InfoChem

Manual

Structure and Reaction Editor

JavaScript Version 3.2

Autumn 2019

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1 Introduction

InfoChem's IC*EDIT* JavaScript editor is an HTML 5 based structure and reaction editor developed for common browsers. Of course, the IC*EDIT* JavaScript version supports all features known by the IC*EDIT* applet and needed by a chemical query editor for structures and reactions.
In addition to the classic IC*EDIT* JavaScript version an enhanced IC*EDIT* JavaScript editor is available based on InfoChem's ICNative / NameToStructure webservices covering additional advanced features like resolution of superatoms, "Convert Name to Structure" functionality, standardization of molecules and others (please see table below).

IC*EDIT* is also available as Windows application and as applet for all platforms supporting Java.
The IC*EDIT* Windows application offers full editing functionalities (chemical as well as display functionalities). The Windows version is a registered OLE-Server and therefore, it allows the integration in MS Office (Word, Excel, Access and PowerPoint) and in any other OLE-Client.

Support of	IC*EDIT* JavaScript editor	Enhanced IC*EDIT* JavaScript editor	IC*EDIT* application
Drawing of structures, reactions and fragments	+	+	+
Atom query features	+	+	+
Bond query features	+	+	+
Reaction query features	+	+	+
R-group query features	+	+	+
Integration in web applications	+	+	-
Superatoms	-	+[1)]	+
Calculation of molecule values, InChIs, InChIKeys and SMILES	-	-	+
Display features	+	+	+
OLE functionalities (MS Office integration)	-	-	+
Automap function	-	+[1)]	+
Standardization of molecules/reactions	-	+[1)]	+
Convert Name to Structure	-	+[1) 2)]	-
Add Hydrogen(s)	-	+[1)]	+

1) Availability is dependent on the licensed options. Please contact us for further licensing information (iceditsupport@infochem.de).

2) NameToStructure webservice and a relational database is required.

2 General Information

This documentation comprises the complete functionality for the IC*EDIT* JavaScript editor including additional properties available by the enhanced IC*EDIT* JavaScript editor like superatoms, “Convert Name to Structure” option and others. Due to licensed options or settings in the IC*EDIT* configuration file your actual IC*EDIT* JavaScript editor may differ from the information given below.

Appearance: Depending on the used configuration of the individual IC*EDIT* JavaScript installation some of the buttons may be hidden or appear in changed order.

Functionality: Depending on the individual configuration for a specific web page, some features may not be available in the IC*EDIT* editor (please refer to the technical documentation for details on the configuration options).

2.1 Toolbars

The JavaScript version of IC*EDIT* has two toolbars. The upper one represents the main toolbar whereas the lower one represents the sub-toolbar.

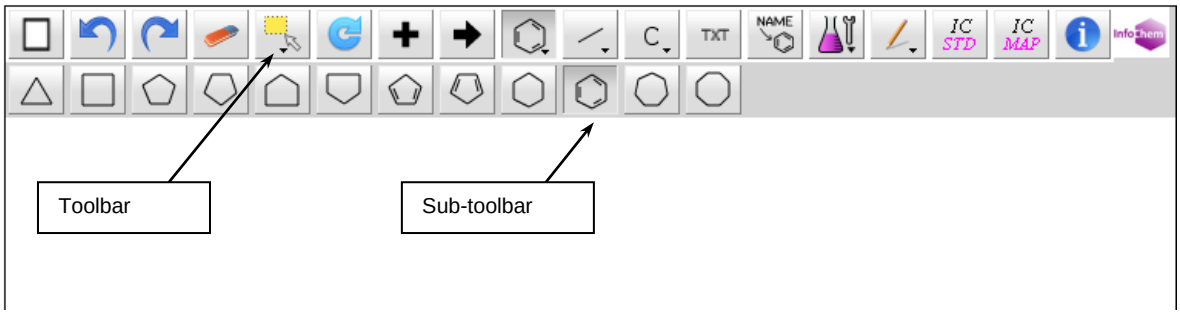


Fig. 1: IC*EDIT* toolbars.

The buttons displayed in the sub-toolbar depend on the selected button of the main toolbar. The buttons from the sub-toolbar show further functionality belonging to the selected main button.

For example the template button  opens the following sub-toolbar:

For a detailed description of the buttons please see chapter 3.

2.2 Context Menus

Context menus are available by right clicking (i) on the drawing area, (ii) on specific bonds, (iii) on specific atoms or (iv) on selected objects. The following features are available within the context menu:

- **Edit:** Opens the “Edit Bond Properties” or “Edit Atom Properties” dialog window. The currently selected atom(s) or bond(s) can now be edited.
- **Copy:** Copies the selected object(s) (into an internal buffer).
- **Paste:** Pastes the selected object(s) (from an internal buffer).
- **Duplicate Object(s):** Duplicates the selected object(s).
- **Delete:** Deletes the currently selected atom(s), bond(s) or object(s) (keyboard shortcut: DEL).
- **Create Chiral Flag:** Creates a chiral flag on the selected molecule(s). Please refer to chapter 4.7 for further details.
- **Group:** Merges multiple selected chemical objects.
- **Ungroup:** Ungroups a selected group of chemical objects.
- **Create Superatom:** Creates a superatom. Please refer to chapter **Fehler! Verweisquelle konnte nicht gefunden werden.** for further details on self-defined superatoms.
- **Expand Superatom:** Expands a selected superatom.
- **Contract Superatom:** Contracts a selected superatom.
- **Add Hydrogen(s):** Fills all atom free sites with explicit hydrogen(s), i.e. additional explicit bond(s) and H atom(s) will be created, which may result in a different hit list when used as substructure query. Please refer to chapter 4.10 for further details.
- **Align:** Aligns the selected objects. Please refer to chapter 4.14 for further details on Alignment.
- **Color:** Provides the opportunity to change the color of the selected object(s).
- **Create No-Structure:** Opens the “No-Structure Properties” dialog window to create a No-Structure label. Please refer to chapter 4.9 for further details on No-Structures.
- **Grid:** Enables or disables grid view of the drawing area.
- **Convert Name to Structure:** Opens the “Convert Name to Structure” dialog window to enter a name to be converted into a structure. Please refer to chapter 4.11 for further details.

Please note: The three methods “Copy”, “Paste” and “Duplicate Object(s)” work only internally within IC*EDIT*. Therefore, you cannot copy/paste from/into other Windows applications via the clipboard.

2.3 Keyboard Shortcuts

The following keyboard shortcuts are supported by the IC*EDIT* JavaScript editor:

- **Ctrl+A**: Selects all objects within the drawing area.
- **Ctrl+C:** Copies the selected object(s) (into an internal buffer).
- **Ctrl+V:** Pastes the selected object(s) (from an internal buffer).
- **Ctrl+Z**: Undoes the last operation.
- **Ctrl+Y**: Redoes the last undone operation.
- **DEL**: Deletes the currently selected atom(s), bond(s) or object(s).

Please note: The three methods “Copy” (Ctrl+C), “Paste” (Ctrl+V) and “Duplicate Object(s)” (Ctrl+D) work only internally within IC*EDIT*. Therefore, you cannot copy/paste from/into other Windows applications via the clipboard.

3 Buttons

Various edit and template buttons are provided in the ICEDIT toolbars. The selected edit or template button is highlighted.

Selected molecule, atom or bond templates can be used to draw the particular object into the drawing area by mouse click. Selected edit buttons can be used to carry out the particular operation.
Please find below a detailed description of all template and edit buttons.

Please note: Depending on the used configuration of the individual ICEDIT JavaScript installation some of the buttons may be hidden or appear in changed order.

3.1 Buttons from Main Toolbar

 Clear screen.
Deletes all objects from the drawing area.

 Undo.
Undoes the last operation (keyboard shortcut: CTRL + Z).

 Redo.
Redoes the last undone operation (keyboard shortcut: CTRL + Y).

 Delete object.
The object(s) (atom, bond, molecule, text) you are selecting with the selection rectangle will be deleted (keyboard shortcut: DEL).

 Select.
The “Select” sub-toolbar contains two select buttons:

For a detailed description see chapter 3.2.1.

 Rotate.

Use this tool to rotate the selected object(s) either clockwise or anti-clockwise.

 Reaction plus.

Adds a reaction plus to the drawing area.

 Reaction arrow.

Adds a reaction arrow to the drawing area.

Please note: Only one arrow per reaction is supported.

 Draw template.

The “Draw template” sub-toolbar consists of the following template buttons:

For a detailed description see chapter 3.2.2.

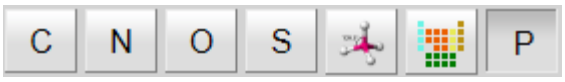
 Draw bond.

The “Draw bond” sub-toolbar contains various standard bond buttons and the “Bond properties” button:

For a detailed description see chapter 3.2.3.

 Draw atom.

The “Draw atom” sub-toolbar contains four atom buttons (configurable), the “Atom properties” button, the “Periodic Table” button and one atom button which shows the last selected atom from the periodic table (here: P-atom).



For a detailed description see chapter 3.2.4.

Draw text.

Activates the text input cursor within the drawing area at the selected position. Please refer to chapter 4.5 for further information.

Name to Structure.

Generates a structure from an entered chemical name. Please refer to chapter 4.11 for further information.


Enhanced chemical functionality.

The “Enhanced chemical functionality” sub-toolbar consists of two Rgroup buttons, two mapping buttons and the “Draw bracket” button.

For a detailed description see chapter 3.2.5.


Draw graphical objects.

Currently, the “Draw graphical objects” sub-toolbar has only one option:


Draw a line.

Standardize the structure.

Standardizes the selected molecule or reaction in accordance with InfoChem’s standardization rules. Please refer to chapter 4.13 for further information.

Automap the reaction.

Mapping numbers and reaction center information will be added automatically to a drawn reaction. Please refer to chapter 4.12 for further information.


Info.

Shows information about IC*EDIT* JavaScript editor and provides a link to open the IC*EDIT* JavaScript manual.

3.2 Buttons from Sub-toolbars

3.2.1 Select Buttons

The “Select” sub-toolbar contains two select buttons:

 Select.

Use this tool either to select a single object or a group of objects in a rectangle. The selected object(s) can then be moved, deleted, copied or edited using the context menu or keyboard shortcuts.

 Select object.

Use this tool to select whole objects at once. Click on a specific object as soon as it is marked by a red frame to select the complete object. The selected object(s) can then be moved, deleted, copied or edited using the context menu or keyboard shortcuts.

3.2.2 Molecule Template Buttons

The IC*EDIT* JavaScript editor provides various structure templates via the molecule template sub-toolbar:

Click in the drawing area to transfer the selected template. By clicking on the desired attachment point at an already existing structure within the drawing area, the template will be connected at the chosen attachment point.

3.2.3 Bond Buttons

The “Draw bond” sub-toolbar contains various standard bond buttons and the “Bond properties” button:

 Draw single bonds or change existent bonds.

Adds a single bond. Either click (i) on a free spot within the drawing area, (ii) on an existing atom or (iii) drag a bond between two atoms. With additional clicks on a single bond, you can convert it into:

(i) a double: one additional click.

(ii) a triple bond: two additional clicks.

(iii) a single bond again: three additional clicks.

Please note: It is only possible to convert a double bond to a triple bond if the valence on the connected atoms is not exceeded. If the valence is exceeded a single bond is drawn instead. In this case a triple bond can be drawn using the “Triple bond” button or the “Edit Bond Properties” dialog window.

 Draw double bonds or change existent bonds to double bonds.

Draws a new double bond or converts an existing bond into a double bond.

 Draw triple bonds or change existent bonds to triple bonds.

Draws a new triple bond or converts an existing bond into a triple bond.

 Draw up wedges or change existent bonds to up wedges.

Draws a new up stereo bond or changes an existing bond into an up stereo bond. An additional click on it changes the direction of the wedge.

Please note: The orientation of up wedges is important for the automatic detection of the stereochemistry (e.g. in case of query features).

 Draw down wedges or change existent bonds to down wedges.

Draws a new down stereo bond or changes an existing bond into a down stereo bond. An additional click on it changes the direction of the wedge.

Please note: The orientation of down wedges is important for the automatic detection of the stereochemistry (e.g. in case of query features).

 Draw a chain.

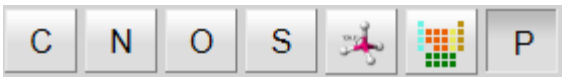
Draws a chain of C-C single bonds.

 Bond properties.

Opens the “Edit Bond Properties” dialog window. Please refer to chapter 4.4.2 for further information about editing bonds.

3.2.4 Atom Buttons

The “Draw atom” sub-toolbar contains four atom buttons (configurable), the “Atom properties” button, the “Periodic Table” button and one atom button which shows the last selected atom from the periodic table (here: P-atom).



 Draw carbon atoms.

Draws a carbon atom or converts an existing atom into a carbon atom. After selection click in the drawing area to place the atom.

 Draw nitrogen atoms.

Draws a nitrogen atom or converts an existing atom into a nitrogen atom. After selection click in the drawing area to place the atom.

 Draw oxygen atoms.

Draws an oxygen atom or converts an existing atom into an oxygen atom. After selection click in the drawing area to place the atom.

 Draw sulfur atoms.

Draws a sulfur atom or converts an existing atom into a sulfur atom. After selection click in the drawing area to place the atom.

 Atom properties.

Use the “Edit Atom Properties” dialog window to define atom properties and atom query features. Please refer to chapter 4.4.1 for further information about editing atoms.

 Periodic Table.

Use the “Periodic Table” dialog window to select another atom type.

Example:

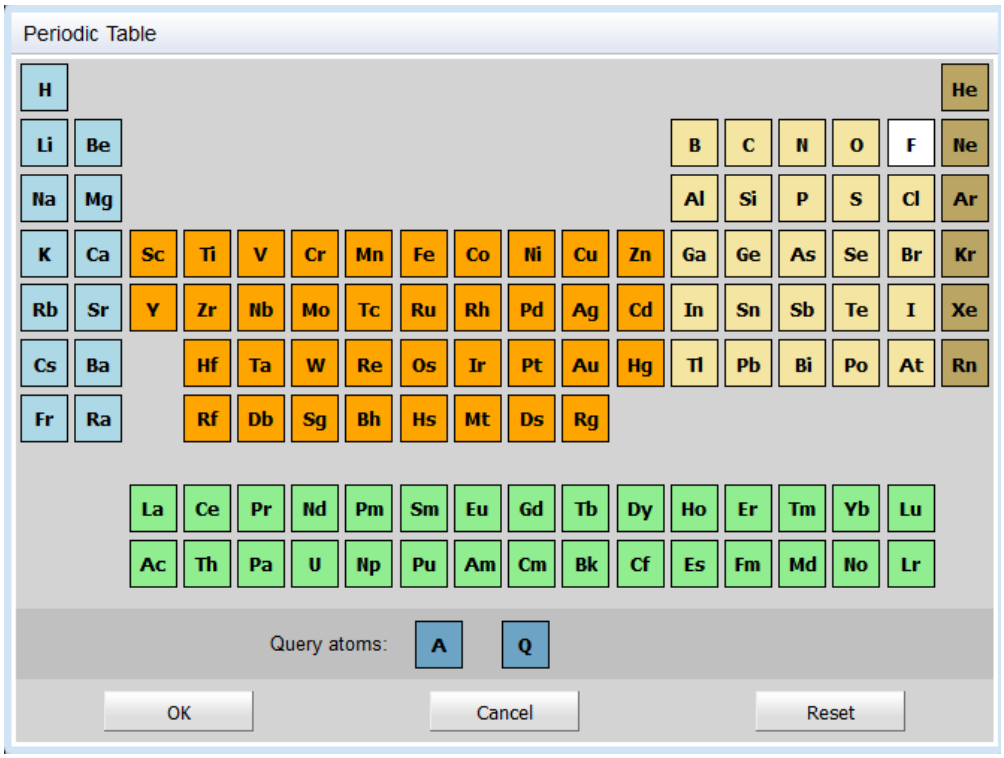


Fig. 2: “Periodic Table” dialog window.

Please select the desired atom and click “OK”. Click in the drawing area to place the atom. The chosen atom type will be displayed as button label on the “Last element” button (to the right of the “Periodic Table” button). For example: Select the Si atom and click “OK”.

The button on the right hand side of the “Periodic Table” button will be updated to “Si” and can be used to draw further Si atoms until the next atom is chosen from the “Peridic Table” dialog window or the editor is closed or refreshed.

3.2.5 Enhanced Chemical Functionality Buttons

The “Enhanced chemical functionality” sub-toolbar contains two Rgroup buttons, two mapping buttons and the “Draw bracket” button.

Define Rgroup.

Draw a core structure and several Rgroups.

First click on the position of the core structure, where you want to have the Rgroup attached. Then click on the connection position of the Rgroups.

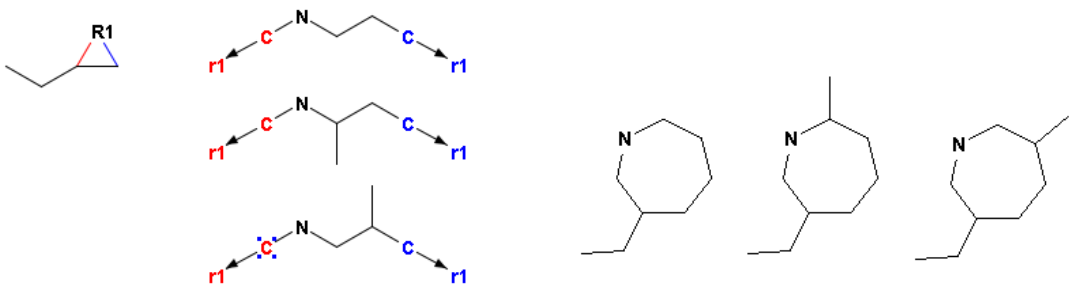
Example:

R-Query resolved single Queries

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

Example:

R-Query resolved single Queries



To change the Rgroup numbering, please click at the object you want to edit and enter the new number with your keyboard. To do this the “Define Rgroups” button must be selected!

 Remove Rgroup.

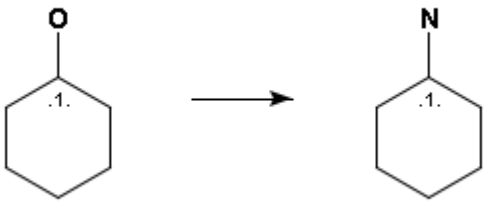
Click single atoms or draw a rectangle to remove the Rgroup information.

 Map atom.

Adds mapping numbers to the atoms you select. In order to do so, please mark the two atoms you want to map at the reactant and product side of the reaction.

Please note: Only mappings of reactant atoms with product atoms are supported. Furthermore, only atoms of the same atom type can be mapped.

Example:



Please note: the enhanced version of the IC*EDIT* JavaScript editor provides automapping functionality via the “Automap a reaction” button. Please refer to chapter 4.12 for further information.

 Remove Mappings.

Click single atoms/bonds or draw a rectangle to remove mappings or reaction center information from multiple atoms/bonds.

 Draw bracket.

Draws a pair of brackets. Please refer to chapter 4.8 for further details.

4 Using the Editor

4.1 Draw Objects

To draw atoms or bonds, click the corresponding button to activate the drawing mode. You can change the alignment of atoms, bonds or templates by dragging the object into the desired direction before releasing the mouse button.

Select the corresponding template button to draw rings and click once into the drawing area for one ring. To fuse rings, click on an existing ring bond. To connect rings as spiro molecules click on a ring atom and drag the object into the desired direction before releasing the mouse button. Otherwise the two rings will be automatically separated by a single bond.

Please note: Rings and bonds will be fused automatically, if the distance between two rings or bonds falls below a certain threshold.

4.2 Select Objects

To select a whole object or parts of it please choose the “Select” button and draw a rectangle covering the desired bond(s) and/or atom(s) and/or object(s). To select one or multiple bonds and/or atoms please click on all desired atoms and/or bonds while the shift button is pressed down.

Or choose the “Select object” button to select whole objects at once.

4.3 Scale Objects

To scale one or more objects please select first the object(s) and then use the double headed arrow in one of the four corners of the selection frame to change the size of the object(s).

4.4 Edit Objects

4.4.1 Edit Atoms

You can change the atom symbol of a selected atom by using the keyboard. Please insert any atom label and press “ENTER”. The input of atom symbols is not case sensitive.
Please note: After drawing a bond, the atom at the end of the bond is selected automatically. This feature facilitates the input of different atom types by simple drawing a bond, typing the atom label and pressing “ENTER”. The keyboard input of charges and isotopes is supported as well:

- For a charged atom please insert an atom symbol, the amount of charge and the charge type respectively (e.g. S2-).
- For isotopic information please insert the isotope number and the atom symbol respectively (e.g. 2H).

In addition, you can change an atom symbol using the “Edit Atom Properties” dialog window. To open the dialog window please use either the “Atom properties” button from the “Draw atom” sub-toolbar, the context menu “Edit Atom(s)” or double-click a specific atom.

Atom properties:

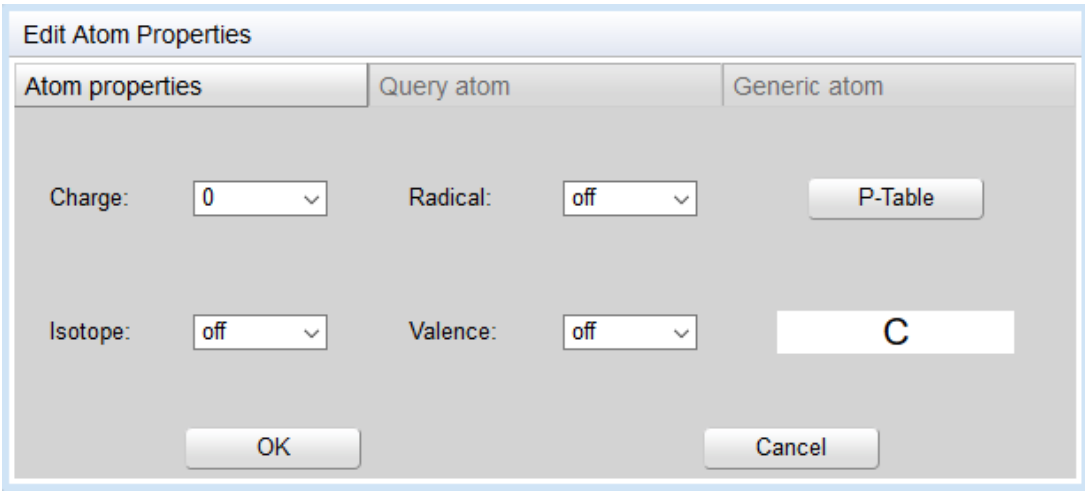


Fig. 3: “Edit Atom Properties” dialog window, main tab.

Use this dialog window to define charge, isotope or radical information and atom valence.

P-Table: Opens a dialog window containing the Periodic Table of the Elements to select any element. Furthermore, this dialog window contains additional buttons for non-standard and query atoms:

- **A:** Draws an A query atom: any atom excluding H.
- **Q:** Draws a Q query atom: any atom excluding H and C.

Query atom:

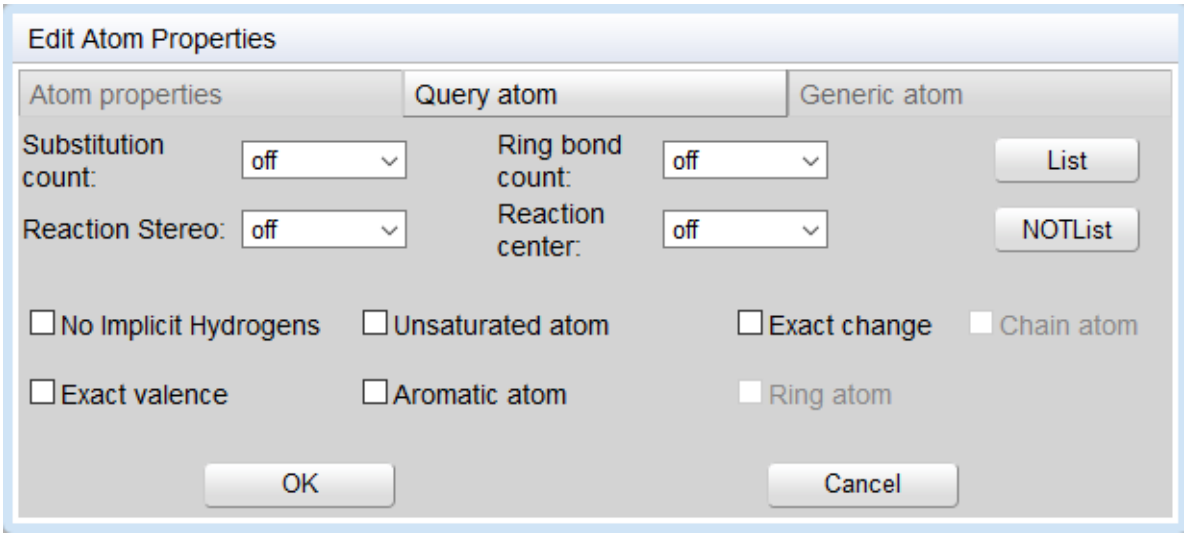


Fig. 4: "Edit Atom Properties" dialog window, Query atom tab.

The following query features are implemented and can be adjusted:

- Substitution count (s0-s6, s*).
- Ring bond count (r0-r4, r*).
- Reaction Stereo (retention, inversion).
- Reaction center (not center, R-center) will be supported in future.
- List: opens the "Periodic Table" dialog window where you can create an atom list for a query.
- NOT List: opens the "Periodic Table" dialog window where you can create a NOT-atom list for a query.

In addition, the following query settings can be adjusted:

- No Implicit Hydrogens (H0).
- Unsaturated atom (u).
- Exact change (ext.).
- Exact valence (ev.).
- Aromatic atom (aa.).

Please read the ICFSE_Tutorial.pdf for further information on the input and use of query features.

Generic atom:

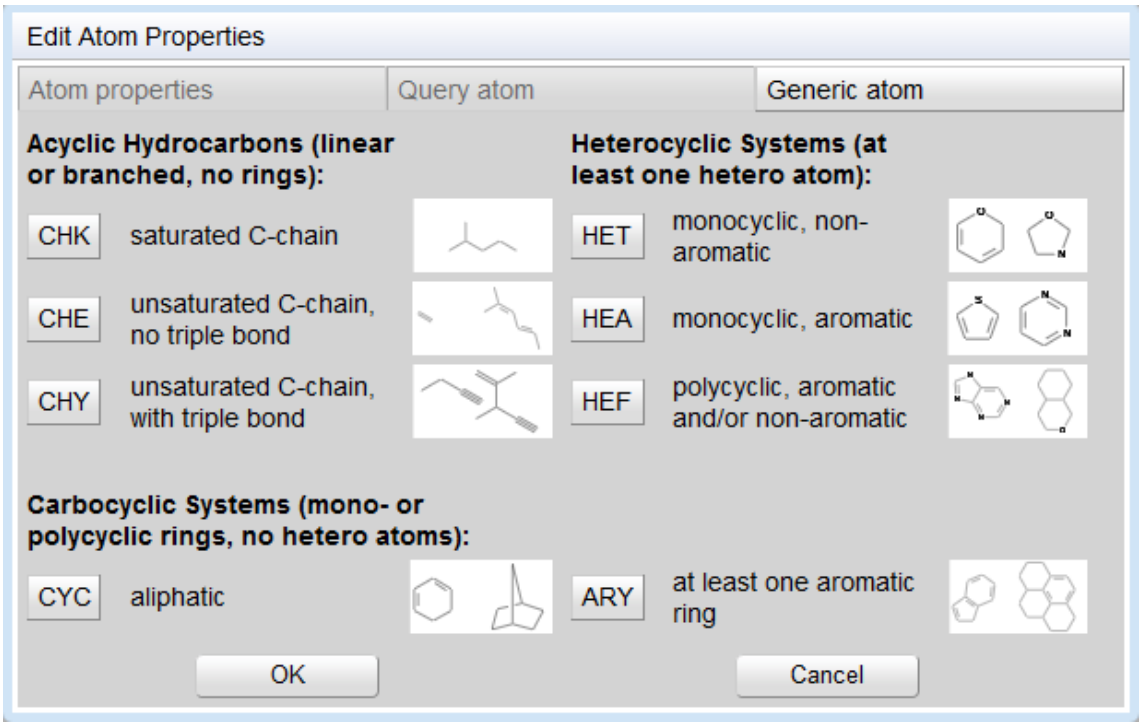


Fig. 5: "Edit Atom Properties" dialog window, Generic atom tab.

Use this dialog window to define generic atoms for Markush queries. The following generic atoms are supported:

Acyclic hydrocarbons:

- **CHK:** any linear or branched saturated carbon chain
- **CHE:** any linear or branched unsaturated carbon chain which contains at least one double bond (triple bonds are not allowed here)
- **CHY:** any linear or branched unsaturated carbon chain which contains at least one triple bond (double bonds are allowed)

Heterocyclic systems:

- **HET:** any non-aromatic monocyclic ring which contains at least one heteroatom
- **HEA:** any aromatic monocyclic ring which contains at least one heteroatom
- **HEF:** any aromatic and/or non-aromatic polycyclic ring which contains at least one heteroatom

Carbocyclic systems:

- **CYC:** any aliphatic non-aromatic mono- or polycyclic ring without heteroatoms
- **ARY:** any aromatic mono- or polycyclic ring containing at least one phenyl ring without heteroatoms

You may also enter generic atoms using the keyboard.

Please note: Generic atoms are not supported by the default configuration of ICEditJS.

4.4.2 Edit Bonds

Select one or several bond(s) and click on the right mouse button. Select “Edit Bond(s)” from the context menu to open the “Edit Bond Properties” dialog window, double-click a specific bond or click the “Bond properties” button from the “Draw Bond” sub-toolbar.

It is possible to change the bond type and to add reaction query features like reacting centers or the topology of the selected bond(s). In addition, the thickness of the selected bond(s) is adjustable in a range of 1 to 10 pixels.

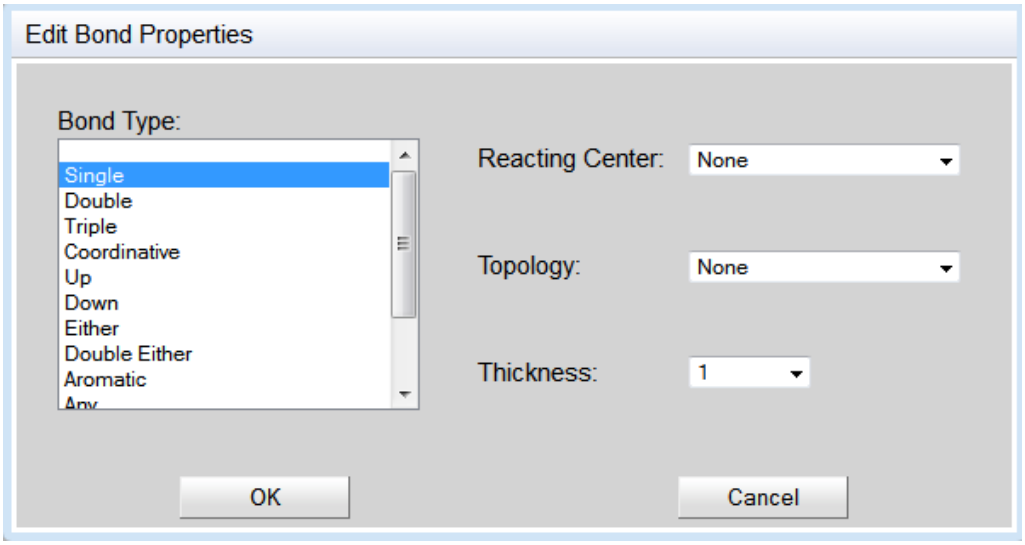


Fig. 6: “Edit Bond Properties” dialog window.

The following bond types are supported:

- Single
- Double
- Triple
- Up
- Down
- Either
- Double Either
- Aromatic
- Any
- Single/Double
- Single/Aromatic
- Double/Aromatic

The following reaction query features are supported:

Reacting Center

 Not Center

 Make/Break & Change

 Change

 Make/Break

 Center

Topology

 Chain

 Ring

4.4.3 Group or Ungroup Chemical Objects

Group

To group multiple chemical objects please select the desired objects and use the context menu item “Group”.

The selected multiple objects are now grouped and will be treated as a unique object, visible at the selection frame which is covering all objects belonging to the created group.

Ungroup

To ungroup a group of multiple chemical objects please select the desired group and use the context menu item “Ungroup”.

Please note: Multiple objects that are grouped act as one unique object.

Example:

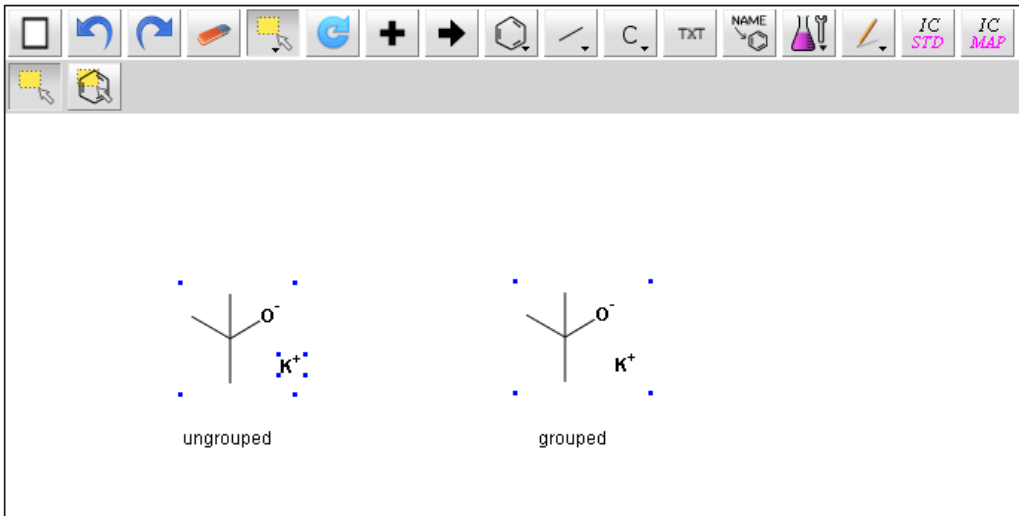


Fig. 7: Ungrouped and grouped objects.

4.5 Insert Text

Please use the “Draw Text” button  from the main toolbar to enter a text string.

To edit any text please double-click the text label (while the “Draw Text” or “Select” button is selected) or right-click the text label to open the context menu and choose “Edit Text” to open the “Edit Text Label” dialog window.

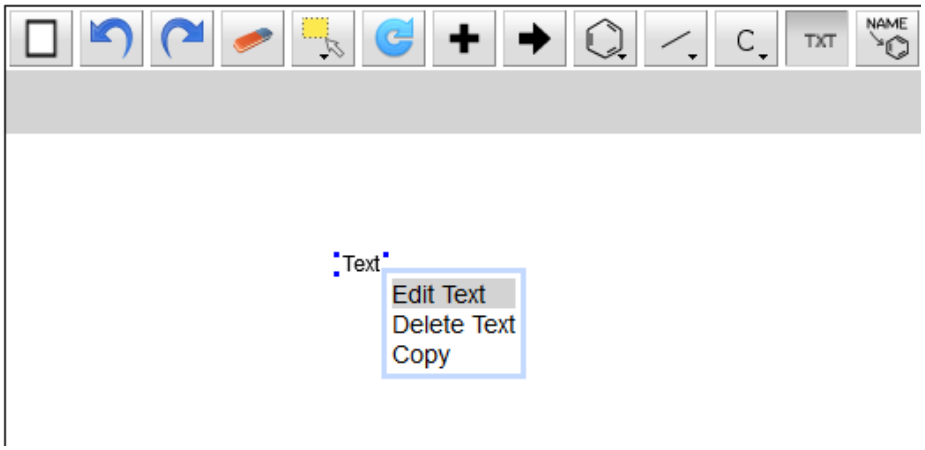


Fig. 8: “Text” context menu.

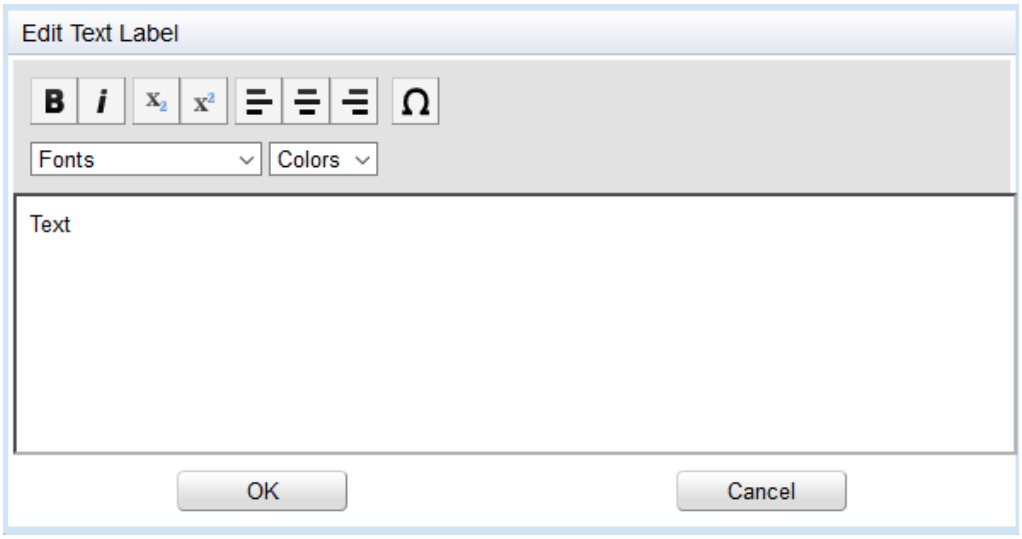


Fig. 9: “Edit Text Label” dialog window.

You can change the font type, style and color as well as the text alignment using the corresponding buttons and drop-down boxes. To add special characters like Greek letters to your text label please click on the “Insert Symbol” button  and select the desired symbol from the “Symbols” dialog window.

4.6 Superatoms

4.6.1 Support of Superatoms

The input and recognition of common superatom labels like COOH, OMe, Cbz, NO_2 is supported by the enhanced IC*EDIT* JavaScript editor (see Introduction for more information and technical documentation for setup information). In the default IC*EDIT* JavaScript version only self-defined superatoms can be created.

4.6.1.1 Input of Superatoms

The superatoms can either consist of (i) a standard abbreviation (Me), (ii) a sequence of elements (COOH), or (iii) a mixture of both (OMe).
If a superatom is recognized the label is shown in default font format (plain style).
Please note: If the label is shown in italic style and/or colored it is not recognized as superatom.

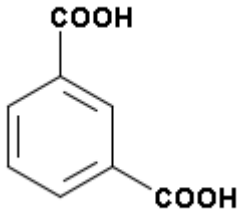
The input of superatoms is case sensitive.

- All atom symbols from superatoms have to be drawn as represented in the Periodic Table of the Elements (e.g. **COOH**, **O**Me, **Si**Me3).
- Abbreviations are case sensitive as well. They are supported in the most common notation (e.g. Me is supported, me or ME is not supported). The standard typing of abbreviations is as follows:
    - Bn, Boc, Bt, Bu, Bz
    - Cbz, Cy
    - EE, Et
    - Fmoc
    - Me, MEM, Mes, MOM, MPM, Ms
    - Naph, NPhth
    - Ph, Piv, PMB, PNB, Pr
    - SEM, Su
    - TBDMS, TBDPS, TBS, TES, Tf, THP, TIPS, TMS, Tol, Tr, Ts

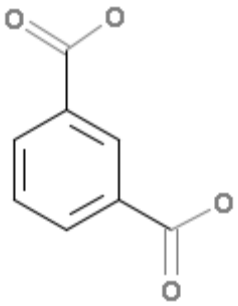
The expanded structure of the superatom is highlighted in gray. The expanded structure parts can be contracted again.

- **Expand a single superatom:** To expand a single superatom select the specific label and use the right mouse button to open the context menu. Choose “Expand Superatom”.
- **Contract a single superatom:** To contract a single superatom select any atom of the specific expanded structure and use the right mouse button to open the context menu. Choose “Contract Superatom”.

Example:



Contracted form

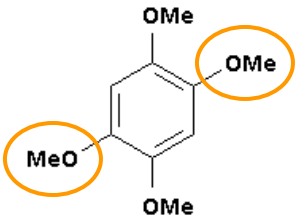


Expanded form

4.6.1.2 Display of Superatom Labels

The display of superatom labels is sensitive regarding the direction of the connection of the superatom to the target molecule.

Example:



On the top, the bottom and the right side of the target molecule the label of the superatom is given in a standard way. The label of the superatom on the left side, however, is in reversed order.
Please note: Abbreviations do not change their order.

Examples:

Left side superatom label	Right side superatom label
MeO	OMe
MeHN	NHMe
HOOC	COOH
TMS	TMS
$H_3C(H_2C)_5$	$(CH_2)_5CH_3$

The label of the superatom is changed automatically according to the direction of the connection to the target molecule in order to represent the connecting atom of the superatom group correctly. E.g. the superatom label input on the left side of a molecule can be COOH and the output changes automatically to HOOC.

Please contact us to receive a full list of supported superatoms (iceditsupport@infochem.de).

4.6.2 Creation of Self-defined Superatoms

Select the desired part of a molecule and choose “Create Superatom” from the context menu to create a self-defined superatom. Enter the desired superatom label into the dialog window and click “OK” to create the superatom.

Example:

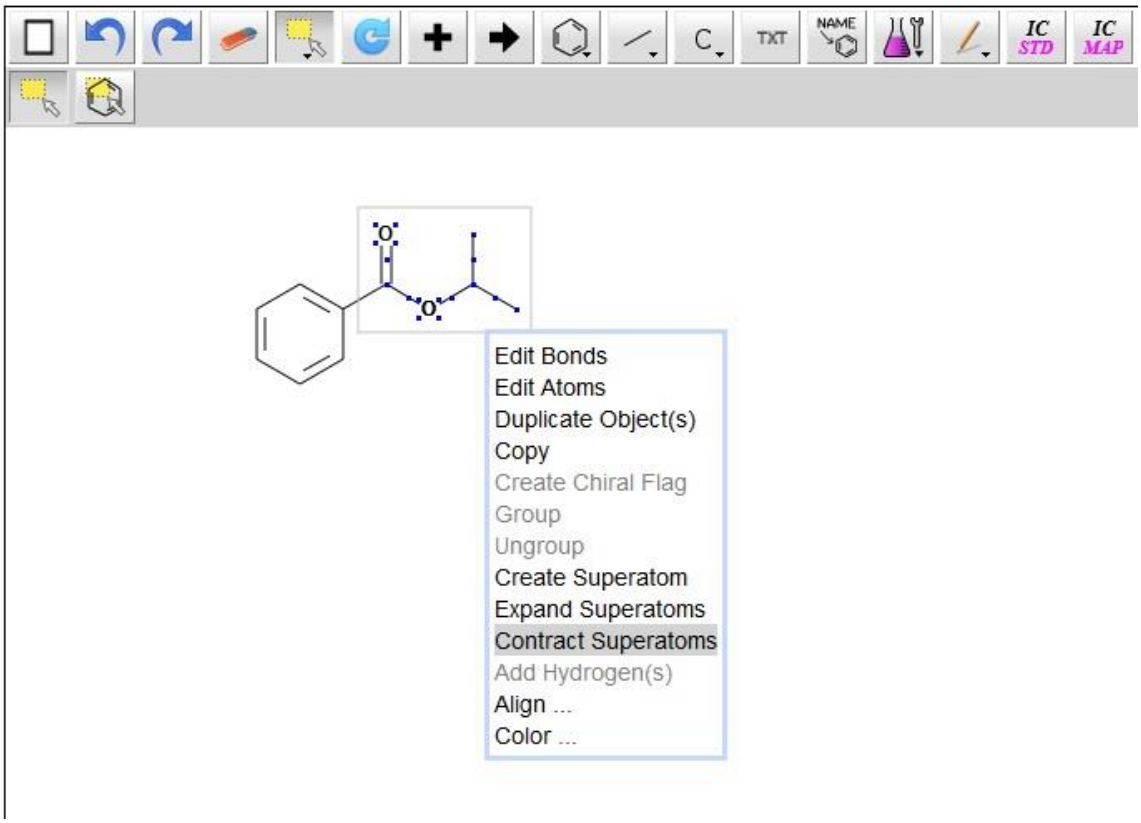


Fig. 10: “Create Superatom” context menu.

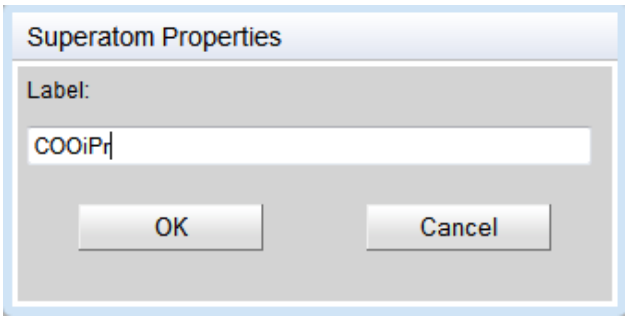


Fig. 11: “Superatom Properties” dialog window.

Result:

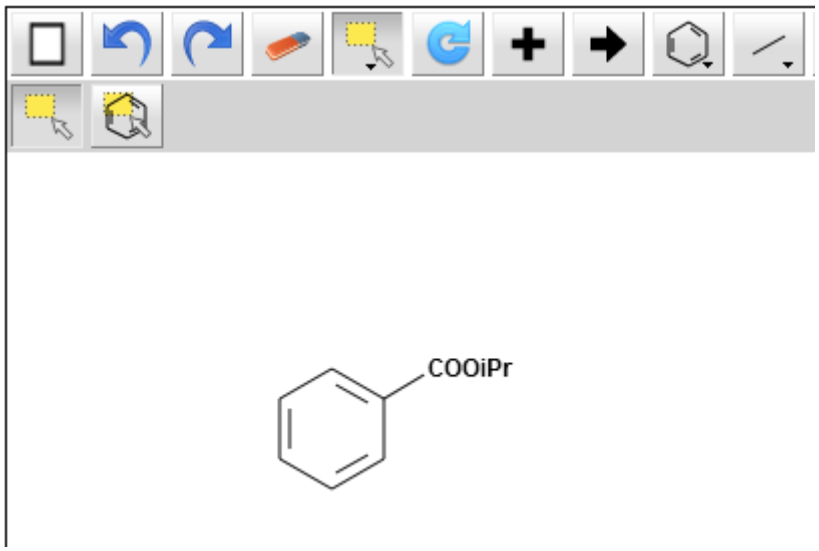


Fig. 12: “Create Superatom” action result.

Please note: A molecule containing a self-defined superatom can be copied like any other usual molecule.

Please note for user of the enhanced version: The self-defined superatom is not added to the internal list of superatoms. Therefore, it is not stored for future use and must be newly-created each time it is used.

4.7 Create Chiral Flag

A chiral flag is used to mark the stereochemistry of the labeled molecule as **absolute**.

To add the chiral flag, please select the molecule you want to label as chiral and use the context menu “Create Chiral Flag”. The labeled molecule is now marked with the text box “chiral”.
To remove the chiral flag, please delete the text box “chiral”. The stereochemistry is no longer marked as absolute.

Example:

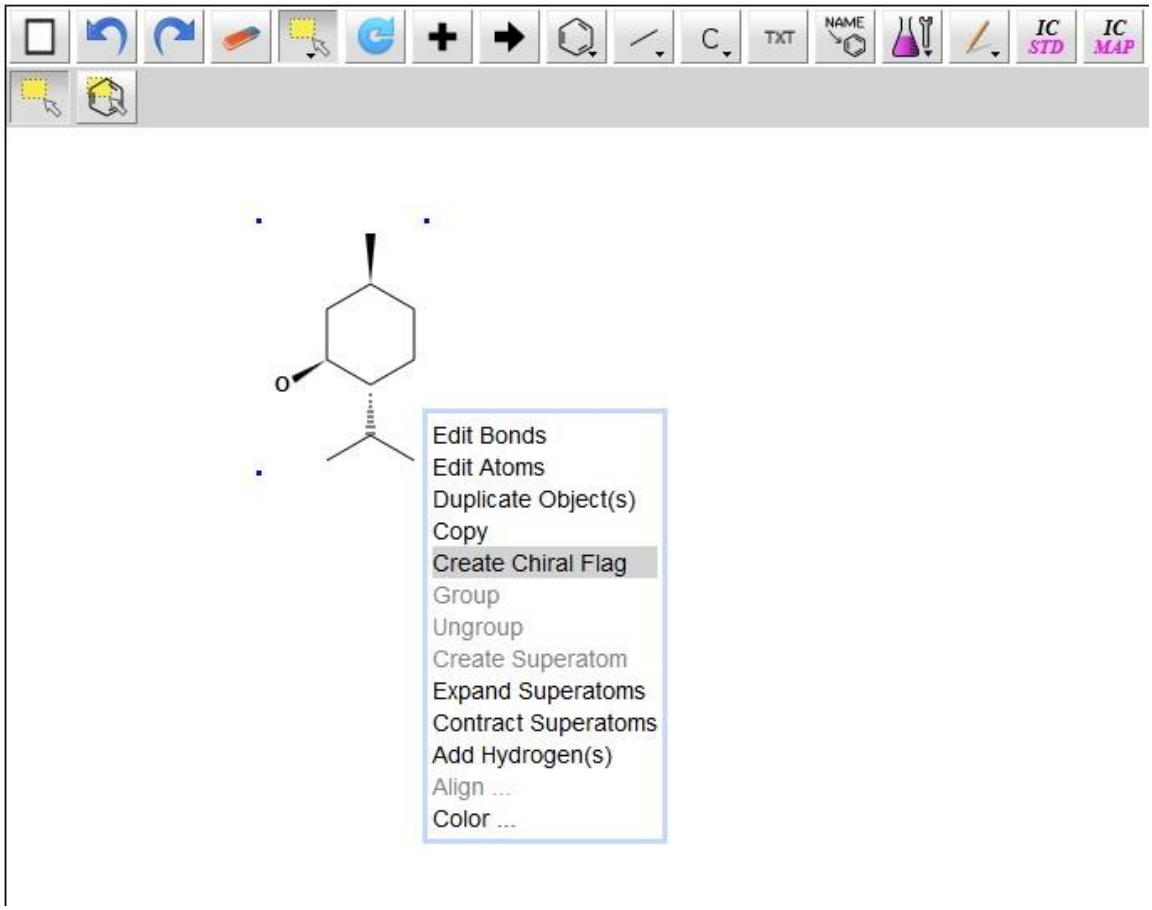


Fig. 13: Context menu item “Create Chiral Flag”.

Result:

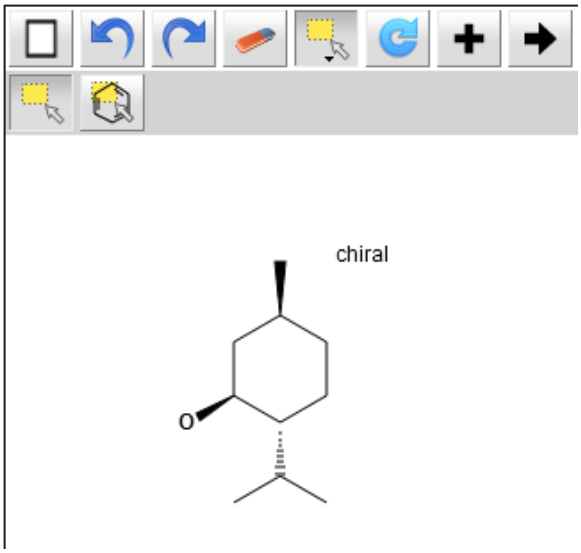


Fig. 14: Molecule labeled as chiral.

4.8 Create Brackets

To draw a bracket, please select the bracket  button from the “Enhanced chemical functionality” sub-toolbar and draw a pair of brackets into the drawing area by using the mouse cursor.

Molecules can only be interpreted correctly if the brackets are drawn properly. The following types of brackets are supported:

- A pair of brackets covering a complete molecule.
- A pair of brackets covering a section in-between a molecule.
  Please note: Both brackets of a pair must cross a bond of the molecule in this case.

Example:

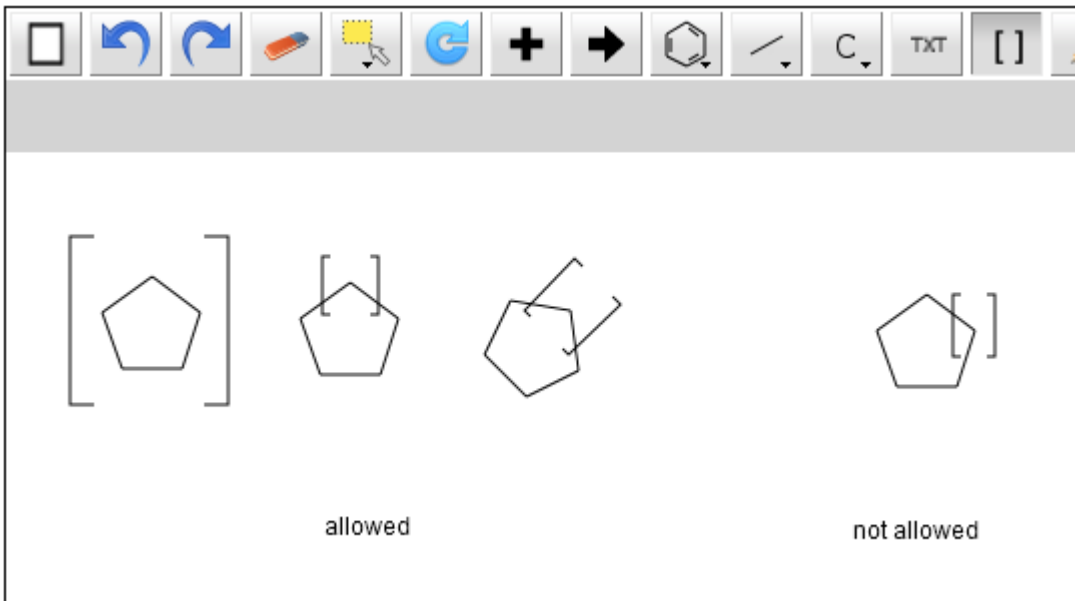


Fig. 15: Allowed/not allowed bracket positions.

You can edit or delete a bracket by using the “Brackets” context menu. To open the “Brackets” context menu, please move the mouse cursor above one bracket until a red frame appears. You can now open the “Brackets” context menu by right-clicking.

Example:

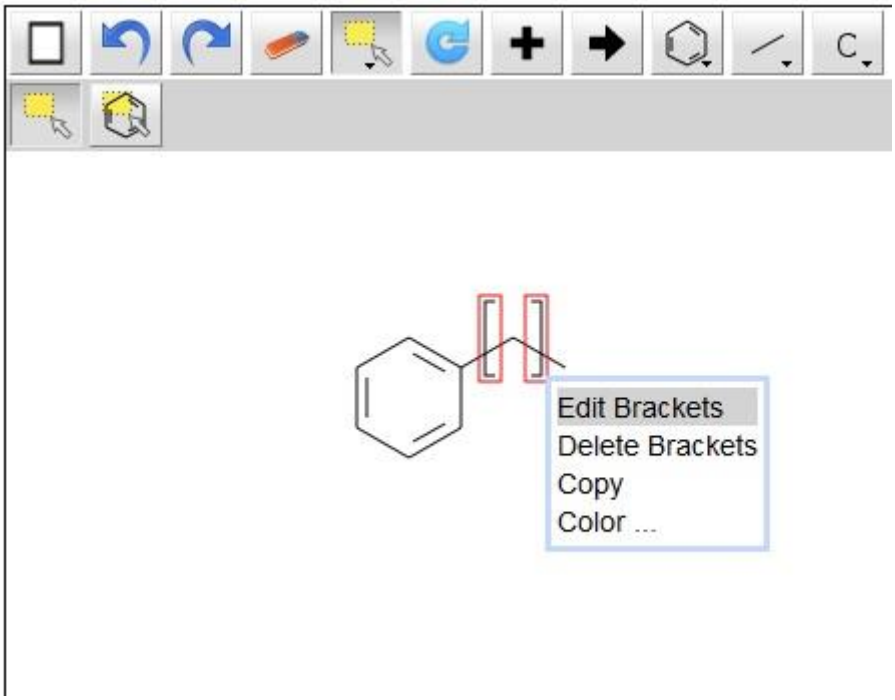


Fig. 16: “Brackets” context menu.

Edit Brackets:

To edit a pair of brackets, choose “Edit Brackets” from the “Brackets” context menu. You can edit (i) the bracket type, (ii) the bracket style or (iii) add display features to the brackets:

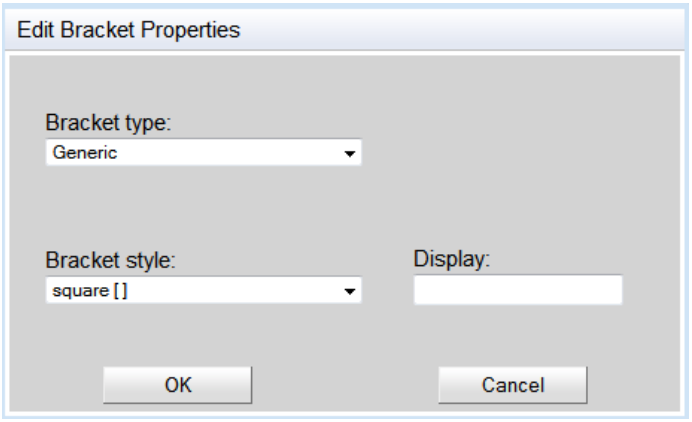


Fig. 17: The “Edit Bracket Properties” dialog window with bracket type “Generic”.

Edit the Bracket Type:

The default bracket type is “Generic”. You can change the bracket type from “Generic” to “Multiple group” or “SRU”.

- **Bracket type - Generic:** A pair of brackets is graphically drawn. No repeating factor is displayed and no repeating factor will be interpreted chemically.
- **Bracket type - Multiple Group:** You can enter any integer beginning with 1. The multiple group information will be interpreted chemically.
- **Bracket type - SRU:** You can enter any value, number, range or free text. The SRU (**S**tructure **R**epeating **U**nit) information is displayed, but will be not interpreted chemically.
  For example: The clamped part is not multiplied, if the “SRU” value is set to 2. However, if the “Multiple group” value is set to 2 the enclosed part is multiplied.

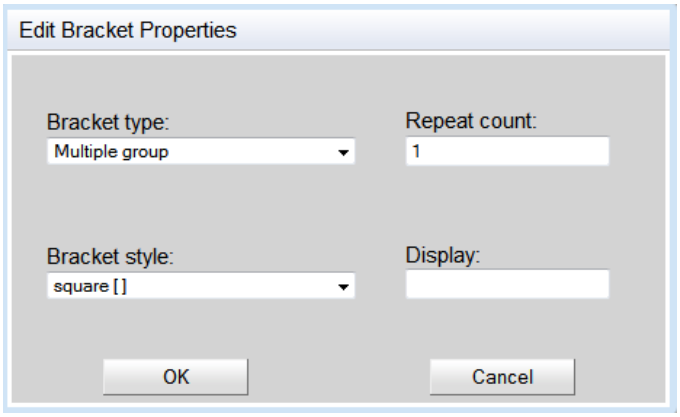


Fig. 18: “Edit Bracket Properties” dialog window with bracket type “Multiple group”.

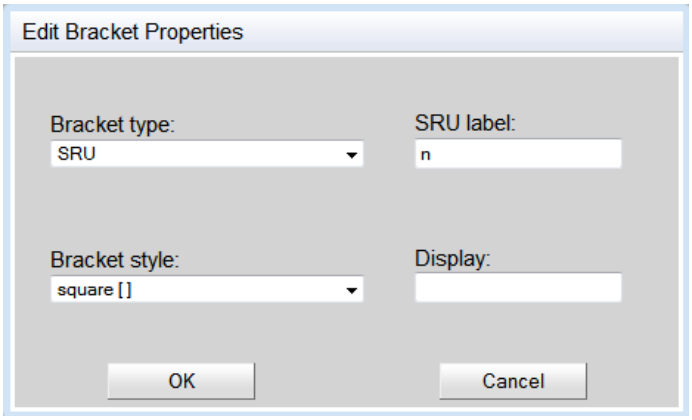


Fig. 19: “Edit Bracket Properties” dialog window with bracket type “SRU”.

Edit the Bracket Style:

The two bracket styles “square” and “round” are supported by the IC*EDIT* JavaScript editor.

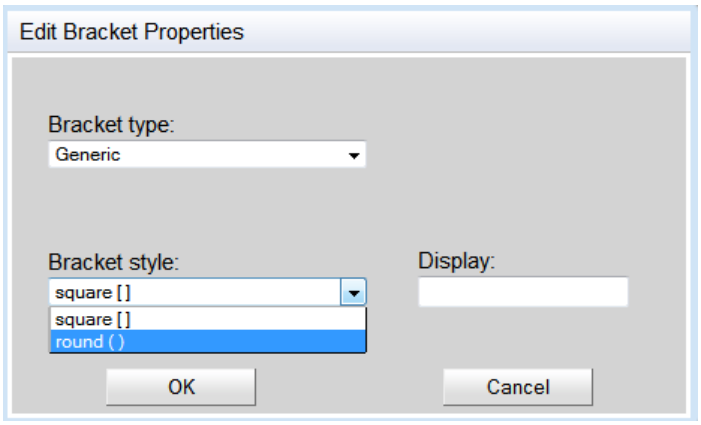


Fig. 20: “Edit Bracket Properties” dialog window with two different bracket styles.

Enter a Bracket Display:

You can enter any additional display information in the “Display“ field. The entered display information is shown on the upper right-hand side of the right bracket pair.

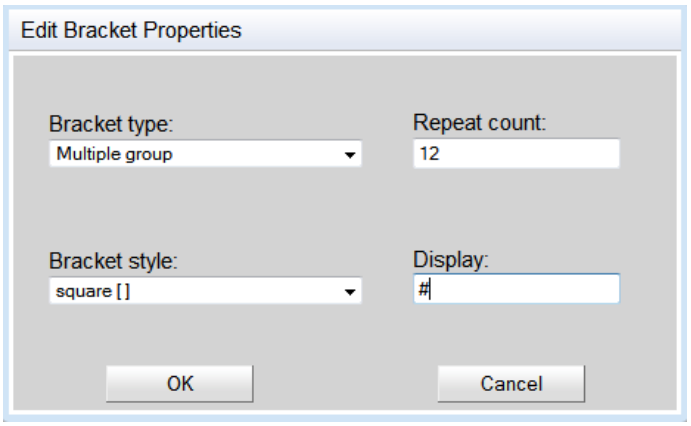


Fig. 21: “Edit Bracket Properties” dialog window with additional display information.

Result:

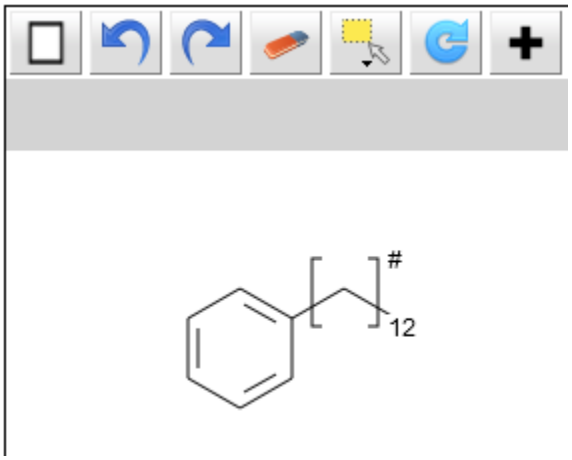


Fig. 22: Molecule with multiple group brackets and display information.

Delete Brackets:

To delete a bracket, please choose “Delete Brackets” from the “Brackets” context menu to remove the whole pair of brackets.

Copy Brackets:

To copy a pair of brackets with its definition, please choose “Copy” from the “Brackets” context menu and paste the defined pair of brackets in the drawing area.

Color:

You have the possibility to change the color of the brackets. Please choose any color given in the sub-menu of the context menu item “Color…”.

4.9 Create a No-Structure

No-Structures are used to enter non-structural components into structure or reaction databases. Some molecules cannot be represented by a drawn structure but do play significant roles in reactions like baker's yeast. In these cases No-Structure labels can be used to insert the molecules into the database. This means the molecule is represented by a No-Structure label (recognized as valid database input) and not by a structure.

Create a No-Structure:

Please use the context menu item "Create No-Structure" to open the "No-Structure Properties" dialog window.

Please enter a desired caption or use the default caption "No-Structure" for your No-Structure. The No-Structure label will be added to the drawing area by clicking "OK".

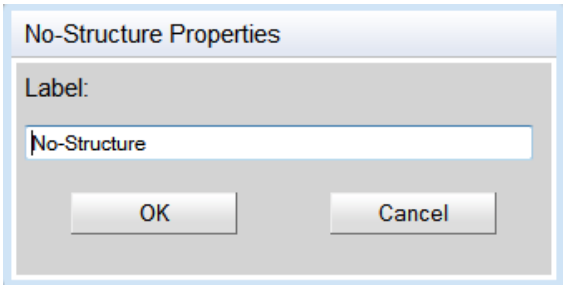


Fig. 23: "No-Structure Properties" dialog window.

Edit or delete a No-Structure:

You can edit or delete a No-Structure by using the "No-Structure" context menu. To open the "No-Structure" context menu, please move the mouse cursor above the No-Structure until a red frame appears. You can now open the "No-Structure" context menu by right-clicking.

Example:

Fig. 24: “No-Structure” context menu.

Color:

You have the possibility to change the color of the No-Structure. Please choose any color given in the sub-menu of the context menu item “Color…”.

Please note: A reaction or molecule containing a self-defined No-Structure can be copied like any other usual molecule.

4.10 Add Hydrogen(s)

The “Add Hydrogen(s)” functionality generates explicit hydrogens to a drawn query structure to generate closed sites.

To add the hydrogen atoms please select a structure and choose “Add Hydrogen(s)” from the object context menu.

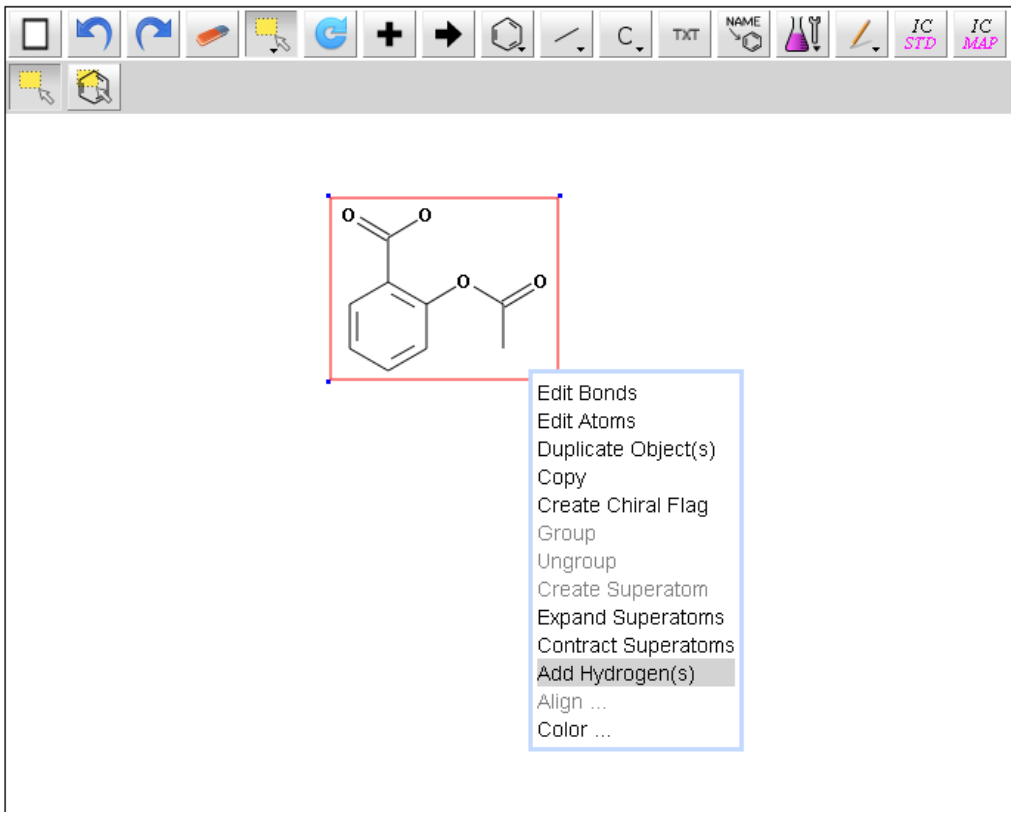


Fig. 25: “Add Hydrogen(s)” functionality.

Result:

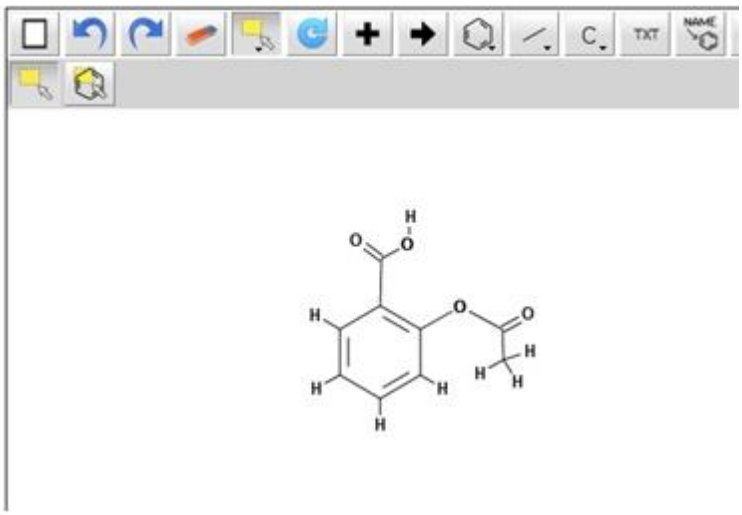


Fig. 26: IC*EDIT* drawing area containing the generated molecule.

Please note: The “Add Hydrogen(s)” functionality does only support single molecules without query features. Multiple (non-grouped) molecules, fragments or query features are not supported yet.

Please note: The “Add Hydrogen(s)” functionality is only supported by the enhanced IC*EDIT* JavaScript editor. For the setup please see the technical documentation.

4.11 Convert Name to Structure

The “Convert Name to Structure” functionality generates a structure from a given name.

To enter a name please open the “Convert Name to Structure” dialog window using the “Name to Structure” button 

or choose “Covert Name to Structure” from the context menu. Please click “OK” to insert the corresponding structure to the ICEDIT drawing area.

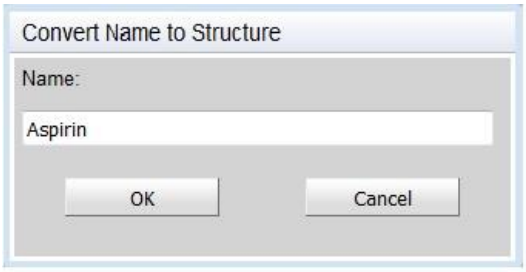


Fig. 27: “Convert Name to Structure” dialog window.

Result:

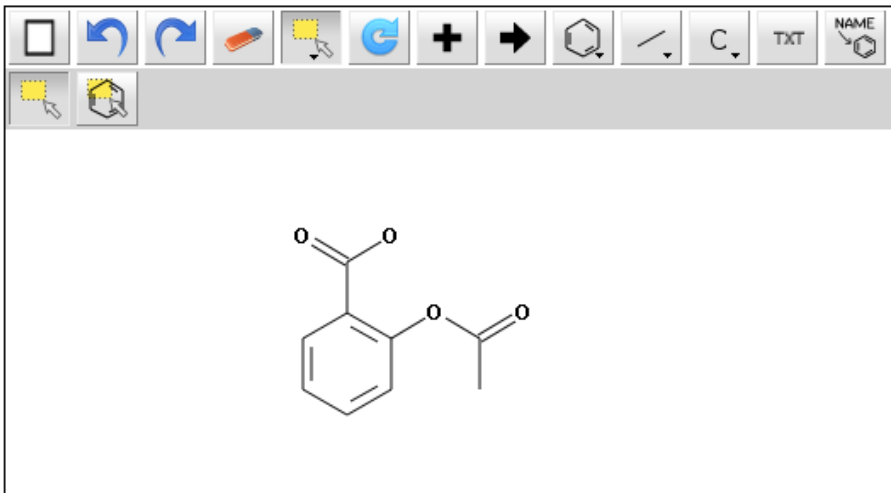


Fig. 28: ICEDIT drawing area containing the generated structure.

The “Convert Name to Structure” functionality comprises systematic nomenclature names (IUPAC and inverted names, i.e. CAS index names) as well as trade-, trivial-, and semi-systematic names. A dictionary-based and a morphology-based (algorithmic) approach are combined to create the chemical structures from names. InfoChem’s dictionary contains more than 28 million chemical names mainly in English and German - plus several other languages for common chemicals. These names correspond to more than 13 million unique structures.

Please note: The “Convert Name to Structure” functionality is only supported by the enhanced ICEDIT JavaScript editor. For the setup please see the technical documentation.

4.12 Automap a Reaction

Please select the desired reaction and click the “Automap the reaction” button  to add mapping numbers and reaction center information automatically to the reaction. To remove the mapping and reaction center information please use the “Remove mappings” button from the button bar  (available in the “Enhanced chemical functionality“ sub-toolbar).
The “Automap the reaction” button automatically maps all possible atoms and automatically adds reaction centers whereas the “Map atoms” button  allows the manual input of mapping numbers (see above).

Please note: The “Automap a reaction” functionality is only supported by the enhanced ICEDIT JavaScript editor. For the setup please see the technical documentation.

4.13 Standardize a Structure/Reaction

Please select the desired structure or reaction and click the “Standardize the structure” button 

to standardize the selected molecule or reaction in accordance with InfoChem’s standardization rules.

For further details on applied standardization rules please refer to the document “Standardization Rules”. Please use the undo button to restore your previously drawn structure/reaction if the standardization does not meet your requirements.

Please note: The “Standardize the structure” functionality is only supported by the enhanced ICEDIT JavaScript editor. For the setup please see the technical documentation.

4.14 Alignment

To align selected objects, please open the context menu and choose the different options given from the window:

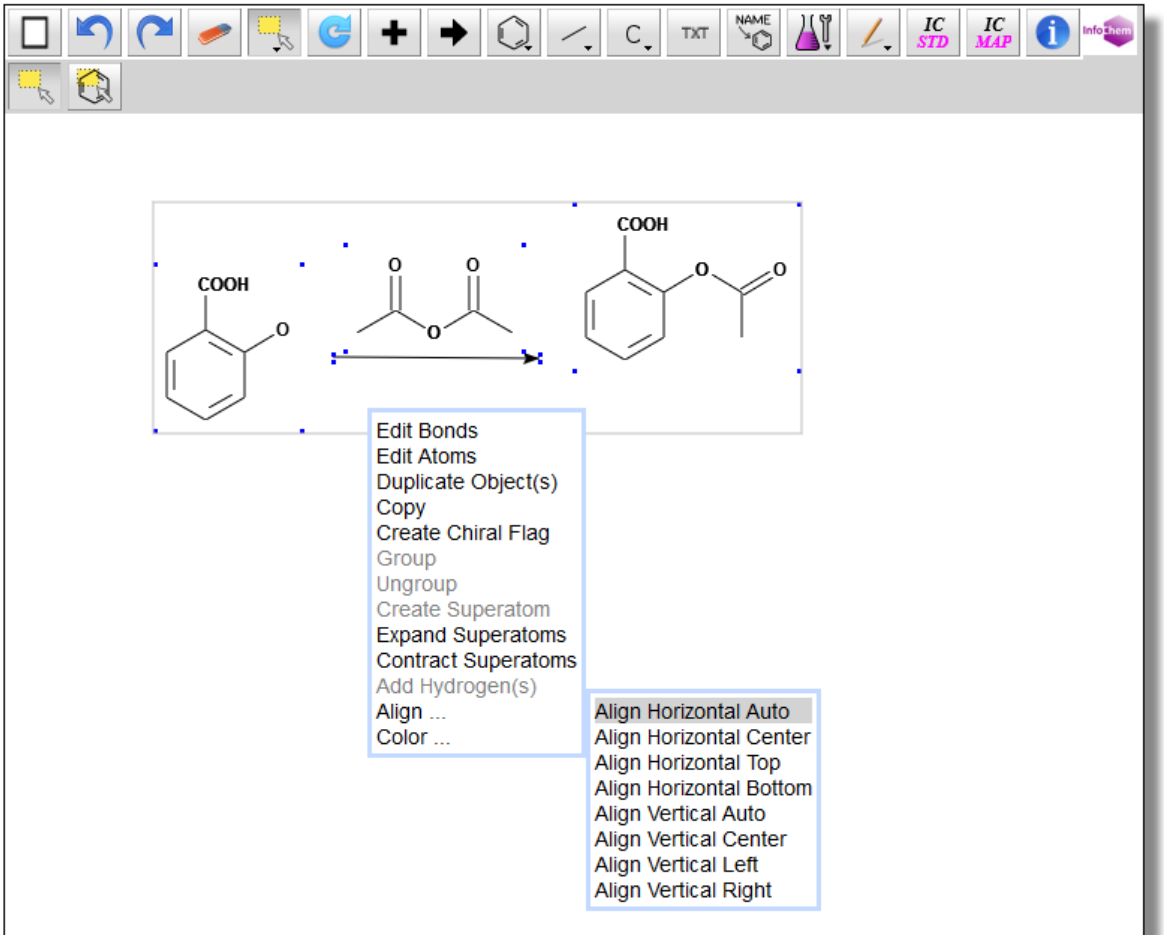


Fig. 29: “Align” context menu.

Result:

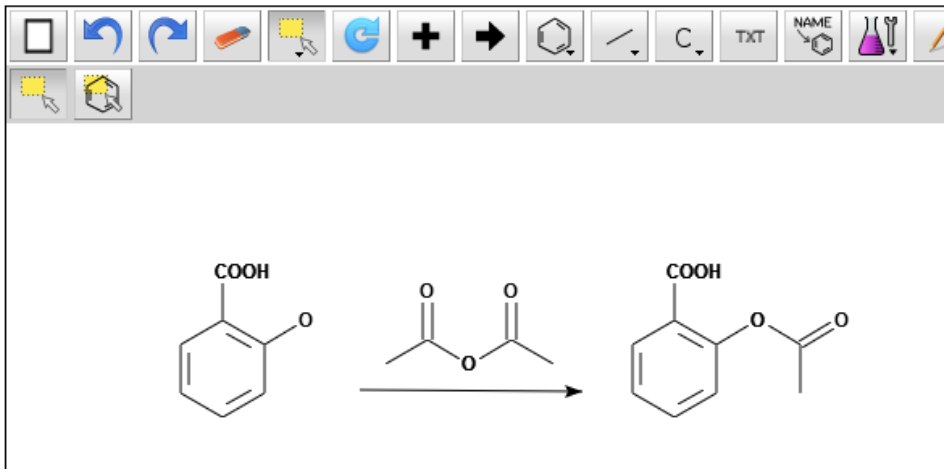


Fig. 30: Result of the horizontal auto alignment.

5 Customer Support

Please contact us to receive technical support or license information:

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