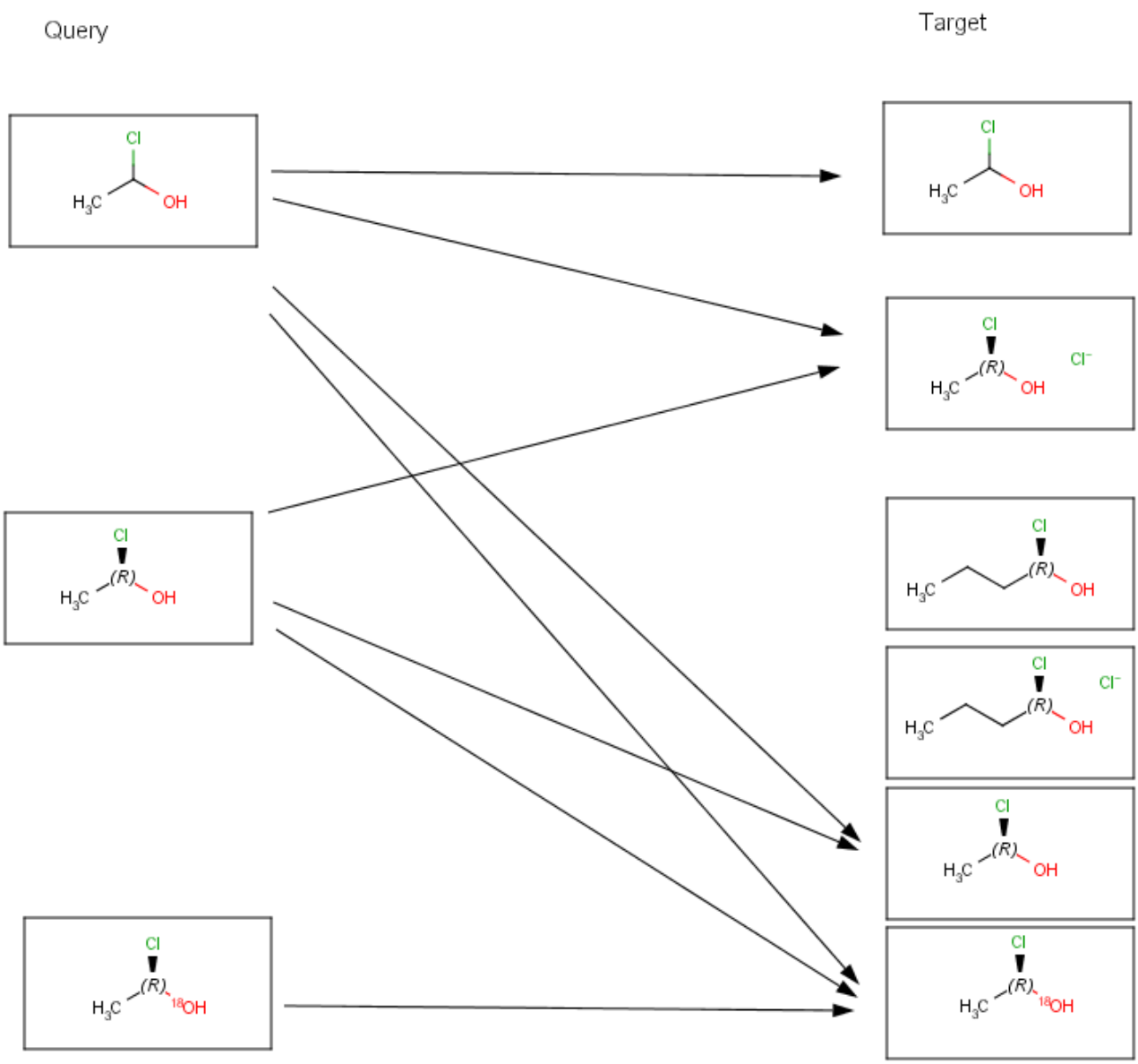
Query	Target	Hit		Remark
		FULL	*DUPLICATE*	
		✓	✓	
		✓	✗	
		✓	✗	
		✓	✗	
		✓	✗	with option DoubleBondStereoMatching set to DBS_MARKED (default)
		✓	✗	(A) denotes aliphatic query property
		✓	✗	
		✓	✓	

The diagrams below show further examples of substructure, full fragment, full and duplicate searches. The arrow between a query and target molecules denotes matching.

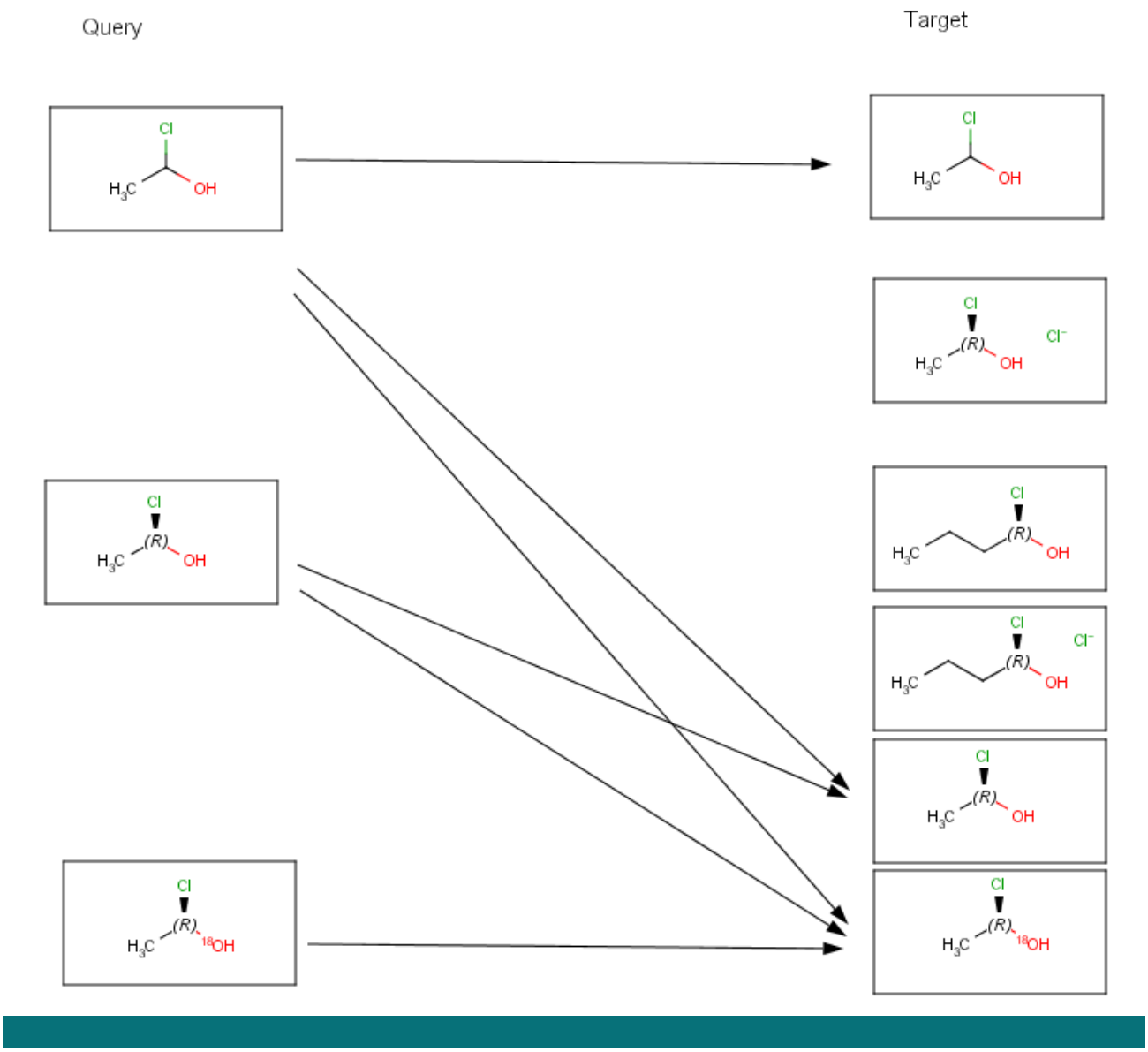
SUBSTRUCTURE search



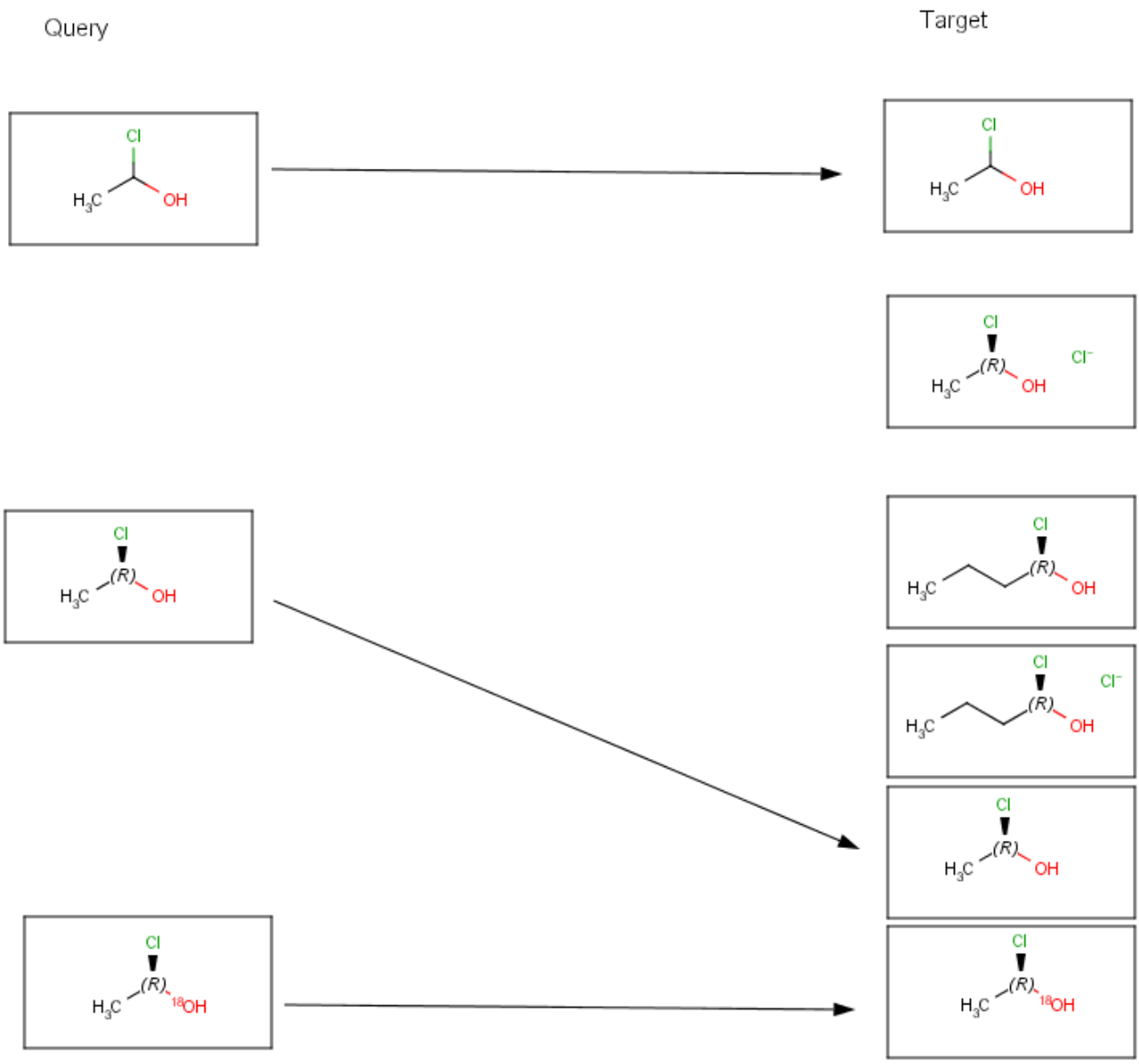
Full fragment search



Full structure search



Duplicate search



Searching in the database

Searching in the database contains a rapid prefiltering step, which screens out many of the targets not matching the query. This step uses chemical hashed fingerprints. To learn more about this step and how to fine-tune fingerprint generation to your needs, see the following document: Parameters for Generating Chemical Hashed Fingerprints

Comparison levels

Graph topology

Graphs consist of *nodes* and *edges*. When we compare structures represented as graphs, the graph patterns must match. Atoms correspond to nodes and bonds are edges.

Atom types

In the case of molecular structures, it is certainly not enough to simply compare the graph patterns, the type of atoms and bonds must be checked as well.

Stereo configuration

Even if both the topology and the type of the corresponding atoms and bonds are matching, we still have to examine the stereochemical configuration. Two molecules having the same kind of atoms connected by the same kind of bonds can be stereochemically different. The relative position of ligands connected to a chiral atom (*R/S* isomers), the enhanced stereo labels on chiral atoms and relative position of atoms located on rings or double bonds (*cis/trans* or *E/Z* isomers) determine the stereochemical configuration of the molecule.