



# Structure Input and Search Documentation

**InfoChem GmbH**

**[www.infochem.de](http://www.infochem.de)**

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## 1. Introduction

### 1.1 About the 'Structure Input and Search Documentation'

This documentation contains instructions for the input of chemical structures and reactions as well as information on the different available search types and parameters to allow database searches that will assist you to easily find the desired objects.

Especially the combination of structure or reaction queries and specific search type parameters leads to tailor-like search queries and therefore to easily accessible professional chemical searches on databases.

Content:

- Chapter 2: Descriptions of available query features on structures (atom and bond query features) are given within this chapter.
- Chapter 3: Query features on reactions are described within this chapter.
- Chapter 4: Information on different search types and parameters is given in this chapter.
- Chapter 5: Basic information on structure handling and database storage is given in this chapter.
- Chapter 6: Advanced stereochemistry information is given within this chapter.

Please note:

This tutorial will be upgraded continuously. Please visit our homepage [www.infochem.de](http://www.infochem.de) to download the latest version.

## 1.2 Input of Structures and Reactions: General Remarks

A proper chemical drawing and editing program is required for the input of chemical structures, reactions and query features for individual search queries. In general the following three different editing programs are supported in the InfoChem web-based products depending on the system used and the access of the editing program.

### 1.2.1 ICEDIT

ICEDIT is a chemical drawing editor developed by InfoChem. It is incorporated in the web-based products as Java applet and therefore no installation is required.

Please click on the button 'Transfer' at the bottom left corner of the editor window to transfer the structure or reaction to the query form when ICEDIT has been launched from the web application.

Please note: The tutorial refers to the ICEDIT Java applet version 1.7.5.9.

### 1.2.2 ISIS/Draw

Users that prefer using ISIS/Draw for the creation of structure and reaction queries in the InfoChem web-based products need to download and install a small software client on their PC, in order to establish the communication with the Symyx editor.

- Internet Explorer: icclient\_setup.zip
- Netscape (only e-Eros users): InfoChem Client.zip

Installation instructions:

1. Download the suitable zip-file from [www.infochem.de](http://www.infochem.de) to any directory on your local computer.
2. Close your web browser.
3. Extract the file and double-click the program file setup.exe.
4. Follow the instructions given by the installation program.
5. When the software is installed, restart your browser.

When ISIS/Draw is launched from the web application, a new transfer mode button will be added

on the upper left corner of the window:



To transfer the query to the web application, please click on this button, or use the menu item 'Chemistry' → 'Query Structure to MRW'.

Please note: The tutorial refers to the ISIS/Draw version 2.5.

### **1.2.3 ChemDraw**

Users that prefer using the ChemDraw plug-in for the creation of structure and reaction queries in the InfoChem web-based products need to have a fully licensed version of ChemDraw or ChemOffice version 6.0, 7.0 or 9.0. Other versions are not supported.

Please click on the button 'Transfer' on the bottom left corner of the editor window to transfer the structure or reaction to the query form when ChemDraw has been launched from the web application.

Please note: The tutorial refers to the ChemDraw Ultra version 7.0.1.

## 2. Query Features on a Molecule

A query feature on a molecule is a definition or a restriction on an atom or a bond that specifies the retrieval of certain types of molecule records from a database.

### 2.1 Atom Query Features

#### 2.1.1 Allow or Exclude Specific Atoms


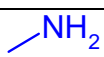
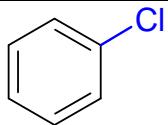
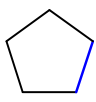
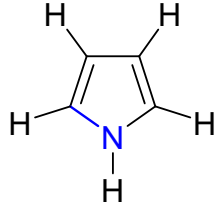
##### 2.1.1.1 ANY ATOM

**Format:** A

**Description**

To allow any atom except hydrogen at a specific position, choose 'A' as atom symbol.

**Example**

Query	Retrieved molecules
—A	
	
	
	
	



**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Open the 'P-Table'.
5. Select 'Query atoms' → 'A'.
6. Click twice 'OK'.

## Alternative Method:

1. Select an atom.
2. Type 'A' on the keyboard.
3. Press 'Enter'.

**Use in ISIS/Draw**

1. Select an atom.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Drop down the 'Symbol' box.
5. Select the atom symbol 'A'.
6. Click 'OK'.

## Alternative Method:

1. Select an atom.
2. Type 'A' on the keyboard.
3. Press 'Enter'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Insert Generic Label' → 'A Any' from the context menu.

## Alternative Method:

1. Choose the 'Text' tool.




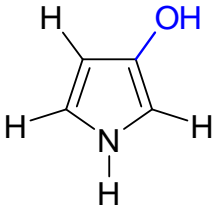
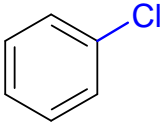
2. Select an atom.
3. Type 'A' on the keyboard.
4. Press 'Enter'.

## 2.1.1.2 Q-ATOM

**Format Q****Description**

To allow any atom *except hydrogen or carbon* at a specific position, choose 'Q' as atom symbol.

**Example**

Query	Retrieved molecules
	
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Open the 'P-Table'.
5. Select 'Query atoms' → 'Q'.
6. Click twice 'OK'.

Or use the alternative method from 2.1.1.1 and enter 'Q'.

**Use in ISIS/Draw**

1. Select an atom.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.

4. Drop down the 'Symbol' box.
5. Select the atom symbol 'Q'.
6. Click 'OK'.

Or use the alternative method from 2.1.1.1 and enter 'Q'.

### ***Use in ChemDraw***

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Insert Generic Label' → 'Q Non-Hydrogen Heteroatom' from the context menu.

Or use the alternative method from 2.1.1.1 and enter 'Q'.

**Please note:** Queries with the query feature 'Q' are currently not supported with higher ChemDraw versions.

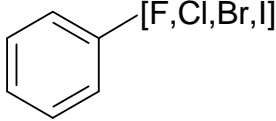
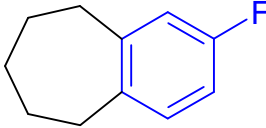
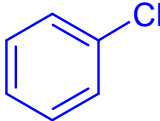
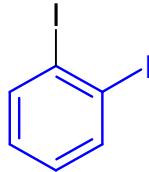
## 2.1.1.3 LIST

**Format** [A,B,C]**Description**

To allow atoms from a list of atoms of your choice at a specific position, choose 'LIST' as atom symbol. Up to 32 different atoms can be selected in a single 'LIST'. Atom 'LIST's with more than 32 atoms are not supported.

Please note: Multiple atom lists per search query are supported.

**Example**

Query	Retrieved molecules
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Select 'List' from the 'Query Atom' window to open the Periodic Table of the Elements.
5. Click an atom symbol to add it to your list of allowed atoms (click an atom symbol a second time to remove it).
6. Click twice 'OK'.

***Use in ISIS/Draw***

1. Select an atom.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Drop down the 'Symbol' box.
5. Select 'List...' to open the Periodic Table of the Elements.
6. Click an atom symbol to add it to your list of allowed atoms (click an atom symbol a second time to remove it).
7. Click twice 'OK'.

***Use in ChemDraw***

1. Select a single atom.
2. Right click the selected atom.
3. Select the option 'Edit Label'.
4. Type the list of desired atom symbols in the atom label box, separated by commas.
5. Tap 'Enter'.

## 2.1.1.4 NOTLIST

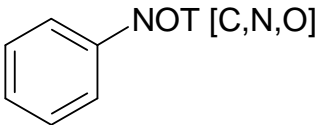
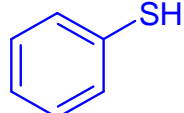
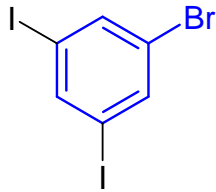
**Format** NOT[A,B,C]

**Description**

To exclude atoms from a list of atoms of your choice at a specific position, choose the 'NOT LIST'. This query feature also specifies no hydrogen atoms. Up to 32 different atoms can be selected in a 'NOT LIST'. Atom 'NOT LIST's with more than 32 atoms are not supported.

Please note: Multiple atom lists per search query are supported.

**Example**

Query	Retrieved molecules
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Select 'Not List' from the 'Query Atom' window to open the Periodic Table of Elements.
5. Click an atom symbol to add it to your list of excluded atoms (click an atom symbol a second time to remove it).
6. Click twice 'OK'.

**Use in ISIS/Draw**

1. Select an atom.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Drop down the 'Symbol' box.

5. Select 'Not List...' to open the Periodic Table of Elements.
6. Click an atom symbol to add it to your list of excluded atoms (click an atom symbol a second time to remove it).
7. Click twice 'OK'.

***Use in ChemDraw***

6. Select a single atom.
7. Right click the selected atom.
8. Select the option 'Edit Label'.
9. Type NOT followed by a space.
10. Type the list of excluded atom symbols in the atom label box, separated by commas.
11. Tap 'Enter'.



## 2.1.2 Specify Explicit Hydrogen Atoms

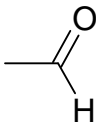
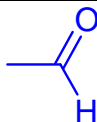
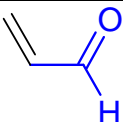
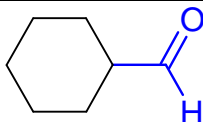
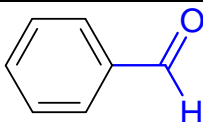
### Description

An explicit hydrogen is a hydrogen atom that is connected to an atom by an explicit bond.

To allow solely hydrogen atoms at specified positions in the structures retrieved, you must draw explicit hydrogens in your search query. You can also draw explicit hydrogens to block substitutions at specific positions in the structures retrieved.

Please note: Implicit hydrogens (hydrogens that are not attached to an atom by a visible bond) are not recognized in a search query.

### Example

Query	Retrieved molecules
	
	
	
	

### Use in InfoChem's Editor ICEDIT

1. Select the drawing tool 'Single Bond'.
2. Draw a single bond from the atom, which you want to have a hydrogen atom attached.
3. Select the atom you want to be defined as the explicit hydrogen.
4. Open the context menu 'Edit Atom' to open the 'P-Table'.
5. Select the atom symbol 'H'.
6. Click twice 'OK'.

Or use the alternative method from 2.1.1.1 and enter 'H'.

**Use in ISIS/Draw**

1. Select the drawing tool 'Single Bond'.
2. Draw a single bond from the atom, which you want to have a hydrogen atom attached.
3. Select the atom you want to be defined as the explicit hydrogen.
4. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
5. Choose the 'Query Atom' tab.
6. Drop down the 'Symbol' box.
7. Select the atom symbol 'H'.
8. Click 'OK'.

Or use the alternative method from 2.1.1.1 and enter 'H'.

**Use in ChemDraw**

1. Select the drawing tool 'Single Bond'.
2. Draw a single bond from the atom, which you want to have a hydrogen atom attached.
3. Select the atom you want to be defined as the explicit hydrogen by right-click.
4. Select the option 'Edit Label'.
5. In the atom label box, type an 'H'.
6. Tap 'Enter'.

Or use the alternative method from 2.1.1.1 and enter 'H'.

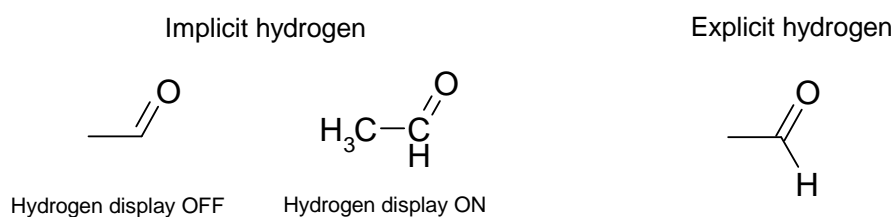
### 2.1.3 Implicit Hydrogen

Implicit hydrogens are no valid query feature!

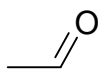
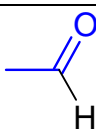
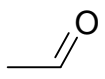
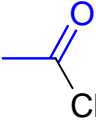
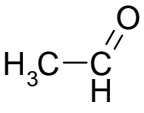
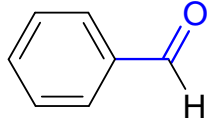
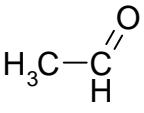
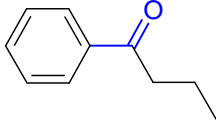
#### Description

An implicit hydrogen is a hydrogen that is either assumed to be present (invisible) or attached to an atom without an explicit bond.

Please note: Implicit hydrogens are not recognized in a search query. If you want to create a search query that allows solely hydrogen atoms at specified positions in the structures retrieved, you must draw explicit hydrogens (see 2.1.2).



#### Example

Query	Retrieved molecules
 Hydrogen display OFF	
 Hydrogen display OFF	
 Hydrogen display ON	
 Hydrogen display ON	

### 2.1.4 Prohibit Hydrogens on an Atom

**Format** (H<sub>0</sub>) or <sup>H</sup>

**Description**

Use this procedure to mark atoms with '(H<sub>0</sub>)' to prohibit any hydrogen attachments to the atom.

**Example**

Query	Retrieved molecules

**Use in InfoChem's Editor ICEDIT**

1. Select the atom on which to prohibit hydrogens.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the check box: 'No implicit Hydrogens'.
5. Click 'OK'.
6. The selected atom is marked with '(H<sub>0</sub>)'.

**Use in ISIS/Draw**

1. Select the atom on which to prohibit hydrogens.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the check box: 'No implicit hydrogens'.

5. Click 'OK'.
6. The selected atom is marked with '(H<sub>0</sub>)'.

***Use in ChemDraw***

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Implicit Hydrogens' → 'Not allowed' from the context menu.
4. The selected atom is marked with <sup>h</sup>.

**Please note:** Queries with the query feature 'Prohibit Hydrogens on an Atom' are currently not supported if ChemDraw is used as input editor.

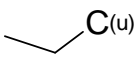
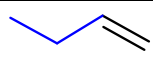
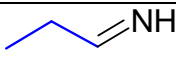
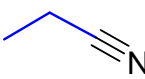
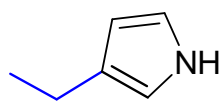
### 2.1.5 Specify an Unsaturated Atom

**Format** (u) or <sup>s</sup>

**Description**

Use this procedure to mark an atom unsaturated '(u)' to specify that the atom must be attached to at least one multiple bond (double, triple, or aromatic bond).

**Example**

Query	Retrieved molecules
	
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select the atom that you want to specify as unsaturated.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the check box: 'Unsaturated atoms'.
5. Click 'OK'.
6. The selected atom is marked with '(u)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as unsaturated.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the check box: 'Unsaturated atoms'.
5. Click 'OK'.
6. The selected atom is marked with '(u)'.

***Use in ChemDraw***

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Unsaturation' → 'Must be present' from the context menu.
4. The selected atom is marked with <sup>s</sup>.

## 2.1.6 Specify the Number of Attachments (Substituents)

This procedure is intended to specify the number of allowed non-hydrogen attachments (substituents) on an atom.

### 2.1.6.1 NO NON-HYDROGEN ATTACHMENTS

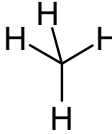
**Format** (s0) or <sup>x0</sup>

#### **Description**

This procedure is intended to specify the number of allowed non-hydrogen attachments (substituents) on an atom as ZERO. The query atom feature '(s0)' allows you to specify that the records retrieved must have NO non-hydrogen attachments at the specified position. All open valences at that position have solely implicit hydrogen atoms. This query feature implies the retrieval of a single atom with attached hydrogens (if any).

Please note: This query feature is not useful for a chemical query, as only single molecules based on the desired atom and a specific amount of hydrogen atoms (if any) would be retrieved. Therefore this query feature is not supported by InfoChem's Search Engine.

#### **Example**

Query	Retrieved molecule
C(s0)	



## 2.1.6.2 ONE NON-HYDROGEN ATTACHMENT

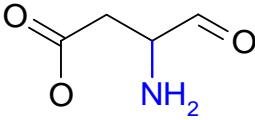
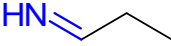
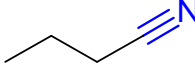
**Format** (s1) or <sup>x</sup>

**Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as ONE. The query atom feature '(s1)' allows you to specify that the records retrieved must have exactly ONE non-hydrogen attachment of any bond type at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
N(s1)	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose 1.
5. Click 'OK'.
6. The selected atom is marked with '(s1)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Drop down the 'Substitution count' box and choose 1.
5. Click 'OK'.
6. The selected atom is marked with '(s1)'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Substituents' → 'Exactly: 1' from the context menu.
4. The selected atom is marked with 'x'.

## 2.1.6.3 TWO NON-HYDROGEN ATTACHMENTS

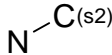
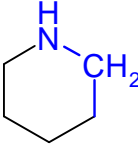
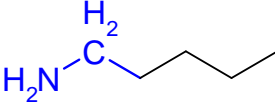
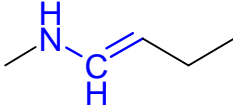
**Format** (s2) or <sup>x2</sup>

**Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as TWO. The query atom feature '(s2)' allows you to specify that the records retrieved must have exactly TWO non-hydrogen attachments of any bond type at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose 2.
5. Click 'OK'.
6. The selected atom is marked with '(s2)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Substitution count' box and choose 2.

5. Click 'OK'.
6. The selected atom is marked with '(s2)'.

***Use in ChemDraw***

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Substituents' → 'Exactly: 2' from the context menu.
4. The selected atom is marked with 'x2'.

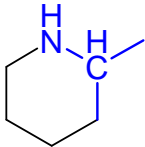
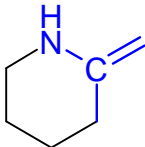
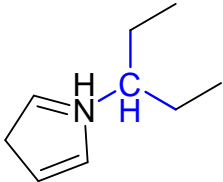
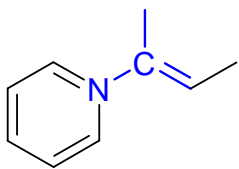
## 2.1.6.4 THREE NON-HYDROGEN ATTACHMENTS

**Format** (s3) or <sup>x3</sup>

**Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as THREE. The query atom feature '(s3)' allows you to specify that the records retrieved must have exactly THREE non-hydrogen attachments of any bond type at the specified position. Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
$\text{N}-\text{C}^{(s3)}$	
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose 3.
5. Click 'OK'.
6. The selected atom is marked with '(s3)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Substitution count' box and choose 3.
5. Click 'OK'.
6. The selected atom is marked with '(s3)'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Substituents' → 'Exactly: 3' from the context menu.
4. The selected atom is marked with 'x3'.

## 2.1.6.5 FOUR NON-HYDROGEN ATTACHMENTS

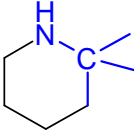
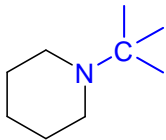
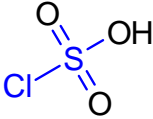
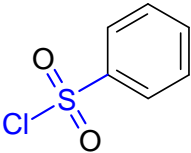
**Format** (s4) or <sup>x4</sup>

**Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as FOUR. The query atom feature '(s4)' allows you to specify that the records retrieved must have exactly FOUR non-hydrogen attachments of any bond type at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
N-C(s4)	
	
Cl-S(s4)	
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose 4.
5. Click 'OK'.
6. The selected atom is marked with '(s4)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Substitution count' box and choose 4.
5. Click 'OK'.
6. The selected atom is marked with '(s4)'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Substituents' → 'Exactly: 4' from the context menu.
4. The selected atom is marked with '<sup>x4</sup>'.



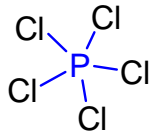
### 2.1.6.6 FIVE NON-HYDROGEN ATTACHMENTS

**Format** (s5)**Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as FIVE. The query atom feature '(s5)' allows you to specify that the records retrieved must have exactly FIVE non-hydrogen attachments of any bond type at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
P(s5)	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose 5.
5. Click 'OK'.
6. The selected atom is marked with '(s5)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Substitution count' box and choose 5.
5. Click 'OK'.
6. The selected atom is marked with '(s5)'.

**Use in ChemDraw**

A substitution count higher than four is not supported.

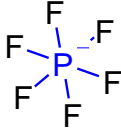
## 2.1.6.7 SIX NON-HYDROGEN ATTACHMENTS

**Format** (s6)**Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as SIX. The query atom feature '(s6)' allows you to specify that the records retrieved must have exactly SIX non-hydrogen attachments of any bond type at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
P(s6)	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose 6.
5. Click 'OK'.
6. The selected atom is marked with '(s6)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Substitution count' box and choose 6.
5. Click 'OK'.
6. The selected atom is marked with '(s6)'.

**Use in ChemDraw**

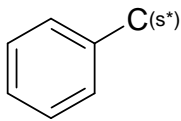
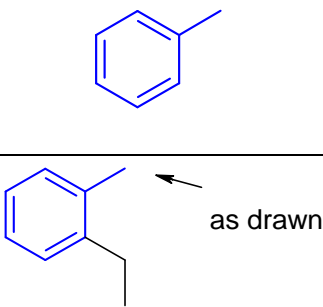
A substitution count higher than four is not supported.

## 2.1.6.8 NON-HYDROGEN ATTACHMENTS 'AS DRAWN'

**Format (s\*)****Description**

Use this procedure to specify the number of required non-hydrogen attachments (substituents) on an atom as EXACTLY THOSE non-hydrogen attachments that you have drawn at the specified position in your query.

**Example**

Query	Retrieved molecules
	

**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Substitution count' box and choose \* (asterisk).
5. Click 'OK'.
6. The selected atom is marked with '(s\*)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having non-hydrogen attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Substitution count' box and choose \* (asterisk).
5. Click 'OK'.
6. The selected atom is marked with '(s\*)'.

**Use in ChemDraw**

The property 'As drawn' is not supported.

## 2.1.7 Specify the Number of Ring Bond Attachments

A ring bond is a bond that is part of a ring structure. Use this procedure to specify the number of allowed ring bonds on an atom.

### 2.1.7.1 NO RING BOND ATTACHMENTS

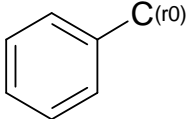
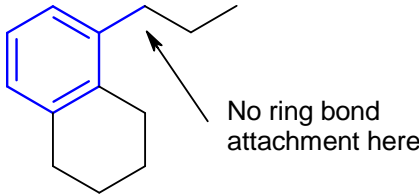
**Format** (r0) or <sup>R</sup>

#### Description

The query atom feature '(r0)' allows you to specify that the records retrieved must have NO ring bond attachment at the specified position. All atoms with this mark must not be part of a ring.

Please note: Count double or triple bonds as one attachment.

#### Example

Query	Retrieved molecules
	

#### Use in InfoChem's Editor ICEDIT

1. Select the atom that you want to specify as having ring bond attachments.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Ring Bond count' box and choose 0.
5. Click 'OK'.
6. The selected atom is marked with '(r0)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having ring bond attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Ring bond count' box and choose 0.
5. Click 'OK'.
6. The selected atom is marked with '(r0)'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Ring Bound Count' → 'No Ring Bonds' from the context menu.
4. The selected atom is marked with '<sup>R</sup>'.

## 2.1.7.2 TWO RING BOND ATTACHMENTS


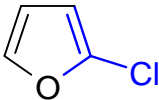
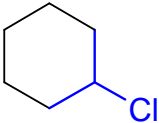
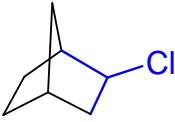
**Format** (r2) or <sup>R</sup>

**Description**

The query atom feature '(r2)' allows you to specify that the records retrieved must have exactly TWO ring bond attachments at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
$\text{Cl}-\text{C}(\text{r}2)$	
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select the atom that you want to specify as having ring bond attachments.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Ring Bond count' box and choose 2.
5. Click 'OK'.
6. The selected atom is marked with '(r2)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having ring bond attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Ring bond count' box and choose 2.
5. Click 'OK'.
6. The selected atom is marked with '(r2)'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Ring Bound Count' → 'Simple Ring' from the context menu.
4. The selected atom is marked with 'R'.

## 2.1.7.3 THREE RING BOND ATTACHMENTS

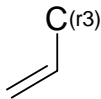
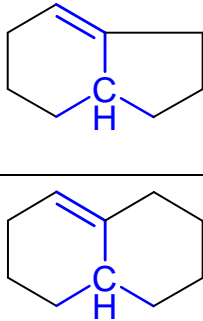
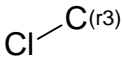
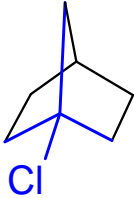
**Format** (r3) or <sup>R</sup>

**Description**

The query atom feature '(r3)' allows you to specify that the records retrieved must have exactly THREE ring bond attachments at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select the atom that you want to specify as having ring bond attachments.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Ring Bond count' box and choose 3.
5. Click 'OK'.
6. The selected atom is marked with '(r3)'.



***Use in ISIS/Draw***

1. Select the atom that you want to specify as having ring bond attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Ring bond count' box and choose 3.
5. Click 'OK'.
6. The selected atom is marked with '(r3)'.

***Use in ChemDraw***

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Ring Bound Count' → 'Fusion' from the context menu.
4. The selected atom is marked with '<sup>R</sup>'.

## 2.1.7.4 FOUR RING BOND ATTACHMENTS

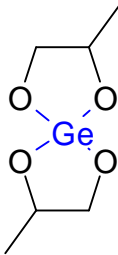
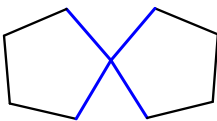
**Format** (r4) or <sup>R</sup>

**Description**

The query atom feature '(r4)' allows you to specify that the records retrieved must have FOUR ring bond attachments at the specified position.

Please note: Count double or triple bonds as one attachment.

**Example**

Query	Retrieved molecules
Ge(r4)	
C(r4)	

**Use in InfoChem's Editor ICEDIT**

1. Select the atom that you want to specify as having ring bond attachments.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Ring Bond count' box and choose 4.
5. Click 'OK'.
6. The selected atom is marked with '(r4)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having ring bond attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Ring bond count' box and choose 4.

5. Click 'OK'.
6. The selected atom is marked with '(r4)'.

***Use in ChemDraw***


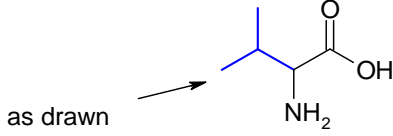
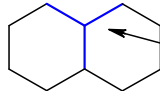
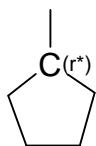
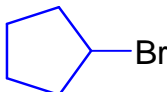

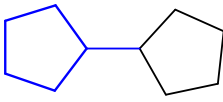
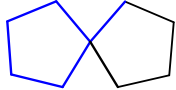
1. Select a single atom.
2. Right click the selected atom.
3. Select 'Ring Bound Count' → 'Spiro or higher' from the context menu.
4. The selected atom is marked with 'R<sub>1</sub>'.

## 2.1.7.5 RING BOND ATTACHMENTS 'AS DRAWN'

**Format (r\*)****Description**

The query atom feature '(r\*)' allows you to specify that the records retrieved must have EXACTLY THOSE ring bond attachments that you have drawn at the specified position in your query.

**Example**

Query	Retrieved molecules
	
	<p>NOTE:</p>  <p>is not retrieved!!</p>
	
	
	
	 <p>is not retrieved!!</p>

**Use in InfoChem's Editor ICEDIT**

1. Select the atom that you want to specify as having ring bond attachments.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Ring Bond count' box and choose \* (asterisk).
5. Click 'OK'.
6. The selected atom is marked with '(r\*)'.

**Use in ISIS/Draw**

1. Select the atom that you want to specify as having ring bond attachments.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Query Atom' tab.
4. Click the 'Ring bond count' box and choose \* (asterisk).
5. Click 'OK'.
6. The selected atom is marked with '(r\*)'.

**Use in ChemDraw**

1. Select a single atom.
2. Right click the selected atom.
3. Select 'Ring Bound Count' → 'As Drawn' from the context menu.
4. The selected atom is marked with 'R'.

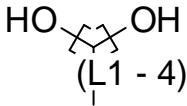
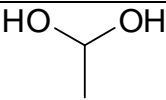
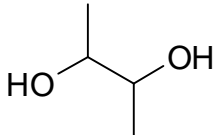
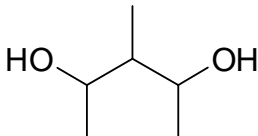
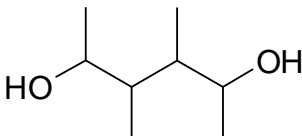
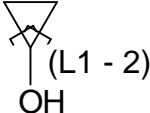

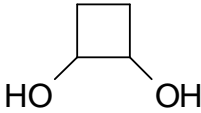
### 2.1.8 Allow Additional Atoms and/or Bonds in a Chain or a Ring

**Format** (L1-*nnn*)

**Description**

The link node query atom feature '(L1-*nnn*)' allows you to specify that the records retrieved may have a variable number of repeating units (1 to *nnn*) in a ring or chain as specified by your query. Supported repeating numbers for MDLCT V2000: 1-999 and MDLCT V3000: 1-32000.

**Example**

Query	Retrieved molecules
	
	
	
	
	
	

**Use in InfoChem's Editor ICEDIT**

Not yet implemented.

**Use in ISIS/Draw**

1. To select a repeating unit, select an atom and its two adjacent ring or chain bonds (the atom that you select can be attached to a substituent by an additional bond).
2. Choose 'Chemistry' → 'Link Node' from the menu.
3. Enter the maximum number of repeating units allowed in your ring or chain. Your number must be a value between 2 and 999 or 32000 (MDLCT V2000: 1-999, MDLCT V3000: 1-32000).
4. Click 'OK'.
5. The selected repeating unit is marked with (L1-10), if 10 is the maximum number of repeating numbers entered.

**Use in ChemDraw**

1. Select the desired atom.
2. Open an atom label text box.
3. Type in the following format: [atom symbol]1-maximum number ([O]1-2).

Please note: Only a single element symbol or a generic nickname is allowed for the input of a link node.

**Please note:** Queries with link node query features are currently not supported with higher ChemDraw versions.

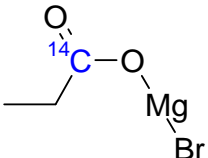
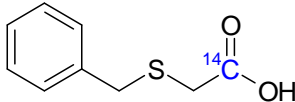
## 2.1.9 Specify a Mass (Isotope) on an Atom

**Format**  $^nX$

### Description

This atom feature allows you to specify that the records retrieved must have the isotopes that you have drawn at the specified position in your query.

### Example

Query	Retrieved molecules
$^{14}\text{C}$	
	

### Use in InfoChem's Editor ICEDIT

1. Select the atom where you want to place the isotope.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Increase or reduce the mass by clicking on the spin buttons of the 'Isotope' box.
5. Click 'OK'.
6. The isotope is displayed as superscript in front of the selected atom.

Or use the alternative method from 2.1.1.1 and enter 'nX'.

### Use in ISIS/Draw

1. Select the atom where you want to place the isotope.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Click the 'Atom' tab.
4. Increase or reduce the mass in the 'Isotope' box by clicking on the arrow.
5. Click 'OK'.
6. The isotope is displayed as superscript on the selected atom.

Or use the alternative method from 2.1.1.1 and enter 'nX'.



***Use in ChemDraw***

1. Open a text box atom label.
2. Insert the isotope number (superscript) in the text label.
3. Insert the atom label (plain) after the isotopic information.
4. Draw other bonds or atoms desired.

### 2.1.10 Specify an Explicit Valence on an Atom

**Format**  $X^{(I,II,III,...)}$

#### Description

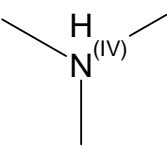

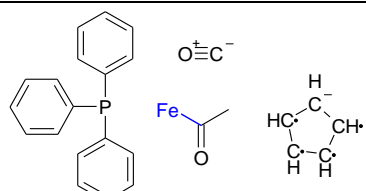
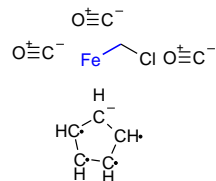
This atom feature allows you to specify that the records retrieved must have exactly the valence that you have specified at the selected position in your query.

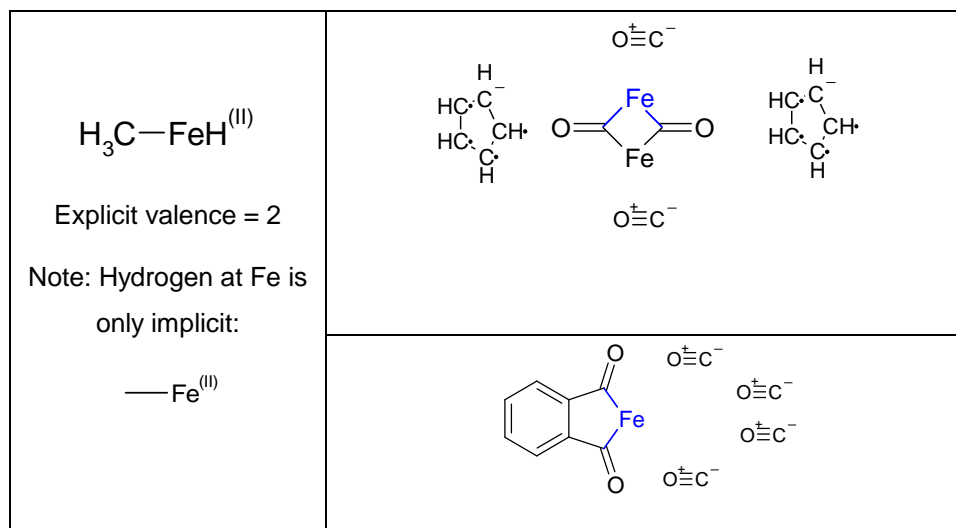
Each atom type has assigned one or more legal standard valence states, e.g. C: 4; N: 3; P: 3,5; S: 2,4,6. When connecting bonds to an atom, always implicit hydrogens will be added to the atom, until the next legal valence state is reached. Transition metal atoms have no standard valence assigned, therefore no implicit hydrogens will be added.

To override the standard valence you may specify an explicit valence to an atom. Only explicit valence settings will be used for retrieving database records with identical valence settings.

Please also refer to chapter 2.1.6 and use this procedure to specify the number of allowed non-hydrogen attachments (substituents) on an atom.

#### Examples

Query	Retrieved molecules
	
<p><math>H_3C-Fe</math></p> <p>Unspecified valence: implicit valence = 1</p> <p>=&gt; Valence in query is set to 1:</p> <p><math>-Fe^{(I)}</math></p>	
	



### Use in InfoChem's Editor ICEDIT

1. Select the atom where you want to place the valence.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Increase or reduce the valence by clicking on the spin buttons of the 'Valence box'.
5. Click 'OK'.

### Use in ISIS/Draw

1. Select the atom where you want to place the valence.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Atom' tab.
4. Click the 'Valence count' box and increase or reduce the value by clicking on an arrow.
5. Click 'OK'.

### Use in ChemDraw

1. Select the atom where you want to place the valence.
2. Right click the selected atom.
3. Select 'Abnormal Valence' → 'Allowed' from the context menu.

It is not possible to specify a specific valence in ChemDraw.

### 2.1.11 Specify a Charge on an Atom

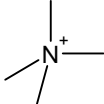

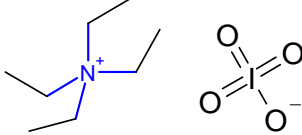
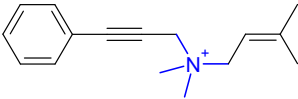
**Format**  $X^{n+}$ ,  $X^{n-}$

#### Description

This atom feature allows you to specify that the records retrieved must have exactly the charge that you have specified at the selected position in your query.

Additional information on salts is given in chapter 5.

#### Examples

Query	Retrieved molecules
	
	
	

#### Use in InfoChem's Editor ICEDIT

1. Select the atom where you want to place the charge.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Increase or reduce the charge by clicking on the spin buttons of the 'Charge' box.
5. Click 'OK'.

Or use the alternative method from 2.1.1.1 and enter ' $X^{n+}$ ', ' $X^{n-}$ '.

#### Use in ISIS/Draw

1. Select the atom where you want to place the charge.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the selected atom.
3. Choose the 'Atom' tab.
4. Click the 'Charge count' box and increase or reduce the value by clicking on an arrow.

5. Click 'OK'.

Or use the alternative method from 2.1.1.1 and enter 'Xn+', 'Xn-'.

***Use in ChemDraw***

1. Select the atom where you want to place the charge.
2. Right click the selected atom.
3. Select 'Edit Label'.
4. Insert the desired atom label and the desired charge.
5. Tab Enter.

Or use the alternative method from 2.1.1.1 and enter 'Xn+', 'Xn-'.

## 2.2 Bond Query Features



### 2.2.1 Specific Bond Type

You can retrieve molecules that allow variations in bond type at specified positions.

**IMPORTANT:** Drawing SINGLE, DOUBLE or TRIPLE bonds in a query structure will only retrieve exactly these bond types at the drawn position. Please use the bond query features 'ANY', 'AROMATIC', 'SINGLE/DOUBLE', 'SINGLE/AROMATIC', 'DOUBLE/AROMATIC' to retrieve aromatic systems or systems with delocalized  $\pi$ -electrons.

Please note: The bonds of six-membered aromatic ring systems and the perimeter bonds of azulenes are stored as aromatic bonds in the database. The bonds of five-membered aromatic rings, however, are stored as single and double bonds and interpreted as aromatic during the search. The differences between five-membered rings and other types of aromatic rings can cause different search results for five- and six-membered rings/azulenes when you use the following bonds in queries: 'SINGLE', 'DOUBLE', and 'SINGLE/DOUBLE' query bonds.

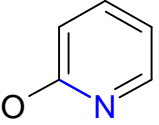
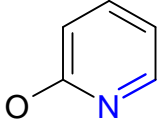
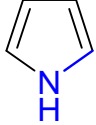
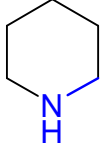
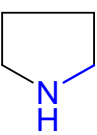
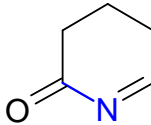
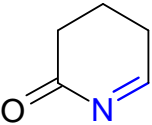
#### 2.2.1.1 ANY BOND

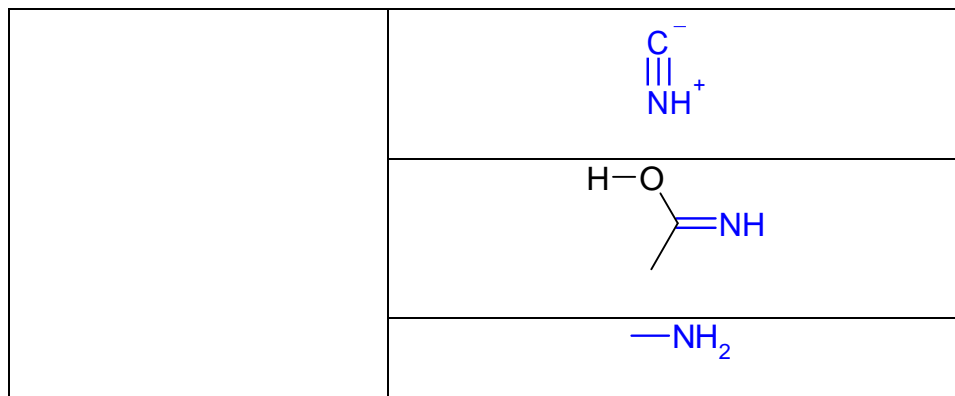
**Format**   Any

#### Description

To allow any bond type at the specified positions in your query, choose 'ANY' bond.

#### Example

Query	Retrieved molecules		
—N			
			
			

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the 'Bond Type' box and select 'Any' from the list.
5. Click 'OK'.




**Use in ISIS/Draw**

1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Click the 'Bond type' box and choose 'Any'.
5. Click 'OK'.

**Use in ChemDraw**

1. Select a bond.
2. Right click the selected bond.
3. Select 'Query' → 'Any' from the context menu.
4. The selected atom is marked with 'Any'.

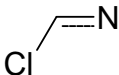

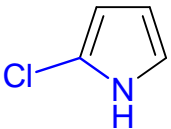
## 2.2.1.2 AROMATIC BOND

**Format**   

**Description**

To allow solely aromatic bonds at the specified positions of your query, choose the 'AROMATIC' bond type.

**Example**

Query	Retrieved molecules
	<div style="text-align: center;">  </div> <hr/> <div style="text-align: center;">  </div>

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the 'Bond Type' box and select 'Aromatic' from the list.
5. Click 'OK'.

**Use in ISIS/Draw**



1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Click the 'Bond type' box and choose 'Aromatic'.
5. Click 'OK'.

**Use in ChemDraw**

1. Select a bond.
2. Right click the selected bond.
3. Select 'Double' → 'Aromatic' from the context menu.



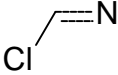
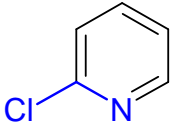
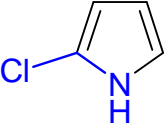
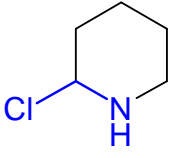
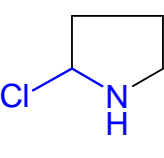
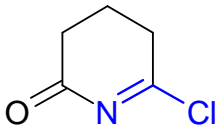
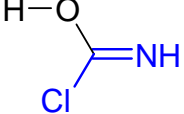
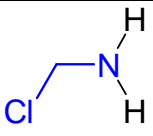
## 2.2.1.3 SINGLE/DOUBLE BOND

**Format**   S/D

**Description**

To allow either single or double bonds at the specified positions of your query, choose the 'SINGLE/DOUBLE' bond type.

**Example**

Query	Retrieved molecules	
		
		
		
		
		

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the 'Bond Type' box and select 'Single/Double' from the list.
5. Click 'OK'.



**Use in ISIS/Draw**

1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Click the 'Bond type' box and choose 'Single/Double'.
5. Click 'OK'.

**Use in ChemDraw**

1. Select a bond.
2. Right click the selected bond.
3. Select 'Query' → 'S/D' from the context menu.
4. The selected atom is marked with <sup>S/D</sup>.

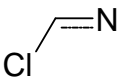

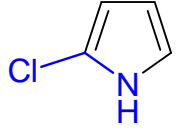
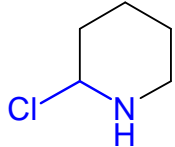
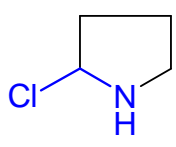
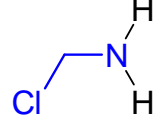
## 2.2.1.4 SINGLE/AROMATIC BOND

**Format**   S/A

**Description**

To allow either single or aromatic bonds at the specified positions of your query, choose the 'SINGLE/AROMATIC' bond type.

**Example**

Query	Retrieved molecules	
		
		
		

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the 'Bond Type' box and select 'Single/Aromatic' from the list.
5. Click 'OK'.



**Use in ISIS/Draw**

1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Click the 'Bond type' box and choose 'Single/Aromatic'.
5. Click 'OK'.

**Use in ChemDraw**

1. Select a bond.
2. Right click the selected bond.
3. Select 'Query' → 'S/A' from the context menu.
4. The selected atom is marked with <sup>S/A</sup>.

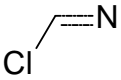

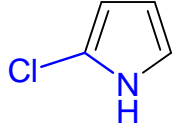
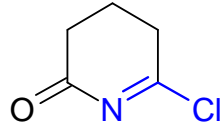
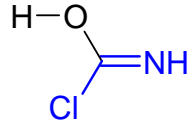
## 2.2.1.5 DOUBLE/AROMATIC BOND

**Format**   D/A

**Description**

To allow either double or aromatic bonds at the specified positions of your query, choose the 'DOUBLE/AROMATIC' bond type.

**Example**

Query	Retrieved molecules	
		
		
		

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the 'Bond Type' box and select 'Double/Aromatic' from the list.
5. Click 'OK'.

**Use in ISIS/Draw**

1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Click the 'Bond type' box and choose 'Double/Aromatic'.
5. Click 'OK'.

**Use in ChemDraw**

1. Select a bond.
2. Right click the selected bond.
3. Select 'Query' → 'D/A' from the context menu.
4. The selected atom is marked with <sup>D/A</sup>.

## 2.2.1.6 Topology (Chain or Ring Bond)

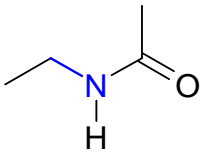
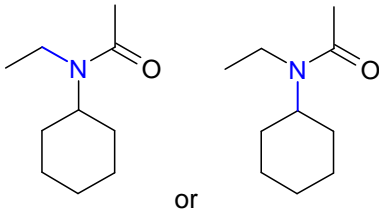
## 2.2.1.7 CHAIN BOND

**Format**  $\text{—Ch—}$   $\text{—Chn}$

**Description**

Use this procedure to mark a bond 'Ch' to specify that the bond must be part of a chain, not part of a ring. The chain may be of any size.

**Example**

Query	Retrieved molecules
$\text{—Ch—N}$	
	

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the spin buttons in the 'Topology' box and select 'Chain'.
5. Click 'OK'.
6. The selected bond is marked with 'Ch'.

**Use in ISIS/Draw**

1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Click the 'Topology' box and choose 'Chain' from the drop down list.

5. Click 'OK'.
6. The selected bond is marked with 'Ch'.

***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Topology' → 'Chain' from the context menu.
4. The selected bond is marked with 'Chn'.



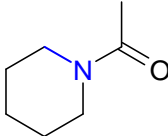
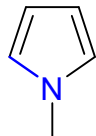
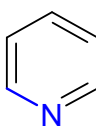
## 2.2.1.8 RING BOND

**Format**  $\text{—Rn—}$   $\text{—Rng—}$

**Description**

Use this procedure to mark a bond 'Rn' to specify that the bond must be part of a ring, not part of a chain. The ring may be of any size.

**Example**

Query	Retrieved molecules
$\text{—Rn—N}$	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select a bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Click the spin buttons in the 'Topology' box and select 'Ring'.
5. Click 'OK'.
6. The selected bond is marked with 'Rn'.

**Use in ISIS/Draw**

1. Select a bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
5. Click the 'Topology' box and choose 'Ring' from the drop down list.

4. Click 'OK'.
5. The selected bond is marked with 'Rn'.

***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Topology' → 'Ring' from the context menu.
4. Click 'OK'.
5. The selected bond is marked with 'Rng'.

### **2.2.2 Allow Additional Atoms and/or Bonds in a Chain or a Ring**

Use a link node to specify the addition of variable numbers of identical repeating units to a ring or chain. See chapter 2.1.8

## 2.3 RGroup Query Features


A RGroup search finds molecule records in a database that contain a desired core structure with defined variable functional groups or structure parts. Instead of performing multiple queries you can combine a parent structure with variable RGroups to use one single query to retrieve the desired records. The RGroup query search can be performed as exact or as substructure search.

Please note: All molecule search operators (except for the XSSEZ search operator see 4.1.2) are supporting RGroup query features. RGroups are not supported in reaction searches.

For example, you can:

1. Specify the structural fragments (such as functional groups or atoms) of your choice at specific sites within a molecule.
2. Exclude structural fragments of your choice at specific sites within a molecule.
3. Specify that the presence of one structural fragment requires the presence of another (RGroup conditions).

### *Use in InfoChem's Editor ICEDIT*

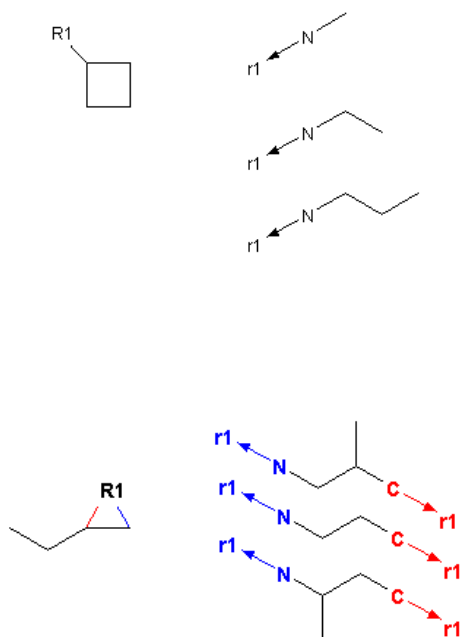
1. Draw a core structure and several RGroups.
2. Select the RGroup query button .
3. First click on the position of the core structure, where you want to have the RGroup attached.
4. Then click on the connection position of the RGroups you want to have attached.

Please note: To specify two different attachments in one RGroup, first define the attachment belonging to the blue bond in the core structure, then define the attachment belonging to the red bond in the core structure.

5. To remove the RGroup Info use the button .

Please note: Input of RGroup Logic is not yet implemented.

Examples for RGroup queries in ICEDIT:



### Use in ISIS/Draw

1. Draw a core structure and several RGroups.
2. Define the RGroups in your core structure:

Select the desired atom and choose 'Chemistry' → 'R-Query' → 'Rgroup Atom'. Select the name of the RGroup to create, such as R1 or R2 and click 'OK'.

3. Specify the attachment point of the RGroup fragments:

To specify the atoms on the RGroup substituent select the desired atom and choose 'Chemistry' → 'R-Query' → 'Attachment' and enter 1 and click 'OK'. To specify a second attachment point, select the second atom on the RGroup substituent, choose 'Chemistry' → 'R-Query' → 'Attachment', and then enter 2 and click 'OK'.

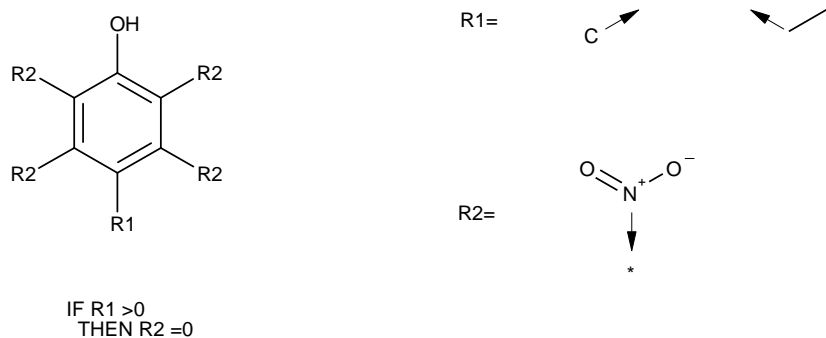
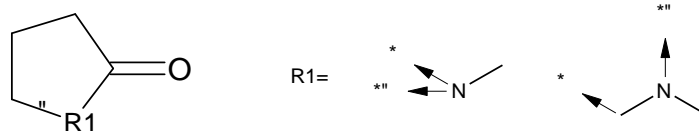
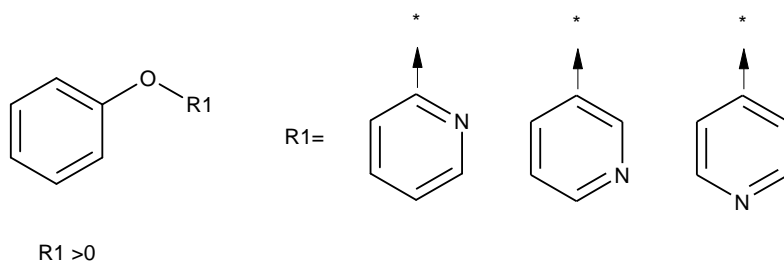
4. You see an arrow that points to an asterisk (\*). If you designated two attachment points, you also see a single quote for the first attachment point and a double quote for the second attachment point.
5. Select all the RGroup members (and their attachment points). Choose 'Chemistry' → 'R-Query' → 'RGroup'. Select the name of the RGroup to create, such as R1 or R2 and click 'OK'. You see the RGroup designation, such as R1= or R2=, next to the RGroup members.

Please note: ISIS/Draw allows the definition of RGroup conditions:

Choose 'Chemistry' → 'R-Query' → 'R-logic'. Enter the desired RGroup number that the conditions apply to in the RGroup#(i) text box. The following parameters can be adjusted:

- Occurrence range: Enter the number of RGroup sites that must be occupied.
- RestH: click the check box to allow non-hydrogen substituents in addition to your defined RGroup that can be attached to the core structure.
- If R(i) then: Enter the number of the dependent RGroup to use the 'If R(i) then' condition.


Examples for RGroup queries in ISIS/Draw:



### Use in ChemDraw

1. Draw a core structure and several RGroups.
2. To define a RGroup: Click the 'Alternative Group' from the 'Show Query Tools' toolbar.



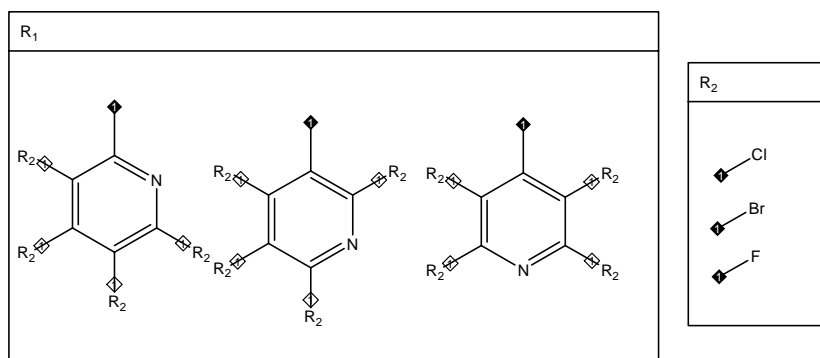
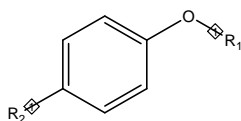
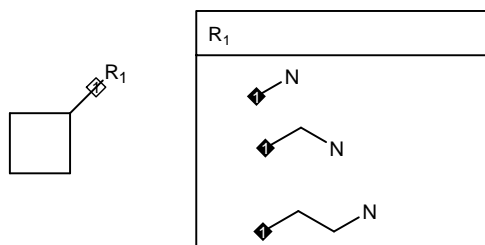
3. Drag the RGroups with the 'Alternative Group' tool. Type a title and use the same label for your RGroup of the core structure (e.g. R1).
4. To specify where the fragments should be attached to the parent structure please define attachment points by selecting the desired atoms with the 'Attachment Point' tool  from the 'Show Query Tools' palette.

Please note: To specify two different attachments in one RGroup, first define the attachment belonging to the bond marked with 1 in the core structure, then define the attachment belonging to the bond marked with 2 in the core structure.

Please note: RGroup Logic definitions can not be entered with ChemDraw.

**Please note:** Queries containing RGroups are currently not supported if ChemDraw is used as input editor.

Examples for RGroup queries in ChemDraw:



## 2.4 Specifying Attached Data

- For an exact search in a molecule database.
- For a substructure search in a molecule database.

Not yet implemented.



## 2.5 Stereochemistry

Please also refer to chapter 6.

### 2.5.1 UP and DOWN BOND

**Format**  and 

#### **Description**

You can create a query with an 'UP' bond or a 'DOWN' bond on the asymmetric center of atoms C, N, O, P, S or Si.

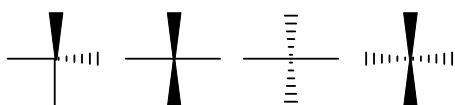
An 'UP' bond or a 'DOWN' bond on the asymmetric tetrahedral center of the above mentioned atoms allows you to retrieve molecules with matching stereochemistry. Without creating a chiral flag for the query, stereochemistry will be treated as relative, i.e. searching the query structure or its mirror image will result in identical hit sets.

Please note: Atom-centered stereo chemistry is defined by up and/or down bonds:



Draw only one stereo bond ('UP' or 'DOWN') per stereo center if possible, otherwise please consider the following examples. If stereochemistry is not absolutely clear, add hydrogens to stereocenters.

The following combinations of 'UP' and 'DOWN' bonds are correct:

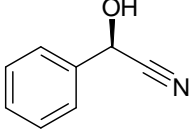
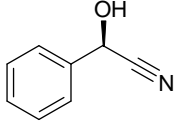
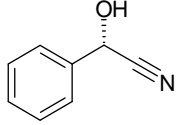
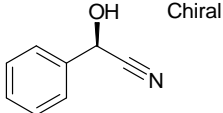
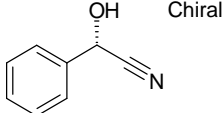
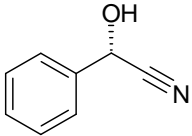
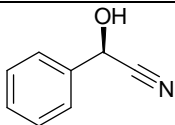
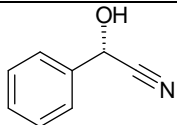
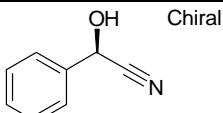
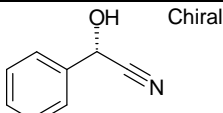


The following combinations of 'UP' and 'DOWN' bonds are INCORRECT:



The direction of the stereo bonds is essential to specify the stereochemical center (the narrow end of the bond specifies the stereo chemical center, the flat end specifies the substituent for this stereochemical center).

**Example**

Query	Retrieved molecules	
		
		
		
		

**Use in InfoChem's Editor ICEDIT**

1. To sprout an 'UP' bond from an atom, choose



To sprout a 'DOWN' bond from an atom, choose



2. Click the atom of your choice, from which the 'UP' or 'DOWN' bond shall be drawn.

You may change the direction of the stereo bond by clicking on the existing stereo bond with the

buttons  or .

**Use in ISIS/Draw**

1. To sprout an 'UP' bond from an atom, choose



To sprout a 'DOWN' bond from an atom, choose




2. Click the atom of your choice, from which the 'UP' or 'DOWN' bond shall be drawn.


You may change the direction of the stereo bond by clicking on the existing stereo bond with the

buttons  or .



Please note: Do not use  for 'UP' bonds and  for 'DOWN' bonds.



**Use in ChemDraw**

1. To sprout an 'UP' bond from an atom, choose .

To sprout a 'DOWN' bond from an atom, choose .

2. Click the atom of your choice, from which the 'UP' or 'DOWN' bond shall be drawn.

You may change the direction of the stereo bond by clicking on the existing stereo bond with the buttons  or .

Please note: Do not use  for 'UP' bonds and  for 'DOWN' bonds.

### **2.5.2 Stereochemistry at Double Bonds**

Not yet supported.

E/Z (cis/trans) configurations drawn in the query will be ignored during searches.

Please note: E/Z configuration is not ignored for exact searches if the XSSEZ search operator is used (see chapter 4.1.2).

### 2.5.3 Chiral flag

**Format** Chiral or ABS

#### Description

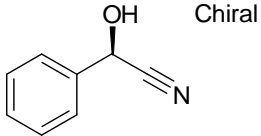
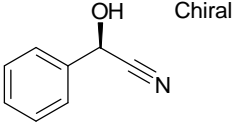
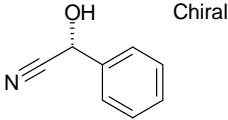
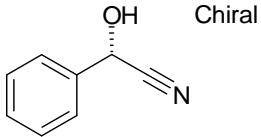
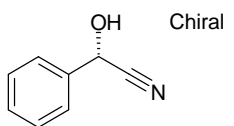
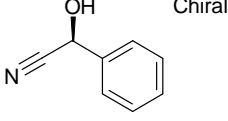
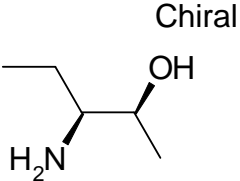
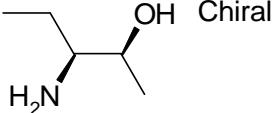
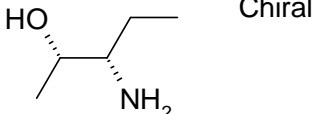
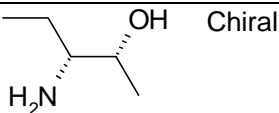
You can create a query with a 'CHIRAL FLAG' on a molecule with at least one asymmetric center or on a molecule that is asymmetric to retrieve solely the absolute stereo configuration but not relative stereo configurations.

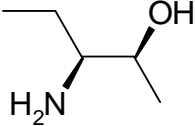
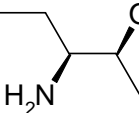
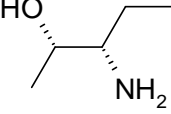
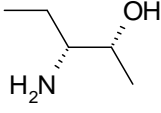
When you create a query without a chiral flag on a molecule that contains at least one asymmetric center or on a molecule that is asymmetric, you retrieve all the relative stereoconfigurations.

The chiral flag eliminates the relative stereoconfigurations.

Please note: Geometrical stereo information (E/Z at double bonds) is currently ignored. However, tetrahedral stereochemistry for the following atoms: C, N, O, S (sulfate and sulfoxide), P, Si, and pentavalent N and P (3 or 4 attachments with 1 double bond) is supported.

#### Example

Query	Retrieved molecules	
1 stereo center: 		
		
2 stereo centers: WITH Chiral flag 		
		
		
	will NOT be retrieved	

Query	Retrieved molecules
2 stereo centers: NO Chiral flag 	 OH Chiral
	 Chiral
	 Chiral will be retrieved

#### **Use in InfoChem's Editor ICEDIT**

1. Select the structure that you want to label as chiral.
2. Choose 'Create Chiral Flag' from the context menu.
3. The structure is marked with 'Chiral'.

#### **Use in ISIS/Draw**

1. Select the structure that you want to label as chiral.
2. Choose 'Chemistry' → 'Create Chiral Flag' from the menu bar.
3. The structure is marked with 'Chiral'.

#### **Use in ChemDraw**

Please note: Although ChemDraw allows the input of stereochemical flags (Racemic **Rac**, Absolute **Abs**, Relative **Rel**) these flags are ignored as query features.

### 3. Query Features on a Reaction

#### 3.1 Specific Query Features on a Reaction

Query Features on a Reaction: A query feature on a reaction is a restriction on (i) reacting centers, (ii) spatial arrangement of stereo bonds or (iii) atoms, that specifies the retrieval of certain types of reaction records from the database.

Reacting Center Query Features: A reacting center is a bond that changes in the reactant and in the product. Markings on the bonds of reactants and products specify exactly which bonds change (or do NOT change). If you do not mark reaction centers, only the “pure” structures (reactant and product) of your query will be searched as substructures in the reaction database, not considering the chemistry of the reaction. Therefore, specifying reaction centers in your query is a method to cut down a large hitlist of “pure substructure hits” to a shorter list of chemically corresponding hits.

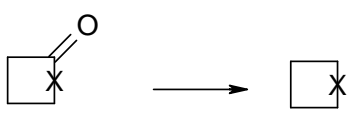
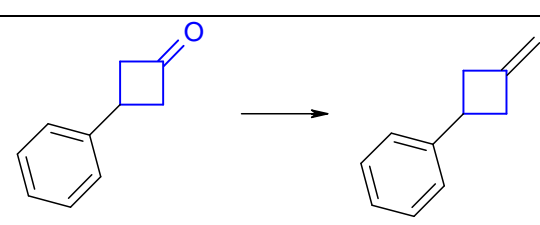
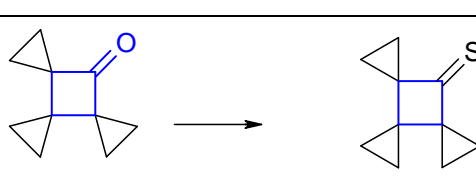
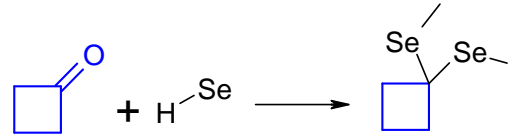
##### 3.1.1 NOT CENTER

**Format**  $\text{---}\times\text{---}$

**Description**

The marked bond must not change.

**Example**

Query	Retrieved reactions
	
	
	

**Use in InfoChem's Editor ICEDIT**

1. Select the bond you want to specify as reacting bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Select 'Not Center' by clicking the spin buttons of the 'Reacting center' box.
5. Click 'OK'.
6. The selected bond is marked with 'x'.

**Use in ISIS/Draw**

1. Select the bond you want to specify as reacting bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Select 'Not Center' from the 'Reacting center' drop down list.
5. Click 'OK'.
6. The selected bond is marked with 'x'.

Alternative method:

1. Click 

ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reactions, you see a message that tells you to use Chem Inspector.

2. Click the bond on which to mark a reacting center. Each time you click the bond, you see a different reacting center mark. Keep clicking the bond until you see the desired reacting center mark: 'x'.

**Use in ChemDraw**

1. Select a bond.
2. Right click the selected bond.
3. Select 'Reaction Center' → 'Not Center' from the context menu.



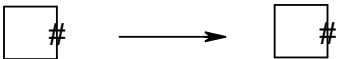
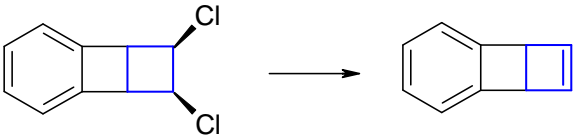
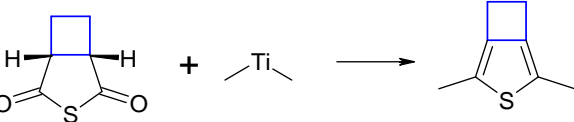
### 3.1.2 CENTER

**Format**  $\text{---\#---}$  Rxn

#### Description

The marked bond changes unspecifically (may be formed or broken or may change its bond order).

#### Example

Query	Retrieved reactions
	<div style="display: flex; flex-direction: column; align-items: center;"> <div style="display: flex; align-items: center; margin-bottom: 10px;">  </div> <div style="display: flex; align-items: center; margin-bottom: 10px;">  </div> <p style="text-align: center;">Bond gets aromatic</p> </div>

#### Use in InfoChem's Editor ICEDIT

1. Select the bond you want to specify as reacting bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Select 'Center' by clicking the spin buttons of the 'Reacting center' box.
5. Click 'OK'.
6. The selected bond is marked with '#'.

#### Use in ISIS/Draw


1. Select the bond you want to specify as reacting bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Select 'Center' from the 'Reacting center' drop down list.
5. Click 'OK'.
6. The selected bond is marked with '#'.

Or use the alternative method from 3.1.1 until the desired reacting center mark '#'.

***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Reaction Center' → 'Center' from the context menu.
4. The bond is marked with 'Rxn'.

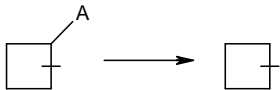
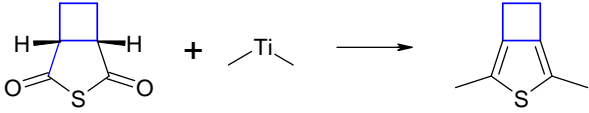
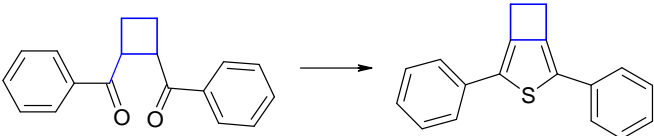
### 3.1.3 CHANGE

**Format**  Rxn

#### Description

The marked bond changes its bond order.

#### Example

Query	Retrieved reactions
	<div style="border-bottom: 1px solid black; padding-bottom: 10px;">  <p style="text-align: center;">Bond gets aromatic</p> </div> <div style="padding-bottom: 10px;">  <p style="text-align: center;">Bond gets aromatic</p> </div>

#### Use in InfoChem's Editor ICEDIT

1. Select the bond you want to specify as reacting bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Select 'Change' by clicking the spin buttons of the 'Reacting center' box.
5. Click 'OK'.
6. The selected bond is marked with 'j'.

#### Use in ISIS/Draw


1. Select the bond you want to specify as reacting bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Select 'Change' from the 'Reacting center' drop down list.
5. Click 'OK'.
6. The selected bond is marked with 'j'.

Or use the alternative method from 3.1.1 until the desired reacting center mark 'j'.

***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Reaction Center' → 'Change' from the context menu.
4. The bond is marked with 'Rxn'.

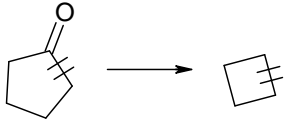
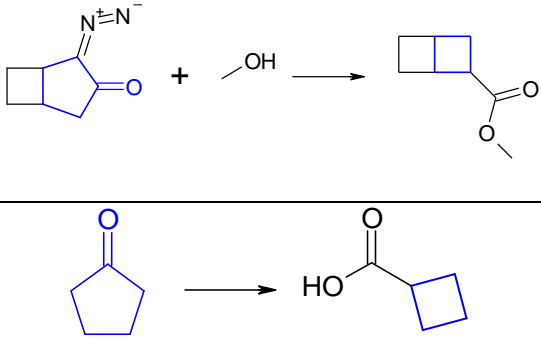
### 3.1.4 MAKE/BREAK

**Format**  Rxn

#### Description

The marked bond is either formed at the product side or broken at the reactant side.

#### Example

Query	Retrieved reactions
	

#### Use in InfoChem's Editor ICEDIT

1. Select the bond you want to specify as reacting bond.
2. Right click the selected bond.
3. Open the context menu 'Edit Bond'.
4. Select 'Make/Break' by clicking the spin buttons of the 'Reacting center' box.
5. Click 'OK'.
6. The selected bond is marked with '||'.

#### Use in ISIS/Draw

1. Select the bond you want to specify as reacting bond.
2. Choose 'Object' → 'Edit Bond' from the main menu or double click the selected bond.
3. Choose the 'Bond' tab.
4. Select 'Make/Brake' from the 'Reacting center' drop down list.
5. Click 'OK'.
6. The selected bond is marked with '||'.

Or use the alternative method from 3.1.1 until the desired reacting center mark '||'.

***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Reaction Center' → 'Make/Break' from the context menu.
4. The bond is marked with 'Rxn'.

### **3.1.5 MAKE/CHANGE**

Please note: This query feature is NOT supported by InfoChem's Search Engine.

#### ***Description***

The marked bond is either formed or broken and changes its bond type.

## 3.2 Stereo Bond Query Features

Inversion and retention tags specify how the stereochemistry of an asymmetric center in a reactant or product changes or does not change in a reaction.

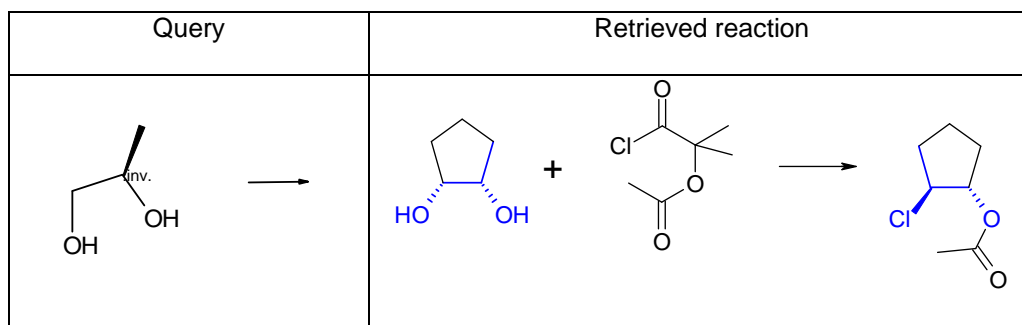
### 3.2.1 INVERSION

**Format** .inv. or T

**Description**

'inv.' specifies that the asymmetric center **INVERTS** its stereo chemical configuration during the reaction.

**Example**



**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Reaction Stereo' box and choose 'Inversion'.
5. Click 'OK'.
6. The selected atom is marked with '.inv.'.

**Use in ISIS/Draw**

1. Select an atom.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the atom.
3. Chose the 'Query Atom' tab.
4. Select 'Inversion' from the 'Reaction Stereo' drop down list.
5. Click 'OK'.
6. The selected atom is marked with '.inv.'.



***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Reaction Stereo' → 'Inversion' from the context menu.
4. The bond is marked with 'T'.

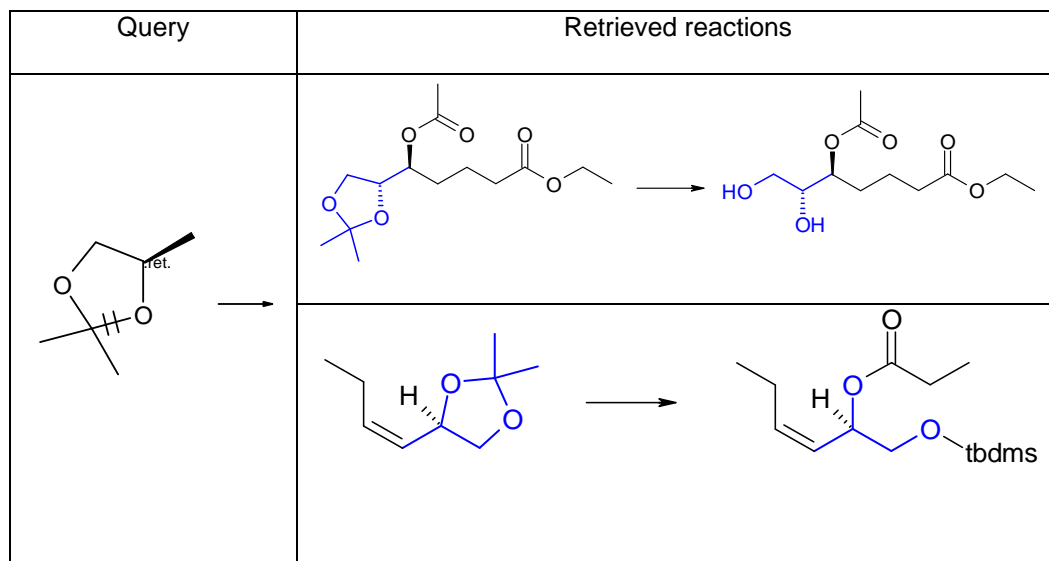
### 3.2.2 RETENTION

**Format** .ret. or T

**Description**

‘.ret.’ specifies that the asymmetric center **RETAINS** its stereo chemical configuration during the reaction.

**Example**



**Use in InfoChem's Editor ICEDIT**

1. Select an atom.
2. Right click the selected atom.
3. Open the context menu 'Edit Atom'.
4. Click the spin buttons of the 'Reaction Stereo' box and choose 'Retention'.
5. Click 'OK'.
6. The selected atom is marked with '.ret.'.

**Use in ISIS/Draw**

1. Select an atom.
2. Choose 'Object' → 'Edit Atom' from the main menu or double click the atom.
3. Chose the 'Query Atom' tab.
4. Select 'Retention' from the 'Reaction Stereo' drop down list.
5. Click 'OK'.
6. The selected atom is marked with '.ret.'.

***Use in ChemDraw***

1. Select a bond.
2. Right click the selected bond.
3. Select 'Reaction Stereo' → 'Retention' from the context menu.
4. The bond is marked with 'T'.

### 3.3 Atom-Atom Map on a Reaction

An atom-atom map on the reaction components in a query specifies exactly which atoms in the reactants correspond to the atoms in the products. You can specify the atoms that must (or must not) change in the transformations that you retrieve.

An atom-atom map eliminates additional, unwanted results from the result of your search.

You can atom-atom map AUTOMATICALLY or MANUALLY. If you map manually, you choose your own correspondence between the atoms in the reactants and in the products.

#### 3.3.1 Automapping a Reaction Query

##### Description

Use this procedure to map all atoms in a reaction automatically (automatic atom-atom mapping is called automapping).

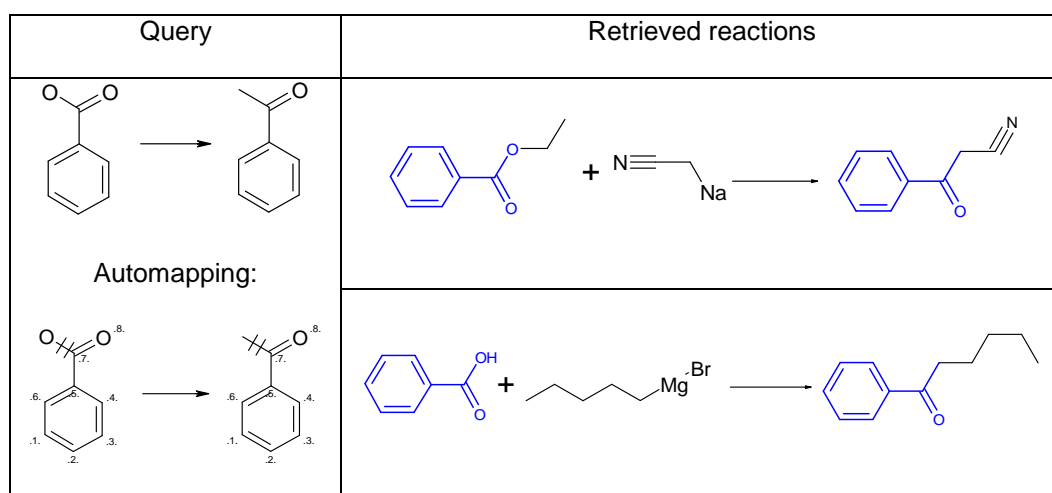
This feature is currently only available for ISIS/Draw as input editor if the InfoChem Map Addin for ISIS/Draw has been installed. For information of how to get the InfoChem Map Addin please contact InfoChem. Support for ICEDIT and SymyxDraw are under development.

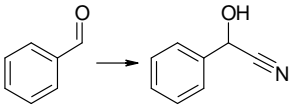
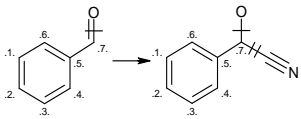
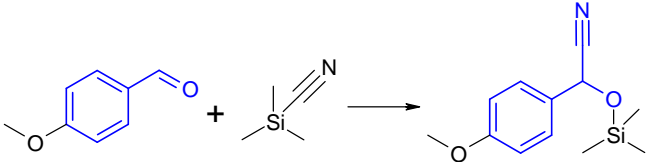
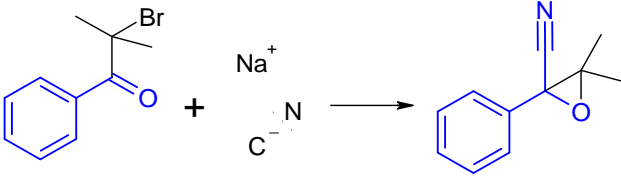
The addin will be activated by using the new automap button.



Your query will be mapped and assigned reaction centers automatically with the automap feature to simplify the input of a RSS query.

##### Example



Query	Retrieved reactions
 <p>Automapping:</p> 	 


### Use in InfoChem's Editor ICEDIT

**Please note:** A licensed version of the ICEDIT application is necessary to use the Infochem autopmap functionality.

Click on the icon . You see the atom-atom maps and reacting centers in the reaction.

Visually inspect the atom-atom maps and reacting centers. If the automatic atom-atom map is incorrect, remove the atom-atom maps and centers and then manually atom-atom map the query.

### Use in ISIS/Draw

Click on the InfoChem's Icon.  You see the atom-atom maps and reacting centers in the reaction.

Visually inspect the atom-atom maps and reacting centers. If the automatic atom-atom map is incorrect, remove the atom-atom maps and centers and then manually atom-atom map the query.

### Use in ChemDraw

1. Draw the reaction you want to map.
2. Select the reactants and products in the reaction.
3. Choose 'Map Reaction Atoms' from the 'Structure' menu.
4. The symbol 'Rxn' appears next to the bonds in the reactant and product that are perceived by the algorithm as being modified by the reaction. These symbols are bond properties that are automatically applied.

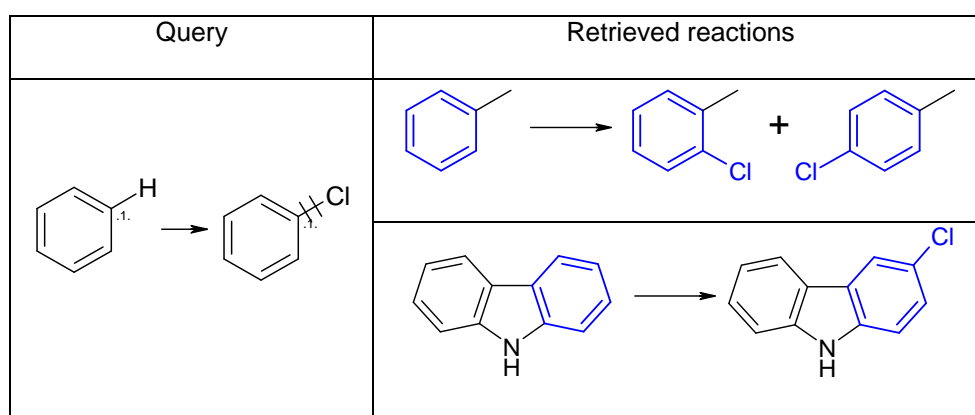
### 3.3.2 Mapping a Reaction Query Manually

#### Description


If you map manually, you choose your own correspondence between atoms in the reactants and in the products. Use the following guidelines to atom-atom map your query correctly:

Always atom-atom map a query that contains an entire reaction (at least a portion of a reactant and at least a portion of a product). Do not attempt to atom-atom map a query that contains solely a reaction component and a reaction arrow. Only map those specific atoms that you see in both the reactants and the products.

#### Example




#### Use in InfoChem's Editor ICEDIT

1. Click 
2. Click an atom in a reactant, and then click the corresponding atom in the product. The mapping numbers (in the form .1.) will be displayed next to the mapped atoms.
3. To map a one-to-many relationship, first click an atom that is marked with an existing atom map. Then, click the corresponding atom.

Please note: You cannot map a many-to-many relationship.

4. To delete single mappings use  and click on the mapped atoms.

#### Use in ISIS/Draw

1. Click 
2. ISIS/Draw checks if the reaction is valid for mapping, and that there is only one reaction present in the sketch. If the reaction is not valid for mapping, or if there are more than one reaction, you see a message that tells you to use Chem Inspector.

3. Click an atom in a reactant, and then click the corresponding atom in the product. The mapping numbers (in the form .1.) will be displayed next to the mapped atoms.
4. To map a one-to-many relationship, first click an atom that is marked with an existing atom map. Then, click the corresponding atom.

Please note: You cannot map a many-to-many relationship.


5. To delete single mappings use  and click on the mapped atoms.

### ***Use in ChemDraw***

To suppress automatic re-mapping:

1. Choose 'Preferences' from the 'File' menu.
2. Deselect 'Automatic Reaction Mapping'.
3. Click 'OK'.

To use the Reaction Atom-Atom Map tool:

1. Click the 'Reaction Atom-Atom Map' tool  from the 'Query' toolbar.
2. Point to the atom in the reactant whose mapping you want to establish.
3. Drag from the reactant atom to the corresponding product atom.
4. To delete single mappings click on one of the mapped atoms.

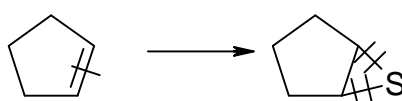
### 3.4 Atom-Atom-Mapping Guidelines

Use the following guidelines to atom-atom map your query correctly:

Always atom-atom map a query that contains an entire reaction (at least a reactant and a product). Do not attempt to atom-atom map a query that contains solely a reaction component and a reaction arrow.

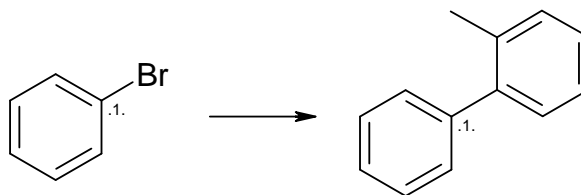
Please note: We strongly recommend that you draw solely the reacting fragments (and use query features where relevant) rather than draw each reactant and product in detail.

Only map those specific atoms that you see in both the reactants and the products. For example, do not map the sulfur atom that you see only in the product:

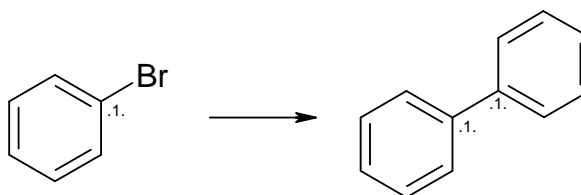


Map them manually:

1. Select a reactant atom and a product atom that you want to specify as atom 1 and map them manually:



2. Select the same atom in the reactant and another atom in the product that you want to specify as atom 1 (a multiple mapping of atom 1) and map them manually:



3. Always atom-atom map a reaction query at last, after you added all other structures, stereochemistry, and/or query features to your query.



## 4. Search Types - Basics

### 4.1 Structure Searches

#### 4.1.1 SSS (Substructure Search)

##### *Description*

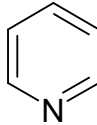
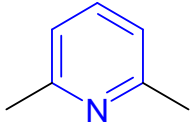
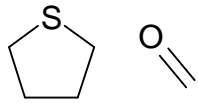
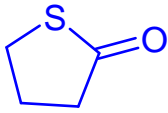
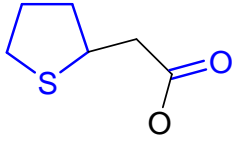
A molecule **Substructure Search** (SSS) finds molecule records in a database that contain your query as a substructure wholly within a larger structure.

Please note: Only two-dimensional substructure representations are supported.

Special feature (by default): Multiple fragments in a single query:

Your substructure query may consist of two or more separated structure fragments. To retrieve molecules that contain all the fragments that you specify in your query, draw each fragment separately, and group all fragments (not necessary if *ICEDIT* is used). The retrieved molecules will contain all fragments of the query (see example).

##### *Example*

Query	Retrieved molecules
	
	 

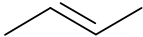

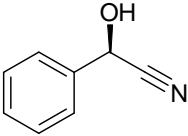
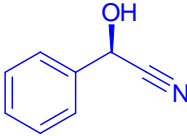
You can also increase the power of a SSS search by the addition of specific restrictions (called query features) on atoms and/or bonds. Several different query features are available (see chapter 2 and chapter 3).

#### 4.1.2 XSSEZ Search (Exact Structure Search, incl. E/Z Stereochemistry)

##### *Description*

An **Exact Structure Search** incl. **E/Z Stereochemistry** (XSSEZ) finds molecule records in a database that match your structure query exactly. For an exact match all stereo information (i.e. R/S and E/Z) and all isotopic labels must match. Any stereo information of your query will be treated as absolute, even without setting the chiral flag for the query structure. Therefore only identical absolute stereochemistry will be retrieved. If you want to retrieve relative stereochemistry, you have to use the relative exact structure search (RXSS, see 4.1.4).

##### *Example*

Query	Retrieved molecules
	
	

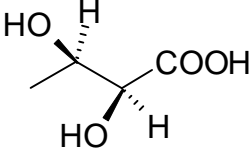
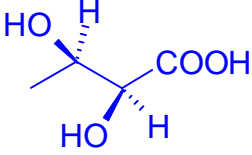
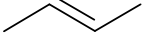


### 4.1.3 XSS (Exact Structure Search)

#### Description

An **Exact Structure Search** (XSS) finds molecule records in a database that match your structure query exactly. For an exact match tetrahedral stereo information (i.e. R/S) and all isotopic labels must match. Any stereo information of your query will be treated as absolute, even without setting the chiral flag for the query structure. Therefore only identical absolute stereochemistry will be retrieved. If you want to retrieve relative stereochemistry, you have to use the relative exact structure search (RXSS, see 4.1.4).

Please note: Geometrical stereo information (E/Z at double bonds) will be ignored during a XSS search. If you want E/Z stereochemistry considered also you have to use the Exact Structure Search incl. E/Z Stereochemistry (XSSEZ, see 4.1.2).

#### Example

Query	Retrieved molecules
	
	
	

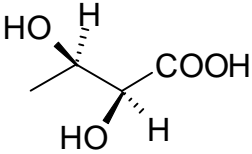
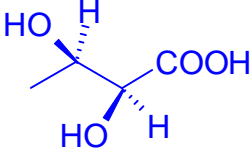
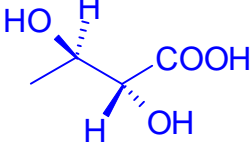
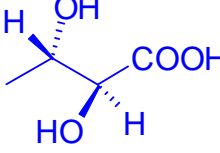
#### 4.1.4 RXSS Search (Relative Exact Structure Search)

##### *Description*

A **Relative Exact Structure Search (RXSS)** finds molecule records in a database that match your structure query exactly. For an exact match tetrahedral stereo information (i.e. R/S) and all isotopic labels must match. Any stereo information of your query will be treated as relative, even when setting the chiral flag for the query structure. Therefore identical absolute and relative stereochemistry will be retrieved. If you want to retrieve only absolute stereochemistry, you have to use the exact structure search (XSS, see 4.1.3).

Please note: Geometrical stereo information (E/Z at double bonds) will be ignored during a RXSS search. If you want E/Z stereochemistry considered also you have to use the Exact Structure Search incl. E/Z Stereochemistry (XSSEZ, see 4.1.2).

##### *Example*

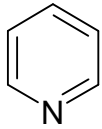
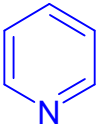
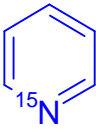
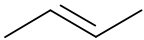


Query	Retrieved molecules
	
	
	

#### 4.1.5 IXSS (Isomer Exact Structure Search, Isomer Search)

##### *Description*

An **I**somer **E**xact **S**tructure **S**earch (IXSS) finds molecule records in a database that are (i) geometric isomers, (ii) stereo isomers or (iii) isotopic isomers of your structure query.

##### *Example*

Query	Retrieved molecules
	
	
	
	

#### 4.1.6 PXSS (Parent Exact Structure Search, Parent Search)

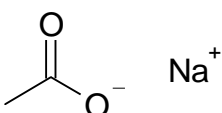
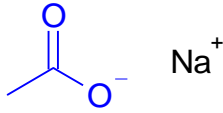
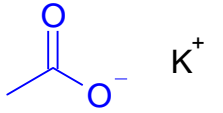
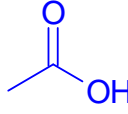
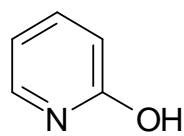
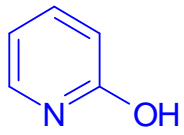
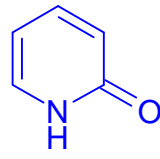
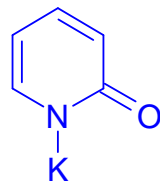
##### Description

A **Parent Exact Structure Search** (PXSS) finds molecule records in a database where the main component of your query is the main component of the hit. With this search you will retrieve (i) salts, (ii) complexes, (iii) identical structures or (iv) tautomeric structures.

Please note:

- If salt queries, consisting of more than one organic component are entered, only the largest (main) organic component is used for parent searching.
- In addition to parents all other salt forms of the main organic component will be found.
- Non-salt organic queries are allowed as well. All salt forms of the organic component will be retrieved (Reverse Parent Search).
- Stereochemistry will be ignored during the search.
- Isotopic labels will not be ignored.

##### Example

Query	Retrieved molecules	
		
		
		
		
		

#### 4.1.7 TXSS (Tautomer Exact Structure Search, Tautomer Search)

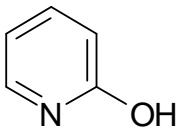
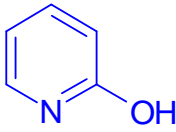
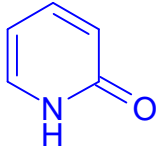
##### **Description**

A **Tautomer Exact Structure Search** (TXSS) finds all isomers, where hydrogens, radicals or metal atoms may be on variable positions, but where the  $\sigma$ -skeleton and the total number of hydrogen atoms must be identical after removing all bonds to metal atoms, all charges and all radical electrons.

Please note:

- Stereochemistry will be ignored during the search.
- Isotopic labels will not be ignored.

##### **Example**



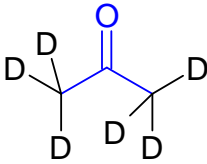
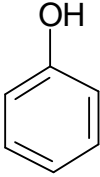
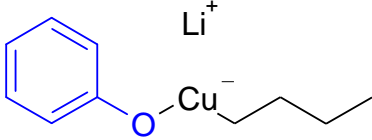
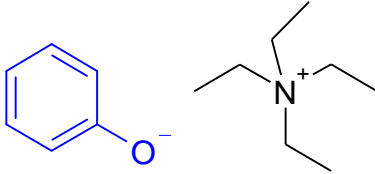
Query	Retrieved molecules
	
	

#### 4.1.8 FlexXSS (Flexible Exact Structure Search, Flex Match)

##### Description

A **Flexible Exact Structure Search** (FlexXSS) retrieves molecules from a database being (i) stereo isomers, (ii) isotopic isomers, (iii) parent substructures and salts, (iv) tautomers or (v) complexes containing the structure(s) you specified in your query as component(s).

##### Example

Query	Retrieved molecules
	
	
	
	

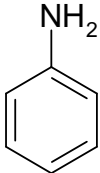
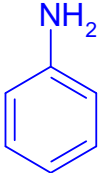
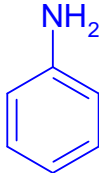


#### 4.1.9 CompXSS (Component Exact Structure Search)

##### *Description*

A **Component Exact Structure Search** (CompXSS) retrieves molecules from a database containing the structure you specified in your query as component.

##### *Example*

Query	Retrieved molecules
	
	ClH 

#### 4.1.10 XSFS (Exact Sum Formula Search)

##### **Description**

An **Exact Sum Formula Search** (XSFS) finds molecule records in a database that contain the formula that you specify in your query.

Your formula query can be:

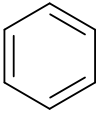
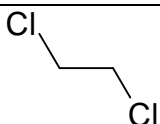
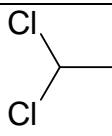
- An exact formula and no other atoms, such as C<sub>6</sub>H<sub>6</sub>O.
- An exact formula containing ranges and no other atoms, such as C(1-6)H(0-99)N(0-5).

Your query can include ranges of atom counts but must include all standard atom symbols, including hydrogens. You can use a single space to separate atoms, but atom symbols must always begin with a capital letter. Multiple occurrences of atom counts will be accumulated.

For example:

- To find phenol or isomers, enter: C<sub>6</sub>H<sub>6</sub>O or C<sub>6</sub>H<sub>5</sub>OH.
- To find ethanol or isomers, enter: C<sub>2</sub>H<sub>6</sub>O or CH<sub>3</sub>CH<sub>2</sub>OH.

##### **Example**

Query	Retrieved molecules
C(1-6)H(1-6)	
	CH <sub>4</sub>
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	
	

#### 4.1.11 SFS (Sum Formula Search)

##### **Description**

A **Sum Formula Search (SFS)** finds molecule records in a database that contain the formula that you specify in your query as sub formula.

Your formula query can be:


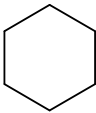
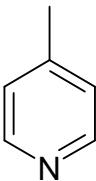
- A sub formula and any additional other atoms, such as C17NO3.
- A sub formula except specific atoms, such as C5N0, where N0 represents zero nitrogens.
- A sub formula containing ranges and any additional other atoms, such as C(1-6)N(0-5).

Your query can include a range of atom counts and typically excludes the hydrogens. You can use a single space to separate atoms, but atom symbols must always begin with a capital letter. Multiple occurrences of atom counts will be accumulated.

For example:

- To find mono sodium salts, enter Na.
- To find molecules that contain six carbons and any number of other atom types, enter: C6.
- To find molecules that contain one to six carbon atoms, zero to five nitrogen atoms and any additional other atom types, enter: C(1-6)N(0-5).

##### **Example**

Query	Retrieved molecules
Na	$\text{Na}^+ \text{OH}^-$
	$\text{Na}^+ \text{O}^-$ 
C6	
	

#### 4.1.12 ISSS Search (Inverse Molecule Substructure Search)

##### *Description*

An Inverse Molecule **S**ubstructure **S**earch (ISSS) finds molecule records in a database which are wholly within your larger query structure.

##### *Example*

Query	Retrieved molecules
 <chem>Cc1cc(C)c(C)n1</chem>	 <chem>Cc1cc(C)ncc1</chem>
	 <chem>c1ccncc1</chem>

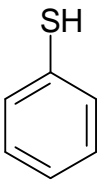
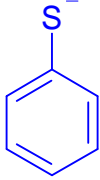
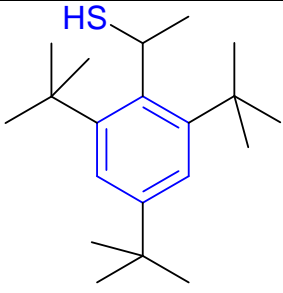
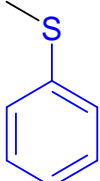
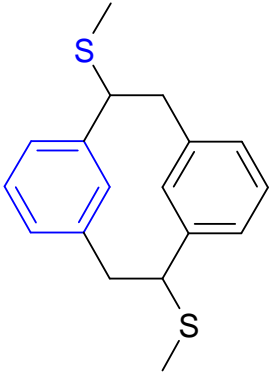
### 4.1.13 MSIMFP (Molecule Similarity Fingerprint Search, Similarity Search)

#### Description

The similarity search operator MSIMFP (**M**olecule **S**imilarity **F**ingerprint Search) finds molecule records in a database that are structurally similar to your query.<sup>1</sup> The desired similarity degree must be defined by a threshold in percent.

Please note: Only the relational operator greater than ('>') is supported for MSIMFP.

#### Example

Query	Retrieved molecules	% Similarity
		100
		80
		68,7
		60

<sup>1</sup> Tanimoto algorithm based on molecule fingerprints.

#### 4.1.14 SSA Search (Structure Search Automatic, All-In-One Structure Search)

##### *Description*

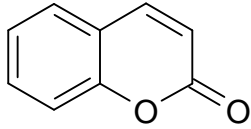
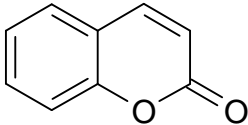
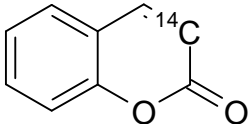
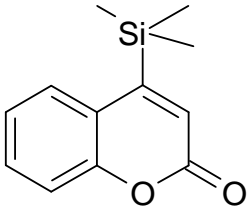
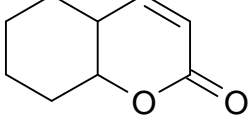
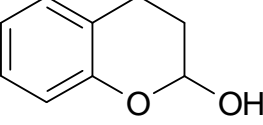
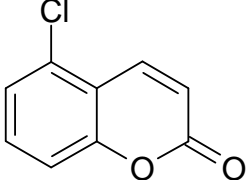
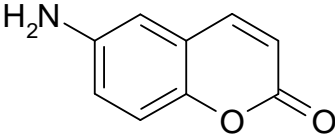
A **Structure Search Automatic (SSA)** finds molecule records in a database that match your query exactly (see 4.1.3: XSS, 4.1.5: IXSS, 4.1.7: TXSS, 4.1.6: PXSS, 4.1.8: FlexXSS) or contain your query as a substructure wholly within a larger structure (see 4.1.1: SSS) or are similar to your query (see 4.1.13: MSIMFP).

**New in V2.8:** Using query features is allowed and will retrieve SSS hits only.

The resulting hits are automatically rated and sorted by decreasing rating:

- XSS hits (rating 600.00)
- iXSS hits (rating 500.00)
- tXSS hits (rating 400.00)
- pXSS hits (rating 300.00)
- FlexXSS hits (rating 200.00)
- SSS hits (rating from 100.00 to 200.00)
- MSIMFP hits (rating from 0.00 to 100.00)

**Example**

Query	Retrieved molecules	Operator
		XSS
		IXSS
		PXSS
		FlexXSS
		FlexXSS
		SSS – 91.66%
	CIH 	SSS – 84.61%

Please note: The maximum number of retrieved hits as well as the percentage of the similarity threshold is adjustable.

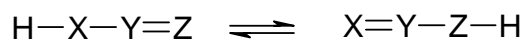
**New in V2.8:** Similarity threshold values 0 – 999 allowed. Can be used to suppress hits from searches with lower rating. E.g. setting a value of 200 will not retrieve SSS hits. Setting a value > 600 will retrieve XSS hits only.



#### 4.1.15 Examples for Structure Search Strategies

##### 4.1.15.1 Tautomer Search using SSS Query Features

You may find all tautomers of a structure by a substructure search using the combination of specific query features. A tautomeric group is defined as:



where

X = C, O, N, S, Se, Te

Y = C, I, P, As, Sb, Cl, Br

Z = O, N, S, Se, Te

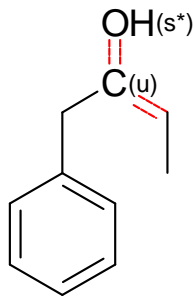
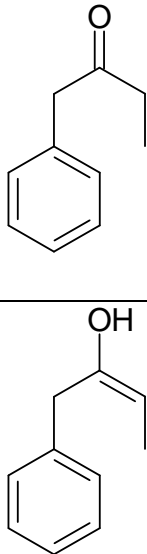
##### 4.1.15.1.1 Chain or Non-Aromatic Ring

The following query features have to be adjusted properly:

- All tautomer bonds ('X-Y', 'X-Z') have to be specified as 'SINGLE/DOUBLE' bonds.
- The 'Y' atom has to be assigned the query feature 'unsaturated atoms' to force a  $\pi$ -electron in this location.
- The atom 'Z' has to be assigned the query feature 'substitution as drawn' to avoid external neighbors in the hit structure.

Please note: Only prototropic tautomerism can be retrieved with this query search.

##### **Example: Keto-Enol-Tautomerism**

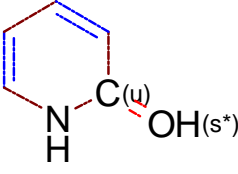
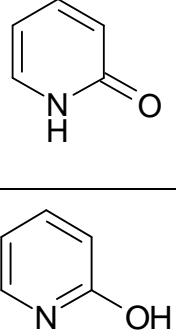
Query	Retrieved molecules
 <p>SINGLE/DOUBLE: red</p>	

#### 4.1.15.1.2 Aromatic Ring

If the tautomeric group is part of an aromatic system ALL bonds of the aromatic systems have to be adjusted as well:

- The tautomeric bond 'X-Y' should be converted to 'ANY' bond.
- The tautomeric bond 'Y-Z' should be converted to 'SINGLE/DOUBLE' bond.
- The 'Y' atom has to be assigned the query feature 'unsaturated atoms' to force a  $\pi$ -electron in this location.
- The atom 'Z' has to be assigned the query feature 'substitution as drawn' to avoid external neighbors in the hit structure.
- All other double bonds should be converted to 'DOUBLE/AROMATIC' bonds.
- All other single bonds should be converted to 'ANY' bonds.

#### Example: Amide-Imidic acid-Tautomerism

Query	Retrieved molecules
 <p>ANY: brown DOUBLE/AROMATIC: blue SINGLE/DOUBLE: red</p>	

## 4.2 Reaction Searches

### 4.2.1 RSS (Reaction Substructure Search)

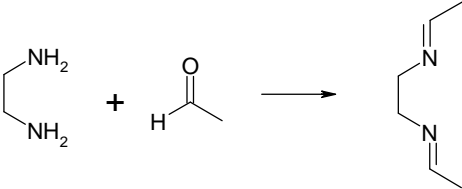
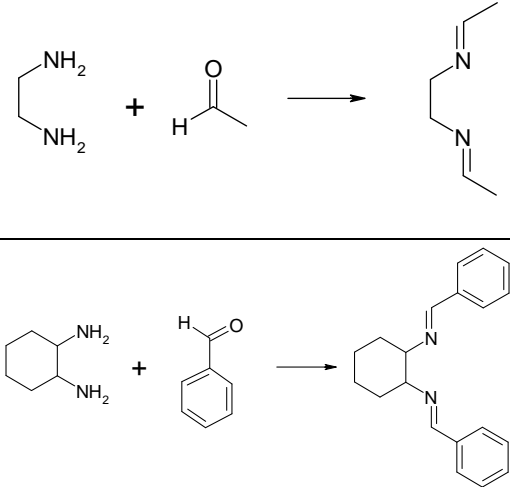
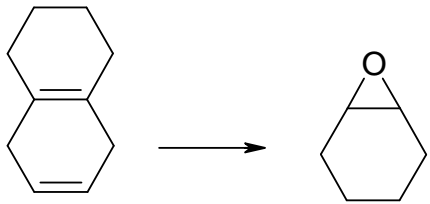
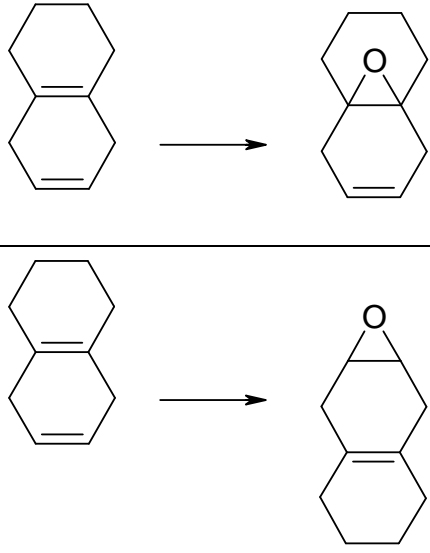
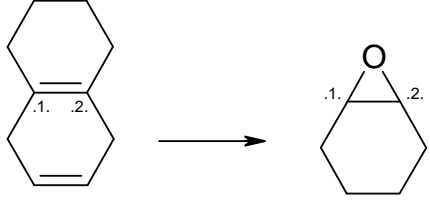
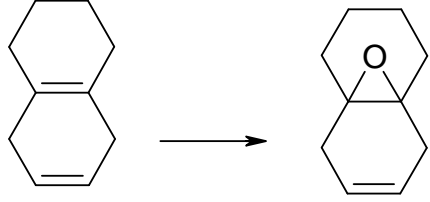
#### *Description*

A **R**eaction **S**ubstructure **S**earch (RSS) finds reaction records in a database that contain your query as a reaction substructure wholly within a larger reaction.

Please note:

- Only two-dimensional representations of reaction substructures are supported.
- You can also increase the power of an RSS search by the addition of specific restrictions (called query features) on atoms, bonds and reaction centers. Several different query features are available (see chapter 2 and chapter 3).
- An atom-atom map on the reaction components in a query specifies exactly which atoms in the reactants correspond to the atoms in the products.
- You can also add hydrogens with explicit bonds (called explicit hydrogens) to your query to block substituents on specific atoms.
- You can also search for an incomplete reaction, e.g. only the reactant or only the product is drawn, but always adding a reaction arrow left (for product search) or right (for reactant search) to the molecule.

**Example**

Query	Retrieved reactions
	
	
	

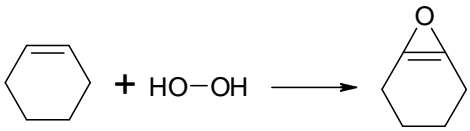
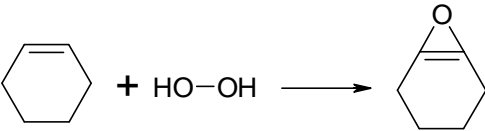
Please note: when using ChemDraw as query structure editor you may get hits for your query, where the first reactant was ignored during the RSS search.

#### 4.2.2 XRS (Exact Reaction Search)

##### *Description*

An **Exact Reaction Search (XRS)** finds reaction records in a database that match your reaction query exactly. For an exact match tetrahedral stereo information (i.e. R/S) and all isotopic labels must match. Any stereo information of your query will be treated as absolute, even without setting the chiral flag for the query structures.

##### *Example*

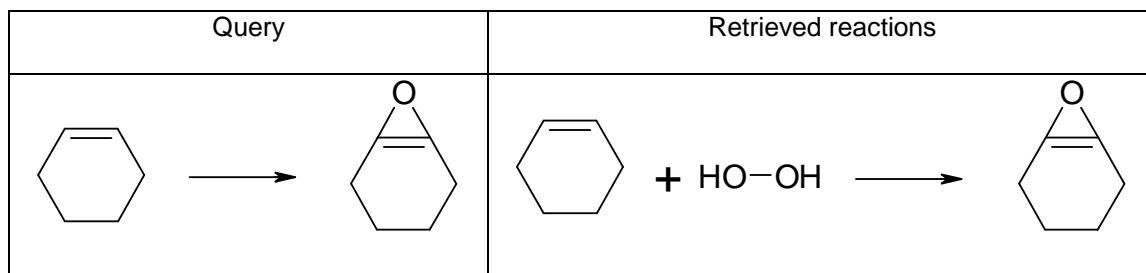
Query	Retrieved reactions
 <p>The query shows a cyclohexene molecule (a six-membered ring with one double bond) reacting with hydrogen peroxide (HO-OH) to form cyclohexane oxide (a six-membered ring with an epoxide group).</p>	 <p>The retrieved reaction is identical to the query, showing cyclohexene reacting with HO-OH to form cyclohexane oxide.</p>

### 4.2.3 XRSSUB (Contains Exact Reaction, Exact Subreaction Search)

#### *Description*

An **Exact Subreaction Search** (XRSSUB) finds always the reaction records in a database that match your reaction query exactly, but additional reactants and products may be found in the reaction records from the database.

#### *Example*



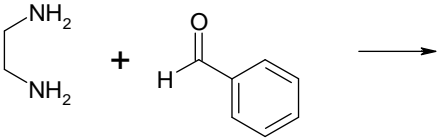
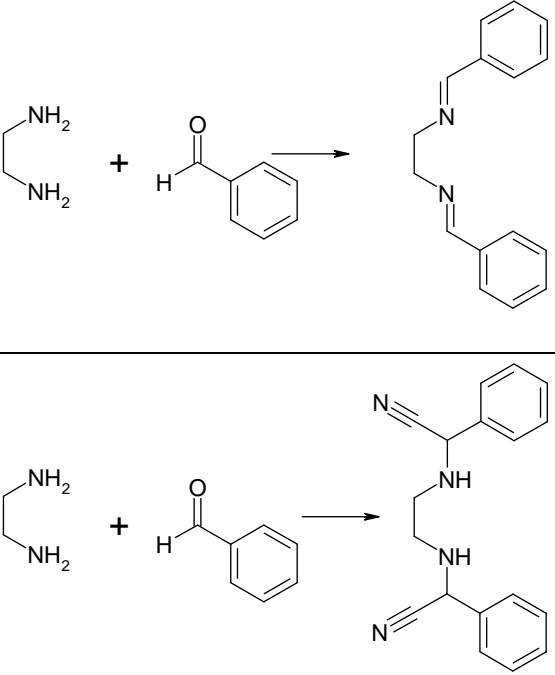
#### 4.2.4 XRSRCT (Contains Exact Reactants, Exact Reactant Reaction Search)

##### Description

An **Exact Reactant Reaction Search** (XRSRCT) search finds always the reaction records in a database that match the reactant or reactants in your reaction query exactly. Additional reactants may be found in the reaction records from the database. The query input must not contain any products.

See also chapter 4.2.16.1 'Role Searches'.

##### Example

Query	Retrieved reactions
	


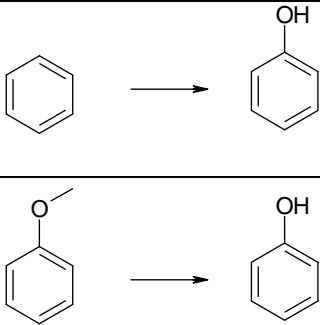
#### 4.2.5 XRSPRD (Contains Exact Products, Exact Product Reaction Search)

##### *Description*

An **Exact Product Reaction Search** (XRSPRD) search finds always the reaction records in a database that match the product or products in your reaction query exactly. Additional products may be found in the reaction records from the database. The query input must not contain any reactants.

See also chapter 4.2.16.1 'Role Searches'.

##### *Example*

Query	Retrieved reactions
	

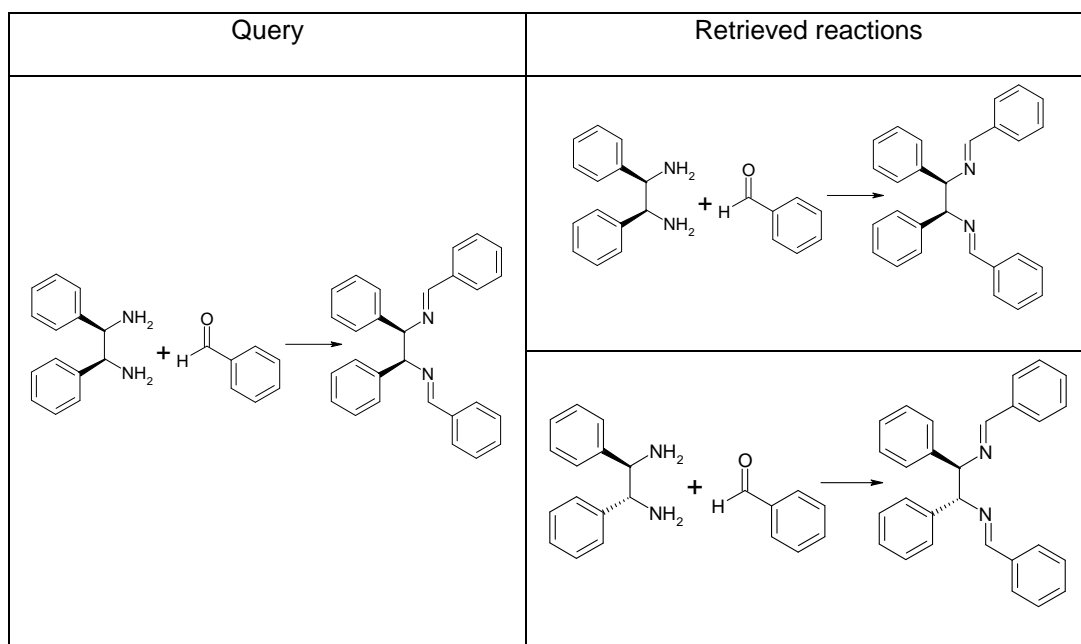


#### 4.2.6 IXRS (Isomer Exact Reaction Search)

##### Description

An **Isomer Exact Reaction Search (IXRS)** finds the reaction records in the database that are (i) geometric isomers, (ii) stereo isomers or (iii) isotopic isomers of your reaction query.

##### Example

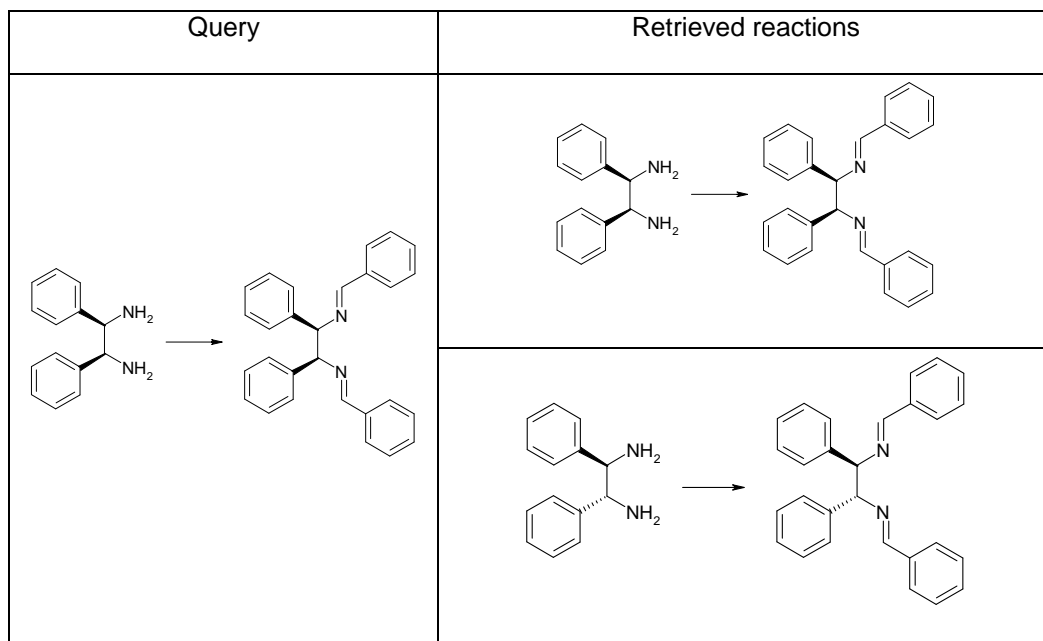


#### 4.2.7 IXRSSUB (Isomer Exact Subreaction Search)

##### Description

An **Isomer Exact Subreaction Search** (IXRSSUB) finds the reaction records in the database that are (i) geometric isomers, (ii) stereo isomers or (iii) isotopic isomers of your reaction query. Additional reactants and products may be found in the reaction records from the database.

##### Example

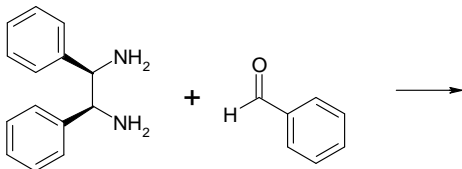
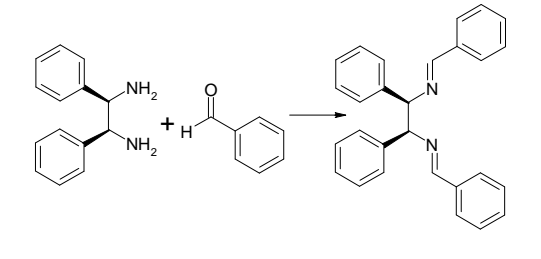
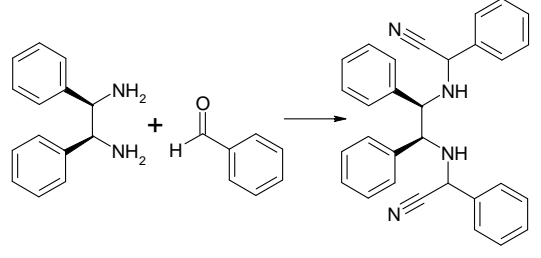
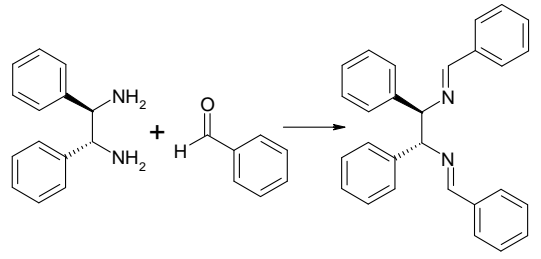


#### 4.2.8 IXRSRCT (Isomer Exact Reactant Reaction Search)

##### Description

An **Isomer Exact Reactant Reaction Search (IXRSRCT)** finds the reaction records in the database that are (i) geometric isomers, (ii) stereo isomers or (iii) isotopic isomers of the reactant or reactants in your reaction query. Additional reactants may be found in the reaction records from the database. The query input must not contain any products.

##### Example


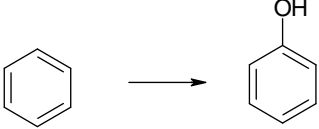
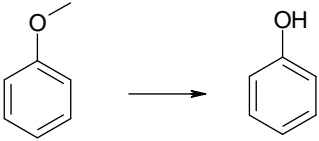
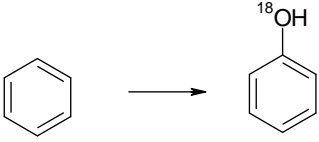
Query	Retrieved reactions
	
	
	

#### 4.2.9 IXRSPRD (Isomer Exact Product Reaction Search)

##### Description

An **Isomer Exact Product Reaction Search** (IXRSPRD) finds always the reaction records in the database that are (i) geometric isomers, (ii) stereo isomers or (iii) isotopic isomers of the product or products in your reaction query. Additional products may be found in the reaction records from the database. The query input must not contain any reactants.

##### Example

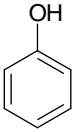
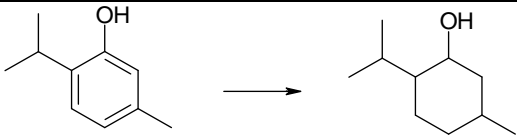
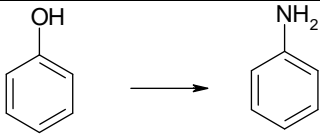
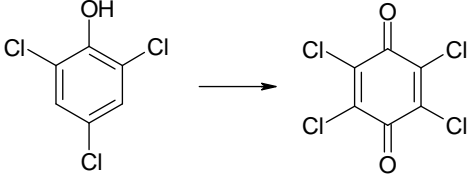
Query	Retrieved reactions
	
	
	

#### 4.2.10 RCTNOTPRD (Reactant NOT Product)

##### *Description*

A **Reactant NOT Product** search (RCTNOTPRD) finds reaction records in the database that contain your query structure as a substructure completely in one or more reactants of the reactions but not as a substructure in the products. The query input as reaction must not contain any products and must contain only one reactant. The query input can also be a single structure.

##### *Example*

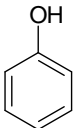
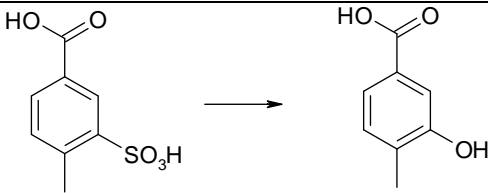
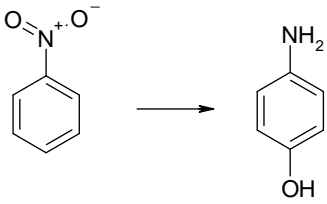
Query	Retrieved reactions
 <chem>Oc1ccccc1</chem>	 <chem>Cc1c(C)c(O)c(C)cc1 &gt;&gt; C1CC(C)C(O)CC1</chem>
	 <chem>Oc1ccccc1 &gt;&gt; Nc1ccccc1</chem>
	 <chem>Oc1c(Cl)c(Cl)cc(Cl)c1 &gt;&gt; ClC1=C(Cl)C(=O)C(Cl)=C1Cl</chem>

#### 4.2.11 PRDNOTRCT (Product NOT Reactant)

##### Description

A **Product NOT Reactant** search (PRDNOTRCT) finds reaction records in the database that contain your query structure as a substructure completely in one or more products of the reactions but not as a substructure in the reactants. The query input as reaction must not contain any reactants and must contain only one product. The query input can also be a single structure.

##### Example

Query	Retrieved reactions
	<div style="display: flex; flex-direction: column; align-items: center;"> <div style="display: flex; align-items: center; margin-bottom: 20px;">  </div> <div style="display: flex; align-items: center;">  </div> </div>

#### 4.2.12 RTS (Reaction Type Search, Similar Reaction Search)

For detailed information and examples please consult the 'CLASSIFY Documentation' (pdf-file) available on our web page ([www.infochem.de](http://www.infochem.de)).

##### 4.2.12.1 RTS\_BROAD (Reaction Type Search Broad)

###### **Description**

A **Reaction Type Search BROAD** (RTS\_BROAD) finds the reaction records in the database that match the BROAD (0-Sphere) reaction type of your reaction query.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

##### 4.2.12.2 RTS\_MEDIUM (Reaction Type Search Medium)

###### **Description**

A **Reaction Type Search MEDIUM** (RTS\_MEDIUM) finds the reaction records in the database that match the MEDIUM (1-Sphere) reaction type of your reaction query.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

##### 4.2.12.3 RTS\_NARROW (Reaction Type Search Narrow)

###### **Description**

A **Reaction Type Search NARROW** (RTS\_NARROW) finds the reaction records in the database that match the NARROW (2-Sphere) reaction type of your reaction query.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

## 4.2.12.4 RTS\_ALL

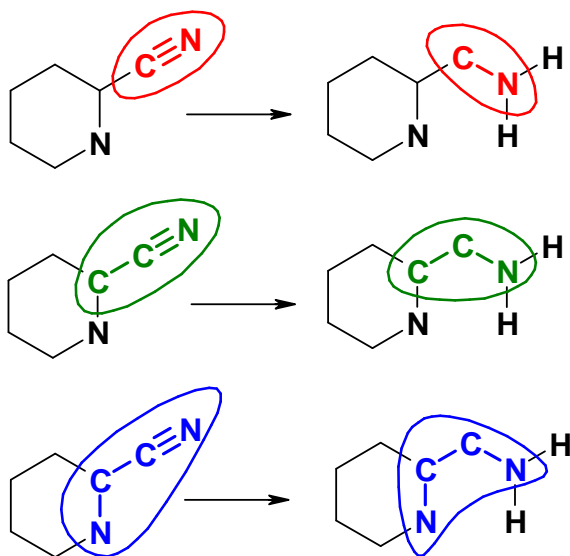
**Description**

A Reaction Type Search ALL (RTS\_ALL) finds the reaction records in the database that match the NARROW, MEDIUM and BROAD reaction type of your reaction query. The hits of the NARROW search will be displayed first, the hits of the BROAD search at last.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

## 4.2.12.5 RTS: Example

**Broad**

Reaction centers only, similar to broadly based substructure search

*large-sized hitlist*

**Medium**

Reaction centers plus alpha atoms, excluding hydrogens

*medium-sized hitlist*

**Narrow**

Reaction centers plus beta atoms, excluding consecutive sp<sup>3</sup>-atoms

*small-sized hitlist*

Further examples and detailed information can be found in the 'CLASSIFY Documentation' on our web page ([www.infochem.de](http://www.infochem.de)).



#### 4.2.13 RXCCluster Search (Reaction Center Cluster Search, Center Cluster Search)

For detailed information and examples please consult the 'CLASSIFY Documentation' (pdf-file) available on our web page ([www.infochem.de](http://www.infochem.de)).

##### 4.2.13.1 RXCCluster\_BROAD

###### **Description**

A Reaction **C**enter **C**luster Search BROAD (RXCCluster\_BROAD) finds the reaction records in the database that contain all BROAD (0-Sphere) reaction center clusters of your reaction query completely or as a subset.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

##### 4.2.13.2 RXCCluster\_MEDIUM

###### **Description**

A Reaction **C**enter **C**luster Search MEDIUM (RXCCluster\_MEDIUM) finds the reaction records in the database that contain all MEDIUM (1-Sphere) reaction center clusters of your reaction query completely or as a subset.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

##### 4.2.13.3 RXCCluster\_NARROW

###### **Description**

A Reaction **C**enter **C**luster Search NARROW (RXCCluster\_NARROW) finds the reaction records in the database that contain all NARROW (2-Sphere) reaction center clusters of your reaction query completely or as a subset.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

#### 4.2.13.4 RXCCluster: Example

Examples and detailed information can be found in the 'CLASSIFY Documentation' on our web page ([www.infochem.de](http://www.infochem.de)).

#### 4.2.14 RSS\_RT (Combined RSS/RTS Search)

For detailed information and examples on Reaction Type Searches please consult the 'CLASSIFY Documentation' (pdf-file) available on our web page ([www.infochem.de](http://www.infochem.de)).

##### 4.2.14.1 RSS\_RT\_BROAD

###### **Description**

A Combined **R**eaction **S**ubstructure **S**earch - **R**eaction **T**ype **S**earch BROAD (RSS\_RT\_BROAD) finds the reaction records in the database that match the BROAD (0-Sphere) reaction type of your reaction query and additionally contain your query as a reaction substructure wholly within a larger reaction.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

##### 4.2.14.2 RSS\_RT\_MEDIUM

###### **Description**

A Combined **R**eaction **S**ubstructure **S**earch - **R**eaction **T**ype **S**earch MEDIUM (RSS\_RT\_MEDIUM) finds the reaction records in the database that match the MEDIUM (1-Sphere) reaction type of your reaction query and additionally contain your query as a reaction substructure wholly within a larger reaction.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

##### 4.2.14.3 RSS\_RT\_NARROW

###### **Description**

A Combined **R**eaction **S**ubstructure **S**earch - **R**eaction **T**ype **S**earch NARROW (RSS\_RT\_NARROW) finds the reaction records in the database that match the NARROW (2-Sphere) reaction type of your reaction query and additionally contain your query as a reaction substructure wholly within a larger reaction.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

#### 4.2.14.4 RSS\_RT\_ALL

##### **Description**

A Combined **R**eaction **S**ubstructure **S**earch - **R**eaction **T**ype **S**earch ALL (RSS\_RT\_ALL) finds the reaction records in the database that match the NARROW, MEDIUM and BROAD reaction type of your reaction query and additionally contain your query as a reaction substructure wholly within a larger reaction. The hits of the NARROW search will be displayed first, the hits of the BROAD search at last.

Please note:

- The query input must contain at least one reactant and one product and must not contain more than one product.
- Query features are not allowed for atoms or bonds of the molecules.

#### 4.2.14.5 RSS\_RT: Example

Examples and detailed information on Reaction Type Searches can be found in the 'CLASSIFY Documentation' on our web page ([www.infochem.de](http://www.infochem.de)).

#### 4.2.15 RSA Search (Reaction Search Automatic, All-In-One Reaction Search)

##### **Description**

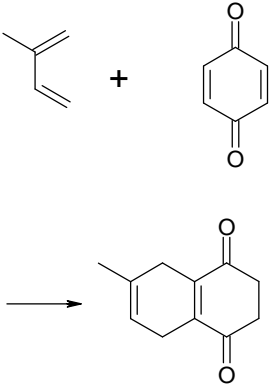
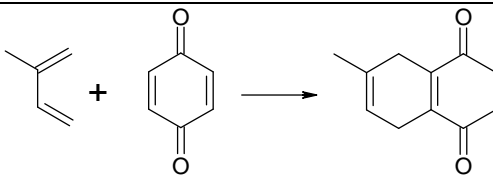
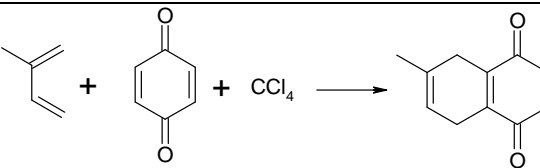
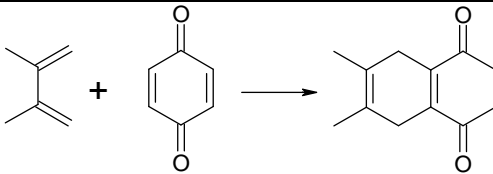
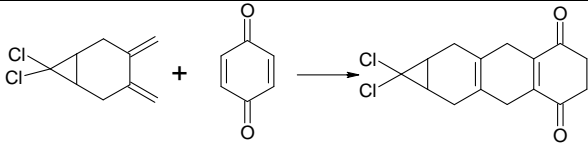
An **Automatic Reaction Search (RSA)** finds reaction records in your database that (i) match your query exactly (see 4.2.2: XRS, 4.2.6: IXRS, 4.2.3: XRSSUB, 4.2.7: IXRSSUB), (ii) match the reaction type of your reaction query and additionally contain your query as a reaction substructure wholly within a larger reaction (see 4.2.14: RSS\_RT), (iii) match the reaction type of your reaction query only (see 4.2.10: RTS) or contain all reaction center clusters of your reaction query completely or as a subset (see 4.2.13: RXCCLUSTER).

**New in V2.8:** Using query features is allowed and will retrieve RSS hits only. Queries containing only products or reactants will retrieve RSS hits only.

The resulting hits are automatically rated by similarity of the query product and the target product and sorted by decreasing rating:

- XRS hits (rating 600.00)
- iXRS hits (rating 500.00)
- XRSSUB hits (rating 420.00)
- IXRSSUB hits (rating 410.00)
- RSS\_RT NARROW hits (rating 330.00 – 331.00)
- RSS\_RT MEDIUM hits (rating 320.00 – 321.00)
- RSS\_RT BROAD hits (rating 310.00 – 311.00)
- RTS NARROW hits (rating 230.00 – 231.00)
- RTS MEDIUM hits (rating 220.00 – 221.00)
- RTS BROAD hits (rating 210.00 – 211.00)
- RXCCLUSTER NARROW hits (rating 130.00 – 131.00)
- RXCCLUSTER MEDIUM hits (rating 120.00 – 121.00)
- RXCCLUSTER BROAD hits (rating 110.00 – 111.00)
- **New in V2.8:** RSS hits (rating 0.00 – 100.00), only if no other search retrieves hits.

**Example**

Query	Retrieved molecules	Operator
		XRS
		XRSSUB
		RSS_RT
		RSS_RT

Please note: The maximum number of retrieved hits is adjustable.

## 4.2.16 Examples for Reaction Search Strategies

### 4.2.16.1 Role Searches

A role search should find your query as a substructure (or as exact structure) in a reaction, where the structure acts as reactant, catalyst, solvent or product according to the role you want to retrieve.

#### **Reactants and Products:**

- As substructure: use RSS (see 4.2.1) and place the reaction arrow accordingly to define the role of the molecule as reactant or as product.
- Exact structure: use the operators XRSRCT and XRSPRD (see chapter 4.2.4 and chapter 4.2.9)

#### **Catalysts and Solvents:**

Please note: in the ICCartridge/ICFSE there is no specific search operator available. Preconditions for role searches for catalysts and solvents are:

- Separate tables for catalysts and solvents in the database structure.
- Implementation of search options 'as catalyst' and 'as product' in the query specification.

For instance InfoChem's web application for MRW offers the search options for catalysts and solvents.

In the ICCartridge environment the role search has to be implemented by a logical combination in the 'where' clause of the 'select' statement on a 'reaction table' and a 'catalyst/solvent table' described above.

- As substructure: use SSS (see 4.1.1) as search operator for your query.
- Exact structure: use XSS (see 4.1.3) as search operator for your query.

### 4.3 Sorting of Hits

The hits retrieved by a query may be sorted by similarity of query and target

#### 4.3.1 Structure Searches

Setting the option SORT\_HITS to YES will sort the hits in the resulting hitlist in descending order of similarity (i.e. mass quotient) of query structure and target. If no query mass is available (e.g. for a query with ANY atoms) the similarity is calculated as quotient of the number of non-hydrogen atoms of query and target.

#### 4.3.2 Reaction Searches

Setting the option SORT\_HITS to YES will sort the hits in the resulting hitlist in descending order of similarity of the query product and the target product. The similarity is calculated as quotient of the number of non-hydrogen atoms of the query product and the target product. When a reaction query has been performed without a query product, the similarity will be 0 and no sorting will be performed.



## 5. Storing and Retrieving Structures in Your Database

When the normalization option has been set for your database, all structures will be automatically normalized during creation of the ICFSE search indices used for retrieving the database hits.

Please see the following table to find out the normalized representation for your structure.

For detailed information and examples please consult the 'Standardization Rules' (pdf-file) available on our web page ([www.infochem.de](http://www.infochem.de)).

### 5.1 General Rules for Bonding of Atoms in Organic Structures

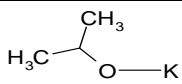
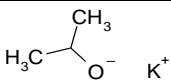
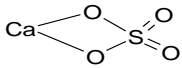
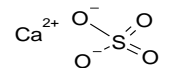


	Group Ia Alkali metals	Group IIa Alkali earth metals	Transition metals and lanthanides, actinides)	Main group elements	Oxygen	Halogens
Group Ia Alkali metals	Covalent	Covalent	Covalent	Covalent	Ionic	Ionic
Group IIa Alkali earth metals	Covalent	Covalent	Covalent	Covalent Exception: bonds between IIa and carbanions of alkenes or alkynes are ionic	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	Covalent
Transition metals (and lanthanides, actinides)	Covalent	Covalent	Covalent	No general rule defined	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	Covalent
Main group elements	Covalent	Covalent Exception: bonds between IIa and carbanions of alkenes or alkynes are ionic	No general rule defined	Covalent	Covalent	Covalent
Oxygen	Ionic	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	Covalent Exception: when a negatively-charged Q=Q-O substructure exist draw ionic	Covalent	Covalent	Covalent
Halogens	Ionic	Covalent	Covalent	Covalent	Covalent	Covalent

## 5.2 Standardization Rules of Functional Groups

### 5.2.1 Separation of Covalent Structures Into Ionic Components

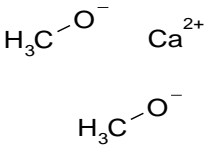
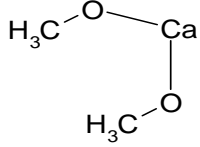
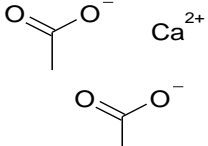
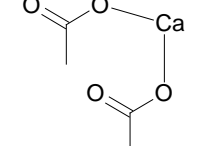
Automatically normalized structures are represented using the standard general rules described in table 5.1.

Therefore some structures drawn covalent will be separated into ionic components, e.g:

Example	Original representation	Normalized representation
Alkali Alcoholates		
Complex ions and Q=Q-O <sup>i</sup> substructures		
Carbon to group IIa		

### 5.2.2 Connecting Ionic Components

On the other hand structures drawn ionic will be converted into covalent structures:

Example	Original representation	Normalized representation
		
		

### 5.2.3 Removing Charge Separations

Charge separations ("Zwitter ions") will be removed:

Example	Original representation	Normalized representation
4-bonded P-Atoms		
3-bonded S-Atoms		
5-bonded S-Atoms		

### 5.2.4 Radicals

$\pi$ -systems represented by radicals will be converted into alternating double bonds:

Original representation	Normalized representation

### 5.2.5 Standardization of Functional Groups

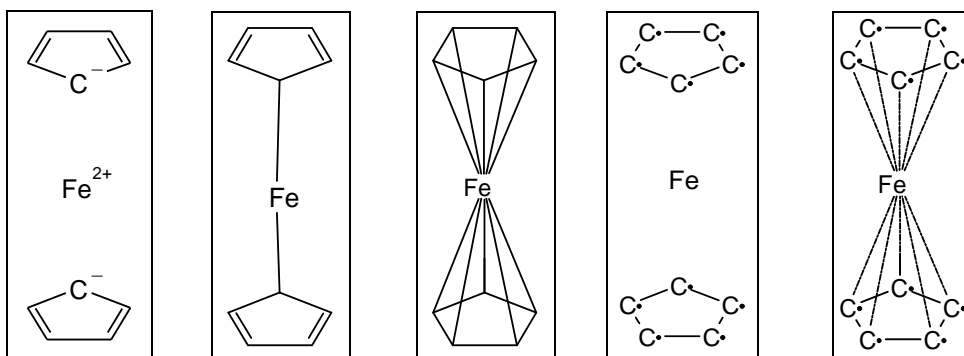
Additionally atoms in an unusual valence state or unusual representations of functional groups will be converted into a normalized representation.

Functional Group	Original Representation	Normalized Representation
5-bonded N-Atoms		
e.g. nitro group		
5-bonded N-Atoms		
5-bonded N-Atoms		
5-bonded N-Atoms		
Enolate group		
Thio-enolate group		
Diazo group		

Diazonium salt		
Azide	$R-N^--N^+=N$	$R-N=N^+=N^-$
Azide	$R-N=N=N$	$R-N=N^+=N^-$
Carbon monoxide	$C^+=O^-$	$C^-=O^+$

### 5.2.6 Special Molecules With Alternative Representations

In the course of time several methods have been used to represent complexes and organometallics, e.g. ferrocene. There are no general rules for normalization defined:



## 5.3 Generic Structures

### IMPORTANT!

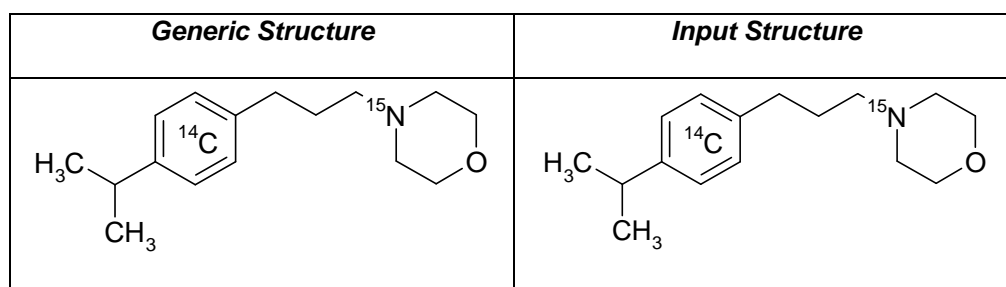
This functionality is only available if the search indices of your database have been created as generic and after installing the InfoChem Client or Middle Ware Component (coming soon) for preparing extended structure representation before importing into the database. Currently this functionality is only available as ISIS/Draw Addin for special user interfaces.

### 5.3.1 Isotopes at Unspecified Positions in Rings

#### Description

To define isotopes at unspecified positions in a ring, draw a single atom and its corresponding mass WITHIN the ring. This mass will be assigned to all atoms of the same type in the smallest ring surrounding the isotope.

#### Example

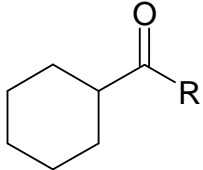
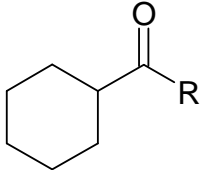
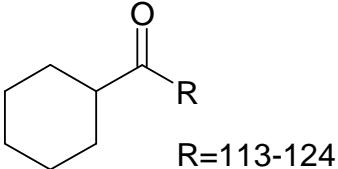
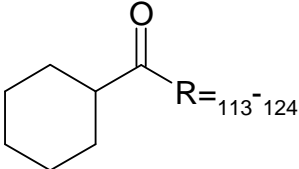


### 5.3.2 Substituents with Unknown Structure

#### Description

To draw unspecified substituents, use the atom type R. You may assign a range for the mass (if known) by typing the range in the text field of the R atom.

#### Examples

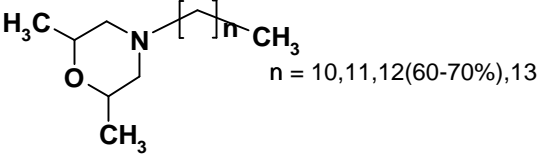
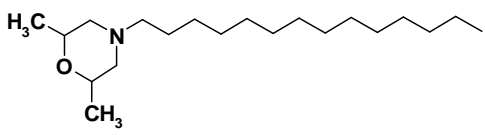
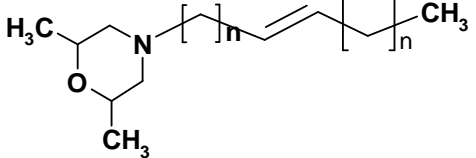
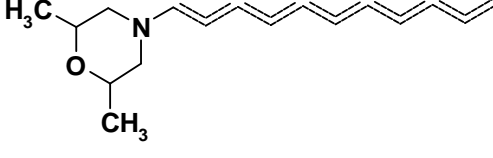
Generic Structure	Input Structure
	
	

### 5.3.3 Variable Side Chains

#### Description

Resolve all brackets and additional explaining text to evaluate the longest chain possible. If this chain shall contain double bonds with unlocalized positions, assign the bond type 'SINGLE/DOUBLE' to all bonds of this chain.

#### Examples

Generic Structure	Input Structure
	
	

### 5.3.4 Substituents with Unspecified Position in Rings and Chains

#### Description

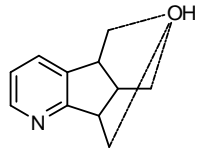
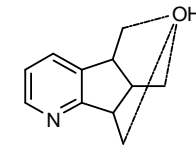
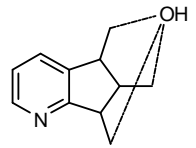
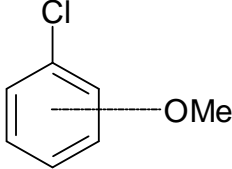
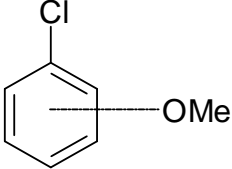
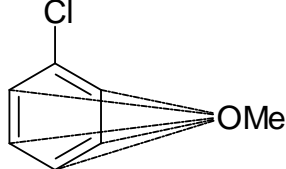
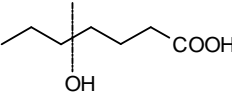
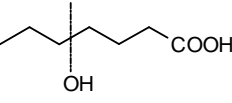
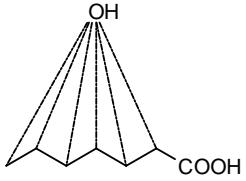
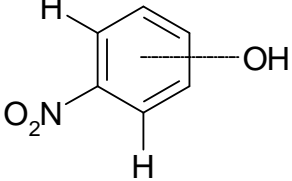
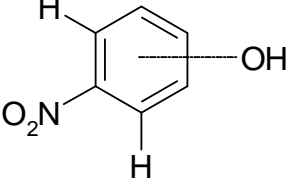
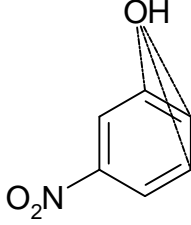
To assign more than one possible position for one substituent, draw a bond from the substituent to each possible position and assign these bonds the bond type 'ANY'.

If the position of the substituent in a ring is not specified, draw a bond with bond type 'ANY' from the substituent to the middle of the ring.

If the position of the substituent in a chain is not specified, draw a bond with bond type 'ANY' from the substituent crossing the chain.

To exclude specific positions among several possible positions, block these positions by adding explicit hydrogens.

#### Examples

Generic Structure	Input Structure	Database Representation <sup>1</sup>
		
		
		
		

<sup>1</sup> The database representation will be generated automatically by the registration software.

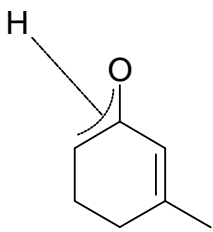
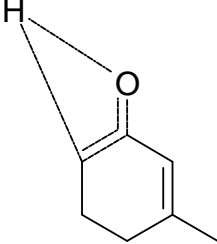
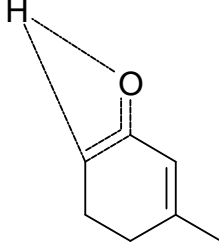


### 5.3.5 Tautomers

#### Description

To draw a mixture of tautomers, select the hydrogen and draw it as substituent with unspecified position (draw 'ANY' bonds from the hydrogen to all possible positions). In addition assign the bond type 'SINGLE/DOUBLE' to all bonds of the  $\sigma$ -skeletal structure.

#### Example

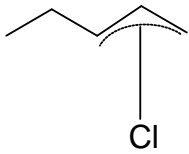
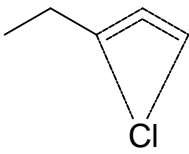
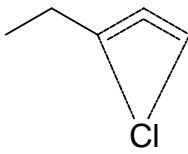
Generic Structure	Input Structure	Database Representation <sup>1</sup>
		

### 5.3.6 Pseudotautomers

#### Description

To draw a mixture of pseudotautomers, select the atom with variable position and draw it as substituent with unspecified position (draw 'ANY' bonds from this atom to all possible positions). In addition assign the bond type 'SINGLE/DOUBLE' to all bonds of the  $\sigma$ -skeletal structure.

#### Example

Generic Structure	Input Structure	Database Representation <sup>2</sup>
		

<sup>1</sup> The registration software will not modify the input structure.

<sup>2</sup> The input structure will not be modified by the registration software.

## 6. Advanced Stereochemistry

IMPORTANT!

This functionality is only available after installing the InfoChem Client or Middle Ware Component (coming soon) for preparing extended structure representation before importing into the database. Currently this functionality is only available as ISIS/Draw Addin for special User Interfaces.

### 6.1 Stereochemical Centers

#### *Description*

Instead of using the chiral flag to specify absolute stereochemistry for a whole molecule, you may specify absolute and relative stereochemistry for single atoms in one molecule.

Select the stereochemical center and add an asterisk (for use in InfoChem's editor ICEDIT, ISIS/Draw or ChemDraw) to the atom symbol to assign absolute stereochemistry.

Use this procedure for absolute stereochemistry only at the following atom types:

C, N, Si, P, S, Ge, As, Sb, B, Sn.

#### *Examples*

'C\*', 'N\*', 'N+\*

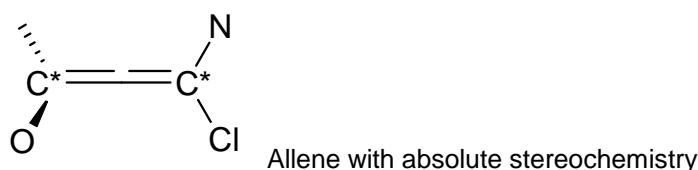
## 6.2 Configuration at Double Bonds

### Description

E or Z configurations are assigned automatically to all double bonds (and higher homologues with odd numbered cumulated double bonds) following the CIP rules.

Configurations at allenes are assigned by specifying UP/DOWN bond at one end of the double bonds. Use an asterisk (for use in InfoChem's editor *ICEDIT*, *ISIS/Draw* or *ChemDraw*) in the atom label additionally to the atom symbol to specify absolute stereochemical configuration.

Please note that wedged bonds have to be drawn in pairs.



For unknown stereochemistry at double bonds, this bond has to be marked explicitly by assigning the bond type 'DOUBLE/EITHER' or by drawing connecting a ligand with an 'EITHER' bond ('WAVY' bond).

### Example

<i>Display Structure</i>	<i>Input Structure</i>	<i>Database Representation<sup>1</sup></i>
	<p>or</p>	

<sup>1</sup> The database representation will be generated automatically by the registration software.