Marvin

Introduction

Marvin is Chemaxon's latest, most advanced drawing solution. It combines the company's well-known chemical intelligence with modern front-end frameworks, resulting in an easy-to-use, clean interface which is capable of converting your thoughts into a visual representation in no time. Our aim was to build an accessible product for everyone so our tool may be used by as many people as possible.

Marvin is the ideal solution for users who do not only want to draw structures easily and efficiently but aesthetically, too. We think that the effort put into research should reflect in the quality of the accompanying drawings. Our goal is to achieve the highest standard in publication quality.

Embeddable and integrable into any web environment through a simple and clean JavaScript API. No hurdles, no lengthy guides to read, just a few lines of code, and your chemical editor is up and running!

Design principles

Fast drawing & analysis

We know very well that the creative process is rarely linear. For this reason, Marvin provides the ability to easily jump between different molecules or handle them at once and gather essential chemical information instantly. Our tool supports users in representing the chemical structures they have in mind by providing the easiest and fastest ways to visualize and digitize their ideas. Think about the canvas as an extension of thoughts.

Publication quality

The aesthetic of any chemical drawing should be in line with the quality and effort put into research. Marvin offers a rich set of tools and graphical objects to make your drawings unique and distinguished, while also fitting the visual requirements of publishers.

Advanced drawing

The feature set of Marvin enables the representation of complex structures and advanced chemical information on the canvas supporting the creation of meaningful drawings. You can easily realize Markush structures, enhanced stereochemical information, polymers and detailed query properties. We believe that quality lies in the details.

Accessibility for everyone

Our tool should be usable by as many people as possible. Our aim was to build an accessible chemical drawing software for everyone.

Easy integration

Embeddable and integrable into any web environment through a simple and clean JavaScript API. No hurdles, no lengthy guides to read, just a few lines of code, and your chemical editor is up and running!

Discover Marvin

Features

A list of all tools and features offered by Marvin.

Shortcuts & Tricks

The list of hotkeys, shortcuts and useful tips for a more convenient drawing experience.

How to? examples

Demonstrative examples on how to use the tools and features of the application.

Comparison with Marvin Sketch and Marvin JS

Review of the innovations and general scope of Marvin compared with our legacy drawing softwares.

Accessibilty

Overview of the accessibility feature set offered by Marvin.

Release notes

List of release notes for Marvin.

Developer resources

Developer and installation guide

Features

Overview of editor

Marvin is equipped with a **Top toolbar** giving place to basic editing options such as the **Undo and Redo**, **Zoom** and **Text editing**. In addition, this is the place to find chemical services to **Calculate** chemical properties, **Clean** structures, switch between **Aromatic and Kekulé** representation of aromatic systems, calculate **CIP stereodescriptors**, show **Explicit hydrogen atoms**, **Import structures** easily and manage the **Export** of the content of the drawing area into images and files.

The **Left toolbar** is the place of the main editing and **Chemical drawing tools**, starting with **Selection** and **Erase**, followed by a wide range of **Chemical bonds**, **Templates**, **Atom toolbar**, **Markush**,**Query Tools** and **Electron tools**. The **Shapes**, **Text tool** and **Scribble line** support the creation of unique, publication quality drawings. In addition, **Marvin** provides a wide set of **Arrow types** and the **Map reaction atoms** feature to support the drawings of various chemical transformations.

At the top left corner of the application the **Main menu** can be found, which, above many other options, gives access to the editor **Settings**. The **Context menu** can be accessed from the drawing area area to organize certain features and editing options, including **Molecule properties**, **Atom properties** and **Bond properties**, which are also available from the **Main menu**. The display of **Atom numbers**, the **Duplication** of selected objects, their **Alignment and distribution** and the **order of layers** can also be set from the **Context menu**.

Setup for local/"offline" usage

It is possible to setup Marvin as a locally hosted application and given a successful license key check occured, it can be used offline.

1. **Please download and install the latest Marvin:**
    1. Make sure to have an installed Java version of 17 or newer on your machine, for example this.
    2. Go to the download page of Chemaxon's Marvin and download the appropriate installer based on the OS you are using: https://download.chemaxon.com/marvin
    3. Run the installer
2. **Setup the license key for Marvin:**
    1. In case you have Chemaxon's license manager installed, please follow these steps (see "Install with GUI")
    2. In case you do not have the license manager installed
        1. Windows:
            1. Go to the "C:\Users<user>\chemaxon" folder
            2. Create a file named "license-manager" with a .properties extension
            3. You need these two lines in the file (where your license key is inserted in place of): server=https://license.chemaxon.com license-key=
        2. Mac:
            1. The same procedure has to be followed as for windows, but the location of the file is: "/root/.chemaxon/license-manager.properties"

    Hints:

    - *Make sure that the extension of the file is ".properties"*
    - *In case of Mac, make sure that textcontent of the file is plain text and not rich text formatted*
3. **Execute the application on your machine:**
    - Windows:
        - Go to "C:\Program Files\Chemaxon\marvinws" (default installation folder)
    - Mac:
        - Go to "Applications\Marvin webservices"

    1. Execute the "run-marvinws.exe" file
    2. After waiting for a few seconds, open your preferred browser and go to http://localhost:8080/
    3. The application is set up and running with default settings.

How "offline" mode is working:

- In case you have Chemaxon's license manager installed: Internet connection is needed when the application is launched to check the validity of the license key. After a successful license check, Marvin can be used for 15 days offline
- In case you do not have the license manager installed: Internet connection is needed every time the application is launched

General tools

Selection tools

Icon	Name	Shortcut
	Rectangle Selection	**Esc**
	Lasso Selection	**Esc**

The editor supports two selection modes: **Rectangle Selection** and **Lasso Selection**. The default mode is the **Rectangle Selection**. Can be used for both single (click) and multiple (drag) selections. Alternatively, double-clicking can be used to select a complete structure.

> The selection tool mode affects the behavior of other tools including the **Erase**, **Define RGroup**, **Variable attachment** and **Color** tool.

When clicking on a bond it will be selected together with the atoms it connects. This is also true when using drag selection. To select a bond without the atoms, hold the Alt/⌥ key and click the bond with the selection tool in hand.

> Additional useful **shortcut**: **Ctrl/⌘ + a** selects the content of the drawing area.

Erase

Icon	Shortcut
	**Delete** or **Backspace** or **fn + Backspace**

The **Erase** tool removes selected objects. Pressing the shortcut when hovering over an object will delete it. Otherwise, when used over an empty part of the drawing area, the shortcut will take the tool in hand. Can be used for both single (click) and multiple (drag) selections.

Undo/redo

Icon	Name	Shortcut
	Undo	**Ctrl/⌘ + z**
	Redo	**Ctrl/⌘ + Shift + z**

Undo revokes the last editing step. The **Redo** button is inactive until the **Undo** button is clicked. It restores the last undone editing step.

Zoom

Icon	Shortcut
	Ctrl/⌘ + scrolling

The default **Zoom** value is 100%. The minimum value is 10% and the maximum is 500%. **Zoom** can be set from the top toolbar dropdown menu at predefined values or by using the plus and minus buttons.

Fit to canvas sets a zoom factor that lets you view the contents of the whole drawing area. This feature can also be accessed using the **Ctrl/⌘ + 1** shortcut.

Fit to selection sets a zoom factor that makes the selected structure fill the viewport.

Attach data

Icon	Name
	Attach data...

The **Attach data** tool can be used on a molecule or fragment selection either from the context menu or from the **Main menu -> Structure** submenu. It offers the opportunity to attach arbitrary textual information to chemical structures, including complete molecules and fragments. This data may include search conditions in queries.

Having a selection in the drawing area that includes no more than one chemical structure, the **Attach data** dialog can be opened from the **Context menu**. It is mandatory to fill out the *Name* and *Value* fields to create an **Attached data**, the *Unit* field and the *Query* operator are optional, the latter being *none* by default. The input fields accept any text or numbers. The *Query* dropdown menu has the following options: *none*, =, <, >, <=, >=, <>, *between*, *like*, *contains*. For more information, see **Query guide**.

As the **Attached data** is added, it appears on the top right corner of the structure. Hovering either the label or the structure, a purple highlight feedback appears on the included structure.

> The attached data can be edited any time by opening the **Context menu -> Edit attached data** dialog from any part of the included structure or the data label.

Clean up reaction

Selected reactions can be cleaned using the **Clean up reaction [Ctrl/⌘ + Shift + x]** action from the selection's context menu. As a result, the **Reaction components**, *i.e.* starting materials, products, plus signs, reaction arrow, reaction agents and reaction conditions are aligned and distributed. Considering a reaction arrow pointing from left to right, compounds that are located on the left side of the arrow are handled as starting materials and those that are located on the right side are handled as products. If more than half of the molecule overlaps with the vertical plane of the arrow it is considered a reaction agent and will be placed over or under the reaction arrow. Textboxes will be placed over and under the arrow if they are overlapping the vertical plain of the reaction arrow.

> This action is only available if at least an arrow and a chemical structure is selected. The **Clean up reaction** is only available if the selection only contains one reaction and only reaction components.

Copy as

Icon	Shortcut
	**Ctrl/⌘ + k**

The contents the drawing area can be copied by selecting the desired elements, then accessing the **Copy as** function either through the selection's context menu or through **Menu -> Copy as**. Copying in the following formats is accessible right away:

- CXON
- MDL Molfile V3000
- PNG (image)
- SMARTS
- SMILES
- SVG (scalable vector graphics)

The **Copy as other format** offers a wider range of formats which are listed in the **Export** section.

Duplicate

Icon	Shortcut
	**Ctrl/⌘ + d**

The selected object (atom, bond, structure, fragment, text or image) may be duplicated in the drawing area from its context menu. Using the **Ctrl/⌘ + c** shortcut will copy the selection to the clipboard.

Bring to Front/Send to back

Icon	Name	Shortcut
	Bring to front	-
	Send to back	-

If a selected object overlaps with other elements in the drawing area, opening its context menu makes it possible to move it *behind* or *in front* of all other objects, making editing more convenient.

Align

When selecting multiple objects in the drawing area, it is possible to **Align** them next to each other or **Distribute** them in even distances horizontally or vertically from the selection's context menu.

Icon	Name
	Left
	Center
	Right
	Top
	Middle
	Bottom
	Distribute horizontally
	Distribute vertically

These actions work automatically when moving objects manually in the drawing area. Upon entering an aligned/distributed state between objects, purple helper guidelines appear and the objects are snapped in that position.

> When holding the Shift button and moving an object, it is fixed on either the horizontal or the vertical axis based on the angle of the movement, supporting the precise movement of already aligned objects.

Text

Icon	Shortcut
	t

The **Text tool** is available from the left toolbar. Clicking in the drawing area with the **Text tool** in hand opens a *dynamically sized* text field for input. Dragging in the drawing area will create a *fixed sized* textbox upon release. Changes made to the text field can be saved by either clicking on an empty part of the drawing area or pressing Esc. Enter can be used for inserting line breaks. When a text field is edited, the following options appear on the top toolbar:

- **Font type** and **size**
- Style elements (**Bold**, **Italic**, **Underline**)
- **Superscript** and **Subscript**
- **Formula** tool: Using the **Formula** tool, the input text is automatically turns to Chemical formula. Existing texts can also be transformed to chemical formula.
- **Symbols**
- **Text color**
- **Highlight color**
- Align options (**Left**, **Center**, **Right**)

> For the **Text color** and **Highlight color** tools, a predefined color palette and the ability to define custom colors are available. See **Create custom colors**.

Shapes

The following **Shapes** are accessible in Marvin from the left toolbar:

Icon	Name	Line Color	Fill color/Opacity/Shadow	Line weight/Line style	Fixed ratio
	Rectangle	✓	✓	✓	NO
	Rounded rectangle	✓	✓	✓	NO
	Ellipse	✓	✓	✓	NO
	Sphere	✓	✓	✓	YES
	Triangle	✓	✓	✓	NO
Arrow object Icon	Arrow	✓	✓	✓	NO
	Star	✓	✓	✓	YES
	Line	✓	✗	✓	NO
	Arc	✓	✗	✓	NO
	Scribble tool	✓	✗	✗	NO
	Cycle	✓	✗	✓/✗	YES
	Recycle	✓	✗	✓/✗	YES
	Flash	✓	✓	✓/✗	YES
	Light	✓	✓	✓/✗	YES
	Explosion	✓	✓	✓/✗	YES

Icon	Name	Line Color	Fill color/Opacity/Shadow	Line weight/Line style	Fixed ratio
	Blocked	✓	✓	✓/✗	YES
	Done	✓	✓	✓/✗	YES
	Electrolysis	✓	✗	✓/✗	YES
	Scissors	✓	✗	✓/✗	YES

Shapes can be placed by selecting them from the toolbar and clicking in the drawing area. In this case they are placed in their default size and ratios. Otherwise, clicking and dragging enables to manually set the dimensions of the shapes during creation. Holding shift during placing a **Rectangle**, **Rounded rectangle**, **Triangle** and **Ellipse** enables the creation of squares, rounded squares, equilateral triangles and circles. Also, when resizing these objects, holding shift will keep the original ratio of the shapes. OTher shapes such as the **Sphere**, **Star**, **Flash**, etc. have fixed ratios, they cannot be distorted, only their size can be set.

When a shape is selected, the following tools may appear on the top toolbar according to the table above:

- **Line Color**: The color of the object's outline can be specified.
- **Fill Color**: The fill color of the object and its opacity can be set and a gray shadow can be also be added.
- **Line Style**: The weight of the outlines can be specified in pixels from 1 to 6. Also, the style of the outlines can be switched between solid and dashed.

> For the **Line color** and **Fill color** tools, a predefined color palette and the ability to define custom colors are available. See **Create custom colors**.
> By defeault, the **Sphere** comes without outlines, the "no line" option being selected in the **Line Color** dropdown menu. The focal point of the sphere can be changed by rotating or flipping the object manually.

Color

Icon	Name
	Color

The **Color** tool, located on the left toolbar, can be used to easily colorize structures and graphical objects on the canvas and to highlight structures and textboxes. Clicking on the tool will reveal a color palette and the *Colorize* and *Highlight* tabs. The former can be used to colorize bonds, atom labels, texts and shapes, while the latter can be used to highlight structural parts and texts.
With the **Color** tool in hand, clicking on an object will take effect. If dragging in the drawing area, the **Color** tool will use the current **selection method** to colorize and highlight objects. Upon releasing the drag, the coloring takes effect. Opposite to the other specific coloring tools such as **Text color**, **Highlight color**, **Line color** and **Fill color** from the top toolbar, the **Color** tool is generic and will affect all eligible objects in the drawing area.

Create custom colors

It is possible to create custom colors in Marvin. When opening the color palette from any of the coloring tools, below the predefined color palette, a *Custom* section is available. Pressing on the Plus button (**+**) will reveal a multifuntional color picker popup. There, the hue and saturation can be set by using the sliders or the color code can be added manually in either Hex or RGB format.
Pressing Apply will add the specified color to the *Custom* section and will be available for every coloring tool in the application. Once custom colors are already available, an *Edit* button appears in the top right corner of the *Custom* section. Pressing *Edit* will enable the removal of custom colors that are no longer needed by clicking on the color icons. Once *Done* is pressed in the top right corner, colors can be selected again for drawing.
If it is enabled by the operator of the application, the custom colors can be saved and remembered by the application upon reopening. If you use Marvin in a browser, the data will be stored in the local storage of the browser by default. For more information on the specifics please check the API documentation.

Image

Icon	Name	Shortcut
	Insert image	**Ctrl/⌘ + i**
	Crop image	-

Clicking on the **Image** icon will open a file browser window. Then, you can select any image file from your local system to add it to the contents of the drawing area. Selected images can be cropped using the **Crop image** tool, accessible either from the top toolbar or the **Context menu** or by clicking twice on the image.

> Crop mode can be left by pressing Enter, Esc, the **Crop image** button or by clicking on an empty part of the drawing area.

Highlight color

Icon	Name
	Highlight color

When a selection contains chemical structures or textboxes the **Highlight color** tool appears on the top toolbar. Selecting a color from the dropdown menu will place a highlight on the selected structure and highlights the selected texts. The highlight can be removed from the same color palette by selecting the *no fill* option.
The size of the highlight depends on the fixed length and the atom label size for bonds and atom labels respectively.

> For the **Highlight color** tool a predefined color palette and the ability to define custom colors are available. See **Create custom colors**.
> If there is a chemical structure highlight on the canvas it can be decided on the **Download image** dialog if it should be included in the exported image.

About Marvin

Information of the version and direct dependencies of the application can be found in the **Main menu/About** dialog. In case a **support ticket** is issued to Chemaxon, please include the content of this dialog as it contains vital information for the development team.

Chemical Drawing tools

Bonds

The following bond types are accessible in Marvin from the left toolbar:

Icon	Name	Shortcut
	Single	**0** and **1***
	Double	**2**
	Triple	**3**
	Up wedge	**w**
	Down wedge	**h** or **Shift + w**
	Wavy	**y**
	Hashed	**Shift + h**
	Dashed	**d**
	Bold**	-
	Dative	-
	Aromatic	-
	Cis or trans	**x**
	Double C/T or unspecified	-
	Single or double	**12**
	Single or aromatic	**14**
	Double or aromatic	**24**
	Any	**Shift + a**
	Coordinate	-

**The '0' hotkey tends to build rings and the '1' hotkey tends to build chains.*
***Besides acting as the other bond tools, **Bold bond** will not overwrite **Double** and **Aromatic bonds** but turns them into their bold versions.*

It is possible to select only bonds without the atoms they are connecting by holding the Alt/⌥ key and clicking on the bond. This feature works in multiselection as well holding Alt/⌥ + Shift together and clicking consecutively on bonds.
Bond color is adjustable, see **Color** tool.

> Holding shift while hovering over an atom with the bond tool in hand offers another angle for placing the bond.
> Shortcuts only works in bond context. Otherwise, press the shortcut key over an empty part of the drawing area to take it in hand.
> When a bond is selected in the drawing area, the top toolbar expands, enabling bond coloring.

Coordinate bond

The **Coordinate bond** can be placed in the drawing area by selecting a group of atoms together with a target atom. If no target atom is selected, the end of the bond is considered a carbon atom. Only one target atom can be selected at once but the selection may contain multiple atom groups. Hovering over any included atom or the bond triggers a purple highlight feedback on the coordination structure. The style of Coordinate bonds in the drawing area can be set from the **Main menu -> Settings -> Coordinate bond**.

Chain tool

Icon	Shortcut
	**Shift + x**

The **Chain tool** facilitates the drawing of longer chains. After taking the tool in hand click and drag in the drawing area to draw alkyl chains. During dragging, the number of chain members is shown at the tooltip.

Templates

The following templates are accessible by default in Marvin from the left toolbar:

Icon	Name	Shortcut
	Benzene	**a**
	Cyclohexane	**6**
	Cyclopentane	**5**
	Cyclobutane	**4**
	Cyclopropane	**v**
	Cyclohexane chair 1	**0**
	Cyclohexane chair 2	**9**
	Cycloheptane	**7**
	Cyclooktane	**8**
	Cyclopentadiene	**z**

By pressing the shortcut key, the corresponding template gets in hand. In bond context, the shortcut action merge the template to the structure in the drawing area. In case a template is in hand, when clicking on atom and dragging the pointer away, the template can be attached to the atom through a single bond, enabling for example the quick drawing of biphenyls.

> Shortcuts **3**, **6** and **7** are working in atom context as well.

Template library

Icon	Shortcut
	**Shift + i**

The **Template library** dialog can be opened from the left toolbar. It contains multiple structural categories with commonly used predrawn structures. Clicking on a template card closes the dialog and takes the appropriate structure into hand that can be placed on the canvas by clicking. The following categories are available by default in Marvin:

- **Aromatics** --> basic and condensed aromatic structures, fullerenes
- **Bicyclics** --> bicyclo alkane rings
- **Conformers** --> structural isomers of cycloalkanes
- **Cycloalkanes** --> a set of cycloalkanes from cyclopropane to ring20
- **Hexoses** --> hexoses displayed in Fischer-projection
- **Supramolecules** --> crown ethers and calixarenes

Atoms

The following atoms can be accessed from the **Left toolbar -> Atoms** combo box:

- **C**
- **H**
- **O**
- **N**
- **S**
- **P**
- **F**
- **Cl**
- **Br**
- **I**

Periodic Table

Icon	Shortcut
	**Shift + p**

Other atoms of the Periodic table can be selected by opening the **Periodic Table** dialog. In the dialog it is possible to create **Atom list** and **NOT list**, see **Query tools**. Also, aliases can be created using the **Text tool**.
When the following atoms are entered using the text tool or by typing when hovering over an atom label, they will be represented as **Abbreviated groups**: **Actinium - Ac, Neptunium - Np, Cerium - Ce, Praseodymium - Pr, Americium - Am**. The appropriate chemical elements can be placed if they are selected from the Periodic table.
Also, it is possible to insert atoms using their shortcuts. Typing an atom label when hovering over the drawing area will take the appropriate element into hand. Typing when hovering over an atom label will exchange it automatically. If one or more atoms are selected, typing will also change their atom labels automatically. If an unavailable atom label is typed, the **Abbreviated groups** input field opens up. The chemical elements can also be accessed from the abbreviated groups library if the exact chemical label is added (*e.g.* **Mg** will reveal Magnesium but **M** will not).

When an atom gets selected in the drawing area, the following new options appear on the top toolbar:

- **Font type** and **size**, which will affect the atom label and the atom properties added to the atom.
- Style elements (**Bold**, **Italic**, **Underline**)
- **Superscript** and **Subscript**
- **Formula** tool: Using the **Formula** tool, the input text is automatically formatted as chemical formula. Existing texts can also be transformed to chemical formula.*
- **Text color** can be used to set colors to atom labels and properties. Also, **CPK coloring** can be used to colorize atoms.

Note that chemical formula is considered a text and thus will not be handled by **Calculations.*

Markush tools

The Markush tools are accessible from the left toolbar, containing the following tools.

RGroup

Icon	Shortcut
R	**r**

The **RGroup** tool lets you place Rgroup labels in the drawing area or on structures with a single click. It is also possible to click on an atom label and dragging the mouse, resulting in a single bond coming from the atom label with an RGroup label on the other end. When using the tool, the application starts the numbering with R1, then automatically increases the number to R2, R3, etc., when placing more labels. The RGroup labels can be renumbered manually by using the **Text tool**. When using the *r* shortcut over an atom label, a simple *R* label will be placed but it is also possible to enter *r1*, *r2*, etc., resulting in the appropriately numbered RGroup label.
In case having at least two bonds connecting to the R-group label and having a corresponding definition, the bonds around the label are numbered in the order of placement indicating their connection pattern on the definition structure.
RGroups are considered eligible for **Enumeration** if a corresponding **definition** is selected with them together.

> The visibility of the ligand order can be changed in **Settings**. Turning the **Show R-group attachment order** on/off will also affect the numbers on the R-group definitions and the Image export.

Define RGroup

Icon	Shortcut
R[]	-

The **Define RGroup** can be used to assign selected structures to the R-group labels. Similarly to the **RGroup** tool, the numbering starts with R1, then the number is automatically increased.
In case of having at least two **RGroup Attachments** on a definition structure, the attachment bonds are numbered in the order of placement indicating their connection pattern on the parent structure.

> The visibility of the ligand order can be changed in **Settings**. Turning the **Show R-group attachment order** on/off will also affect the numbers around the R-group labels and the Image export.

RGroup Attachment

Icon	Shortcut
	-

The **RGroup Attachment** bond visualize the point of attachment between a definition and the parent structure. Note that the wavy end of the RGroup attachment bond is not considered an atom but represents the connection of the RGroup label with the parent structure. For an efficient drawing experience it is suggested to start drawing of RGroups with placing the attachment point first. For more detailed examples see the **Examples page**.

Variable attachment

Icon	Shortcut
	-

The **Variable attachment** tool is the **Marvin** version of the **Position variation** known from **Marvin Sketch** and **Marvin JS**. It enables the representation of atoms and groups connecting to various points of a parent structure. The involved atoms and bonds are highlighted with a patch and give hover feedback.
There are two ways to create Variable attachments in Marvin. The tool can be activated from the left toolbar **Markush tools**. In this case, the tool uses the current selection method and during selection of a molecule or fragment a live feedback shows the content of the Variable attachment upon releasing the selection. The other way is to create the desired selection simply by using the selection tool and then open the context menu and press the **Add variable attachment** button. In the **Main menu -> Structure** submenu the Add variable attachment button may be found that acts the same way as the context menu button.

> The representation of the highlight patch can be changed in **Settings**. In the Variable attachment submenu the reprsentation may be set to **Color highlight**, **Gray highlight**, or **No highlight**.

The **Variable attachment** bond may be moved and the length and angle may be modified by dragging the inside endpoint of the bond. The outside end of the bond may be edited with arbitrary atoms and complex structures.

> The editor recognises if there is a **Variable attachment** group in the drawing area and offers to include the highlight patch during Image export. The default setting may be changed in **Settings**, in the Variable attachment submenu.

Variable attachments are eligible for **Enumeration**.

Charge

Icon	Name	Shortcut
	Increase Charge	+
	Decrease Charge	-

Charge can be set on atoms by taking the **Increase Charge** and **Decrease Charge** tools in hand and clicking on the atom. Any additional click will either increase or decrease the charge.
Charge can also be set from the **Main menu -> Atom** submenu and the **Context menu**, see **Atom properties**.

> The display of **Charge** can be set from **Settings**.

Brackets

The following **Brackets** can be drawn in Marvin from the left toolbar:

Icon	Name

Icon	Name
[ ]	Square bracket
( )	Round bracket
}	Curly bracket

The shortcut **Shift + t** will take the most recently used bracket type into hand. The **Square brackets** and **Round brackets** can be used to create **S-groups**.

Creating S-groups

When a bracket is placed on a chemical structure, an input field pops up enabling the addition of a repetition value that will appear in the bottom right corner of the bracket. Based on the structure and the value, the bracket will be automatically categorized into a repeating unit type.
The value can be edited anytime by double clicking on the bracket or the label or by opening the Bracket properties dialog. A purple feedback highlight appears on the structure when placing, resizing or relocating the bracket indicating the structural part that will be embraced by the bracket upon release. Purple dots mark the attachment points of the bracket.

S-group definitions and rules

The following repeating unit types are available in **Marvin**, for examples see the **Examples page**.

Repeating unit type	Structural conditions[1]	Value conditions
Copolymer (co)	No structural restrictions	Only "co" is accepted
Custom group	No structural restrictions	Any input, included blank is accepted
Graft (grf)	The bracket has even number of crossing bonds on either side (e.g. 1-1, 2-2, etc)	Only "grf" is accepted
Link node	The bracket embraces exactly one atom with 1-1 crossing bonds on either side	Range of integers starting from 1 (*e.g.* 1-4)
Modification (mod)	The bracket has even number of crossing bonds on either side (e.g. 1-1, 2-2, etc)	Only "mod" is accepted
Monomer (mon)	Cannot have crossing bonds on the brackets	Only "mon" is accepted
Multiple group	No structural restrictions	Positive integer (*e.g.* 4)
Repeating unit	The bracket is placed around a fragment that has at least one crossing bond	Must contain range of positive integers[2] ; additionally it can contain other ranges and positive integers; e.g. "2-4", "2-4, 6-9, 11"
SRU polymer	The bracket has even number of crossing bonds on either side (e.g. 1-1, 2-2, etc)	Single letter of the english alphabet (*e.g.* n; m)

[1]*Crossing bonds are bonds that are cut by the bracket or land outside the bracket area.*

[2]*Range can start from 0.*

{info}

- Link node and Repeating unit are eligible for **Enumeration**.
- If the bracket does not fit into any S-group types, it will be categorized as a **Custom group**.
- Hovering either the bracket or the structure, a purple highlight feedback appears on the included structure and a tooltip shows the **Repeating unit type**.

Nesting rules

The following table shows the rules for nesting S-groups into each other. The green tick and red cross indicate if an S-group listed in the column can contain an S-group listed in the row. For example the **Monomer (mon)** type cannot contain a Copolymer (co) but can contain an **SRU polymer**.
A rule of thumb for reading the table is that S-groups that require to have crossing bonds on the bracket cannot contain S-groups that are not allowed to have crossing bonds. Thus, these two main takeaways can be defined:

- **Copolymer (co)** cannot be nested inside any other S-group.
- **Monomer (mon)** cannot be nested in SRU-like polymer types (**Graft (grf), Link node, Modification (mod), Repeating unit, SRU polymer**) as they all require to have one or more crossing bonds (*i.e.* are placed on a fragment), while **Monomer (mon)** cannot have crossing bonds by definition.

Inner groups below ↓	Copolymer (co)	Custom group	Graft(grf)	Link node	Modification (mod)	Monomer (mon)	Multiple group	Repeating unit	SRU polymer
Copolymer (co)	✗	✗	✗	✗	✗	✗	✗	✗	✗
Custom group	✓	✓	✓	✓	✓	✓	✓	✓	✓
Graft(grf)	✓	✓	✓	✓	✓	✓	✓	✓	✓
Link node	✓	✓	✓	✓	✓	✓	✓	✓	✓
Modification (mod)	✓	✓	✓	✓	✓	✓	✓	✓	✓
Monomer (mon)	✓	✓	✗	✗	✗	✓	✓	✗	✗
Multiple group	✓	✓	✓	✓	✓	✓	✓	✓	✓
Repeating unit	✓	✓	✓	✓	✓	✓	✓	✓	✓
SRU polymer	✓	✓	✓	✓	✓	✓	✓	✓	✓

Bracket properties

It is possible to set the properties of S-groups from the **Bracket properties** dialog. The dialog can be opened when the S-group is created by clicking on the icon next to the input field or, if the bracket is already placed on the canvas, right clicking on it will show a **Bracket properties** button that will open the dialog.

- **Bracket type**: The S-group type can be selected. Note, that certain S-groups have structural limitations, thus, only the enabled types can be selected from the list, based on the structure embraced by the brackets.
- **Value, range**: Defines the repetition value of the S-group that will be displayed at the bottom right corner of the bracket. Note, that certain S-groups have limitations on what repetition values are enabled.
- **Bracket style**: Sets the shape of the bracket.
- **Repeat pattern**: Defines if the repeating pattern of repeating structural units is either/unknown (eu), head-to-tail (ht) or head-to-head (hh). Note, that this property is only available for SRU and Repeating unit types. The selected repeating patterns will appear at the top right corner of the bracket:

Repeat pattern	Label*
Head-to-tail	-
Head-to-head	hh
Either/unknown	eu

**The default label is Head-to-tail, which is not displayed on the bracket.*

For more details check the S-group definitions and rules.

The color of the bracket and the labels can be specified using **Text Color** and **Line Color** from the top toolbar upon selection or by using the **Color tool**. In addition, the position of the labels can be manually set in a vertical manner alongside of the bracket.

Graphical brackets

When a bracket is placed in the drawing area and no chemical strcuture is involved, it is considered a graphical bracket. The color of the bracket can be specified using **Line Color** from the top toolbar or the **Color tool** and its size can be customized using the edit points appearing upon selection.

> Holding shift during placing **Brackets** enables the creation of square shaped objects. Also, when resizing brackets, holding shift will keep the original ratio of the bracket.

Reaction components

Arrows

The following **Arrows** are available in Marvin from the left toolbar:

Icon	Name
→	Single
⇌	Equilibrium
⇄	Unbalanced equilibrium
⇝	Rearrangement arrow

Icon	Name
	Resonance
	Open
	Dashed
	Crossed
	Hashed
	Retrosynthesis
	Curved
	Half-headed curved
	Circular
	Single electron flow
	Double electron flow

The arrows can be placed by simply clicking or dragging inside the drawing area with an arrow in hand. In the former case, the arrow will be placed in default length, while dragging enables the dynamic sizing of the arrow. Once an arrow is placed, its direction can be switched by either clicking on it with the arrow in hand or opening its context menu by right click and pressing the *Change direction* button. The length and orientation of the arrows can be changed using the edit points provided at the beginning and the end of the arrow and by rotating it.

Icon	Name
	Change direction

The type of the arrows placed in the drawing area can be changed from the context menu or by taking the desired arrow type in hand from the left toolbar and clicking on the arrow once. The color of the object's outline can be specified using **Line Color** from the top toolbar or by using the **Color tool**.
Single and **Double electron flow** arrows are handled as special types. See details below.

> Using the shortcut **e** will take the most recently used arrow type into hand. Holding shift during placing **Circular arrow** enables the creation of circle shaped arrows. Also, when resizing arrows, holding shift will keep the original ratio of the object.

Electron flow arrows

The **Single** and **Double electron flow** arrows can be used to represent electron movements in the drawing area. They are located on the left toolbar in the **Arrows** subtoolbar. After picking up the tool, the arrow can be created by clicking on an eligible starting point and either dragging the arrow to the target (creating a more rounded arrow) or just clicking on it (creating a more flat arrow). Clicking on the arrow reveals an edit point that can be used to change its curve.
The following objects are eligible starting points for the electron flow arrows:

Starting point	Single electron flow	Double electron flow
Monovalent radical	Can host **one** arrow	n/a
Divalent singlet radical	Can host **two** arrows	Can host an arrow
Divalent triplet radical	Can host **two** arrows	Can host an arrow
Trivalent doublet radical	Can host **three** arrows	Can host an arrow
Trivalent quartet radical	Can host **three** arrows	Can host an arrow
Lone pair	Can host **two** arrows	Can host an arrow
Bond	Can host **two** arrows	Can host an arrow

The electron flow arrows can target any natural atoms and any type of bonds and can be created inside a molecule or between the atoms and bonds of different molecules. **Atom lists**, **NOT lists**, **Query atoms**, **Homology groups**, **RGroup labels**, contracted **Abbreviated groups** and **Aliases**, however, are not eligible targets for electron flow arrows.

Plus sign

Icon	Shortcut
+	-

Plus sign can be accessed from the left toolbar. Placing a **Plus sign** between reagents or products indicate that they participate in a chemical reaction.
When a **Plus sign** is placed in the drawing area, the color of the object's outline can be specified using **Line Color** from the top toolbar.

> Imported reactions that do not contain plus signs, are automatically replaced by the editor.

Map reaction atoms

Icon	Shortcut
•→•	-

The **Map reaction atoms** tool enables the manual creation of atom mappings on the canvas. When having the tool in hand, clicking on an atom label will assign the lowest available atom map number to that atom. If clicking and dragging from an atom with the tool in hand, a blue line will appear between the starting atom and cursor, indicating, that a mapping pair can be created. Releasing the drag over an atom of another molecule will create a mapping on both atoms with the same number. If the drag is started from an atom that already had an atom map number, that number will carried over to the target atom.
If an atom number is hovered or selected and enter is pressed, the value can be manually changed. When editing is over the changes can be applied by pressing Enter, Esc or simply clicking out on the canvas area.
When an atom number is hovered by the cursor, it will be highlighted along with all the other atom map numbers having the same value.

> Atom map numbers are exported into MDL file formats such as MOL V2000, MOL V3000, RXN and SD files.

Electron tools

Add radical

The **Add radical** tool can be used to equip atoms with radicals by click, giving access to monovalent, divalent triplet and trivalent quartet radicals. Divalent singlet radical can only be created by selecting **Context menu -> Radical -> Divalent singlet** and adding another radical using the **Add radical** tool enables the creation of trivalent doublet radicals.
If having three radicals on an atom, using the tool sets the radical state to Off, removing the unpaired electrons.

> All radical types can be set directly from the atom's context and main menu through the **Radical submenu**.

Add lone pair

The **Add lone pair** tool can be used to add one to four lone pairs around an atom. When having four lone pair around an atom, upon clicking a fifth time on it, all lone pairs are removed. The position of a lone pair can be customized by grabbing and relocating it manually when having the **selection tool** in hand.

Abbreviated groups

Icon	Name
⇕	Expand
⇕	Contract
⇱	Ungroup

There are a few ways to add **Abbreviated groups** to the drawing area. First, hovering over an atom and starting typing results in the appearence of an input field and a suggestion list of search hits. This list contains the available abbreviated groups that can be selected by clicking on them or pressing enter. The list is automatically filtered upon typing. Note that **chemical elements** are also accessible from this library when typing exact matches.
The **Text tool** can also be used to overwrite an atom label with an abbreviated group's name (in this case the suggestion does not appear). It is also possible to add abbreviated groups in multiselection of atoms.
Finally, the content of the suggestion list is available from the top toolbar, using the **Search bar**, where even the underlying structure can be inspected as a thumbnail before selecting and placing it on the canvas.

Expand/Contract/Ungroup abbreviated groups

Once an **Abbreviated group** is in the drawing area, it can be **Expanded** from its **Context menu** to show the cleaned underlying structure. In expanded state the attachment points of the abbreviated group are revealed offering a convenient way to create the desired chemical connections with other structures. As long as the **Abbreviated group** is chemically unchanged it can be **Contracted** from its **Context menu**. It is possible to attach bonds to the contracted label as they are automatically connected to the available attachment points. The connection pattern can always be revealed by expanding the abbreviated group.

Upon modifying the chemical content of the structure (*e.g.* adding or removing atoms and bonds, changing the stereochemical information), the abbreviated group is automatically ungrouped and cleaned. It is possible to manually ungroup an abbreviated group from its context menu by using the **Ungroup** command.

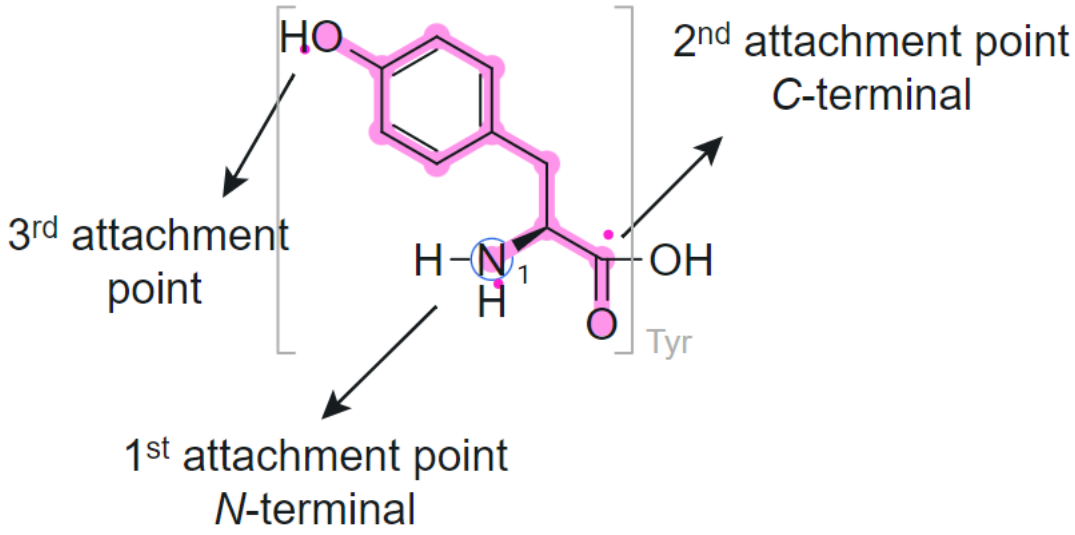
> The expand, contract and ungroup actions work on multiselection of abbreviated groups as well if no other structure or shape is included in the selection.

Display of abbreviated groups

Hovering any part of the expanded abbreviated structure triggers a purple highlight feedback, indicating the structural content of the group. Also a bracket preview appears around the group displaying the label of the contracted group in the bottom right corner. The purple dots on certain atoms indicate the abbreviated group's attachment points, where chemical structures can be attached to it. If the abbreviated group has more than one attachment point, hovering over these atoms reveal their connection index on the pointer. When connecting bonds to a contracted abbreviated group with multiple attachment points, they are used up starting with the attachment point having the index *1* followed by *2*, etc. The connection pattern can be revealed by expanding or ungrouping the abbreviated group.
The abbreviated groups are displayed according to the style settings of the application both in contracted and expanded state. In case the font type or size is modified manually in either state of the group, it will not be altered by the changes of the style settings.

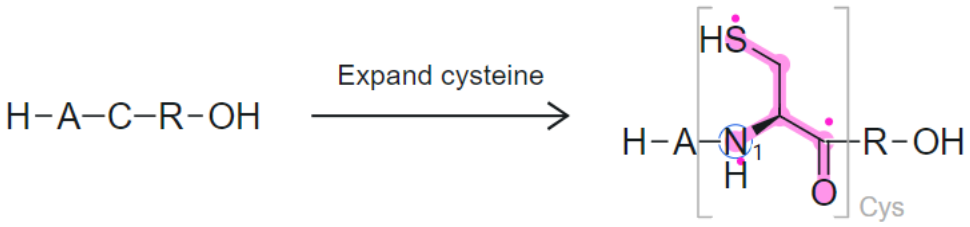
Representation of amino acids and peptides

Alpha amino acids are handled in **Marvin** as a special set of abbreviated groups having multiple attachment points. Their connection indexes are sorted as follows: *N*-terminal attachment point **connection index *1***, *C*-terminal attachment point **connection index *2*** and the third attachment point if available **connection index *3***.



Unlike as in the case of regular abbreviated groups, bonds attached to the contracted amino acid labels are not neccessarily placed in the order of the connection indexes. Following the conventional representation of peptides, attaching a bond from the left side of the amino acid's contracted label is always considered an *N*-terminal connection and a bond attached from the right side of the label is considered a *C*-terminal connection. If the amino acid has a third attachment point (e.g. tyrosine, cysteine), it will only be used up in contracted state if the amino acid already has two bonds occupying the terminal attachment points. The connection pattern and the underlying structure can always be revealed and modified in expanded state.

> The expand, contract and ungroup actions work on multiselection of amino acids and peptides. In the case of peptides, the selection on the molecule can include any other structural parts such as side-chain modifications or terminal groups, in order to support the convenient work with peptides.



Also, in expanded state the attachment points can be used up manually in any desired manner.

The connecting bond between amino acids used as **abbreviated groups** is handled as a special bond type. It is displayed as a single bond but is constrained into horizontal and vertical orientations, broken in 90 degree angles to fit the peptide chain.
If other than single bond types are used to create connections between amino acids, they will be automatically turned into this representation. If the amino acids are ungrouped, they are handled as regular structures, thus any desired bond types can be used between them.
It is possible to create crosslinked and cyclopeptides. For that, simply pick up any bond type and connect the appropriate amino acids. If a contracted amino acid is overloaded with bonds it turns to an alias, thus, its bonds will not be constrained into horizontal and vertical orientations.

Import options for amino acids and peptides

The most convenient way to import amino acids and peptides is through the **Search bar** input field on the top toolbar. For peptides, both 1-letter and 3-letter amino acid input is accepted:

- 1-letter peptide abbreviations using capitalized letters: **MARVIN**
- 3-letter peptide abbreviations, only the first letter is capitalized: **MetAlaArgValIleAsn**

Standalone amino acids can be imported as an **abbreviated group** through the abbrevation suggestion list, using the text tool or the top toolbar's search bar. Otherwise, as a name to structure feature, amino acids can be imported as standard structures using their IUPAC or traditional names.

Peptide display options

The visual representation of the **amino acid** labels can be switched between **1-letter** and **3-letter** options, if handled as abbreviated groups. This can be changed individually by hovering/selecting one or more amino acids and right clicking on the selection to reveal its context menu. Inside, a **Peptide display** submenu is available, where the display of the amino acids can be switched between the 1-letter and 3-letter options. This setting is also available on a selection from the **Main menu -> Structure -> Peptide display** submenu.
In the **Main menu -> Structure -> Peptide display** submenu, the **Amino acids per line** submenu can be accessed, where a list of predefined options are available for wrapping peptide chains. The **...** button opens a dialog for custom values to be added.

Create abbreviated group

Icon	Name
	Create abbreviated group...
	Custom abbreviated group

In **Marvin** it is possible to create custom abbreviated groups that will be listed in the **Custom abbreviated groups**. This action is available on selections of a whole molecule or an undivided fragment by opening the selection's context menu or from the **Main menu -> Structure** submenu. Clicking on the button will reveal a dialog with the cleaned preview of the selected structure and the numbered attachment points if there are any. After typing in a unique name of 3 to 15 characters, the custom abbreviated group can be saved and it becomes available from either the suggestion list (see above) or the **Search bar**. A profile icon is used to support the quick recognition of the custom groups.
In case a whole molecule is selected the abbreviated group will not have attachment points, although the expand/contract/ungroup actions will work. When fragment selections are used for the creation of custom abbreviated groups, the cut bonds are considered attachment points and they are numbered as indicated by the preview. Every eligible bond type is considered a single attachment point, thus, cutting a single or a double bond is handled the same way and indicated as one attachment point. As a result, the attachment points can host any bond types without being ungrouped, although, **valence errors** are marked on the abbreviated group as well. Custom abbreviated groups act the same way as built-in groups, see placement, display. For more detailed examples see the **Examples page**.
If ineligible structural elements are included in the selection, the **Create abbreviated group** action will not be available. Ineligible structural elements are all **Markush tools**, **Query tools**, **S-groups**, **built-in abbreviated groups**, **coordinate complexes**. Regarding the **atom properties**, charges and radicals are enabled to be included in a custom abbreviated group, atom numbers and stereolabels, such as CIP stereodescriptors and enhanced stereo labels are, however, considered ineligible properties.

Custom abbreviated groups

You may find and manage your custom abbreviated groups created by the **Create abbreviated group** action in the **Main menu -> Settings -> Custom abbreviated groups** dialog in alphabetical order. From the dialog it is possible to take an abbreviated group in hand in contracted state using the **Insert** button and then place it on the canvas or a chemical structure. When a custom abbreviated group is selected, the *Rename* and *Delete* buttons appear on their card enabling to rename or remove the abbreviated group. In case there are no custom abbreviated groups saved, then the dialog gives instructions on how to populate the list.
If it is enabled by the operator of the application, custom abbreviated groups can be saved and remembered by the application upon reopening. If you use Marvin in a browser, the data will be stored in the local storage of the browser by default. For more information on the specifics please check the API documentation.

Merge and split components

Icon	Name
	Merge components
	Split components

When multiple chemical structures are selected the **Merge components** action appears in the selection's **Context menu** and becomes enabled in the **Main menu -> Structure** submenu. Merged components are handled as one molecule *e.g* receives a single **Molecule level stereo label**, gets complete selection to a double click and the **Calculations** selection gives a single data box for a complete selection. This feature offers the opportunity to handle salts and other molecular groups in **Marvin**. Hovering any part of the merged structure, a purple highlight feedback appears on every member of the group enclosed in a bracket preview.
The **Split components** action is available from the merged components **Context menu** or **Main menu -> Structure** submenu and separates the merged components to individual chemical structures.

> The **Merge and Split components** actions are available if the selection contains only chemical structures.

Stereochemical representations

Chan-Ingold-Prelog (CIP) stereodescriptors

The **CIP stereodescriptors** can be turned on from the top toolbar, using the **Show Stereo** button.

Molecule stereo

In **Marvin**, the **Molecule stereo labels** can be assigned to any chiral molecules from either the **Main menu -> Structure submenu** or the molecule selection's **Context menu**. The default setting is **Absolute** and it can be changed to **Mixture**. In the **Stereochemistry options** dialog, the visibility and name of the stereochemical flags can

be set.
There can only be either a **Molecule stereo flag** or **Enhanced stereo flags** assigned to a molecule. If switching from the enchaned stereo representation to molecule stereo flag, the enhanced stereo information is lost. Using the **Undo and Redo** buttons restores the previous stereodescriptors.

Enhanced stereo

Enhanced stereo descriptors can be assigned to chiral atoms. By default, all chiral atoms are considered *abs* and this label can be changed from the **Context menu** to *and* and *or* labels. There can only be either a **Molecule stereo flag** or **Enhanced stereo flags** assigned to a molecule.
When having multiple chiral centers in the molecule and turning from **Molecule stereo label** to **enhanced labels**, the remaining chiral atoms are automatically equipped with **enhanced labels** by the following rules:

Molecule stereo label	Selected atom enhanced stereo label	Remaining chiral atoms enhanced stereo labels
Absolute	*abs*	*abs*
Absolute	*and/or*	*abs*
Mixture	*abs*	*and1*
Mixture	*and/or*	*and1*

Geometric transformations

Resize

Graphical objects and images can be resized using the edit points appearing upon selection. This option is available for **Shapes**, **Brackets**, **Arrows**, **Plus sign**, **Text box**, **Images** and **Scribbles**.

Rotate in 2D

When an object is selected the appearing rotate icon indicates that it can be rotated in 2D. This option is available for **molecular structures**, **Shapes**, **Brackets**, **Arrows**, **Images** and **Scribbles**.

Mirror & Rotate

Icon	Name	Shortcut
	Mirror horizontal	**Alt/⌥ + h**
	Mirror vertical	**Alt/⌥ + v**
	Rotate horizontal	-
	Rotate vertical	-
	Mirror group	-
	Rotate group	-

When selecting chemical structures in the drawing area, the **Mirror & rotate** submenu appears in the **Context menu**. The **Mirror/Rotate horizontal** and **Mirror/Rotate vertical** actions mirror or rotate the selection in 180° around a horizontal or vertical axis in the plane of the drawing. This feature is feasible on complete molecules and fragment selections.
The **Mirror group** and **Rotate group** options appear when the selected fragment is only connecting to the rest of the structure through one connection point. In that case, the connecting bond acts as the axis for the geometrical transformation.

> The **mirror** transformation results in the **inversion** of the stereocenters. The **rotate** transformation results in the **retention** of the stereocenters.

Query tools

Query Atoms

The following **Query Atoms** are available from the left toolbar:

Icon	Name
A	Any non hydrogen
AH	Any atom
Q	Hetero atom
QH	Hetero atom or hydrogen
M	Metal
MH	Metal or hydrogen
X	Halogen

Icon	Name
XH	Halogen or hydrogen

Homology groups

Icon	Name
ALK	**Homology groups**

In the left toolbar, the following **Homology groups** are available from the opening dialog. The definitions can be found at the **Homology groups** page. The homology groups are displayed in the drawing area with their long names. If the atom label is edited manually and the abbreviation is added, upon finishing editing the abbreviation is switched to the corresponding long name.

Name	Abbreviation
Actinide	ACT
AlkaliMetal	AMX
Alkenyl	CHE
Alkyl	CHK
Alkynyl	CHY
AnyAtom	-
AnyGroup	XX
Aryl	-
Carboalicyclyl	CYC
Carboaryl	ARY
Carbocyclyl	-
CarbonChain	-
Cyclyl	-
Fusedheteroalicyclyl	-
Fusedheteroaryl	-
Fusedheterocyclyl	HEF
Haloalkyl	-
Halogen	HAL
Heteroalicyclyl	-
Heteroaryl	-
Heterocyclyl	-
Heteromonoalicyclyl	HET
Heteromonoaryl	HEA
Heteromonocyclyl	-
HeteroSubstitutedAlkyl	HSA
Hydroxyalkyl	-
Lanthanide	LAN
Metal	MX
OtherMetal	A35
Protecting	PRT
RingSegment	-
TransitionMetal	TRM
UnknownGroup	UNK

Atom lists/NOT lists

In the **Periodic table** dialog, **Atom lists** and **NOT lists** can be created and assigned as an atom label. Atom lists are eligible for **Enumeration**

Query bonds

The list of **Query bonds** available in **Marvin** are listed in **Bonds**.

Atom query properties

The following **Atom query properties** are available in **Marvin**:

Name	Abbreviation	Eligible values	Collision of values
Total H count	H	Empty, 0-99	MIXED
Implicit H count	h	Empty, 0-99	MIXED
Connections	X	Empty, 0-99	MIXED
Smallest ring size	r	Empty, 0-99	MIXED
Ring count	R	Empty, 0-99	MIXED
Unsaturated	u	Yes/No	No
Ring bond count	rb, rb*	Off, As drawn, 0-99	Off
Substitution count	s, s*	Off, As drawn, 0-99	Off
Aromaticitiy	a, A	Off, Aromatic, Aliphatic	Off
SMARTS*	n/a	Any string	MIXED

> *For more information on how SMARTS queries are handled see the **Query guide**.

Atom query properties can be assigned to atoms in multiselection mode as well. When there is a collision of values between atom query properties in multiselection, the dialog shows the above values. In these situations, applying a modification of the values will result in unified values on the atoms. For example, two atoms are selected, one of the having *X1* and the other having *X3*, the dialog displays *MIXED* in the *Connections* field. Setting the value to '2' and applying the modification will result *X2* on both atoms.

Valence

In **Marvin** custom valence values can be assigned to atoms from the **Main menu -> Atom -> Valence** submenu or the selection's context menu. There is a range of predefined values from 0 to 8 that can also be assigned in multiselection of the same type of atoms. Custom values can also be added for individual atoms.

Bond properties

When there is a selection in the drawing area that includes bonds, **Bond properties** become accessible from the **Main menu -> Bond** submenu or the **Context menu**.

Topology

The **Topology** value is **Undefined** by default and may be switched to **In ring** or **In chain** from the selection's context menu or the **Main menu -> Bond -> Topology** submenu.

> Setting **Topology** is enabled in mixed selection as well.

Reacting center

The **Reacting center** value is **Undefined** by default and the following values may be set.

Icon	Name
-	Undefined
#	Center
|	Make or break
||	Change
|||	Make and change
×	Not center

> Setting **Reacting center** is enabled in mixed selection as well.

Atom properties

When there is a selection in the drawing area that includes atoms, the **Atom properties** become accessible from the **Main menu -> Atom** submenu or the **Context menu**.

Charge

The **Charge** can be selected from predefined values or custom values can be used by clicking on the "**...**" icon. The selected values can be modified using the **Charge** tool.

> Setting **Charge** is enabled in mixed selection as well but custom charge can only be assigned in single selection.

Enhanced stereo

The **Enhanced stereo** labels can be assigned to any chiral atoms. The toggle button in the submenu is a global on/off button for **Stereochemical labels** in the drawing area.

> In multiselection, it is possible to set enhanced stereo labels, choosing from the predefined label set.

Isotope

For natural elements, an **Isotope** may be selected. The default setting is **Off** indicating a natural mixture of isotopes. Predefined values may be selected from the submenu or custom values can be added by clicking on the "**...**" icon.

> In multiselection, the **Isotope** option is only available when selecting atoms of the same type.

Periodic table

The **Periodic table** tool is available from the **Atoms** combo box as well.

Radical

The default setting of **Radical** is **Off** and it can be switched to the following states from the atom's context menu and if selected, from the main menu:

- **Off**
- **Monovalent**
- **Divalent singlet**
- **Divalent triplet**
- **Trivalent doublet**
- **Trivalent quartet**

On the left toolbar, the **Electron tool** can be used to add radicals manually to an atom.

> Assigning radicals is enabled in mixed selection as well.

Atom numbering

Icon	Name
123	**Add atom numbers**

In Marvin it is possible to assign numbers to atoms. There is two main method to do that: generating **Generic numbers** or **IUPAC numbers**. These numbers can be **overwritten manually** to any numbers, letters and special characters. If an atom or molecule already has numbers, using any method to generate numbers will remove the existing ones. Naturally, undo can be used to revert such an action.

> Numbers are not updated automatically upon modifying the structure. If You desire to regenerate numbers, one of the above methods should be applied.
>
> > **Abbreviated groups** in contracted and expanded state can be numbered independently from each other. For example, if a number is assigned to the contracted label of the abbreviated group, upon expansion of the group the underlying structure is not numbered.

Generic numbers

It is possible to assign positive integer numbers to atoms in the drawing area that starts from 1 on each molecule. When an atom is hovered or selected, opening the context menu with right click will reveal the **Add atom numbers** submenu and inside the **Generic numbers** button. Pressing the button will assign the lowest available number to the atom in that molecule (upon selection, the action is also available from the **Main menu -> Atom -> Add atom numbers** submenu). When multiple atoms or complete molecules are selected the numbers are assigned automatically from 1 in each molecule based on the order of placement of the atoms. The numbers can be deleted by the **Erase** tool or by selecting and deleting them using **shortcuts**. Also, atom numbers are removed if the atom label is exchanged.

> **Merged components** are considered a single molecule when assigning atom numbers. In case an atom number is deleted and then reassigned again, it may be different from the original value as the lowest available number will be assigned to the selected atom.

IUPAC numbers

In contrast to **Generic numbers**, IUPAC numbers can be generated only on full molecule selections from the selection's Context menu or the Main menu. Pressing the **IUPAC numbers** in the **Add atom numbers** submenu will assign atom numbers based on the IUPAC naming algorythm.

Customize atom numbers

Any atom number (*i.e.* generic and IUPAC numbers) can be modified manually to any desired value. Numbers, letters and special characters are accepted. Custom atom numbers are saved and will be kept during copy/paste actions or upon reopening a file. Selecting atoms with custom atom number values and pressing either the **Generic numbers** or **IUPAC numbers** button will reset the numbers to positive integers based on the application's numbering algorythm.

The atom numbers can be colorized independently from the atom label by using the **Color Tool** or in selection mode from the top toolbar, using the **text color** tool. Also, they can be moved around the atom labels to arbitrary positions.

The visibility of the atom numbers in the drawing area can be turned Off/On from **Main menu -> Settings** using the **Show atom numbers** toggle button. If this toggle is turned Off, the **Add atom numbers** action will not be displayed in the context menu and will be disabled in the main menu.

Chemical calculations & services

Calculations

Icon	Name	Shortcut
MW	**Calculations**	**Ctrl/⌘ + Shift + c**
	Copy text	n/a

Activation of the **Calculations** tool enables the quick and convenient retrieval of advanced chemical calculations on structures. Selecting a chemical entity with the Calculations turned on will instantly reveal a list of calculation results according to the **Calculations settings**. The databox can be persisted in the drawing area using the **pin** button and then it can be relocated manually. Structural changes such as overwriting atom labels, changing bonds, adding or removing structural elements from the selection will update the data content of the pinned box. Pinned boxes will be displayed on exported images. Upon clicking the pin button again the box disappears. Right clicking on the box will reveal its Context menu, where the calculation settings submenu and the **Copy text** button can be found. The Copy text action will copy the calculation results onto the clipboard as unformatted text.

Calculation settings

The list of calculations available in **Marvin** can be found in the **Visibility settings**. Using the toggles in the Settings, the various calculations can be turned On/Off that will affect all newly placed boxes. The content of the pinned boxes can be modified by right clicking on the box and entering the **Calculations** submenu. These changes will only affect that specific databox from where the local settings were opened.
The *Formula*, *Molecular weight* and *Exact mass* values are calculated on both complete molecule and fragment selections as well. The other properties are calculated only on full molecule selections.

Clean

Icon	Name	Shortcut
2D	Clean	**Ctrl/⌘ + Shift + k**
	Clean to scaffold	-
3D	Clean 3D	-

Marvin provides three cleaning option for chemical structures:

- **Clean** standardizes irregular bond angles and bond lengths in 2D matching the current style settings.
- **Clean to scaffold** attempts to align molecules according to their core structures to provide a common orientation and eventually support the convenient overview of a set of molecules.*
- **Clean 3D** will return the 3D structure for the molecule based on Dreiding force field.

In case there is a selection on the canvas, the clean action will only be applied to the selected structures. Note, that **Clean** can also be used on fragments, while **Clean to scaffold** and **Clean 3D** can only be applied on whole structures.

*This feature is in experimental status, improvements can be expected in later versions.

Aromatize/Dearomatize

Icon	Shortcut
	Alt/⌥ + k

The **Aromatize** service transforms the molecule from Kekulé representation to aromatic representation by using the general aromatization method.
The **Dearomatize** service transforms the molecule from aromatic representation to Kekulé representation. (This method does not check by default if Hückel's rule is valid.)
Pressing the button successively, the function converts the structure from Kekulé to aromatic form back and forth. If there is a selected aromatic ring in the drawing area, the aromatize and dearomatize method works only for the selected structure.

Show stereo

Icon	Shortcut

Icon	Shortcut
	Shift + s

The **Show stereo** service assigns the *R* or *S* label to chiral centers and the *E* or *Z* label to unsymmetrical double bonds.

Add or remove explicit H

Icon	Shortcut
	Ctrl/⌘ + Shift + h

Adds or removes hydrogen atoms to/from the selected structures or fragments. If there is no active selection, changes apply to every atom in the drawing area.

Search bar

The **Search bar** is located on the top toolbar of the application as an input field. It can be used to quickly access structures and tools and also, it acts as a name to structure service.

Searching for structures and tools

Typing input in the Search bar will reveal an automatically filtered list of hits grouped into categories. Selecting a hit will take the appropriate tool in hand ready to use in the drawing area. The following categories can be accessed from the input field:

- Chemical elements
- Query atoms
- Homology groups
- Abbreviated functional groups
- Templates
- Editing tools (e.g. bonds, reaction arrows, template library)
- Dialog windows (e.g. Stereochemistry options, Style settins)

The input is checked for prefix matching, thus will be compared with the beginning of the names of the items. Chemical elements are filtered for their label, therefore will only be displayed on 1 and 2 character inputs. Query atoms are filtered for either their label or their long name.

> Abbreviated functional groups and templates have a thumbnail next to their names where an enlarged preview of the structure can be revealed upon hovering.

Name to structure

The **Name to structure** service can be accessed as an input field for importing structures based on their names or chemical file formats. Common names, drug names and acronyms are suggested by the editor upon input in the **Insert molecule** category. Also,adding an exact input and then pressing enter will import the corresponding structure. The following inputs are supported: *IUPAC*, *common names*, *drug names*, *acronyms*, *SMILES*, *SMARTS*, *CAS Registry Numbers®* and *CXON*. Also, peptides can be imported using 1-letter or 3-letter amino acid abbreviations. For more information see the **Import options for amino acids and peptides** section.

> For more information about the underlying technology, see **Name to Structure**.

Structure to Name

Icon	Name
IUPAC	**Structure to name**
	Copy text

The **Structure to Name** action can be reached on a selection of a single or multiple full molecules from either the **Main Menu -> Structure** submenu or the **Context menu** by right click. The generated name is placed under the selected structures. Upon modification of the chemical structure, the name is automatically updated to match the new compound. It can be removed by the **Erase** tool or by selecting the name and removing it by shortcut.
Upon selecting the name, styling tools appear on the top toolbar to customize the font type, size, style, color and highlight of the name. These formattings are kept if the complete structure is duplicated or copied and pasted. Upon changing the structure or duplicating only a fragment of it, only the full text stylings are kept.
The IUPAC name can be partially or fully copied by entering the name as a regular textbox. In addition, upon opening the context menu of the name, the **Copy text** button is available, that copies the unformatted name onto the clipboard. The name itself cannot be changed manually on the canvas.

Expand generic structure

Icon	Name
	Expand generic structure

It is possible to enumerate generic structures in **Marvin** into the drawing area or export the results in an SDFile. The following chemical entities are eligible for enumeration:

- Markush structures including **RGroups with definition** and **Variable attachment**

- Repeating unit and link node **S-groups**
- **Atom lists**
- **Bond lists**

In order to use this feature, a complete molecule that contains the enumerable groups has to be selected and then the **Expand generic structure** submenu appears in the selection's context menu and the **Main menu -> Structure** submenu. Pressing the **Paste to canvas (up to 50)** button will generate up to 50 resulting structures in the drawing area. If the enumeration provides more than 50 structures, the results can be exported in an SDFile. This option is also available from the Expand generic structure submenu. If the number of results exceeds 1000 structures, only the first 1000 will be exported in the SDFile.

> If only a fragment is selected of the RGroup definition together with the corresponding RGroup containing molecule, it is still considered eligible for enumeration. In this case, only the selected parts of the definition will be used for the enumeration.

Predict NMR spectrum

In **Marvin** it is possible to predict 1H or 13C NMR spectrum for a single, selected structure. If a structure is selected, NMR prediction can be requested either from the **Main menu/Structure/NMR Prediction** submenu or by right clicking on the selection and NMR Prediction will be readily available from the appearing menu. Once 1H or 13C NMR prediction button is pressed, a side panel appears at the right side of the window with the appropriate NMR spectrum.
Chemical shifts are displayed in ppm on top of the peaks. It is possible to zoom in to the spectrum and pan it around to inspect the peaks in more detail. When a peak is hovered, it will be distinguished with a purple highlight. Pressing the **X** button in the top right corner of the spectrum or clicking outside will remove the side panel.

Check and fix structures

Icon	Name	Shortcut
	**Check structure**	Alt/⌥ + s

Marvin offers a handful of structure checkers and - if available - fixers to highlight incorrect structure display and tackle the found issues. Checker mode can be initiated by pressing the **Main menu/Structure/Check structure** button or by pressing Alt + s or by having a selection including chemical content, opening the **Context menu** by right clicking inside the selection and pressing the **Check structure** button.
As a result, a floating dialog will pop up in the upper right corner of the window, giving information on the current status of the checker and the fixer:

- *Select whole molecule(s) to check* in case there is no active selection on the canvas
- *No errors found on selection* in case the checkers found the structures correct
- *Checker service is not available* in case the service cannot be used (*e.g.* network connection issue, bad request, etc.)
- This dialog also hosts the list of the found issues and the available fixers

When an issue is found on the drawings, the affected atoms and bonds get a red outline to highlight the location of the issues. In case fixers are available for structural errors and they are selected for fixing, the affected atoms and bonds get a transparent red highlight patch. This visual feedback indicates which structural parts will be subject of the fixes.

The following checkers and fixers are available in Marvin:

Checker	Fixer
Ring Strain Error	-
Non-standard Wedge Scheme	Yes
Non-stereo Wedge Bond	Yes
Incorrect Tetrahedral Stereo	Yes
Molecule Charge	Yes
Overlapping Atoms	Yes
Overlapping Bonds	Yes
Bond Length	Yes
Bond Angle	Yes

Valence error

In **Marvin**, the **Valence error** is indicated by a red, dashed ellipse around the atom label.

> The visibility of the valence error can be changed in **Settings**.

Autosave document

It is possible in Marvin to automatically save the content of the drawing area continuously during editing. The most recently autosaved file can be reopened from the **Main menu** by pressing the **Reopen latest** button. The tooltip of the button reveals the date of the saved file. If it is enabled by the operator of the application, the autosave can be used. If you use Marvin in a browser, the data will be stored in the local storage of the browser by default. For more information on the specifics please check the API documentation.

Import/Export

Import

Open

The **Open** dialog can be reached from the **Main Menu** to open files. **Marvin** supports the CXON and MRV chemical file formats and **JPG**, **PNG**, **SVG** and **BMP** image file formats for import.

> The **Name to structure** field supports a wide range of chemical notation languages for import.

Insert

The **Insert [Ctrl/⌘ + i]** dialog can be reached from the **Main Menu** to open image files. The **listed** image file formats are supported by **Marvin**. Also, the **Image** button from the left toolbar opens the **Insert** dialog.

> The **Insert** dialog can be opened using the **Ctrl/⌘ + i** shortcut as well.

Export

Download as file

Icon	Name	Shortcut
	Download	-
	Download as file	**Ctrl/⌘ + s**

The **Download** button enables the export of the drawing area in a chemical file format. **Marvin** supports the following file formats.

- CXON
- MRV
- MDL Molfile
- SMILES
- SMARTS
- InChI
- InChIKey
- MDL Molfile V3000
- CDX
- SKC
- MDL SDF
- MDL RDF
- MDL RXN

> The **Copy as** option also offers **PNG** and **SVG** image formats.

Pressing the **Export** button downloads the data in file format, while the **Source** button copies the data onto the clipboard.
Download can also be reached from the **Main Menu**.

Download as image

Icon	Name
	Download as image

The **Download** button enables the export of the drawing area in an image file format. **Marvin** supports the export of images in **JPG**, **PNG**, **SVG**, **WebP** and **TIFF**. The width and height of the exported image can be set.
If there is an active selection in the drawing area, the **Selected area only** options enables the export of the corresponding part of the drawing area.
In addition, if there is a **Variable attachment** group in the drawing area and the visibility of the variable attachment highlight is turned On, then the **Include variable attachment highlight** option enables the export of the **Variable attachment** highlight on the image. Similarly, if there is a multiple substituted Rgroup with an RGroup definition on the canvas and the visibility of the RGroup attachment order is turned On, the **Include R-group attachment order** checkbox appears in the image export dialog. In case there is a chemical structure highlight on the canvas, it can be decided to be included in the exported image from the dialog.

Visibility settings

In the **Main menu -> Settings** submenu, various visibility options are available. These settings affect the schemes in the drawing area and the imported structures as well. In addition, the most prominent visibility settings, namely **Use CPK coloring**, **Show valence errors**, **Molecule visualization** and **Style settings** can be accessed from the **Context menu** by clicking on an empty part of the canvas.
If it is enabled by the operator of the application, these settings can be saved and remembered by the application upon reopening. If you use Marvin in a browser, the data will be stored in the local storage of the browser by default. For more information on the specifics please check the API documentation.

> In case there is a selection on the canvas, the visibility settings context menu can be opened outside the selection, from an empty part of the canvas.

Charge

The display of **Charge** may be set to **Default** or **Circled**.

Calculations

The display of newly placed **calculation** databoxes can be set. The following calculations are available in **Marvin**:

Calculated on every selection:

- Formula
- Molecular weight
- Exact mass

Calculated only on full molecule selections:

- m/z
- logP
- pKa
- Elemental analysis
- logS
- tPSA
- IUPAC name

This setting will affect all newly placed boxes on the canvas and will not modify the content of the pinned databoxes.

Peptide display

The visual representation of the **amino acid** labels can be switched between **1-letter** and **3-letter** options.
Under the **Amino acids per line** submenu a list of predefined options are available for wrapping peptide chains. The **...** button opens a dialog for custom values to be added.

Coordinate bond

Three display option are available for the **Coordinate bonds**:

- **Solid**
- **Hashed**
- **Dashed**

Variable attachment

The display of the **Variable attachment** highlight color may be set to **Color highlight** or **Gray highlight**. The display of the **Variable attachment** highlight color may be set to **Color highlight** or **Gray highlight**.

Molecule visualization

The display of chemical structures in the drawing area may be set from the **Molecule visualization** dialog to the following visibility options:

- **No implicit hydrogens**
- **Skeletal** (*default*)
- **Implicit hydrogens on terminals and heteroatoms**
- **Heavy atoms without implicit hydrogens**
- **Structural**

Stereochemistry options

The display and visibility of **Molecule level and enhanced stereochemical flags** can be customized in **Marvin**. From the **Stereochemistry options** dialog, the visibility of molecule level stereochemical notations and atom level enhanced stereo notations can be switched between **On** and **Off**. Also the selective display of 'chiral' and 'not chiral' flags and their names can be changed from the dialog.

The following *Chiral* flag names are available:

- **Absolute**
- **Chiral**

The following *Not chiral* flag names are available:

- **Mixture**
- **Racemic**
- **Relative**
- **Not absolute**
- **Not chiral**

> The selected Chiral and Not chiral flag names are effective to the whole drawing area.

The global visibility of molecule level and atom level chiral flags can also be set from the **Context menu -> Enhanced stereo** submenu and, if complete molecules are selected, from the **Context menu -> Stereo** submenu.

Style settings

From the **Style settings** dialog, the following structural display options can be set: From the **Style settings** dialog, the following structural display options can be set:

- **Bond spacing** -> sets the distance between double and triple line bonds in percentages of the bond length.
- **Fixed length** (unit: points)* -> sets the bond length between the atoms.
- **Width** (unit: points) -> sets the bond width.
- **Bold width** (unit: points) -> sets the bold bond width.
- **Margin width** (unit: points) -> sets the amount of space around the atoms that is masked out of the connecting bonds.
- **Hash spacing** (unit: points) -> sets the distance between bond hashes. Only affects the **Down wedge bond** and the **Hashed bond**.
- **Atom font and properties** -> sets the default font type for atom labels and atom and bond properties.
- **Atom label size** -> sets the default size for atom labels and atom and bond properties.

Commonly used scientific journal styles with predefined settings are provided in the editor in a dropdown list. Currently, the following journals can be accessed from the menu:

- **ACS 1996 (default)**
- **Wiley**
- **Advanced Synthesis and Catalysis**
- **RSC**
- **Nature**
- **CellPress**
- **Synthesis/Synlett**

Custom styles can also be defined by selecting **Custom style** from the predefined style list and by changing the settings. If it is enabled by the operator of the application, custom styles can be saved and remembered by the application upon reopening. If you use Marvin in a browser, the data will be stored in the local storage of the browser by default. For more information on the specifics please check the API documentation.

When there is a conflict between style settings during import, a **Style options** dialog pops up enabling manual resolution of the conflict. Selecting *Use Imported* will apply the style settings of the imported structures, while *Keep Original* will force the imported structure to adapt to the style settings of the drawing area.

> The effect of the modifications can be checked instantly on the dynamically changing example structure.
> The applied settings will not affect the atom fonts and/or label sizes which were set uniquely in the drawing area. *The Fixed length also scales graphical objects proportionally. Objects included are **Shapes**, **Brackets**, **Arrows**, **Plus sign**, **Text boxes**, **Images** and **Scribble lines**.

CPK coloring

CPK coloring of atoms can be switched between **On** and **Off**.

Atom numbering

The visibility of the **Atom numbers** can be set by the **Enable atom numbers** toggle button, affecting the whole drawing area. When turned on, all existing atom numbers are visible. Switching the toggle to **Off** hides the atom numbers but they are remembered by the application, thus, turning the toggle button back **On** will reveal them again.

R-group attachment order

The visibility of the RGroup ligand order around the **RGroup labels** and the **RGroup attachments** can be set using the **Show R-group attachment order** toggle button.

Valence errors

The visibility of the **Valence errors** can be set using the **Show valence errors** toggle button.

Variable attachment highlight

This switch icon sets the general visibility of the highlight patch of **Variable attachments** between **On** and **Off**.

Shortcuts & tricks

Notable new features

Calculations

The **Calculations** feature enables fast access to the most important information about molecules. Formula, molecular weight and exact mass are now only a click away from you. Check out how to use **Calculations** tool in **Features**.

Scribble tool

The **Scribble tool** enables you to create handmade notes and shapes on the canvas to visualize your thoughts and ideas. This feature supports being creative and thinking outside the box making your drawings unique and special. Check out **Scribble tool** in **Features**.

Customize labels

Marvin enables you to manually move and customize the style of not only the atom labels but also **Atom properties** such as stereo notations, charges or query propertes according to your needs.

Accessible application

Based on the **Web Accessibility Initiative** guidelines **Marvin** supports the accessible use of the application including keyboard navigation and screen reader compatibility. For more information check out the available shortcuts and keyboard commands below.

Shortcuts

General shortcuts

Shortcut	Action
Ctrl/⌘ + a	Select all canvas content
Ctrl/⌘ + o	Open file (Replace)
Ctrl/⌘ + i	Insert file/image (Add)
Ctrl/⌘ + s	Export file
Ctrl/⌘ + k	Copy as
Ctrl/⌘ + x	Cut
Ctrl/⌘ + z	Undo
Ctrl/⌘ + Shift + z	Redo
Ctrl/⌘ + scrolling	Zoom in/out
Delete / Backspace / fn + Backspace	Erase
Ctrl/⌘ + c	Copy
Ctrl/⌘ + v	Paste
Ctrl/⌘ + d	Duplicate
Ctrl/⌥ + drag	Duplicate selected structure
Double click	Select whole structure
Esc	Selection tool
Alt/⌥ + h	Mirror horizontal
Alt/⌥ + v	Mirror vertical
Ctrl/⌘ + Shift + x	Clean up reaction
Space + drag	Pan the canvas
Ctrl/⌘ + 1	Fit to canvas

Canvas context shortcuts

These shortcuts can be used when the canvas is in focus.

The following shortcuts get the appropriate bond on the tooltip:

Shortcut	Bond
1	Single
2	Double
3	Triple
w	Upper wedge
h / Shift + w	Down wedge
y	Wavy
Shift + h	Hashed
d	Dashed
x	Cis or trans
12	Single or double
14	Single or aromatic
24	Double or aromatic
Shift + a	Any

The following shortcuts get the appropriate template on the tooltip:

Shortcut	Template

Shortcut	Template
a	Benzene
z	Cyclopentadiene
v	Cyclopropane
0	Cyclohexane chair 1
9	Cyclohexane chair 2
8	Cyclooktane
7	Cycloheptane
6	Cyclohexane
5	Cyclopentane
4	Cyclobutane

The following shortcuts open a dialog or get a tool in hand:

Shortcut	Template
Shift + x	Chain Tool
r	RGRoup
+	Positive charge
-	Negative charge
Shift + t	Brackets
e	Arrows
t	Text
Shift + i	Template library
Shift + p	Periodic table

Services:

Shortcut	Tool
Ctrl/⌘ + Shift + c	Calculations on/off
Ctrl/⌘ + Shift + k	2D clean
Alt/⌥ + k	Aromatize/Dearomatize
Ctrl/⌘ + Shift + s	Show stereo
Ctrl/⌘ + Shift + h	Add or remove explicit H
Alt/⌥ + s	Check structure

Atom context shortcuts

These shortcuts can be used when an atom is in focus or selected.

Shortcut	Tool
0	Single bond left orientation
1	Single bond right orientation
4	Upper wedge bond
5	Down wedge bond
3	Benzene
6	Cyclohexane
7	Cyclopentane
2	Acyl group*
Shift + click	Selects multiple atoms
+	Increase charge
-	Decrease charge
Enter/type	Edit label

> *It adds an acyl group to primary/terminal atoms and an oxo group to secondary atoms

Bond context shortcuts

These shortcuts can be used when a bond is in focus or selected.

The following shortcuts change the bond type:

Shortcut	Tool
1	Single
2	Double
3	Triple
w	Upper wedge
h / Shift + w	Down wedge
y	Wavy
Shift + h	Hashed
d	Dashed
x	Cis or trans
12	Single or double
14	Single or aromatic
24	Double or aromatic
Shift + a	Any

The following shortcuts merge the appropriate template to the structure:

Shortcut	Template
a	Benzene
z	Cyclopentadiene
v	Cyclopropane
0	Cyclohexane chair 1
9	Cyclohexane chair 2
8	Cyclooktane
7	Cycloheptane
6	Cyclohexane
5	Cyclopentane
4	Cyclobutane

Other shortcuts:

Shortcut	Action
Alt/⌥ + click	Selects bond without its atoms
Alt/⌥ + Shift + click	Selecting multiple bonds without atoms

Text context shortcuts

These shortcuts will affect text contents.

Shortcut	Action
Ctrl + b	Bold
Ctrl + i	Italic
Ctrl + u	Underline
Ctrl + ,	Subscript
Ctrl + .	Superscript

Keyboard navigation

Toolbar navigation

Shortcut	Action
TAB	Navigate between the toolbars and the canvas.
Left/Right arrows	Navigate between top toolbar objects and open/close sub toolbars from the left toolbar.
Up/Down arrows	Navigate between left toolbar objects.
Enter/Space	Open/close menus and sub toolbars and activate/deactivate top toolbar services.
Esc	Close menus and sub toolbars.

Main menu and Context menu navigation

Shortcut	Action
Up/Down arrows	Navigate between menu items.
Left/Right arrows	Open/close submenu.
Enter/Space	Select menu item.
Esc	Close menu.

Dialog window navigation

Shortcut	Action
TAB	Enter dialog and navigate between dialog fields and buttons.
Up/Down arrows	Open and navigate inside lists and the elements of the **Periodic table**.
Enter/Space	Open lists and select item.
Esc	Close lists and close the dialog.

Entering canvas

Shortcut	Action
TAB	Enter canvas.
Ctrl/⌘ + Left arrow	Select the top visible object and navigate between objects from top to bottom.
Ctrl/⌘ + Right arrow	Navigate between objects from bottom to top.
Enter	Enter selected chemical structure by placing the focus on the top left atom.
Arrows	Move the selected object on the canvas

Navigation inside structures

Shortcut	Action
Arrows	Move the focus around the molecule's atoms and bonds. Move the selected object (atom/bond/molecule/graphical object).
Shift + arrows	Move the selected object (atom/bond/molecule/graphical object) faster.
Ctrl/⌘ + Enter	Select the atom/bond in focus
Shift + Space	Open Context menu.
Shift + Enter	Move back from atom selection to focus.
Enter	Open text editing mode on the atom in focus/selection.
Alt/⌥ + Right/Left arrow	Rotate the selected object 1 degree clockwise and counter clockwise
Shift + Alt/⌥ + Right/Left arrow	Rotate the selected object 15 degrees clockwise and counter clockwise
Esc	Remove the focus/selection and get the **Selection tool** in hand.

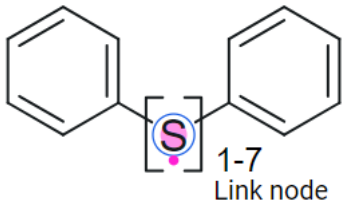
Examples

Create S-groups

The behavior of S-groups in **Marvin** is described in the **Features** chapter.

Link node

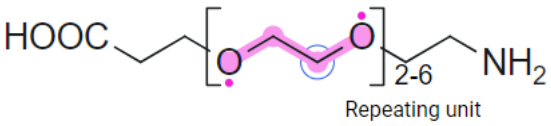
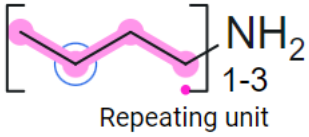
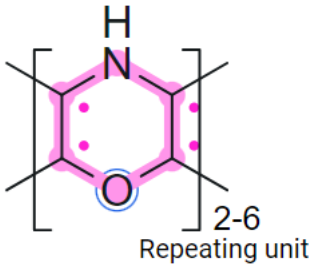
- **Structural conditions**: The bracket is placed around one atom that has two connecting and crossing bonds
- **Value conditions**: Range of integers starting from 1 (*e.g.* 1-4)



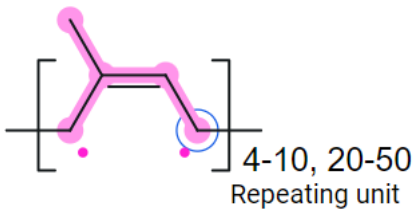
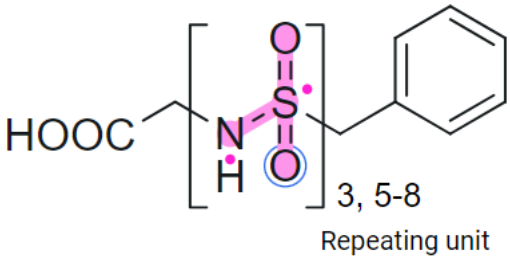
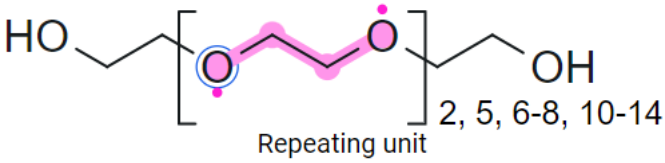
Repeating unit

- **Structural conditions**: The bracket is placed around a fragment with either 1-1 or 2-2 bonds crossing both brackets OR only one of the brackets has crossing bonds
- **Value conditions**: It must have at least one range of integers and then other ranges and positive integers are accepted (*e.g.* 0-4; 1-3, 6-8; 3-5, 8; 2, 4-6)

Structural conditions

Description	Example
One attachment point on each bracket	
Only one attachment point	
Two attachment points on each bracket	

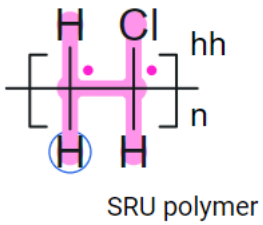
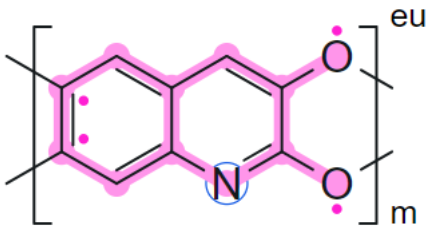
Value conditions

Description	Example
Value is multiple ranges	
Value is a mix of a range and a number	
Value is a mix of ranges and numbers	

SRU Polymer

- **Structural conditions**: The bracket is placed around a fragment with either 1-1 or 2-2 bonds crossing both brackets
- **Value conditions**: One letter of the english alphabet (*e.g.* n; m)

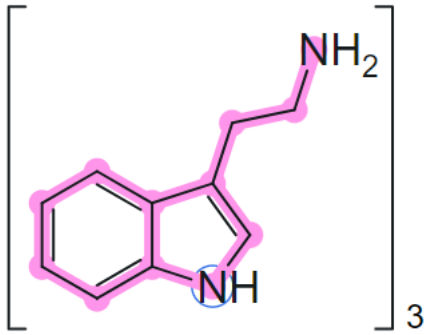
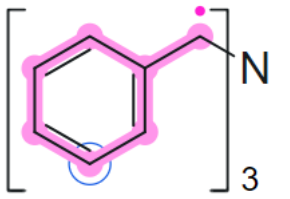
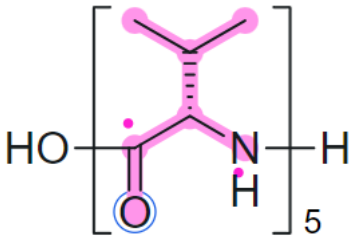
Structural conditions

Description	Example
One attachment point on each bracket	 SRU polymer
Two attachment points on each bracket	 SRU polymer

Multiple group

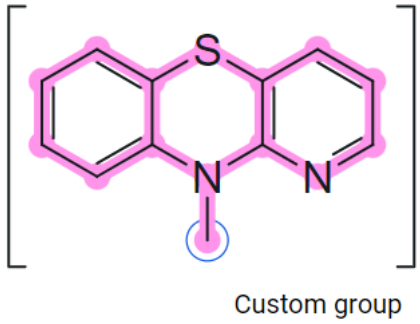
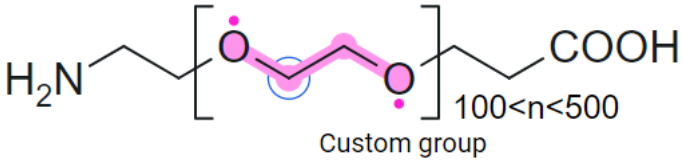
- **Structural conditions**: The bracket is placed around a complete molecule with no attachment points or a fragment with arbitrary number of crossing bonds
- **Value conditions**: Positive integer (*e.g.* 4)

Structural conditions

Description	Example
No attachment points	 Multiple group
Only one attachment point	 Multiple group
Arbitrary number of attachment points	 Multiple group

Custom group

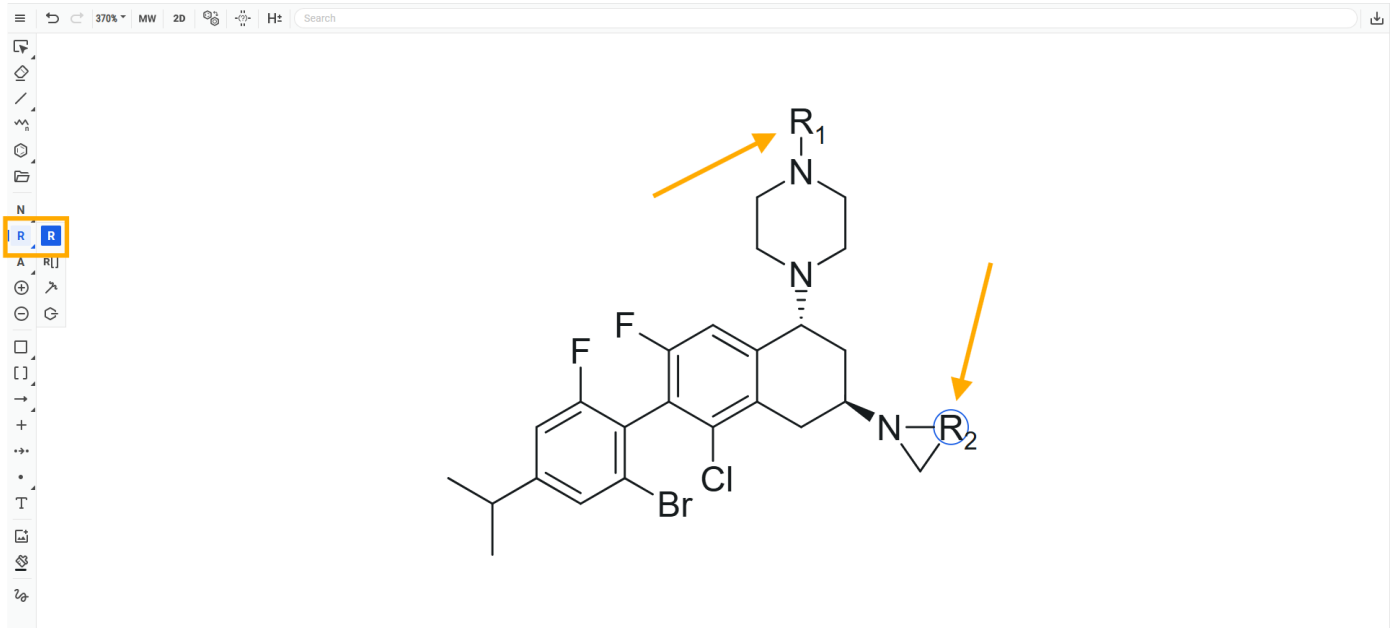
- No structural and value conditions. All S-groups that are not fitting in the above listed categories are considered Custom groups.

Description	Example
No attachment points, no value	
Arbitrary number of attachment points, special value	

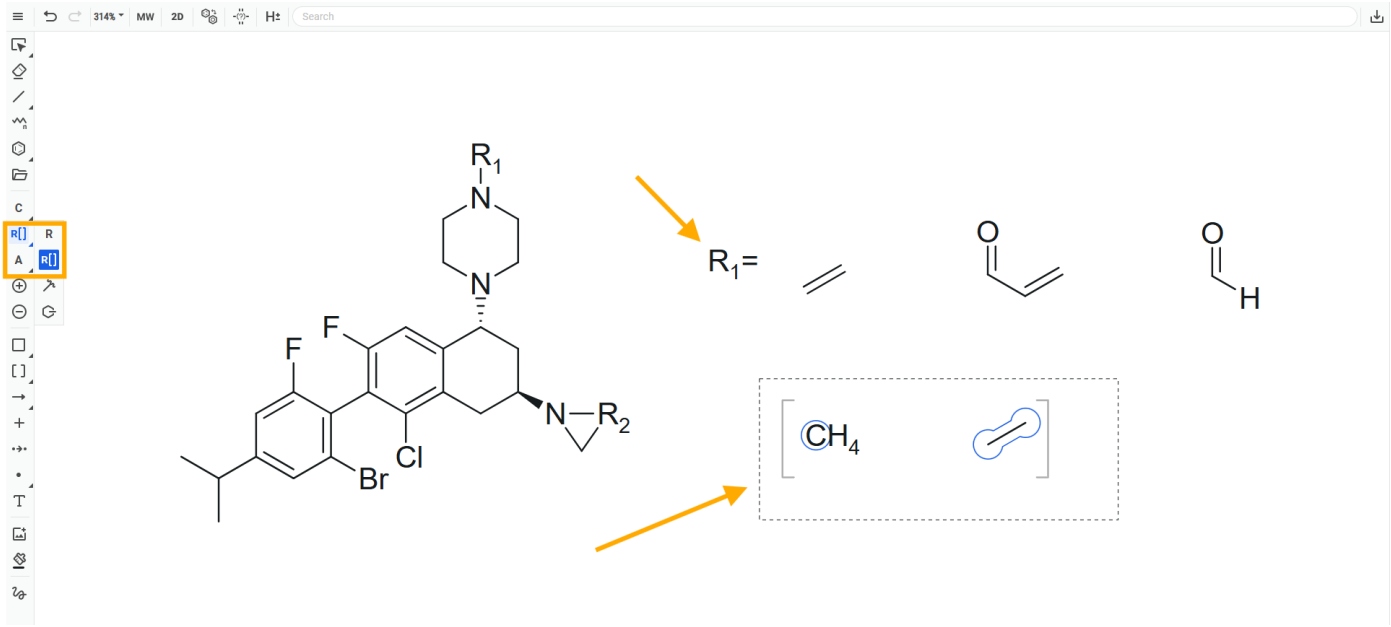
Create RGroup attachments

The behavior of the RGroup, the corresponding definition and the RGroup attachment point is described on the **Features** chapter.

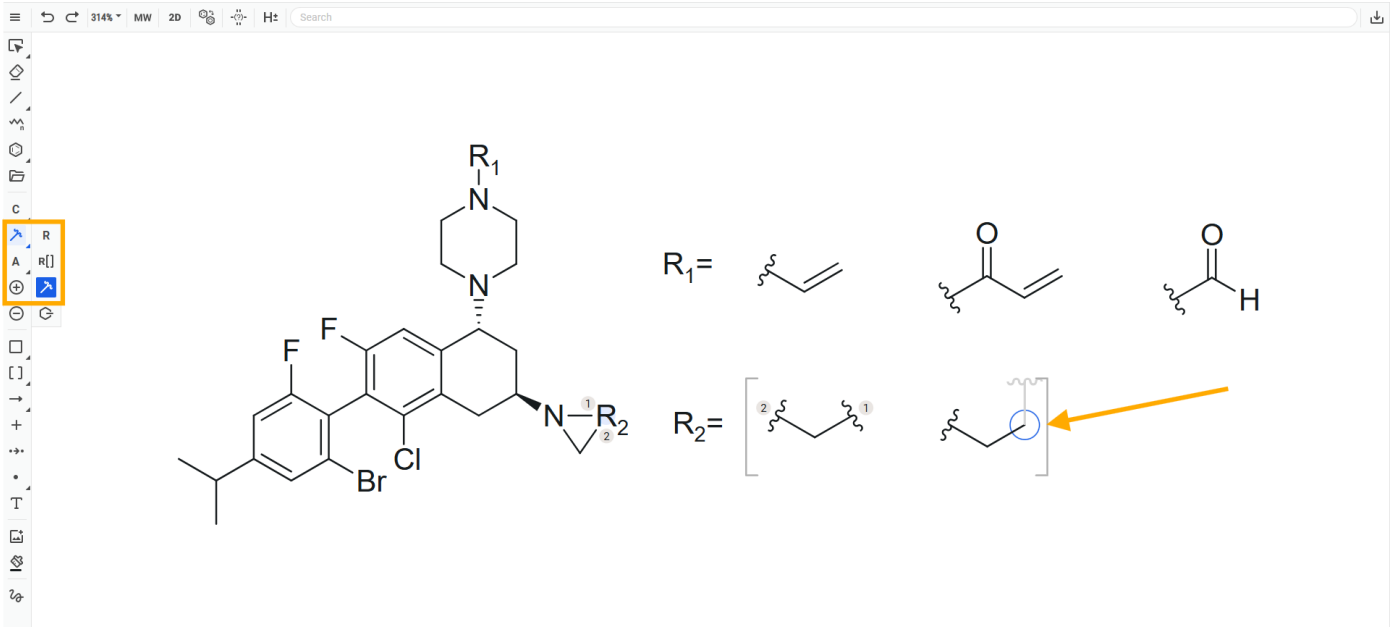
In this example a generic structure is created on which the variable positions are marked with the *R1* and *R2* RGroup labels using the RGroup tool.



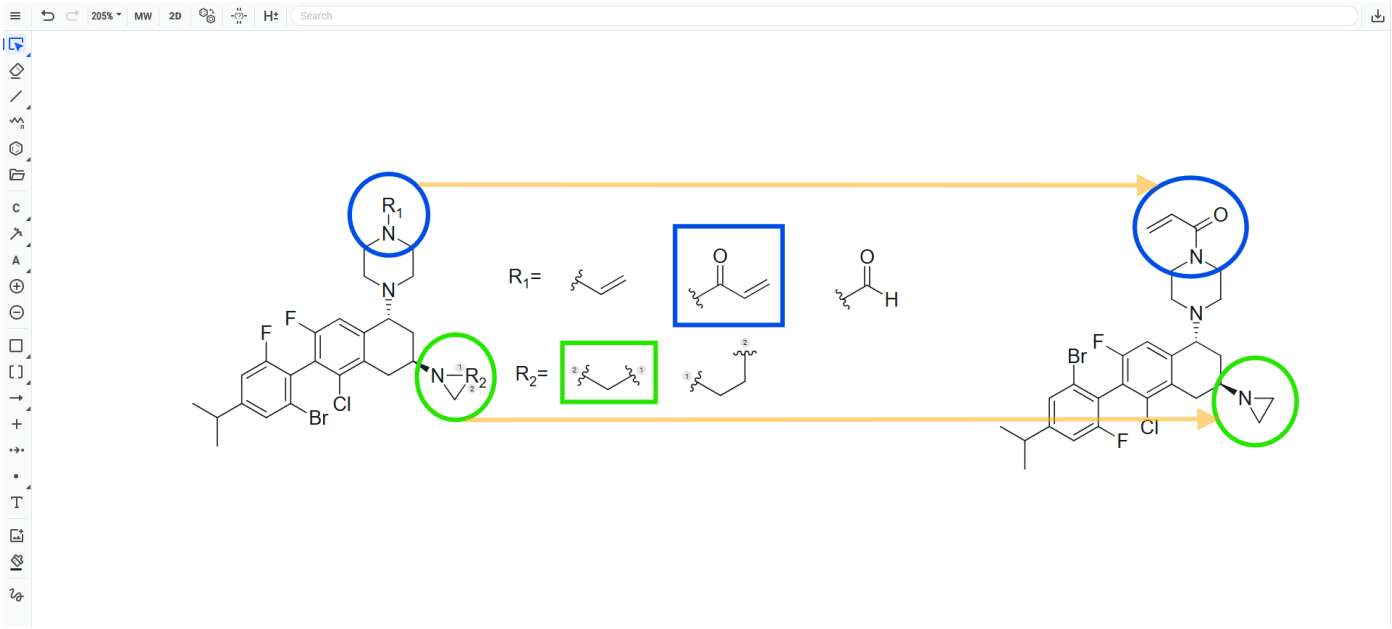
Then, the Define RGroup tool is picked and the depicted molecules are selected with it to create the definitions to the RGroup labels.



Using the RGroup Attachment tool, the attachment point on the definition's molecules can be marked, thus, the scheme can be unequivocally resolved. Note that as the *R2* label has two connections on the generic structure, they are numbered automatically both there and on the definition so that the underlying structure could be clearly defined. The order of the numbers is consistent with the order of placement of the bonds on the canvas.



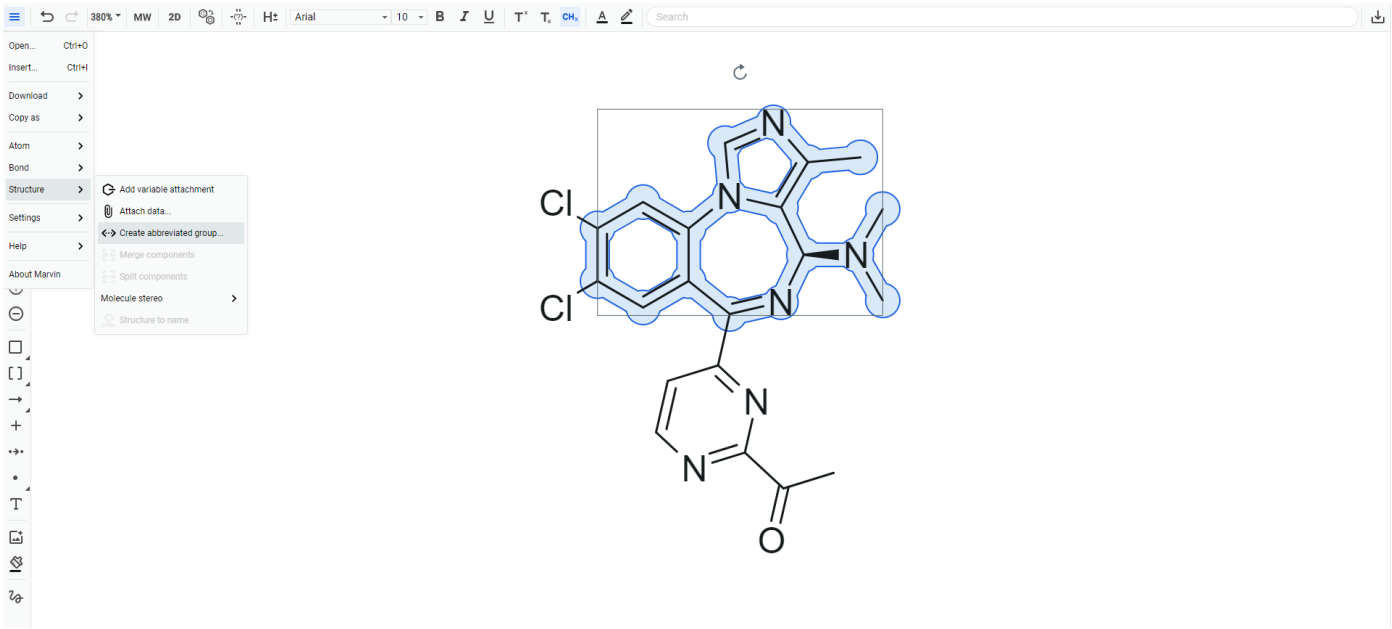
After enumeration of the structure, let's observe one of the generated structures more closely! The *R1* label is exchanged with the acrylic group and the *R2* label with the *-CH2-* group. One should note, that the RGroup attachment bond on the definition molecule only marked the connection of the RGroup label with the neigbouring atoms, it did not added any atoms to the structure.



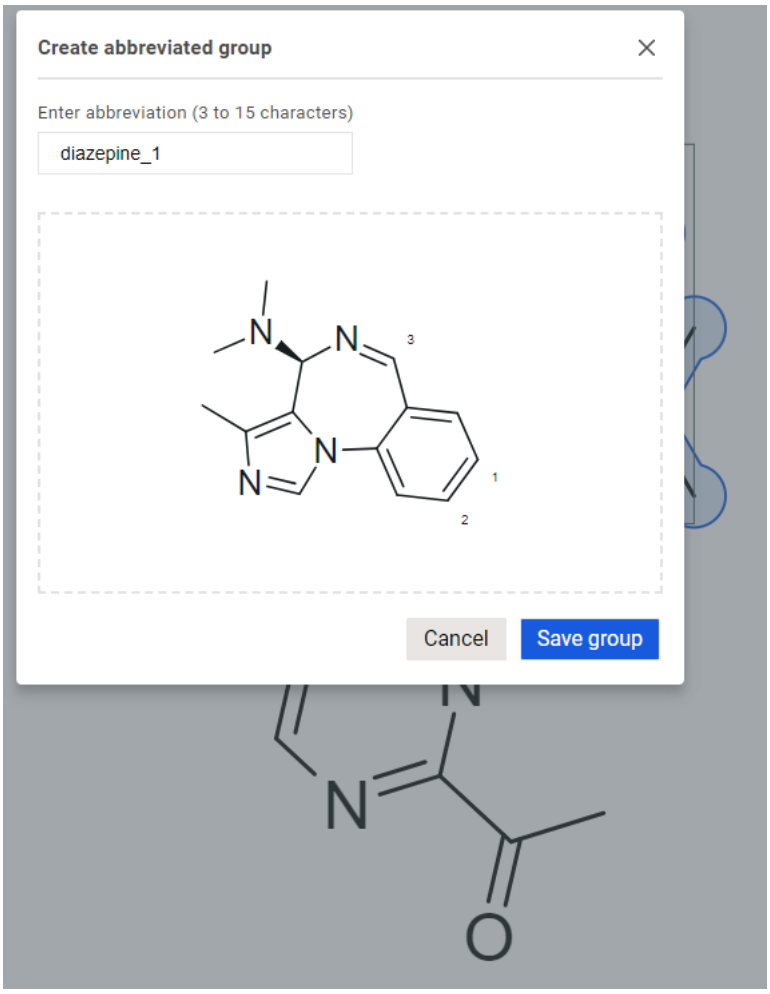
Create abbreviated groups

The behavior of abbreviated groups in **Marvin** is described in the **Features** chapter.

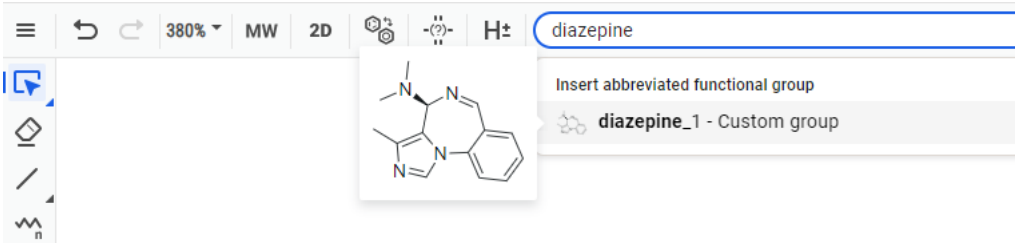
To create a custom abbreviated group an eligible selection has to be made on a chemical structure. In this example a heterocyclic core is selected as the desired abbreviated group. The selection cuts the single bonds to the chlorine atoms and the connection to the pyrimidine ring. Those atoms will be considered attachment points in the created group.

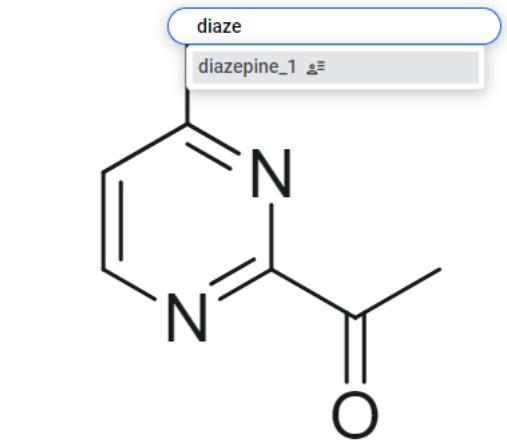


In the appearing dialog, the selected structure is displayed in cleaned status as it will appear on the canvas when expanded or ungrouped. The attachment points are numbered, in this example from 1 to 3. If an eligible name is added in the input field, the group can be saved.

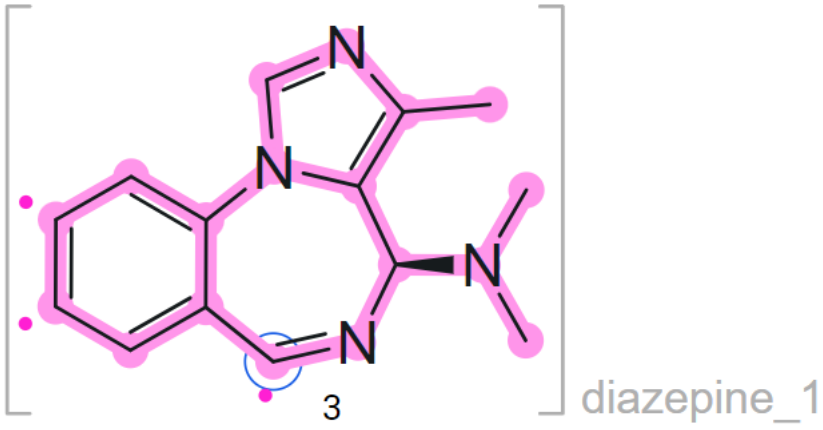


The saved group will appear in the Search bar's suggest list and in the abbreviated groups suggest list, indicated by a profile icon and can be placed on the canvas.





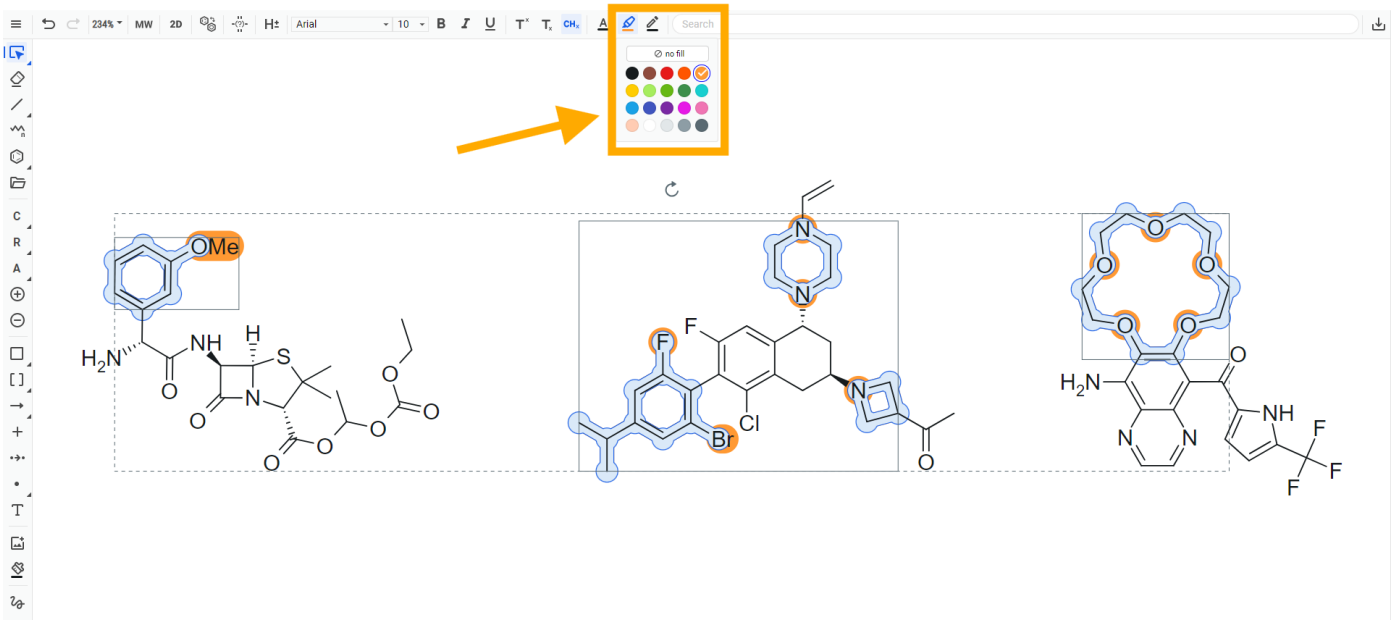
Upon expanding and hovering the created group, the structure is having a purple highlight feedback and the attachment points are marked by purple dots and their corresponding number. The name of the group is displayed in the bottom right corner of the preview of the bracket.



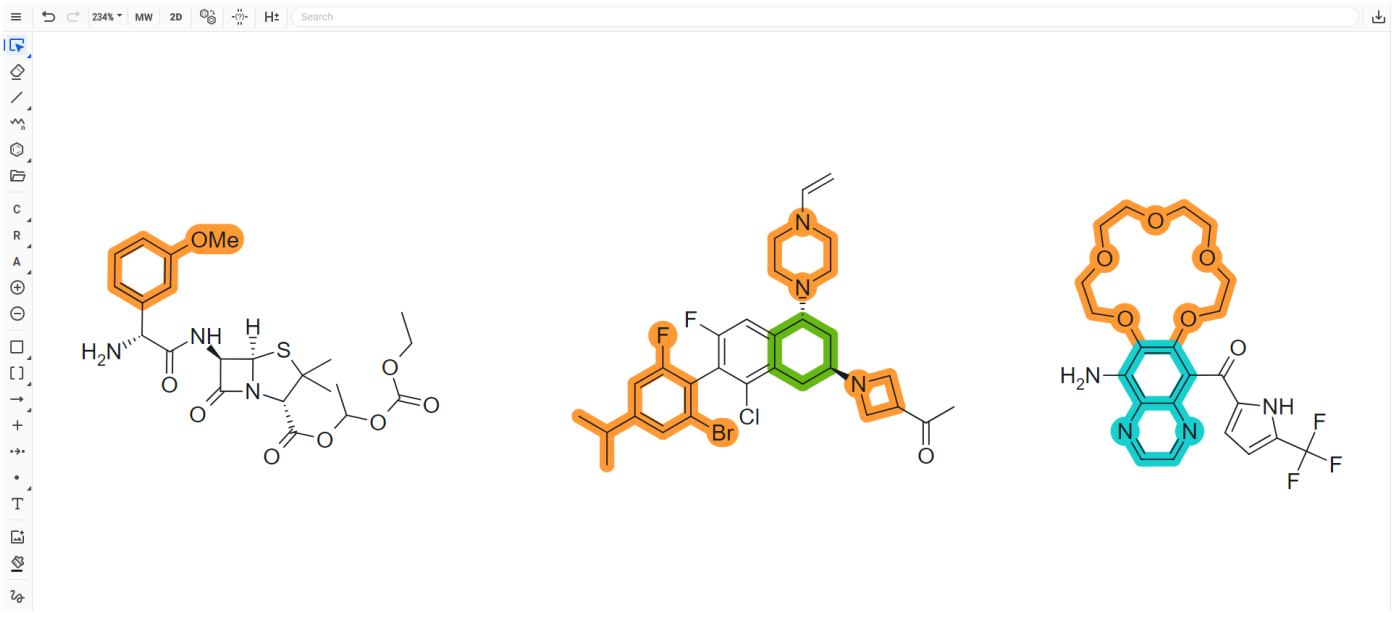
Highlight chemical structures

The behavior of the highlight color tool in **Marvin** is described in the **Features** chapter.

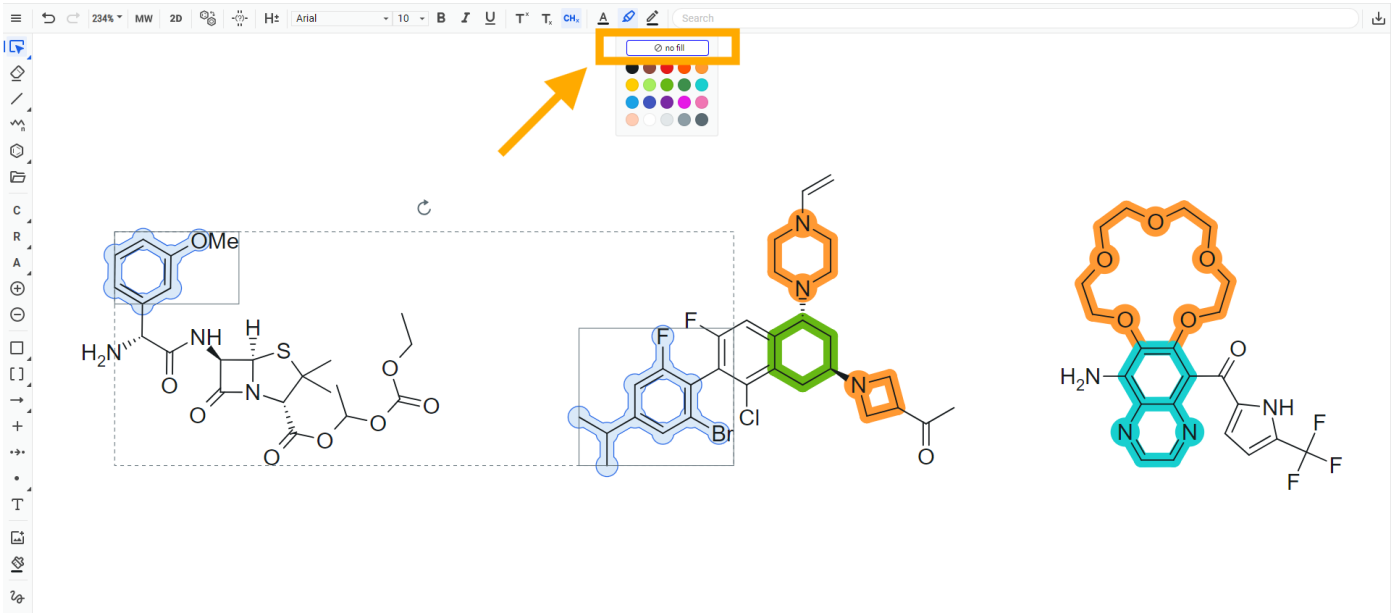
When a selection includes chemical structures, the highlight color tool appears on the top toolbar. Clicking on it will reveal a color palette that can be used for highlighting atom labels and bonds.



Choosing a color will place the highlight on the selected structures.



The highlight can be removed from the structures by selecting them and chossing the *no fill* option from the palette.



Comparison with Marvin Sketch and Marvin JS

To provide an easy-to-use publication tool for chemical figures, **Marvin** comes with a wide range of features to facilitate drawing and enhanced visuals. Meanwhile, our legacy web-based drawing tool, Marvin JS, continues to support workflows involving advanced chemical intelligence.

For a detailed overview, see the comparison tables between **Marvin**, **Marvin JS** and **Marvin Sketch** further below.

Publication quality

Feature	Marvin	Marvin JS	Marvin Sketch
Coloring and highlighting options for atoms, bonds and shapes	YES	no	no
Advanced text editor with highlight and list options*	YES	no	no
Scribble/free hand line	YES	no	no
Predefined and custom drawing templates	YES	no	YES
Wide range of arrows, bonds, shapes, symbols and brackets	YES	no	YES
Import/export and crop multiple image formats	YES	no	no

> *Coming soon

Fast drawing & analysis

Feature	Marvin	Marvin JS	Marvin Sketch
Search bar for templates, chemical elements and tools	YES	no	no
Setting atom and bond properties in multiselection	YES	YES	no
Alignment and distribute guidelines to easily organize objects	YES	no	no
Single click access to webservices and calculations	YES	YES	no
Display calculation results on canvas	YES	no	no

Detailed feature comparison

Coloring and highlighting options for atoms, bonds and shapes

Feature	Marvin	Marvin JS	Marvin Sketch
Coloring bonds and atom labels	YES	no	YES
Coloring atom properties	YES	no	no
Highlighting bonds and atom labels	YES	no	no
Customize colors	YES	no	YES

Advanced text editor with highlight and list options

Feature	Marvin	Marvin JS	Marvin Sketch
Change font type & size	YES	no	YES
Align text	YES	no	YES
Bulleted list*	YES	no	no
Coloring text	YES	no	YES
Highlight text	YES	no	no
Formula tool	YES	no	no

> *Coming soon

Additional arrow types, shapes and brackets

Feature	Marvin	Marvin JS	Marvin Sketch
Dashed arrow	YES	no	YES
Crossed arrow	YES	no	YES
Retrosynthesis arrow	YES	no	YES
Curved arrow	YES	no	YES
Circular arrow	YES	no	no
Unbalanced equilibrium arrow	YES	no	no
Rearrangement arrow	YES	no	no
Rectangles, ellipse, line	YES	no	YES
Sphere, triangle, star, arc	YES	no	no
Advanced shapes (*e.g.* scissors, lightbulb, electrolysis)	YES	no	no
Dashed style for shape strokes	YES	no	no
Line weight for shape strokes	YES	no	YES
Shadow for shapes	YES	no	no
Round and square brackets	YES	no	YES
Curly bracket	YES	no	no

Import/export and crop multiple image formats

Feature	Marvin	Marvin JS	Marvin Sketch
Copy/paste image	YES	no	no
Crop image	YES	no	no
Save selection as image	YES	no	no
Save as JPEG	YES	YES	no
Save as PNG, SVG, WebP, TIFF	YES	no	no

Accessibility

Keyboard navigation in Marvin

Marvin supports keyboard navigation in the application giving access to the main menu, context menu, dialog windows and the toolbars to enable the usage of the features, services and settings in the application. The drawing area and its content can be accessed by keyboard including navigation and edit of chemical structures. For more information about the available shortcuts and actions see **Shortcuts**.

Using Marvin with screen readers

Supported content

The application supports Users with screen readers to access the content of the main menu, context menu, dialog windows and the toolbars.
We are continously working on extending the supported items in **Marvin** including the content of the drawing area.

Screen readers

The following screen readers are suggested to be used:

- NVDA for Microsoft Windows
- VoiceOver for MacOS

History of changes

September 1st, 2025: Marvin 25.3.3

Features

- **Fixers** for structure errors have been added.
- **Fixable structure errors are marked** on the canvas.
- It is now possible to create **nested S-groups** to represent complex polymers.
- **Templates** can now be placed by **sprouting** from an atom.
- The list of **available S-group types** have been extended.
- It is now possible to **clean structures based on their common scaffolds**.

Improvements

- **Dependency versions** are included in the application's specification on the UI.
- **Performance improvements** have been implemented to provide a **more seamless user experience**.
- It is now possible to insert clickable **links** into textboxes.
- The **NMR prediction** feature has been improved.

May 6th, 2025: Marvin 25.1.58

Features

- **1H and 13C NMR prediction** is now available.
- **Structure checker issues** are **marked** on the structures
- It is now possible to **clean and rotate structures in 3D**.
- A **new shape** has been added.
- The **Clear canvas** feature has been implemented.

Improvements

- **Responsivity of the application** has been significantly improved.
- The **2D Clean** service has been improved.

March 13th, 2025: Marvin 25.1.7

Features

- **Custom colors** can now be created.
- The **Map reaction atoms** tool has been upgraded.
- **S-group** functionality has been upgraded.
- The **position** and **color of the S-group labels can be customized**.
- **Arrow direction** can be changed quickly.
- **IUPAC names** can be saved.
- Functionalities on **multiple abbreviated functional group** selection has been extended.

Improvements

- **Peptide handling** has been improved.
- The **Contextual menu** has been reorganized.
- **Text editing** has been improved.
- **Visual representation of aromatic systems** has been enhanced.
- The context menu of the **Calculation box** has been improved.

November 15th, 2024: Marvin 24.3.126

Features

- It is now possible to create and manage **custom abbreviated functional groups**.
- **Autosave** has been implemented.
- **Advanced calculations** are now available.
- **IUPAC numbers** can now be assigned to molecules.
- **Markush structures, atom lists and S-groups** can be **enumerated** either on the **canvas or SDFiles**.
- It is now possible to **highlight structures**.
- Most prominent **visibility settings** can be accessed from the **context menu**.
- The **Atom query properties** dialog is extended with a **SMARTS input** field.
- It is now possible to **search for tools and named molecules in the Search bar**.
- **Paste button** is added to the menus.

Improvements

- The **display** of the **pinned calculation boxes** on the canvas and exported images has been **refined**.
- **New symbols** have been added.
- The **Copy as** submenu has been improved.
- **Display** of atoms hosting **radicals** has been changed.
- **Responsivity of the dialog windows** has been improved.

September 9th, 2024: Marvin 24.3.13

Security vulnerabilities have been fixed.

September 5th, 2024: Marvin 24.3.12

Features

- The **Search bar** feature has been implemented, enabling a **quick access to chemical elements, query atoms, abbreviated functional groups, templates and homology groups**.
- It is now possible to **generate IUPAC names for molecules**.
- The **visibility settings** of the software can now be **stored in the local storage** of the browser.
- A new, improved **atom numbering method** has been implemented.
- The **font types, font size** from the top toolbar, the left **sub toolbars** and the **wrapped top toolbar** can now be accessed and navigated through by keyboard as part of the **accessibility feature set**.
- The **Context menu** and the **Dialog windows** can be opened and navigated through using the keyboard as part of the **accessibility feature set**.
- The **Template library** tool has been introduced that lists an **extended set of predrawn structures** organized in multiple structural categories.
- Commonly used **scientific journal styles with predefined settings** are available now from **Style settings** dialog.
- It is now possible to **create and save Custom journal styles**.
- When a **conflict** between **document style settings occurs during import** a dialog pops up enabling **manual resolution**.
- Adjusting the **Fixed length** in the Style settings now **affects graphical objects** proportionally.
- **Peptide representation** in the application has been implemented.
- **S-group brackets** can now be **resized** and **relocated manually**.
- **Solid and dashed bond styles** has been introduced for the display of **Coordinate bonds**.
- The arrow types have been extended by the **Rearrangement arrow**.
- New shapes such as **Rounded rectangle, Triangle, Star**,**Arc** and **Spehere** are added and a **new set of unique items**, such as flash, light or electrolysis were added.
- **Solid, hashed and dashed bond styles** has been introduced to **display Coordinate bonds**.
- It is now possible to add **Shadow** to certain **shapes**.
- It is now possible to **assign Atom query properties in multiselection**.
- The **Formula & Molweight box is automatically extended** if applied on a full structure.
- It is now possible to **export images in TIFF format**.
- The **Cut** feature has been implemented.
- **Shortcuts** have been implemented for **rotation** and **faster movement** on the drawing area.
- **Horizontal** and **vertical constraint movement** is implemented.
- **Distribution guidelines** now appear on manual movement of structures and graphical objects.
- It is now possible to use **atom shortcuts and abbreviated groups in multiselection**.
- **All radical types** are now available from the **Main and Context menu**.
- **Chemical elements** can be **accessed from the abbreviated groups library**.

Improvements

- The **Single and Double electron flow arrows** can now be exported into **CXON** files.
- **Validation of S-group types** has been extended and refined.
- The **aromatic ring now inherits** the kekule structure's **color** after inviting aromatize service.
- The **direction of single bonds placed by shortcuts** have been refined.
- The typing of **two-letter atom shortcuts** has been refined.
- Behavior of the **Reaction clean up** has been improved.
- The **screen reader** compatibility of the **Homology groups dialog**, **toolbars** and the **drawing area** has been improved.
- **Responsivity of the preview structure** in the **Style settings dialog** has been improved.
- The **display of the Homology groups on the canvas** has been refined.
- **New shortcuts** have been implemented, including quick access to **webservices, tools and dialogs**.
- The placement of the calculation boxes has been improved.
- The **context and main menu** have been **restructured** to serve **better user experience**.

April 5th, 2024: Marvin Pro 24.1.1

New features

- **Brackets** can now be used to represent S-groups on chemical structures such as **repeating units, multiple groups, SRU polymers, link nodes and custom groups**.
- **Coordinate bond** and **Dative bond** are now available from the Bond toolbar.
- It is now possible to **Attach data** to chemical structures.
- It is now possible to **represent salts** on the canvas using the **Merge components** action.

- **Single and double electron flow arrows** can now be drawn to represent electron movements.
- **Multiple attachment point abbreviated groups** can now be placed on the canvas including amino acids.
- The document style settings options are extended with **Margin width and Fixed length**.
- It is now possible to set from API a **confirmation dialog**, when the change of stereochemical labels would cause **stereochemical data loss**.
- The **content of the pinned Formula & Molweight data box** now dinamically **follows structural changes**.
- **Lone pairs** can now be **relocated manually**.
- It is now possible to **Clean up reactions** from the Context menu.
- Selected objects can now be **Distributed** on the canvas in even distances.
- The **location and display of unique atom numbers** can now be customized.
- The dropdown **menus can now be scrolled** if they do not fit into the browser window.
- **New accessibility features** have been added, including accessing and navigating through chemical structures by keyboard.
- The **font size of atom labels and atom/bond properties** can be set globally.
- **Single curly brackets** can now be placed on the canvas.
- Supported **chemical file formats** are extended with **SDF, RDF and RXN**.

Improvements

- The **TAB key** can now be used to put the focus on **dropdown menus**.
- **Standalone carbon atoms** placed on the canvas are represented with their implicit hydrogen atoms.
- **Lone pair placement** has been refined.
- The **placement of** certain **elements** having the **same labels as abbreviated groups** has been fixed.
- The **display of arrow heads** has been refined.

Februray 2nd, 2024: Marvin Pro 23.17.1

New features

- The **publication quality display of the fittings of single, bold and wedge bonds** has been implemented.
- **Unique numbers** can now be assigned to **atoms** with the possibility of customized location and color.
- The **Electron tool** has been introduced including the **Add radical** and **Add lone pair** features.
- The query bonds are now fully complete with the implementation of the **Double Cis/Trans or unspecified bond**.
- The query tools are expanded with the introduction of **Homology groups**.
- The **Style settings** dialog has been equipped with an **adaptive preview structure**.
- The **Font type and size of atom labels and atom/bond properties** can be set globally.
- It is now possible to set the **visibility of the Variable attachment highlight** on the canvas.
- The **Formula & molweight box** can now be **pinned to the canvas** and the **text content can be copied**.
- It is now possible to colorize elements by switching to **CPK color display** of atoms in the main settings.
- The **Mirror & rotate** action is expanded with the **Mirror group and Rotate group** actions.
- The application's **top toolbar is now customizable from API**.
- **New accessibility features** have been added, including navigation of the toolbars and dropdown menus with keyboard, hoverable tooltips and screen readers can now recognize the toolbars and the content of the dialogs.

Improvements

- The **performance** of the application has been **improved**.
- The **style of the stereodescriptors** and **bond topology** labels are refined.
- The application can now **handle molecules separately** if they are **imported together**.

November 23rd, 2023: Marvin Pro 23.16.0

New features

- It is now possible to assign **Molecule stereo label** to structures and **import/export** the **stereochemical information in CXON, MRV and Mol V3000** files.
- Switch icons are introduced to set the **visibility of stereochemical flags and valence error**.
- A **Stereochemistry options** dialog has been implemented that enables the **customization of the visibility and name of the stereochemical flags**.
- The **Map reaction atoms** tool has been implemented, enabling the creation of reaction mapping.
- **Variable attachment bonds** can be added from the Markush tools and the **highlight** can be set to **colored or gray** versions. **Image export** can be set to contain the variable attachment highlights or not.
- It is now possible to assign advanced **Query properties** and **Custom valence** values to atoms.
- Molecules can now be **Mirrored and Rotated** from the context menu.
- **Crop image** tool has been introduced.
- Document **Style settings** have been implemented to **set the display properties of structures**. Bond spacing, bond width, bold bond width and hash spacing can be changed.
- The editor's **left toolbar is now customizable from API**.
- Brackets have been extended with the **Round bracket** graphical object.
- It is now possible to draw **Retrosynthesis arrow**.
- **RGroup attachment ligand order** is introduced.
- Imported reaction schemes are now automatically supplemented with **Plus signs**.
- It is now possible to **draw regular sized shapes** such as circles and squares by holding down the shift key.

Improvements

- The **performance** of the editor has been **significantly improved**.

- **2D Clean** now works with **RGroup attachment points**.
- **Dashed line** representation has been refined.

September 5th, 2023: Marvin Pro 23.12.32

New features

- It is now possible to draw query structures with **Aromatic bond** and **Cis or trans bond** through the left toolbar, main menu and context menu.
- **RGroup attachment bond** can now be placed on atoms from Markush tools in the left toolbar.
- Natural and custom **Isotopes** can be added through the main menu and the context menu.
- **Valence checker** is now introduced to give feedback about valence errors and its visibility can be disabled manually from the main menu settings.
- **Mono- and diradicals** can now be added to atoms through the main menu and the context menu.
- It is now possible to draw **Equilibrium and Unbalanced equilibrium arrow**.
- **Bold bond** is added to the tools and now it is possible to **bold double bonds** as well.
- **Query properties for bonds** such as **topology** and **reacting center** now can be added through the main menu and the context menu.
- **Aromatize/Dearomatize** tool now works with nitrogen containing heterocycles.
- **Image export** now works **on selections** as well.
- It is now possible to place **Molecule stereo labels** Absolute and Racemic on structures.
- It is now possible to **customize** the available **structure templates of the left toolbar from API**.
- New **API option** is introduced **to place imported structures in the middle** of the canvas.
- **CXON file format** introduced some **breaking changes** that may affect older CXON files.
- It is now possible to **import/export enhanced stereochemical properties in MRV** files.

Improvements

- **Enhanced stereo labels and visibility** now can be set from the atom context menu.
- **Absolute configuration** is automatically detected.
- The **properties of multiselected bonds** now can be changed.
- **Mixed atom and bond properties are visible in the context menu** when multiselecting atoms and bonds.
- The default **positioning and graphical representation of the enhanced stereo labels** have been refined.
- **Representation of charges** can be changed through the main menu.
- **Custom positions of charges and labels** are now **stored in CXON** files.
- **Curved and circular arrow properties** are now **stored in CXON** files.
- **Templates have been reorganized**.
- The **design and positioning of the icons** on the toolbar and in the context menu have been **improved**.
- In the **context menu** a **checkmark** is now **showing the type of** the selected **bond**.
- When a new **bond overlaps** with an existing structure they are now **automatically merged together**.
- **Query atom tooltips have been renamed** to make them more easy to understand.
- **Square brackets** representation has been **refined**.

Marvin Developer Guide

Overview

Marvin consists of both backend and frontend components, each of which must be installed and configured to enable full functionality.

- The **backend** (Marvin Web Services) is a SpringBoot application that provides RESTful API endpoints for operations such as transforming, converting, exporting, and analyzing chemical structures.
- The **frontend** is a React application, which can be seamlessly embedded into HTML or integrated with other frontend frameworks like Vue or Angular.

Our distribution packages bundle both components, tailored for specific platforms (Windows, Mac, Linux, and Docker image as well), making them easy to install or deploy. In these packages, the backend runs an instance of Marvin Web Services SpringBoot app, while the frontend is served as static content.

The two components rely on each other and are tied to together through a secure communication:

- The Marvin frontend is granted a valid license by the backend, without which it remains disabled and shows an error message.
- The Marvin Web Services backend only accepts requests coming from and signed by a Marvin frontend, and cannot therefore be used outside the context of Marvin editor.

Quickstart

The following steps will guide you through the easiest installation process, in which most settings and configurations are left untouched.

You can skip steps 1-2. if you already have Java installed, and steps 4-5 if you already have your license key and license-manager configuration ready.

Step	Windows	macOS	Linux
1. Make sure at least Java 17 is installed Test it with `java -version` in a terminal:	`Win + R`, type `cmd` and hit Enter	`Applications > Utilities > Terminal`	`Ctrl + Alt + T`
2. Get Temurin OpenJDK if necessary here			
3. Get and run installer from our download page	64 bit .exe	.dmg	.deb (Debian/Ubuntu) .rpm (Fedora)

Step	Windows	macOS	Linux
4. Get your own license key from your account			
5. Create a license settings with the following content (replace license key)	`C:/Users/<username>/Chemaxon/license-manager.properties`	`/root/.chemaxon/license-manager.properties`	`/root/.chemaxon/license manager.properties`
`server=https://license.chemaxon.com license-key=<LICENSE_KEY>`			
6. Start the Marvin WS service	execute `C:\Program Files\Chemaxon\marvinws\run-marvinws` (available in Start Menu)	`launchctl start marvinws`	`sudo systemctl start marvinws` *
7. Open Marvin in your browser: http://localhost:8080			

* `marvinws` is supposed to be automatically enabled and running on Linux after installation. Test it with `sudo systemctl status marvinws`

Installation and integration

- Installing the Marvin Web Services
- Integrating Marvin UI Editor

Marvin Web Services

Overview

The Marvin Web Services is the backend component for Marvin. The Marvin editor (frontend component) heavily relies on it for full functionality. It has two main roles:

1. It serves most computation-heavy functionalities for the user-interface, which would be unfeasible or ineffective to run in the end-users' browser (e.g. transforming chemical models, 2d-clean-up, chemical calculations).
2. It acts as a license server for the frontend component. The purchased license key is installed only along the Marvin Web Services. The fronted component makes a license request to the backend during initialization, and will refuse every user action unless the backend responds and confirms a valid license key.

The Marvin Web Services backend only accepts requests coming from and signed by a Marvin frontend, and cannot therefore be used outside the context of Marvin editor.

Marvin Web Services is a stateless service: it does not store incoming requests, and it also does not forward any content to external services. What happens in Marvin backend, stays in Marvin backend.

Software requirements

- Windows, Linux or macOS
- Java 17. Eclipse Temurin is officially recommended.

Hardware requirements

At least 2GB RAM. The default size of maximum Java heap size (`-Xmx`) is set to 2GB.

Installation

Platform-specific installers

All the distributed installer packages contain both the backend (Marvin Web Services) and the frontend component (Marvin user interface) as static content.

The following platform-specific installers automatically copy the files to the default installation directory, and create a system-level service called MarvinWS:

- `.deb` for Debian / Ubuntu
- `.rpm` for Fedora
- `.exe` for Windows *
- `.dmg` for macOS.

* For installing Marvin WS as a service on Windows, you'll have to run `marvinws/marvinws.exe --install` after running the above installer package.

Alternatively, you can choose to extract and run the executable zip archive on Windows, or the tar.gz archive on Linux/macOS.

Running the server

- If you have installed Marvin WS as a system service (using a platform-specific installer), you can start, stop, restart it with specific system-specific commands:
  - `sudo systemctl start marwinws` on Linux
  - `launchctl start marvinws` on macOS
  - `Start-Service -Name marvinws` on Windows
- Execute directly `./run-marvinws` or `run-marvinws.exe` located the installation directory

- For detached mode, execute `./marvinws start` or `marvinws.exe start` located in the installation directory. The same executable is also capable of stopping, restarting or reporting status on the service.

Docker

The `marvinws` docker image can be found in registry `hub.chemaxon.com` under in the repository `cxn-docker-release/chemaxon/`

In order to get your credentials to the registry, please visit our download page and select **CLI with docker**.

The provided docker image is built on Temurin JDK, with a default user `cxnapp`, and default entry point `/app/marvinws/run-marvinws`.

Quickstart with docker

1. Login to the registry
   `docker login -u <username> -p <password> hub.chemaxon.com`
2. Pull the latest image
   `docker pull hub.chemaxon.com/cxn-docker-release/chemaxon/marvinws:latest`
3. Run the image
   1. Make sure to map the default port 8080 to one of the hosts' ports (e.g. `-p 8080:8080`)
   2. Make sure to map the license file or license settings as an external resource (for details, see below).
      `-v path/to/license-file:/home/cxnapp/.chemaxon/license.cxl`
      or
      `-v path/to/license-key-config:/home/cxnapp/.chemaxon/license-manager.cxl`
   3. Full run command
      `docker run --name marvin -d -v /home/user/license.cxl:/home/cxnapp/.chemaxon/license.cxl -p 8080:8080 hub.chemaxon.com/cxn-docker-release/chemaxon/marvinws`
4. Verify that the docker container is up and running
   `docker logs marvinws`
5. You can access the running editor at http://localhost:8080.

Alternative ways to pass license to the docker container

- set an environment variable with `-e CHEMAXON_LICENSE_SERVER_KEY=<license-key>`
- pass a JVM parameter `-Dchemaxon.license.serve.key=<license-key>`
- map the Chemaxon home directory (`.chemaxon`) or the license/configuration file (see above)
- use Docker secrets

License installation

Marvin needs a valid license (license file or license key see below). If you are unsure how to obtain your license, please contact us.

Background

1. License key has to be installed on the server that hosts the Marvin Web Services backend.
2. The Marvin frontend requests a license from the Marvin Web Services during initialization via a signed RESTful request. In case the backend-frontend communication is not properly configured, or the server rejects the license request coming from the browser, the Marvin user interface will be inactive with an error message.

Installing a license file

Put the Marvin license file under `<userhome>/chemaxon/licenses/` (on Windows) or `<userhome>/.chemaxon/licenses/` (on Linux or macOS) folder.

Installing a license key

License key configuration has to be in `license-manager.properties`, in `<userhome>/chemaxon/` (on Windows) or `<userhome>/.chemaxon/` (on Linux or macOS) folder, in the following way (make sure to replace <LICENSE_KEY> with your actual license key):

```
server=https://license.chemaxon.com
license-key=<LICENSE_KEY>
```

You can get your license key from your account.

The license key configuration will use Chemaxon's Central License Server (instead of a local license file), therefore the server where Marvin WS is hosted needs to be able to connect the configured license server through the internet.

Further information

For further information on the license installation, please visit our corresponding documentation page or contact Sales, or our Support.

Troubleshooting

If you are encountering issues during license installation (e.g. the user interface does not detect any valid license), please check the following.

- Verify that the Marvin Web Services are up and running, for example, `sudo systemctl status marvinws` on Linux, `launchctl list | grep marvinws` on macOS, or `Get-Service -Name "marvinws"` on Windows in case you are running Marvin Web Services as a system service. Alternatively, you can check the log file, located by default in `logs/mjsws.log` (inside the installation directory), unless configured otherwise.
- Verify that the Marvin Web Services can access the license file or key, by checking the `License file information` section in the log file (`logs/mjsws.log`).
- Make sure your license has not expired. If you are uncertain, please contact Sales, or our Support.
- If you have recently upgraded or re-installed the license, you might need to restart the Marvin Web Services.
- Make sure that the frontend editor is configured to reach the backend at the proper URL, and can connect to the server. This can be verified with the Network tab of the Developer tools (e.g. F12 on Chrome).
- If your frontend and backend are hosted on different domain, and the license request is denied because of the CORS policy, you'll have to make sure to configure CORS in the backend, or set up a reverse proxy

License Server Certificate Error

If the Marvin backend fails to start and the following error appears in `logs/mjsws.log`:

```
PKIX path building failed: sun.security.provider.certpath.SunCertPathBuilderException: unable to find valid certification path
to requested target
```

This indicates that the Java Virtual Machine (JVM) cannot validate the SSL certificate of ChemAxon's license server (`https://license.chemaxon.com`). To resolve this:

- **Add the certificate manually**: Download the license server's certificate and import it into your system's keystore. Refer to this guide for instructions.
- **Use the system trust store**: Start the application with the following JVM parameter to use the system's trust store: `-Djavax.net.ssl.trustStoreType=WINDOWS-ROOT`
- **Check for SSL filtering by firewall**: Some firewalls intercept SSL traffic, modifying the certificate chain. Temporarily disable your firewall and try connecting to `https://license.chemaxon.com`. If this resolves the issue, update the firewall settings accordingly.

Configuring backend

Configuration file `application.properties` is available under the installed `marvinws/config/` folder. In `application.properties` file you can set the followings:

Option name	Default value
server.port	8080
logging.file.name	`./logs/mjsws.log`
spring.application.name	marvin-js-mini

For more settings possibilities, see the spring documentation page.

Configuring Cross Origin Policy

By default, it is allowed to access the web services from every origin. If you want to limit which JavaScript applications can access the web services, configure the following default values in `application.properties` accordingly:

```
endpoints.cors.allowed-headers=*
endpoints.cors.allowed-methods=*
endpoints.cors.allowed-origin-patterns=*
endpoints.cors.max-age=1800
```

You can set a list of values by separating the individual values with a comma. For more information, see CORS.

Forbid CORS

The following setting accepts same-origin requests only.

```
endpoints.cors.allowed-headers=
endpoints.cors.allowed-methods=
endpoints.cors.allowed-origin-patterns=
```

Allow CORS on Two Origins

To enable cross-origin calls from specific domains only, like origin1.com and origin2.example.com:

```
endpoints.cors.allowed-headers=*
endpoints.cors.allowed-methods=*
endpoints.cors.allowed-origin-patterns=http://origin1.com, http://origin2.example.com
endpoints.cors.max-age=1800
```

Enabling HTTPS

By default, the REST endpoints use plain HTTP as a transport. You can switch to HTTPS easily, by adding a certificate to your configuration. You can either create a new file, that contains the SSL configuration, for example, *skipper.yml*, or amend your `application.properties` file with the same information.

You can reference the SSL configuration file as well as the original application.properties file together by using the following parameter: `--spring.config.location=skipper.yml,application.properties`

```
server:
  port: 8443                                    (1)
  ssl:
    key-alias: yourKeyAlias                     (2)
    key-store: path/to/keystore                 (3)
    key-store-password: yourKeyStorePassword    (4)
    key-password: yourKeyPassword               (5)
    trust-store: path/to/trust-store            (6)
    trust-store-password: yourTrustStorePassword (7)
```

Alternatively, the same information can be appended to the `application.properties` configuration file:

```
server.port=8443                                    (1)
server.ssl.key-alias=yourKeyAlias                   (2)
server.ssl.key-store=path/to/keystore               (3)
server.ssl.key-store-password=yourKeyStorePassword  (4)
server.ssl.key-password=yourKeyPassword             (5)
server.ssl.trust-store=path/to/trust-store          (6)
server.ssl.trust-store-password=yourTrustStorePassword (7)
```

1. As the default port is 7577, you may choose to change the port to a more common HTTPS-typical port.
2. The alias (or name) under which the key is stored in the keystore.
3. The path to the keystore file. Classpath resources may also be specified, by using the classpath prefix: `classpath:path/to/keystore`.
4. The password of the keystore.
5. The password of the key.
6. The path to the trust store file. Classpath resources may also be specified, by using the classpath prefix: `classpath:path/to/trust-store`.
7. The password of the trust store.

For more details, see spring configuration-security.

Protection against unauthorized use

According to our End User License Agreement (EULA), clients with restricted access to Marvin are responsible for securing backend endpoints against unauthorized use, ensuring that only licensed end-users can access the REST API. This includes, for example, hiding the endpoints behind a reverse proxy or implementing an authentication layer.

Required headers for Marvin backend-frontend communication

The Marvin backend only processes REST requests that are signed by the Marvin frontend. This is achieved by setting the `x-cxn-api-signature` header to a token generated by the frontend. If the backend is deployed behind a reverse proxy or if REST headers are subject to filtering, ensure that the `x-cxn-api-signature` header is explicitly allowed and forwarded to the backend.

Marvin editor UI (frontend)

The Marvin editor is a React-based JavaScript application, that operates in the client-side browser, supporting all major browsers. It allows users to create, edit, and transform chemical structures while facilitating seamless communication with the host application via its JavaScript API. Additionally, it supports both a single-page mode and multiple integration options for higher-level web applications.

JavaScript API

Marvin has a rich and flexible JavaScript API that allows the embedding page to interact with the editor dynamically. The full documentation can be accessed here.

Integrating the Marvin editor

Embedding into HTML

To achieve full functionality, you'll need to load the following sources as scripts in your HTML:

- `marvin.js` - The Marvin bundle
- `react` and `react-dom`, located in `lib/react.production.min.js` and `lib/react-dom.production.min.js`
- helper JavaScript code located in `marvin-scripts`. These might not be necessary, depending on the use-case, and can be substituted with other, custom implementation.
  - `marvinLocalStorage.js` for reading & writing the editor state into the Browser's local storage
  - `marvinWebserviceSettings.js` for the default backend configuration

- `marviniFrameClient.js` (optional) for embedding Marvin as an iframe

A global `marvin` variable is provided by the `marvin.js` source, through which the JavaScript API can be used. To initiate the editor, invoke the `createMarvin()` function, while specifying the `id` of the HTML element where the UI will be loaded. An optional, second parameter allows for passing configuration settings. Most importantly, the webservice endpoints have to be specified, without which the UI will not be usable.

```
<head>
  <script src="libs/react.production.min.js"></script>
  <script src="libs/react-dom.production.min.js"></script>
  <script src="marvin-scripts/marvinWebserviceSettings.js"></script>
  <script src="marvin-scripts/marvinLocalStorage.js"></script>
  <script src="marvin.js"></script>
</head>

<body>
  <div id="marvin-0"></div>
  <script>
    marvin.createMarvin("marvin-0", {
      webServiceSettings: getDefaultMarvinWebserviceSettings(),
      calculationSettings: {
        ...getDefaultMarvinCalculationSettings(),
      },
    });
  </script>
</body>
```

The `createMarvin` function returns with a promise of a `Marvin` object, through which one can interact with that specific instsance's JavaScript API, for example:

```
var globalMarvinRef;

marvin
  .createMarvin("marvin-0", {
    webServiceSettings: getDefaultMarvinWebserviceSettings(),
    calculationSettings: {
      ...getDefaultMarvinCalculationSettings(),
    },
  })
  .then((marvin) => {
    globarlMarvinRef = marvin;
  });

//...

console.log(globalMarvinRef.isEmpty());
```

An `index.html` example page is provided in the distribution package to illustrate default integration.

NPM package

For any custom project, Marvin can be used as an NPM package, accessible in our NPM registry.

To get your npm credentials, visit our download page, and select `CLI with npm`. If you follow the steps outlined there, you will be able to install Marvin simply by:

`npm install @chemaxon/marvin` `npm install @chemaxon/marvin-examples`

Framework-specific integration

Since Marvin is a pre-compiled React component, it is possible to integrate it directly into various frontend frameworks. Framework-specific integration examples can be found in our public GitHub repo for:

- React
- Vue
- Angular

Integrating with Marvin Web Services (backend)

The client-side Marvin editor heavily relies on the Marvin Web Services, for two main purposes:

- Certain calculations, analyses or chemical transformations (e.g. import and export in various file formats), which would be unfeasible or ineffective to run in the end-users' browser, are requested from the Web Services via its RESTful API.
- The client-side Marvin is granted the license by the backend component. The purchased license key is installed only along the Marvin Web Services. The fronted component makes a license request to the backend during initialization, and will refuse every user action unless the backend responds and confirms a valid license key.

Frontend and backend hosted together

All distributed installer packages for Marvin Web Services include the complete frontend library as static content. The default landing page (index.html) is accessible directly on the same domain as the backend at the default path (e.g., http://localhost/index.html). By default, the provided JavaScript code and HTML pages are configured to communicate with the backend's RESTful API on the same origin.

When the backend and frontend components are hosted on the same domain, it eliminates the complexity of making cross-origin requests from the client-side to the backend, thereby making CORS and the use of iframes, which rely on the browser's postMessage API, unnecessary.

Hosting backend and frontend on different domain

In certain use cases, it is necessary that the Marvin UI frontend be used on a domain where the Marvin Web Services are hosted.

Configure HOST in Marvin frontend settings

When embedding the Marvin UI into HTML, The `createMarvinPro()` method allows for passing a `MarvinProSettings` object, in which you can specify the `webservicesSettings` and the `calculationSettings` with the full URLs of the endpoints exposed by Marvin Web Services (take care to replace `<HOSTNAME>`):

```
marvin.createMarvin(document.getElementById("marvin-div-id"), {
  webServiceSettings: {
    licenseServiceURL: "<HOSTNAME>/rest-v1/license/grant",
    clean2dServiceURL: "<HOSTNAME>/rest-v1/jws/structure/clean",
    aromatizeServiceURL: "<HOSTNAME>/rest-v1/jws/structure/aromatize",
    cipStereoServiceURL: "<HOSTNAME>/rest-v1/jws/stereo/cip",
    molConvertServiceURL: "<HOSTNAME>/rest-v1/jws/molconvert",
    hydrogenizeServiceURL: "<HOSTNAME>/rest-v1/jws/structure/hydrogenize",
    enumerateServiceURL: "<HOSTNAME>/rest-v1/jws/markush/enumerate",
    tiffServiceURL: "<HOSTNAME>/rest-v1/jws/image/convert/tiff",
    searchServiceURL: "<HOSTNAME>/rest-v1/jws/search",
  },
  calculationSettings: {
    endpoints: [
      {
        endpointName: "Marvin",
        endpointURL: "<HOSTNAME>rest-v1/jws/calculator/calculate",
      },
      {
        endpointName: "MarvinNamingIUPAC",
        endpointURL: "<HOSTNAME>/rest-v1/jws/molconvert",
      },
    ],
  },
});
```

For simplicity, in the distributed packages, you will find a helper script `marvin-scripts/marvinWebserviceSettings.js`. In that, the paths of all the endpoints are pre-configured, and you only have to replace the `HOST` variable:

```
const HOST = "<HOSTNAME>";
```

Take care that the script is properly loaded in your html (like in the provided HTML example pages):

```
<script src="marvin-scripts/marvinWebserviceSettings.js"></script>
```

Since you are accessing the REST api endpoints from a different domain, you might run into issues with CORS policy. In this case, consult with the configure CORS above.

Use iframe

You can take advantage of Marvin's iframe API to embed the frontend editor on a different domain from where the backend is hosted. This way, you will only need to copy the content of `marvin-scripts/` directory to your server where your webapp lives, and make sure import `marvinIframClient.js`:

```
<script src="marvin-scripts/iFrameClient.js"></script>
```

In your HTML, you have to create an iframe and import `iframe_marvin.html` from the remote host as its source. Take care that this html file needs to be available for your webapp. When the page is loaded, you have to explicitly create the editor the same way as with direct integration, but this time, the API will be that of the iframe client.

When creating the Marvin editor inside your iframe, you have to repeat the configuration of the REST endpoints outlined in Configure HOST in Marvin frontend settings. The easiest way, again, is to import `marvinWebserviceSettings.js`, overwrite `HOST` and use the helper functions.

```
<iframe id="iFrame" src="<HOSTNAME>/iframe_marvin.html" class="marvin"></iframe>

<!--...-->

<script>
  let iFrame = document.getElementById("iFrame");
  let iFrameClient = createMarvinIFrameClient(iFrame);
  iFrame.addEventListener("load", onLoad);

  function onLoad() {
      iFrameClient.createMarvin("marvin-0", { //The ID of the HTML element needs to be the same as in iframe_marvin.html in the
remote host
          webServiceSettings: getDefaultMarvinWebserviceSettings(),  //make sure you load the marvinWebservicesSettings.js
      }
  }
</script>
```

Syling consideration

Minimum size

Please be avare that the Marvin UI editor has a minimum size of 700x450px. The editor will refuse to shrink below that.

CSS style collision

The Marvin editor currently does not have specific safeguards against CSS style collisions with the host application. This may lead to unintended layout issues in Marvin. If such anomalies occur, the recommended solution is to wrap Marvin with an iframe.

Further integration examples

The distributed package contains integration examples for various workflows, for example:

- How to embed a fixed size or a resizable Marvin into a web application
- How to import and export chemical content through the API
- How to get notified when the content of the canvas changes
- How to customize the toolbars, how enable or disable buttons
- How to enable autosave, so the last changes can be opened easily

...and many more. To access the integration examples, please go to our download page, and download platform specific package according to your needs. Alternatively, find the `marvin-examples` package in our NPM registry:

```
npm install @chemaxon/marvin-examples
```

License installation

License only needs to be installed on the server where the Marvin Web Services backend is hosted. The Marvin editor frontend is granted a license by the backend at initialization. If the backend-frontend communication is configured properly, license installation needs no further action on the frontend.