MarvinSketch User's Guide

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Marvin User's Guide

Introduction to MarvinSketch

MarvinSketch is an advanced chemical editor for drawing chemical structures, queries and reactions. It has a rich (and growing) list of editing features, is chemically aware and is able to call ChemAxon's structure based calculation plugins for structures on the canvas.

Rich editing:

- wide range of file types supported: MOL, MOL2, SDF, RXN, RDF (V2000/V3000), SMILES, SMARTS/SMIRKS (recursive), MRV, InChi, CML, PDB, etc.
- Copy and paste between different editors
- Abbreviated groups
- Pre-loaded structure templates and "My Templates"
- Fog effect in 3D viewing mode
- 3D editing
- 3D geometry and conformer generation
- 2D cleaning and conformer generation
- Advanced query features (generic atoms and bonds, atom lists/not lists, query properties, pseudo atoms, multiple groups, Link nodes, etc.)
- Creating and editing molecule sets (without a database)
- Multipage documents and printing support
- Drawing and formatting shapes, arrows and text boxes
- Structure annotation
- User definable customisable styles (colours, structure representations, etc.)

Chemically aware

- Structure based calculations can be called directly from MarvinSketch. For a complete listing of functions please see the Calculator Plugins section
- Error checking (valence and reaction error checking)
- Structure query design (R-logic, SMARTS properties, etc.)
- Isotopes, charges radicals, lone pairs and aliases are supported
- Manual and automapping for reaction drawing
- Advanced stereochemistry functions (E/Z double bonds, R/S chirality, ABS/OR/AND enhanced stereo, etc.)

Cross platorm delivery

- Marvin can run on all major operating systems, it is available in the following distributions:
  - **Java Applets** can easily be implemented into Java enabled web pages without the need for the user to install software or plugins
  - **Java Beans** can be directly installed to give standalone desktop applications and can also be used to integrate Marvin into Java based applications
  - **Java Web Start** enables web delivery of end user applications
  - **.NET package** makes it available to integrate Marvin into .NET applications

Installation & System Requirements

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1. Marvin Applets or Marvin Beans?

Marvin is separated to two packages depending on how you want to use it

- **Marvin Applets** for the web developer
- **Marvin Beans** for the chemist's desktop and for the software developer

Marvin Applets are tools for building chemical web pages, which are compatible with most browsers (Chrome, Firefox, Internet Explorer, Safari, Opera, etc.). They offer access from/to JavaScript and are customizable by applet parameters.
Note, that the applets are signed that allows the same feature set as the applications.

Marvin Beans are easy-to-install applications for the desktop *and* tools for integrating Marvin capabilities into any application.

2. System Requirements

2.1. Marvin Applets

- Java distributed by Oracle (or Apple's Mac OS X built-in Java)
- Version: Java 1.6.0_13 or higher
- Java 2 enabled browser

2.2. Marvin Beans for Java

- Java distributed by Oracle (or Apple's Mac OS X built-in Java)
- Version: Java 1.6.0_13 or higher

2.3. Marvin Beans for .NET

- .NET framework 3.5 SP1. Please note that .NET framework 4 does not include the version 3.5.

2.4. How to get Java?

You can download **Java** from Oracle's official site or contact your OS manufacturer.

If you use **Mac OS X**, probably Java is already installed on your machine. If not, select **Java** in the **Software Update** center to install or update.

Which Java do I need?

- You need **Java Runtime Environment (JRE)** installed on your system to run applications and applets.
- To develop applications and applets, you need the **Java Development Kit (JDK)**, which includes the **JRE**.
- Version: Java 1.6.0_13 or higher

Testing Java

- If you are not sure whether Java is installed or not on Windows, you can check it the following way:

  1. Select *Command Prompt* from the *Accessories* sub-menu in the *Start* menu.
  2. Type the following commands in the opened Command Prompt window: *java -version*
  3. You will get the following error message if Java is not available on your machine:

     ```
     'java' is not recognized as internal or external command, operable program or batch file
     ```

     If Java is installed, the version number of Java will be printed:

     ```
     java version "1.6.0_24"
     Java(TM) SE Runtime Environment (build 1.6.0_24-b07)
     Java HotSpot(TM) 64-Bit Server VM (build 19.1-b02, mixed mode)
     ```

- You can **test** whether Java is working on your computer on Oracle's official testing site, too.

2.5. How to get .NET framework?

.NET framework 3.5 SP1 is included in Windows 7 by default. For other Windows OS you can download the .NET framework from Microsoft's official site.

- .NET framework 3.5
- .NET framework 3.5 Service Pack 1

3. Installation

3.1. Marvin Applets

1. Download the Marvin Applets package according to your platform from the Marvin download page. (`.tar.gz` is recommended for Unix-like platforms, `.zip` for others).
2. You need a web server on the machine where you would like to install the Marvin Applets package (because applets work properly only through HTTP protocol). If there is no web server on the target machine, we suggest to use Tomcat.
3. Extract `marvin-all-VERSION.tar.gz` (in Unix or in Mac OS X) or `marvin-all-VERSION.zip` (in MS Windows) in the parent directory of "marvin", where `VERSION` is the current version number.
4. Modify the settings of the web server if the directory of Marvin is not accessible from the web server root. Then restart it (if it is necessary) to validate new settings. (Consult with the manual of the web server how to do it.)
5. Open the `index.html` file in a browser.

Removing any binary (*jar* or *zip*) or configuration (*properties* or *xml*) **file** from the applet **package** can **cause** unexcepted **error or limitation in the usage.**

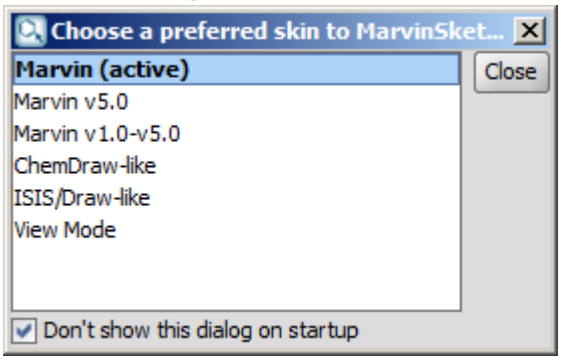
3.2. Marvin Beans for Java

Download the package according to your platform from one of the links below:

- **Download Marvin for End Users** to install desktop applications
- **Download Marvin for Developers** to use the tools for application development

Notes:

- After installation, at the first launch of MarvinSketch, a dialog asks the user to select the desired skin for the GUI configuration:



- The selected **configuration** can be changed later any time.

3.2.1. Windows

If you have a 64-bit Windows, you can choose both the normal (32-bit) Marvin Beans installer or its 64-bit version.

The following table helps you to choose which installer can you use on your platform.

Installer	32-bit Windows		64-bit Windows		
	without Java	with Java	without Java	with 32-bit Java	with 64-bit Java
marvinbeans-VERSION-windows.exe	NO	YES	NO	YES	NO
marvinbeans-VERSION-windows_with_jre.exe (bundled with 32-bit Java)	YES	YES	YES	YES	YES
marvinbeans_VERSION-windows_64bit.exe	NO	NO	NO	NO	YES

If you have a 64-bit Windows, follow the instructions in the 64-bit Windows section.

1. Double-click on **`marvinbeans-VERSION-windows.exe`** or **`marvinbeans-VERSION-windows_with_jre.exe`** to install.
2. You can add the `bin` folder of Marvin Beans to the PATH environment variable to be able to run Marvin applications from any directory in the command line. Details about editing environment variables is described in Windows Help.

Notes:

- Please **make sure to close all running Marvin applications before starting the installer** otherwise it may not be able to perform the installation correctly (overwriting certain `.jar` files is not possible if they are being used by a running application).
  Running applications may include:
  - Marvin desktop applications
  - MS-Office documents where Marvin Objects are being edited
  - Running applications where Marvin is embedded, like Instant JChem

  In this image, you can see an error message displayed during installation. Checking the running processes you can find that `marvinOLEServer.exe` is running, which means that an MS-Office document is just using

Marvin.

- You can run the installer in **silent/non-interactive mode**, which means that in case Marvin is already installed, it will be overwritten with the update without the need of checking the "OK" and "Next" buttons on the installer dialogs. To enable this mode, use the `-q` option (for example open the command prompt with `cmd.exe` and type "`marvinbeans-5_3_0.exe -q`").

64-bit Windows

System requirements: 64-bit Windows system having an installed Java for 64-bit architecture.

1. After downloading **marvinbeans-VERSION-windows_64bit.exe**, take a double-click on the downloaded file (accept running if Windows expects verification).
2. Installer is started: go through the installation wizard. The installer will setup the 64-bit version of JChem_NET_API automatically (that is wrapped into the installer).

Notes:

- JChem_NET_API is required to be able to insert Marvin OLE (embedded object) into MS-Office document or transfer it between Marvin and the MS-Office applications.
- Earlier versions of MS-Office suites are not available in 64-bit format. If your Office does not support 64-bit platform, you cannot use the OLE functionality of 64-bit version of Marvin. In this case, install 32-bit version of Marvin Beans and JChem_NET_API that can incorporate with 32-bit Office applications.
- When you edit an embedded Marvin Object in Office, the editor can be different depending on the platform.
  - MS-Office 32-bit requires 32-bit JChem .NET API for Marvin embedding. It uses 32-bit .NET implementation of MarvinSketch unless 32-bit Marvin Beans package is installed. In this case, it prefers the 32-bit Java implementation.
  - MS-Office 64-bit requires 64-bit JChem .NET API for Marvin embedding. The 64-bit .NET implentation of MarvinSketch is used in all cases.
- See further notes in 32-bit Windows section: here.

3.2.2. MAC OS X

1. Double-click **`marvinbeans-VERSION-macos.dmg`** to install.
2. You can add the `bin` folder of the Marvin Beans folder to the PATH to be able to run Marvin applications from any directory in command line.

Notes:

- Requires Mac OS X 10.0 or later
- The compressed installer should be recognized by Stuffit Expander and should automatically be expanded after downloading. If it is not expanded, you can expand it manually using StuffIt Expander 6.0 or later.
- If you have any problems launching the installer once it has been expanded, make sure that the compressed installer was expanded using Stuffit Expander. If you still have problems, please contact our technical support.
- You can run the installer in **silent/non-interactive mode**, which means that in case Marvin is already installed, it will be overwritten with the update without the need of confirmation. To enable this mode, use the `-q` option.

3.2.3. Linux / Solaris

1. Open a shell and **`cd`** to the directory where you downloaded the installer.
2. Type the following to install: **`sh marvinbeans-VERSION-linux.sh`** (or **`sh marvinbeans-VERSION-linux_with_jre.sh`** depend on which package has been downloaded).
3. You can add the `bin` subdirectory of the Marvin Beans directory to the PATH to be able to run Marvin applications from any directory.

Notes:

- If the installer does not start, check whether **JAVA_HOME/bin** is in PATH (where JAVA_HOME is the directory of Java).
  To check it, type the "**which java**" command that shows the location of the Java launcher. You should get something like this:

  ```
  /usr/java/jdk1.6/bin/java
  ```

  If Java is missing from PATH, you will see something like that:

  ```
  /usr/bin/which: no java in (/usr/java/jdk1.6/bin:/opt/apache-ant-
  1.6.1/bin:/usr/kerberos/bin:/usr/local/bin:/bin:/usr/bin:/usr/X11R6/bin:/home/vertset/bin)
  ```

- You can run the installer in **silent/non-interactive mode**, which means that in case Marvin is already installed, it will be overwritten with the update without the need of confirmation. To enable this mode, use the `-q` option. If you are in terminal mode (GUI is not accessible), we recommend to use this option.

3.2.4. Other Platforms

1. Go to the directory where **`marvinbeans-VERSION.zip`** was downloaded then uncompress the zip file.
2. You can start applications via scripts or batch files that you can find in the `marvinbeans/bin` directory.

Notes:

- You need an expander which can handle `zip` extension.
- Batch files (`bin/*.bat`) have to be initialized before the first use. Set the `MARVINBEANSHOME` variable in the files to the full path of the directory where Marvin Beans is located.

3.2.5. How to uninstall?

Use the uninstaller to remove Marvin Beans from your machine. If you give the **-q** command line parameter by running the uninstaller, it will run in silent mode (no GUI, non-interactive mode).

- **Windows:** Double click on `uninstall.exe` in the Marvin Beans's home folder or select Marvin Beans from the *Add / Remove programs* list on *Control Panel*.
- **OS X:** Double click on `ChemAxon Marvin Beans Uninstaller` in the Marvin Beans' home directory.
- **Linux / Solaris:** Launch the `uninstall` script in the Marvin Beans' home directory.

3.2.6. Additional package

Who needs this package?

Install `marvinbeans-lib-VERSION-signed.zip` only if you need the *signed version* of the Marvin Beans package.
If you would like to launch Marvin applications via Java Web Start from your server, you will need the signed version for security reasons.
Please note that this archive can only be used as an extension of the already installed Marvin Beans package.

Installation

1. Check the product version of the Marvin Beans package you have already installed. You can find the product version of your installed disribution in the *Help > About dialog* or in the `version.properties` file located in the Marvin Beans installation directory.
2. Download the additional package for exactly the same version: **marvinbeans-lib-VERSION-signed.zip**.

3. Create a backup of the **lib** sub-directory of your Marvin Beans package.
4. Extract the **marvinbeans-lib-VERSION-signed.zip** archive file into the Marvin Beans directory. Your extractor tool (e.g. *unzip* or *WinZip*) may ask confirmation to update all files by unwrapping. In this case let it overwrite all. This operation will update the jar files (overwrite them with the signed versions) in the **lib** sub-directory of the installed Marvin Beans package.

3.3. Marvin Beans for .NET

The Marvin Beans package for .NET platform can be downloaded from this link.

4. Version Number

From the Marvin version 5.7, in the file name of any downloadable artifacts, an identifier appears that indicates the internal build number of the file. This identifier begins with _b and continous with a number. It is automatically generated and help to identify the file in the build system of ChemAxon.

MarvinSketch Application Options

Version 6.1.7

The Marvin Beans package contains the MarvinSketch application.

Usage

msketch [*options*] [*files or URLs...*]

Options

`-h` `--help`	Print command line help
`-`	Import a structure from standard input
`--debug`	Verbose debugging messages for cut/copy/paste and drag & drop
`--imageImportServiceURL=[URL]`	Specifies the URL of an image import service for the Sketcher to use.

You can also pass options to Java VM when you run the application from command line.

Examples

1. Start MarvinSketch with an empty sketcher window:

```
msketch
```

2. Start MarvinSketch by loading two molfiles in two windows:

```
msketch caffeine.mol l-adrenaline.mol
```

MarvinSketch Parameters and Events

License Management

This documentation contains detailed instructions about licensing ChemAxon products.

For the online version please visit this link: http://www.chemaxon.com/marvin/help/licensedoc/index.html

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MarvinSketch Graphical User Interface

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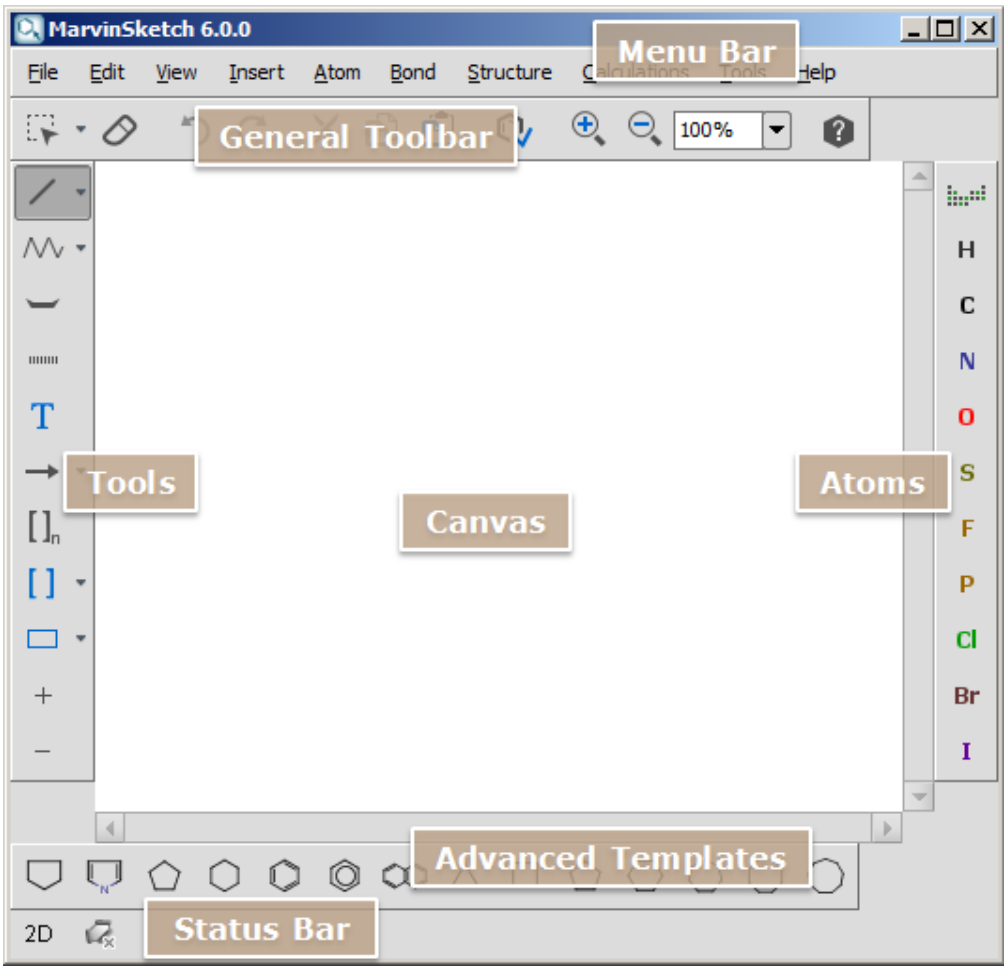
The default layout of the MarvinSketch user interface is shown in the following picture.



It consists of the following primary components:

- Menu Bar: It is located at the top of the main frame, containing menu titles that describe the content of each menu.
- Canvas: This is the main area where chemical structures, queries and reactions are drawn.
- General Toolbar: This toolbar contains buttons for freqently used commands.
- Tools Toolbar: Contains basic elements for stucture drawing like bond, chain, reaction arrow, graphics, etc.
- Atoms Toolbar: Location of the most freqent atom types and the Periodic System button.
- Advanced Templates Toolbar: This special toolbar is a container of structure templates. The templates are rotatable by pressing and holding down the left mouse button while dragging.
- Status Bar: Shows file status, contains navigation buttons and the dimension button.
  The Status Bar appears at the bottom of the main frame, and unlike toolbars, it cannot be customized or moved.
  Some buttons of the Status Bar appear dynamically when you invoke the corresponding command, like enabling multipage molecular documents.

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http://www.chemaxon.com/marvin

Canvas of MarvinSketch

The canvas is the main area where chemical structures, queries and reactions are drawn.

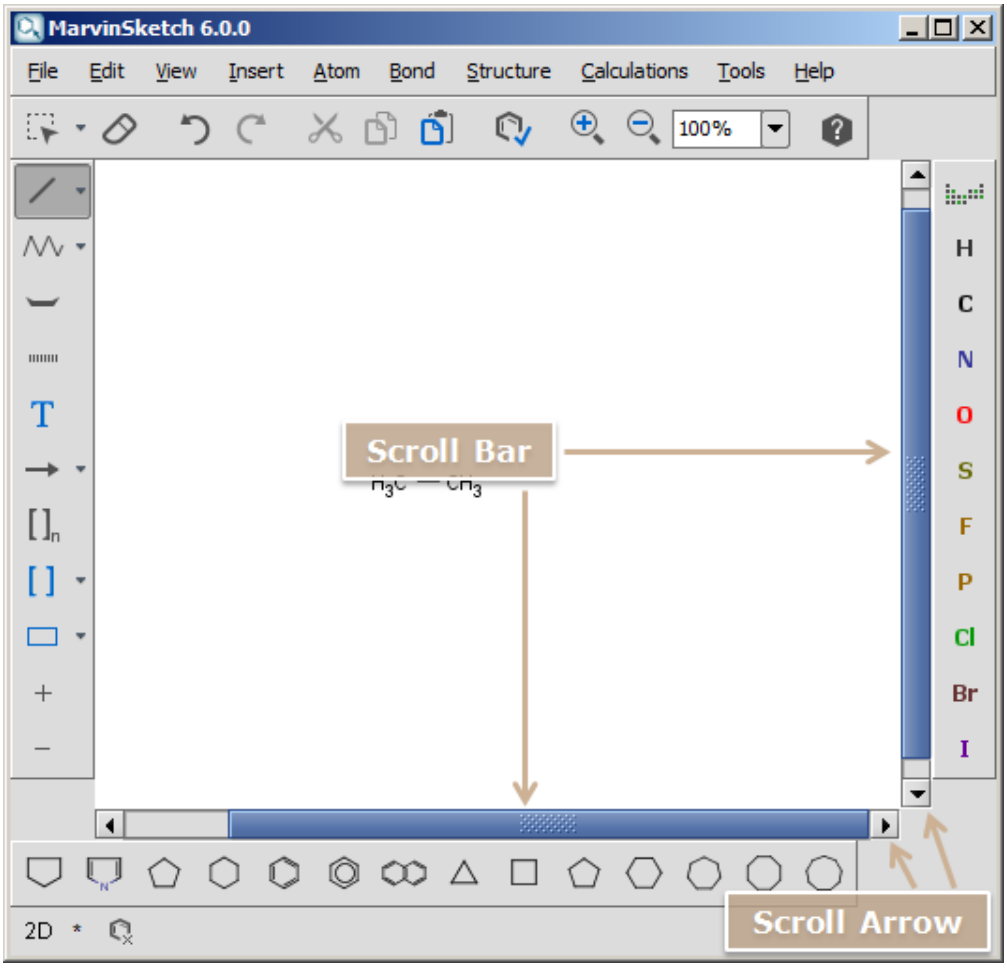
Basic Navigations

Zooming the Canvas

To zoom in or out on the canvas, you can choose the Zoom In, Zoom Out or Zoom Tool of General Toolbar. The View Menu has also options to change the magnification of the canvas. If you have a mouse with a wheel, you can also use Ctrl+Mouse Wheel to zoom in or out on the canvas. When using Ctrl+Mouse Wheel to zoom, the actual position of the cursor will define the center of zooming.

Scrolling the Canvas

Drawing on the canvas activates the horizontal and vertical scroll bars. To move the canvas click the Scroll Arrow of the scroll bar or drag the Scroll Box to scroll the canvas in the preferred direction. You can also use the appropriate Arrow Key of your keyboard to move the canvas. Note: Moving the Canvas with Arrow Keys works only when no selection is made or everything is selected on the Canvas. When an item is selected on the canvas, the Arrow Keys will move the marked object. Ctrl+Arrow key can be used to move the canvas in this case. Shift+Arrow keys will move the selected items in greater units. The undo operation recalls the former direction of these movements. If you have a mouse with a wheel, use the Mouse Wheel to scroll the canvas up or down and use Shift+Mouse Wheel to scroll the canvas left or right.



Menus of MarvinSketch

The Menu Bar contains almost all commands that are available in MarvinSketch.
The main menus are groups of functionally similar commands shown in the following picture:

File Menu
: The File menu contains the available file operations, such as New, Open, Save, Print, and Close. (Note that the unsigned Swing applets contain only a subset of these functions.)

Edit Menu
: The Edit menu contains general clipboard operations like Copy and Paste, structure selecting and deleting commands, as well as Marvin-specific editing options.

View Menu
: The View menu allows you to alter the way the molecule is displayed without modifying the structure file itself. You can change the molecule display type, background color, color scheme, error highlighting, etc. See also: Structure Display Options.
The view menu also contains operations to change the graphical user interface.

Insert Menu
: The Insert menu allows drawing structure templates, bonds, reaction arrows, graphics, text boxes, and more on the canvas. See also: How To Draw Graphic Objects and Text Boxes.

Atom Menu
: Contains all atom related properties such as charge, atom radicals, maps, and many more.

Bond Menu
: Allows changing the type of a bond, and makes bond properties available like bold, topology, reacting center, etc.

Structure Menu
: Provides chemical functions relating to structures like molecule cleaning, aromatization, reaction-handling, naming and more.

Calculations Menu
: Contains the available Calculator Plugins.

Tools Menu
: Contains the available Services.

Help Menu
: Provides information about using the program, technical details and license management.

Full Menu Reference

File Menu

New > Clear Desk	Removes the structure being on the canvas including all fragments and graphical objects.
New > New Window	Opens another MarvinSketch window.
Open	Loads your saved molecule file into Marvin and discard any unsaved changes to the molecule you were previously working with.
Insert File	Inserts your saved molecule file into the canvas whitout erasing its former content.
Save	Saves the molecule to the same file it was opened from and in the same format. If you are working with a new molecule, Save will function as Save As.
Save As	Saves the molecule in a different location or with a different file name or format.
Import Name	Opens the Source window in IUPAC Name format, and enables you to enter directly a IUPAC Name and convert it to structure.

Import Image	Tries to convert an image file to a structure using OSRA.
Export to Image	Exports the molecule to the required location in the required image format.
Find Structure Online > Find Structure in ChemSpider	If ChemSpider contains the structure, it opens the records in your default browser.
Find Structure Online > Find Structure in Chemicalize	If Chemicalize.org contains the structure, it opens the records in your default browser.
Find Structure Online > Find Structure in PubChem	If PubChem contains the structure, it opens the records in your default browser.
Print	Prints an image of the current molecule.
Document Style	Changes atom and bond drawing properties in the document.
Multipage Settings	Creates a multipage molecular document that helps to work with large drawings by dividing them into pages.
Recent	Lists of recently used file names.
Close	Finishes working with the currently open molecule.
Exit	Saves GUI settings, preferences and My Templates before exiting the application.

Edit Menu

Undo	Reverses the last command or the last entry you typed.
Redo	Reverses the action of the last Undo command.
Cut	Removes and copies the selection to the clipboard.
Copy	Copies the selection to the clipboard.
Copy As	Copies the selection to the clipboard in the specified format.
Copy As Smiles	Copies the selection to the clipboard in SMILES format.
Paste	Inserts the contents of the clipboard at the location of the cursor, without replacing selection.
Select All	Selects the structure being on the canvas including all fragments and graphical objects.
Delete	Removes the selection from the canvas.
Transform	These transformations affect the molecular coordinates. Note: The structure will be saved with the altered coordinates.
Transform > Drag Selection	Moves selection on the canvas with changing coordinates.
Transform > Rotate in 2D	Rotates selection in the plane of the canvas with changing coordinates.
Transform > Rotate in 3D > Around arbitrary axis	Rotates selection in 3D around an axis defined by two atoms selected by the user.
Transform > Rotate in 3D > Around X axis	Rotates selection in 3D around a horizontal axis placed in the canvas.
Transform > Rotate in 3D > Around Y axis	Rotates selection in 3D around a vertical axis placed in the canvas.
Transform > Rotate in 3D > Around Z axis	Rotates the selection in 3D around an axis perpendicular to the canvas.
Transform > Rotate in 3D > Free 3D rotation	Rotates selection in 3D with changing coordinates. Compare it to the Rotate in 3D transformation of View Menu, which affects only the position of observation.
Transform > Rotate in 3D > Group rotation	The selected group rotates around the bond that connects it to the molecule.
Transform > Switch Transformation	Changes transformation mode from Drag to Rotate in 2D, Rotate in 2D to Rotate in 3D, while Rotate in 3D to Drag.
Transform > Flip > Flip Horizontally	Flips the selected object(s) horizontally, preserving the configuration of all enantiomers.
Transform > Flip > Flip Vertically	Flips the selected object(s) vertically, preserving the configuration of all enantiomers.
Transform > Flip > Rotate 180° in Canvas	Rotates the selected object(s) on the canvas plane, preserving the configuration of all enantiomers.
Transform > Flip > Group Flip	Rotates the selected structure group by 180° around an axis set on the bond connecting the selection to the rest of the molecule. Stereocenters in the molecules are retained, the wedge bond styles change to keep the stereo information.

Transform > Mirror > Mirror Horizontally	Mirrors the selected object(s) horizontally, inverting the configuration of all enantiomers.
Transform > Mirror > Mirror Vertically	Mirrors the selected object(s) vertically, inverting the configuration of all enantiomers.
Transform > Mirror > Mirror to Canvas Plane	Mirrors the selected object(s) to the canvas plane, inverting the configuration of all enantiomers.
Transform > Mirror > Group Mirror	Mirrors the selected group if it has only one connecting bond to the structure.
Transform > Invert > Invert to geometric center	Reflects the selected fragment(s) through the geometric center point.
Transform > Invert > Invert to an arbitrary center	Reflects the selected fragment(s) through the chosen point in any fragment (an atom).
Transform > 3D plane	Rotates the molecule to place the selected 3 atoms into the plane of the canvas.
Object > Bring to Front	Brings the selected object in front of all others.
Object > Send to Back	Places the selected object behind all others.
Object > Align	Aligns the centers of the selected objects horizontally or vertically on the canvas.
Object > Distribute	Distributes the selected objects horizontally or vertically in the space defined by the furthermost objects.
Object > Align and Distribute	Performs alignment and distribution horizontally or vertically.
Template Library	Organized collection of template molecules can be edited.
Source	You can alter a molecule by directly editing its source in the Edit Source Window. You can view and edit the source in any of the supported file formats.
Preferences	The Preferences dialog window allows you to change many of the MarvinSketch display settings, including look & feel, error highlighting, and object visibility.

View Menu

Mouse Mode > Sketch	The Sketch mode allows drawing into the canvas.
Mouse Mode > Zoom	Zoom the content of the canvas by dragging the mouse without modifying atom coordinates.
Mouse Mode > Rotate in 3D	Spin the structure around its central point in 3 dimension with the help of the mouse without modifying atom coordinates. Compare it to the Free 3D rotation of Edit Menu, which affects the molecular coordinates.
Mouse Mode > Reset View	Restores the starting view as modified by rotation and zoom.
Zoom Level	Allows you to select a magnification percentage from the list or to type a custom percentage.
Structure Display > Atom Symbols in 3D	Sets atom symbol visibility in 3D mode. Note that in 3D mode, atoms may become invisible in Wireframe and Stick mode by hiding atom symbols.
Structure Display > Wireframe	Displays bonds as thin lines, and atoms (except Carbon) as symbols.
Structure Display > Wireframe with Knobs	Displays bonds as thin lines, Carbon atoms as knobs, and other atoms as symbols.
Structure Display > Stick	Displays bonds as thick lines, and atoms (except Carbon) as symbols.
Structure Display > Ball and Stick	Displays bonds as thick lines, atoms as shaded balls, and atoms (except Carbon and Hydrogen) as symbols on balls.
Structure Display > Spacefill	Displays atoms as large shaded balls, and atoms (except Carbon and Hydrogen) as symbols on the balls.
Structure Display > Quality > Low Quality	Disables line anti-aliasing.
Structure Display > Quality > High Quality	Enables line anti-aliasing.
Colors > Monochrome	Displays all atoms with default drawing color.
Colors > CPK	Displays all atoms with Corey-Pauling-Kultun colors.
Colors > Shapely	This color scheme is based on RasMol's shapely color scheme for nucleic and amino acids.
Colors > Group	Coloring atoms based on PDB residue numbers.

Colors > Atom/Bond Sets	Colors atoms and bonds according to the color of the pre-defined set they belong to.
Colors > Background	Sets custom background color with adjusted default drawing color.
Colors > White Background	Sets the background color to white and the default drawing color to black.
Colors > Black Background	Sets the background color to black and the default drawing color to white.
Stereo > R/S Labels > All	Always show atom chirality (R/S).
Stereo > R/S Labels > Absolute Stereo	Show atom chirality if chiral flag is set for the molecule or the atom's enhanced stereo type is absolute.
Stereo > R/S Labels > None	Do not show atom chirality (R/S).
Stereo > E/Z Labels	Toggles the display of absolute double bond stereo configuration labels. Bonds known to have an (E) or (Z) configuration will be marked as such.
Stereo > Absolute Labels	Toggles the display of the Absolute label if the chiral flag is set on the molecule.
Implicit Hydrogens > On All	View hydrogens by symbol on all atoms. This option is disabled in Spacefill and Ball & Stick display modes.
Implicit Hydrogens > On Hetero and Terminal	View hydrogens by symbol on hetero and terminal carbon atoms. This option is disabled in Spacefill and Ball & Stick display modes.
Implicit Hydrogens > On Hetero	View hydrogens by symbol on hetero atoms only. This option is disabled in Spacefill and Ball & Stick display modes.
Implicit Hydrogens > Off	Disable hydrogens by symbol on all atoms.
Peptide Display > 1-letter	View peptide sequence with 1-letter aminoacid codes.
Peptide Display > 3-letter	View peptide sequence with 3-letter aminoacid codes.
Advanced > Atom Numbering > Off	Disable the visibility of atom indices.
Advanced > Atom Numbering > Atom Number	Enable the visibility of unique internal atom indices. The indices are continuous starting from 1.
Advanced > Atom Numbering > IUPAC Numbering	Enable the visibility of IUPAC numbering of atoms in a molecule. It is synchronized with the numbering of "Structure to name" option.
Advanced > Atom Properties	Toggles the visibility of atom properties.
Advanced > Atom Mapping	Toggles the visibility of atom mapping labels.
Advanced > Graph Invariants	Toggles the display of graph invariants (canonical labels).
Advanced > Bond Lengths	Toggles the display of bond lengths in Angstroms on the middle of the bonds.
Advanced > Lone Pairs	Toggles the display of lone pairs.
Advanced > R-groups	Toggles the display of R-group definitions.
Advanced > R-logic	Toggles the display of R-logic definitions.
Advanced > Valence	Toggles the display of valence numbers. Default setting is On.
Advanced > Ligand Error	Toggles the display of ligand errors. Default setting is On.
Pages > Fit Page Width	Adjusts the width of the current page to the width of the canvas.
Pages > Fit Page Height	Adjusts the height of the current page to the height of the canvas.
Pages > Fit Page	Adjusts the current page so that the whole current page will be placed centralized within the canvas.
Pages > Previous Page	Goes to the previous page of multipage molecular document.
Pages > Next Page	Goes to the next page of multipage molecular document.
Pages > First Page	Goes to the first page of multipage molecular document.
Pages > Last Page	Goes to the last page of multipage molecular document.
Pages > Goto Page	Goes directly to a specific page by entering a number in the appearing dialog window.
Open MarvinSpace	Launches a MarvinSpace window containing the current molecule from the Sketcher.
Toolbars > Toolbars	Sets the visibility of individual toolbars.
Menubar	Sets the visibility of the main menubar.
Status Bar	Sets the visibility of the status bar.
Editor Style > Configurations	Lists the available configurations, and allows quick switch.
Editor Style > Configuration	Configurations are GUI alternatives storing whole menu, toolbar and popup

Settings	personalizations. This makes easy to define and quickly change the GUI for various purposes like sketching, publishing, teaching, etc.
Editor Style > Reset Current Configuration	Removes all local modifications made on the active GUI configuration. Note that this action cannot be undone.
Editor Style > Customize	Customization allows you to personalize the GUI of MarvinSketch including menus, toolbars and keyboard shortcuts.

Insert Menu

Template Library	Organized collection of template molecules.
Groups	The full list of Abbreviation Groups.
New Structure	Opens a new MarvinSketch window to add new fragments to tha canvas without having to change e.g. the 3D view mode.
Bond > Single	Places Single type bond on the canvas.
Bond > Double	Places Double type bond on the canvas.
Bond > Triple	Places Triple type bond on the canvas.
Bond > Aromatic	Places Aromatic type bond on the canvas.
Bond > Single Up	Places Single Up type wedge bond on the canvas.
Bond > Single Down	Places Single Down type wedge bond on the canvas.
Bond > Single Up or Down	Places Single Up or Down type wedge bond on the canvas.
Bond > Double Cis or Trans	Places Double Cis or Trans query type double bond on the canvas.
Bond > Double C/T or Unspec	Places Double C/T or Unspec query type double bond on the canvas.
Bond > Single or Double	Places Single or Double type bond on the canvas.
Bond > Single or Aromatic	Places Single or Aromatic type bond on the canvas.
Bond > Double or Aromatic	Places Double or Aromatic type bond on the canvas.
Bond > Any	Places Any type bond on the canvas.
Bond > Coordinate	Places Coordinate type bond on the canvas.
Chain > Chain	Places a carbon chain on the canvas. The number of carbon atoms can be increased or decreased by dragging the mouse. The chain drawing direction is mirrored based on the direction of the mouse movements.
Chain > Curved Chain	Places a curved carbon chain on the canvas. The direction of the chain growth follows the mouse path. The number of carbon atoms can be increased or decreased by dragging the mouse. The chain drawing direction is mirrored based on the direction of the mouse movements.
Arrow > Single Reaction Arrow	Places a Single Reaction Arrow object on the canvas.
Arrow > Retrosynthetic Arrow	Places a Retrosynthetic Arrow object on the canvas.
Arrow > Equilibrium Arrow	Places an Equilibirum Arrow object on the canvas.
Arrow > Two-headed Arrow	Places a Two-headed Arrow object on the canvas.
Arrow > Single Arrow	Places a Single Arrow graphical object on the canvas.
Arrow > Graph. Retrosynthetic Arrow	Places a Retrosynthetic Arrow graphical object on the canvas.
Arrow > Graph. Equilibrium Arrow	Places an Equilibrium Arrow graphical object on the canvas.
Arrow > Resonance Arrow	Places a Resonance Arrow graphical object on the canvas.
Arrow > Curved Arrow	Places a Curved Arrow graphical object on the canvas.
Arrow > Dashed Arrow	Places a Dashed Arrow graphical object on the canvas.
Arrow > Crossed Arrow	Places a Crossed Arrow graphical object on the canvas.
Bracket > Parentheses	Places a Parentheses object on the canvas.
Bracket > Square Brackets	Places a Square Brackets object on the canvas.
Bracket > Braces	Places a Braces object on the canvas.
Bracket > Chevrons	Places a Chevrons object on the canvas.
Electron Flow > 1 Electron	Places an electron flow arrow object on the canvas representing one-electron transfer.
Electron Flow > 2 Electrons	Places an electron flow arrow object on the canvas representing two-electron

	transfer.
Graphics > Line	Places a Line object on the canvas.
Graphics > Single Arrow	Places a Single Arrow graphical object on the canvas.
Graphics > Graph. Retrosynthetic Arrow	Places a Retrosynthetic Arrow graphical object on the canvas.
Graphics > Graph. Equilibrium Arrow	Places an Equilibrium Arrow graphical object on the canvas.
Graphics > Resonance Arrow	Places a Resonance Arrow graphical object on the canvas.
Graphics > Curved Arrow	Places a Curved Arrow graphical object on the canvas.
Graphics > Dashed Arrow	Places a Dashed Arrow graphical object on the canvas.
Graphics > Crossed Arrow	Places a Crossed Arrow graphical object on the canvas.
Graphics > Polyline	Places a Polyline object on the canvas.
Graphics > Rectangle	Places a Rectangle object (Square object in case the Shift button is pressed) on the canvas.
Graphics > Rounded Rectangle	Places a Rounded Rectangle object (Rounded Square object in case the Shift button is pressed) on the canvas.
Graphics > Ellipse	Places an Ellipse object (Circle object in case the Shift button is pressed) on the canvas.
Text	Places a Text object on the canvas. Allows changing text properties on the appearing toolbar.

Atom Menu

Stereo > R/S > Off	Removes the absolute stereo configuration from a chiral atom along with the marking wedge bond.
Stereo > R/S > R	Sets the absolute stereo configuration on a chiral atom to R, marking it with wedge bond.
Stereo > R/S > S	Sets the absolute stereo configuration on a chiral atom to S, marking it with wedge bond.
Stereo > Reaction > Off	Sets the stereo configuration of the atom not to be considered during the reaction.
Stereo > Reaction > Inversion	Sets the stereo configuration of the atom to be inverted during the reaction.
Stereo > Reaction > Retention	Sets the stereo configuration of the atom to be retained during the reaction.
Stereo > Enhanced	See Stereo Documentation for details.
Charge	Allows you to change the charge of any atom between [-128, 128]. The number of implicit hydrogens will be adjusted if possible to accommodate the new charge. Valence errors will be highlighted in red.
Valence	Allows you to change the valence of any atom between [0, 8].
Radical > Off	Removes the radical designation from an atom.
Radical > Monovalent	Sets Monovalent radical center.
Radical > Divalent	Sets Divalent radical center.
Radical > Divalent Singlet	Sets Divalent radical center with singlet electronic configuration.
Radical > Divalent Triplet	Sets Divalent radical center with triplet electronic configuration.
Radical > Trivalent	Sets Trivalent radical center.
Radical > Trivalent Doublet	Sets Trivalent radical center with doublet electronic configuration.
Radical > Trivalent Quartet	Sets Trivalent radical center with quartet electronic configuration.
Isotope	Sets or changes the isotope number of the selected element, or resets the default atom (no isotope) when it is set to Off.
Map	Sets map labels/identifiers on the selected atoms that do not change while altering the molecule. They are useful when dealing with reactions, and can be saved in SMILES and MDL formats.
R-group	Changes the selected atom to an R-group label. R-groups symbolize alternative substituents.
R-group Attachment	The selected atom becomes the attachment point for the substituent.
R-group Attachment Order	Changes the order (numbering) of the attachment points.
Link Node	Specifies query structures containing rings or chains of variable size.

Periodic Table	Shows Periodic Table and query/atom property drawing window.
Edit Properties	Specifies the property of an atom.
Add S-group attachment	If the selected atom is part of an S-group, you can specify an attachment point.
Remove S-group attachment	Removes the highest-numbered attachment point from an atom of an S-group.

Bond Menu

Type > Single	Changes the selected bond type to Single.
Type > Double	Changes the selected bond type to Double.
Type > Triple	Changes the selected bond type to Triple.
Type > Aromatic	Changes the selected bond type to Aromatic.
Type > Single Up	Changes the selected bond type to Single Up.
Type > Single Down	Changes the selected bond type to Single Down.
Type > Single Up or Down	Changes the selected bond type to Single Up or Down.
Type > Double Cis or Trans	Changes the selected bond type to Double Cis or Trans.
Type > Double C/T or Unspec	Changes the selected bond type to Double Cis/Trans or Unspec.
Type > Single or Double	Changes the selected bond type to Single or Double.
Type > Single or Aromatic	Changes the selected bond type to Single or Aromatic.
Type > Double or Aromatic	Changes the selected bond type to Double or Aromatic.
Type > Any	Changes the selected bond type to Any.
Type > Coordinate	Changes the selected bond type to Coordinate.
Bold	Changes the selected bond to Bold. See details on bold tool application.
Hashed	Changes the selected bond to Hashed.
Topology > None	Unsets the bond topology property.
Topology > In Ring	Sets a bond property so that when the molecule is used as a query, the specified bond must be in a ring to score a hit.
Topology > In Chain	Sets a bond property so that when the molecule is used as a query, the specified bond must be in a chain to score a hit.
Reacting Center > None	Unsets reacting center query feature of the selected bond.
Reacting Center > Center	Sets reacting center query feature on the selected bond: the bond takes part in the reaction.
Reacting Center > Make or Break	Sets reacting center query feature on the selected bond: the bond is created or disappears in the reaction.
Reacting Center > Change	Sets reacting center query feature on the selected bond: the bond remains in the reaction, but its bond type changes, for example from single to double.
Reacting Center > Make and Change	Sets reacting center query feature on the selected bond: currently it works exactly as "Center".
Reacting Center > Not Center	Sets reacting center query feature on the selected bond: the bond must not change in the reaction.
Stereo Search	Uses stereo configuration of the specified double bond when this molecule is used as a query.
Regenerate Bonds	Generate bonds for an XYZ structure with a different bond length cut-off.
Align > Horizontally	Alters the molecule so that the selected bond is oriented horizontally.
Align > Vertically	Alters the molecule so that the selected bond is oriented vertically.
Ligand order	Changes the order of the attachment of R-group ligands.
Edit Properties	Bond properties can be edited from this menu.

Structure Menu

Clean 2D > Clean in 2D	Calculates new 2D coordinates for the molecule.
Clean 2D > Hydrogenize Chiral Center	Adds an explicit hydrogen atom to a chiral center having no terminal atoms when 2D cleaning is performed.
Clean 2D > Clean Wedge Bonds	Arranges the wedge bonds of the molecule in 2D.
	Calculates new 3D coordinates for the molecule. Clean3D builds up conformers of

Clean 3D > Clean in 3D	fragments from which the best, i.e. the lowest energy conformer is given back. The quality of the structures is measured by a simple energy function (Dreiding type molecular mechanics).
Clean 3D > Cleaning Method > Fine Build	Fine Clean3D builds up conformers of fragments to find low energy conformer. Leaves failed fragments intact.
Clean 3D > Cleaning Method > Fine with Hydrogenize	The build process always adds explicit hydrogens to the structures which are removed if not present in the original molecule. This option prevents the removal of extra hydrogen atoms, otherwise gives the same results than Fine build.
Clean 3D > Cleaning Method > Fast Build	Fast clean, which if fails, performs fine clean. It accepts any generated structure, and it is the default behavior of the Clean3D function.
Clean 3D > Cleaning Method > Build or Optimize	Builds 3D structure for non-3D molecules and just optimizes the 3D molecules with the Dreiding force field.
Clean 3D > Cleaning Method > Gradient Optimize	Optimizes with the Dreiding force field using the actual structure as starting geometry.
Clean 3D > Display Stored Conformers	Allows you to choose one of the possible conformer structures which were calculated via the Conformers plugin.
Directed Merge > Assign Atoms	Chooses the atoms of the fragments to be merged.
Directed Merge > Merge	Merges the fragments at the atoms set.
Add > Add Explicit Hydrogens	Adds explicit H atoms instead of the current implicit ones. Explicit hydrogens are displayed with atoms joining its neighbor while implicit hydrogens are displayed by atom symbols only.
Add > Data	Attaches data like stoichiometry coefficient to the molecule.
Add > Absolute Stereo (CHIRAL)	Sets chiral flag for the molecule.
Add > Multi-Center	Adds a multi-center attachment point representing a group of atoms.
Add > Position Variation Bond	Create a variable point of attachment to represent a connection point to a group of atoms.
Remove > Explicit Hydrogens	Removes explicit H atoms and increases the number of implicit hydrogens.
Remove > Data	Removes attached data from the molecule.
Remove > Absolute Stereo (CHIRAL)	Removes the chiral flag of the molecule.
Edit data	Changes a previously attached data like stoichiometry coefficient of the molecule.
Edit properties	Bond properties can be edited from this menu.
Aromatic Form > Convert to Aromatic Form	Transforms the molecule to aromatic representation using the transformation method set.
Aromatic Form > Conversion Method > Basic	Basic aromatization method is described here.
Aromatic Form > Conversion Method > General	General aromatization method is described here.
Aromatic Form > Conversion Method > Loose	Loose aromatization method is described here.
Aromatic Form > Convert to Kekulé Form	Transforms the molecule to non-aromatic representation.
Group > Group	Creates a custom S-group, R-group or Repeating Unit with Repetition Ranges.
Group > Frequency Variation	Creates a Repeating Unit with Repetition Ranges.
Group > Merge Brackets	Creates a bracket that crosses two bonds.
Group > Edit Group	Modifies the properties of the selected group (restricted to 4 types: generic, component, monomer, mer).
Group > Contract Group	Contracts all groups to its abbreviations.
Group > Expand Group	Displays the full structure instead of the abbreviations.
Group > Ungroup	Removes all abbreviated group associations from the molecule.
Reaction > Merge	

Reactants	Merges the selected fragments to a reactant, product or agent.
Reaction > Unmerge Reactants	Removes selected fragments from a previously merged reactant, product or agent.
Mapping > Map Atoms	Inserts map numbers of the selected atoms.
Mapping > Reaction Mapping Method > Complete	All atoms in the reaction are mapped.
Mapping > Reaction Mapping Method > Changing	Only those atoms are mapped that have changing bond. Either the bond order changes, or new bond is created, or bond is deleted. Orphan and widow atoms are included.
Mapping > Reaction Mapping Method > Matching	Maps all matching atoms in the reaction (Daylight style mapping). A reaction atom is called matching if it is not an orphan/widow atom: it exists on both sides of the reaction.
Mapping > Unmap Atoms	Removes map numbers of the selected atoms.
Attribute > R-Logic	Allows setting additional R-group conditions such as occurrence, rest H and if-then expressions to R-groups in the R-logic dialog window.
Structure to Name > Place IUPAC Name	Inserts IUPAC Name onto the canvas.
Structure to Name > Generate Name	Generates IUPAC and/or Traditional Name.
Name to Structure	Opens the Source window in IUPAC Name format, and enables you to enter directly a IUPAC Name and convert it to structure.
Markush Enumeration	Generates a whole or a subset of the library of a generic Markush structure.
Check Structure	Checks and corrects chemical structures. See Structure Checker in MarvinSketch for more details.
Auto Check	Toggles auto checking of structures while drawing.

Calculations Menu

Elemental Analysis	Calculates the elemental composition of the molecule.
Protonation > pKa	Calculates the pKa values of the molecule.
Protonation > Major Microspecies	Draws molecular microspecies at given pH.
Protonation > Isoelectric Point	Calculates gross charge distribution of a molecule as function of pH.
Partitioning > logP	Calculates the octanol/water partition coefficient.
Partitioning > logD	Calculates the octanol/water partition coefficient at any pH.
Charge > Charge	Calculates the partial charge value of each atom.
Charge > Polarizability	Calculates the polarizability of each atoms.
Charge > Orbital Electronegativity	Calculates electronegativity of each atoms.
Charge > Dipole Moment Calculation	Calculates the electric dipole moment of the molecule
NMR > CNMR Prediction	Predicts ^{13}C NMR chemical shifts of the molecule.
NMR > HNMR Prediction	Predicts ^{1}H NMR chemical shifts of the molecule.
NMR > NMR Spectrum Viewer	Opens and displays JCAMP-DX NMR spectral file.
Isomers > Tautomers	Generates two dimensional tautomers of the molecule.
Isomers > Stereoisomers	Generates all possible stereoisomers of the molecule.
Conformation > Conformers	Generates selected number of conformers or the lowest energy conformer of a molecule.
Conformaton > Molecular Dynamics	Calculates the configurations of the system by integrating Newton's laws of motion.
Conformation > 3D Alignment	Overlays drug sized molecules onto each other in the 3D space.
Geometry > Topology Analysis	Provides characteristic values related to the topological structure of a molecule.

Geometry > Geometry	Provides characteristic values related to the geometrical structure of a molecule. It can calculate steric hindrance and Dreiding energy.
Geometry > Polar Surface Area (2D)	Provides estimation of topoligical polar surface area (TPSA).
Geometry > Molecular Surface Area (3D)	Calculates van der Waals or solvent accessible molecular surface area.
Predictor	Predicts molecular properties based on its structure. The method is based on QSAR algorithm using a multiple linear regression model and a least squares fitting.
Other > H Bond Donor/Acceptor	Calculates atomic hydrogen bond donor and acceptor inclination.
Other > Huckel Analysis	Calculates localization energies L(+) and L(-) for electrophilic and nucleophilic attack at an aromatic center.
Other > Refractivity	Calculates molar refractivity of the molecule.
Other > Resonance	Generates all resonance structures of the molecule.
Other > Structural Frameworks	Calculates Bemis and Murcko frameworks and other structure based reduced representations of the input structures.

Tools Menu

Services	Provides accessibility to previously integrated third-party calculations*.

Help Menu

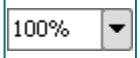
Help Contents	Shows MarvinSketch User's Guide.
Licenses	Starts ChemAxon License Manager where you can manage the licenses of all ChemAxon products.
About MarvinSketch	Shows MarvinSketch product information and technical details.

Toolbars of MarvinSketch

The toolbars provide buttons that access some of the frequently used commands in the menus. To activate a command, click its toolbar button. If a command is unavailable, its button appears grayed-out.

Note: Place the mouse cursor over a toolbar button to see the tooltip describing its use.

General Toolbar

	Rectangle Selection	Allows selection in rectangle mode on mouse drag.
	Lasso Selection	Allows selection in lasso mode on mouse drag.
	Structure Selection	Allows selection in structure selection mode on mouse drag. With this selection mode only whole fragments can be selected.
	Erase	Removes all structures upon selection.
	Undo	Reverses the last command or the last entry you typed.
	Redo	Reverses the action of the last Undo command.
	Cut	Removes and copies the selection to the clipboard.
	Copy	Copies the selection to the clipboard.
	Paste	Inserts the contents of the clipboard at the location of the cursor, without replacing selection.
	Check Structure	Checks and corrects chemical structures. See Structure Checker in MarvinSketch for more details.
	Zoom In	Increases the canvas's magnification.
	Zoom Out	Decreases the canvas's magnification.
	Zoom Tool	Changes the canvas's magnification to a specific value. It can also do autoscale using named values: All, Selection. This is supplemented with 'Scaffold' and R-group(s) when there is a defined R-group on the canvas.
	Help Contents	Shows MarvinSketch User's Guide.

Tools Toolbar

The tools consist of various command groups. The tools having chemical meaning (like bond or reaction arrow) are drawn in black lines, while strictly graphical objects are in blue. You can place for example only ONE reaction arrow on the canvas, but as many graphical arrows as you wish and they will look completely identical.

	Insert Bond	Places various bond types on the canvas.
	Insert Chain	Places a carbon chain on the canvas. The number of carbon atoms can be increased or decreased by dragging the mouse. Selection of straight or curved chain drawing is available.
	Bold Tool	Thickens the selected bond. See details on bold tool function.
	Hashed Bond Tool	Makes the selected bond hashed. It only retains single original bond type.
	Insert Text	Places a Text object on the canvas. Allows changing text properties on the appearing toolbar.
	Insert Reaction Arrow	Places various reaction arrow objects on the canvas.
	Create Group	Creates a custom abbreviation group.
	Insert Brackets	Places brackets, parentheses, chevrons or braces on the canvas.
	Insert Graphics	Places various graphical objects on the canvas.
	Increase Charge	Increases the charge of the selected atom. The number of implicit hydrogens will be adjusted if possible to accommodate the new charge. Valence errors will be

		highlighted in red.
–	Decrease Charge	Decreases the charge of the selected atom. The number of implicit hydrogens will be adjusted if possible to accommodate the new charge. Valence errors will be highlighted in red.

Atoms Toolbar

	Periodic Table	Shows Periodic Table and query/atom property drawing window.
H	Insert Hydrogen	Places Hydrogen atom on the canvas.
C	Insert Carbon	Places Carbon atom on the canvas.
N	Insert Nitrogen	Places Nitrogen atom on the canvas.
O	Insert Oxygen	Places Oxygen atom on the canvas.
S	Insert Sulfur	Places Sulfur atom on the canvas.
F	Insert Fluorine	Places Fluorine atom on the canvas.
P	Insert Phosphorus	Places Phosphorus atom on the canvas.
Cl	Insert Chlorine	Places Chlorine atom on the canvas.
Br	Insert Bromine	Places Bromine atom on the canvas.
I	Insert Iodine	Places Iodine atom on the canvas.

Chemical Toolbar

This toolbar contains chemical functions and it is not visible by default.
To make it visible, choose **View > Toolbars > Chemical**.

	Clean 2D	Calculates new 2D coordinates for the molecule.
	Clean 3D	Calculates new 3D coordinates for the molecule. Clean3D builds up conformers of fragments from which the best, i.e. the lowest energy conformer is given back. The quality of the structures is measured by a simple energy function (Dreiding type molecular mechanics).
	Convert to Aromatic Form	Transforms the molecule to aromatic representation using the transformation method set.
	Convert to Kekulé Form	Transforms the molecule to non-aromatic representation.

Markush Toolbar

This toolbar contains funtions that help to work with Markush structures and it is not visible by default.
To make it visible, choose **View > Toolbars > Markush**.

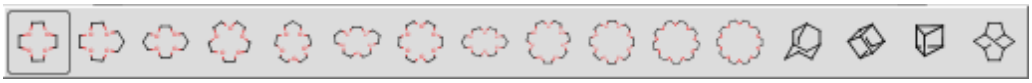
	Position Variation Bond	Creates a variable point of attachment to represent a connection point to a group of atoms.
	Frequency Variation	Creates a Repeating Unit with Repetition Ranges.
	R-group attachment	Adds an attachment to the structure.

Advanced Templates Toolbar

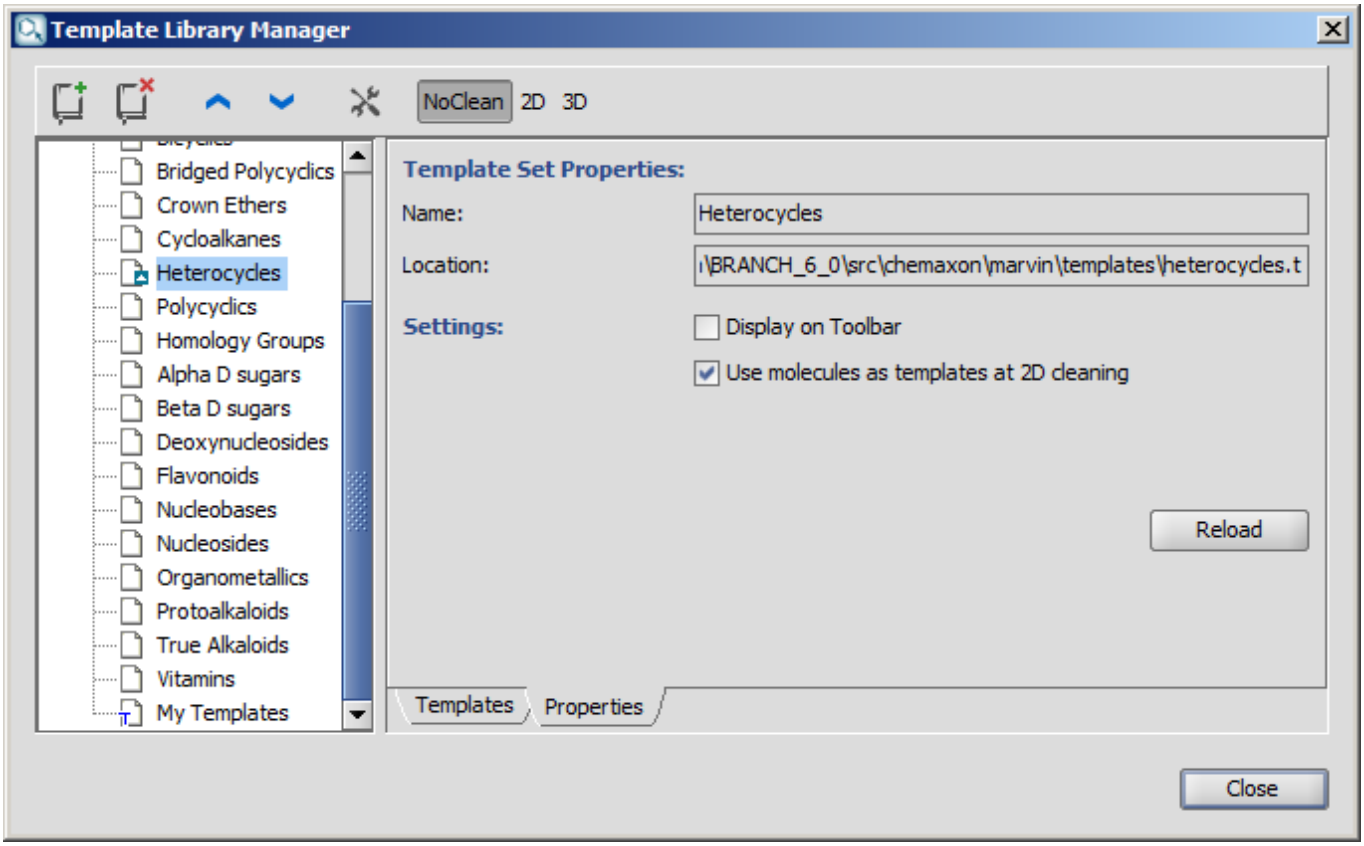
This toolbar contains special buttons holding structure templates.
Additional functions of this toolbar:

1. **The toolbar can show different template groups.**
   - General and My Templates:

   - Crown Ethers and Bridged Polycyclics:

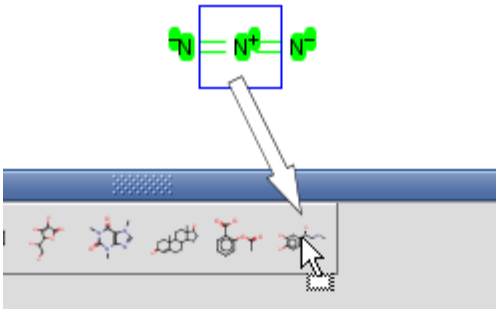


   - To control which template sets are displayed on the toolbar, use the Properties panel in the Template Library (Ctrl+t):

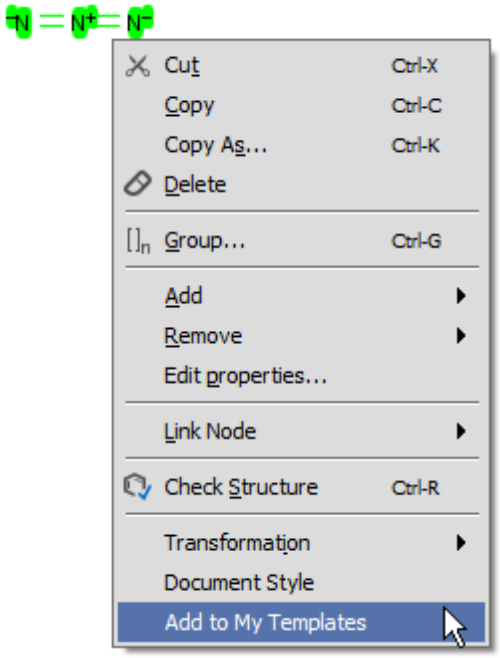


     Checking the 'Use molecules as templates at 2D cleaning' checkbox will effect the structures containing that template during cleaning of the structure: the default cleaning form is overwritten by the template structure. This way, you can cutomize your drawings: add or draw a set of templates and check this option.

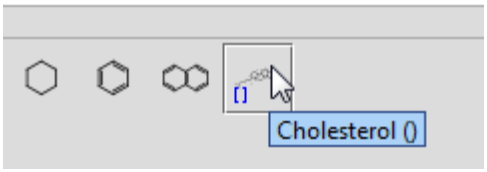
2. **Any structure can be added to the My Templates group.**
   - Using Drag & Drop to the toolbar



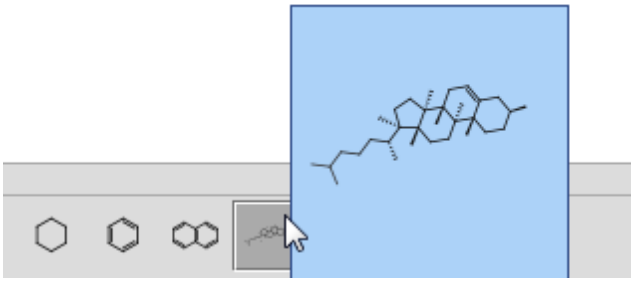
   - Using the Pop-up menu



3. **Set the name of the new template.**
   - Right-click on the template icon on the template toolbar and select **Properties**.
   - Set the name and/or the abbreviation of the template in the Template Properties box.
   - After that the template is identified with its name and/or abbreviation.



4. **Templates without a name**
   - If the template does not have a name, hovering the cursor over its icon on the template toolbar magnifies the image on the icon. This improves the visibility of the template icon, especially for big structures.



5. **The template can be removed from the toolbar.**
   - Right-click on the template icon and select **Remove** to remove the template from the toolbar and from the My Templates list.

Simple Templates Toolbar

If you only wish to use the 6 generic template structures without additional functions, you can use the Simple Templates Toolbar. This toolbar is not visible by default. To make it visible, choose **View > Toolbars > Simple Templates**.

	Cyclopentane (house)
	Pyrrole
	Cyclopentane
	Cyclohexane

	
	Benzene
	Naphthalene

3D editing Toolbar

	Maps atoms to merge.
	Merges assigned atoms.
	Alters the coordinates of the molecule in order to put the 3 selected atoms of the molecule onto the plane of the canvas.
	Adds new fragment to the canvas.

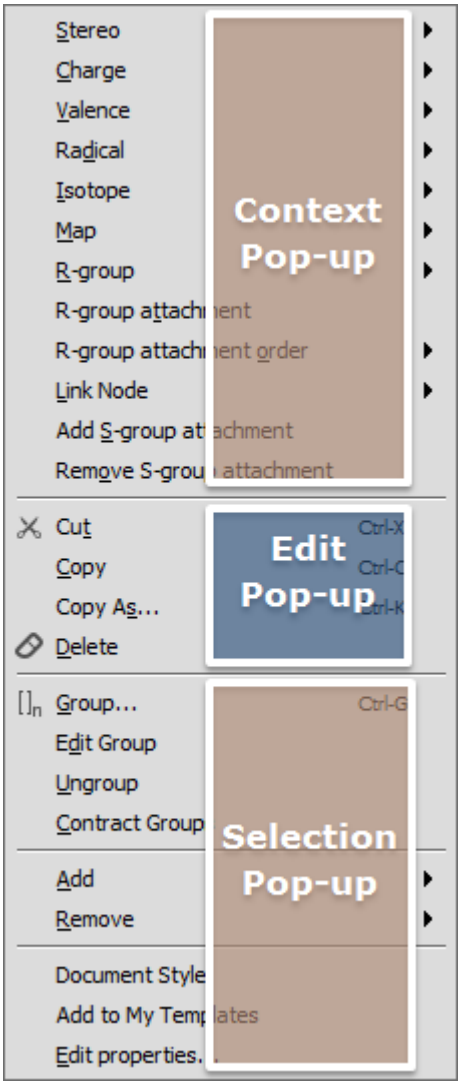
Pop-up Menus of MarvinSketch

There are four pop-up menus (also called context or right-click menus) available in MarvinSketch:

- Atom Pop-up Menu
- Bond Pop-up Menu
- Object Pop-up Menu
- Edit Pop-up Menu

These popup menus do not require the corresponding atom, bond or object to be selected, however there are some additional menu elements that appear only when they are selected.

Please note that when a pop-up menu appears, it is usually the combination of these menus. For example when selecting an atom and pressing the right mouse button, a popup menu appears that contains elements of the context pop-up menu,in this case the Atom Pop-up Menu, the Edit Pop-up Menu, and the Selection Pop-up Menu.



Atom Pop-up Menu

The Atom pop-up menu appears when you right-click on an atom on the canvas. It contains options for atom-specific activities that also can be accessed from the Atom Menu.

Menu Item	Description
Stereo	Assigns reaction stereo labels or enhanced stereo labels to atoms. See the Enhanced stereo specification for details.

Charge	Applies a charge between [-128,128] to the atom. Marvin will let you set any of these values on any atom, highlighting the Valence Errors in red upon completion. In other words, Marvin will allow you to set a charge of -5 on hydrogen, despite the fact that this is chemically impossible.
Valence	Allows you to change the valence of any atom between [0, 8].
Radical	Sets the selected atom as a radical. You can select the type of radical - monovalent, divalent, divalent singlet, divalent triplet, trivalent, trivalent doublet, trivalent quartet. The Off option removes the radical designation.
Isotope	The Isotope submenu contains a list of the isotopes of the selected element, dynamically generated based on the selected atom. Select an isotope to set or change the isotope number or choose Off to reset the default atom type (no isotope).
Map	Set map labels/identifiers on the selected atoms that do not change while altering the molecule. They are useful when dealing with reactions, and can be saved in SMILES and MDL formats.
R-group	Changes the selected atom to an R-group label. R-groups symbolize alternative substituents.
R-group attachment	Adds R-group attachment point to the selected atom.
R-group attachment order	Defines the order of the R-group or deletes R-group attachment point.
Link Node	Link node specifies rings or chains of variable size.
Add S-group attachment	Creates an attachment point on the selected atom of an S-group.
Remove S-group attachment	Removes the last attachment point from the selected atom of an S-group.

Bond Pop-up Menu

The bond pop-up menu appears when you right-click on a bond within the molecule. It allows you to make a number of changes to the selected bond. It contains options for bond-specific activities that also can be accessed from the Bond Menu.

Menu Item	Submenu Items	Description
Type	Single	Changes the selected bond type to Single.
	Double	Changes the selected bond type to Double.
	Triple	Changes the selected bond type to Triple.
	Aromatic	Changes the selected bond type to Aromatic.
	Query bond types	Changes the selected bond to a bond type (Single Up, Single Down, Single Up or Down, Double Cis or Trans, Double C/T or Unspec, Single or Double, Single or Aromatic, Double or Aromatic, Any) for use in a query.
	Coordinate	Changes the selected bond type to Coordinate.
Bold		Thickens the selected bond.
Hashed		Changes the selected bond hashed.

Topology		The following options can be set as bond property when the molecule is used as a query.
	None	Removes defined bond topologies.
	In Ring	The specified bond must be in a ring to score a hit.
	In Chain	The specified bond must be in a chain to score a hit.
Reacting Center		The following bond property options can be set in case of drawing reaction search queries. See Reacting center bond for further query feature descriptions.
	None	Removes added bond property.
	Center	Specifies that the bond takes part in the reaction.
	Make or Break	The assigned bond can form or disappear in the reaction.
	Change	The assigned bond remains and can alter during the reaction.
	Make and Change	The assigned bond can form, break,or change its type during the reaction.
	Not Center	The assigned bond can not be the reaction center.
Stereo Search		Uses stereoconfiguration of specified double bond when the molecule is used as a query.
Arrange	Bring to Front	Brings the selected bond in front of the others.
	Send to Back	Sends the selected bond to the back of the others.
Align	Horizontally	Orients the selected bond horizontally.
	Vertically	Orients the bond vertically.

Object Pop-up Menu

This menu appears when the context is a graphical object like Text, Bracket, or other Graphics.

Menu Item	Description
Bring to Front	Brings the selected object in front of all others.
Send to Back	Places the selected object behind all others.

Edit Pop-up Menu

The Edit pop-up menu appears when you right-click on open canvas space. In case there is an atom, bond or graphic object under the cursor, the appearing pop-up menu contains the elements of the Edit Pop-up Menu merged with the pop-up menu of the selected element.
Edit pop-up menu items include:

Menu Item	Description
Cut	Removes and copies the selection to the clipboard.
Copy	Copies the selection to the clipboard.

Copy As	Copies the selection to the clipboard in the specified format.
Paste	Inserts the contents of the clipboard at the location of the cursor, without replacing selection.
Select All	Selects the structure being on the canvas including all fragments and graphical objects.
Group	Creates an abbreviated Group from the selected substructure. See the S-groups section for more information on creating and using Groups.

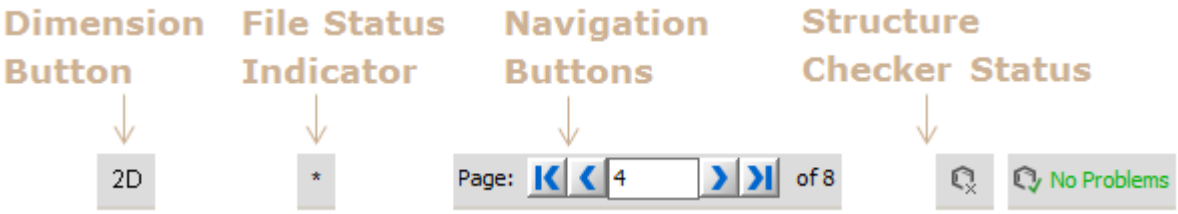
Pop-up elements upon Selection

Menu Item	Description
Add/Remove Explicit Hydrogens	Switches explicit H atoms to implicit ones and vica versa. Explicit hydrogens are displayed with atoms joining its neighbor while implicit hydrogens are displayed by atom symbols only.
Add/Remove Map Atoms	Adding atom maps is an automatic assignment of map numbers to all selected atoms of a reaction by using the automapper tool.
Add/Remove Data	Attach/Remove data like stoichiometry coefficient to the molecule.
Add/Remove Absolute Stereo (CHIRAL)	Sets/Removes chiral flag for the molecule.
Add Multi-Center	Add a multi-center attachment point representing a group of atoms.
Add Position Variation Bond	Create a variable point of attachment to represent a connection point to a group of atoms.
Link Node	Specifies query structures containing rings or chains of variable size.
R-Logic	Allows setting additional R-group conditions such as occurrence, rest H and if-then expressions to R-groups in the R-logic dialog.
Transformation > Drag Selection	The selected part of the molecule can be moved by dragging the mark box with your mouse or with the proper arrow keys.
Transformation > Rotate in 2D	The selection can be rotated in the plane of the canvas with changing coordinates.
Transformation > Rotate in 3D	The selected part of the molecule will be rotated according to the chosen rotation mode.
Transformation > Switch Transformation (space)	You can switch between dragging or 3D rotating the selected molecular parts by hitting the space bar.
Transformation > Flip	Flips the structure on the canvas. The submenu allows you to choose horizontally or vertically.
Transformation > Mirror	Flips the object horizontally, inverting tetrahedral stereochemistry. The submenu allows you to choose horizontally or vertically.
Transformation > Invert	Reflects the selected fragment(s) through the geometric or arbitrary center.
Document Style	Change atom and bond drawing properties.
Add To My Templates	Adds the selected structure to the "My Templates" group that appears in the Template Library and on the Advanced Templates Toolbar.

Status Bar of MarvinSketch

The Status Bar appears at the bottom of the main frame, and unlike toolbars, it cannot be customized or moved.

The Status Bar consists of 3 parts:



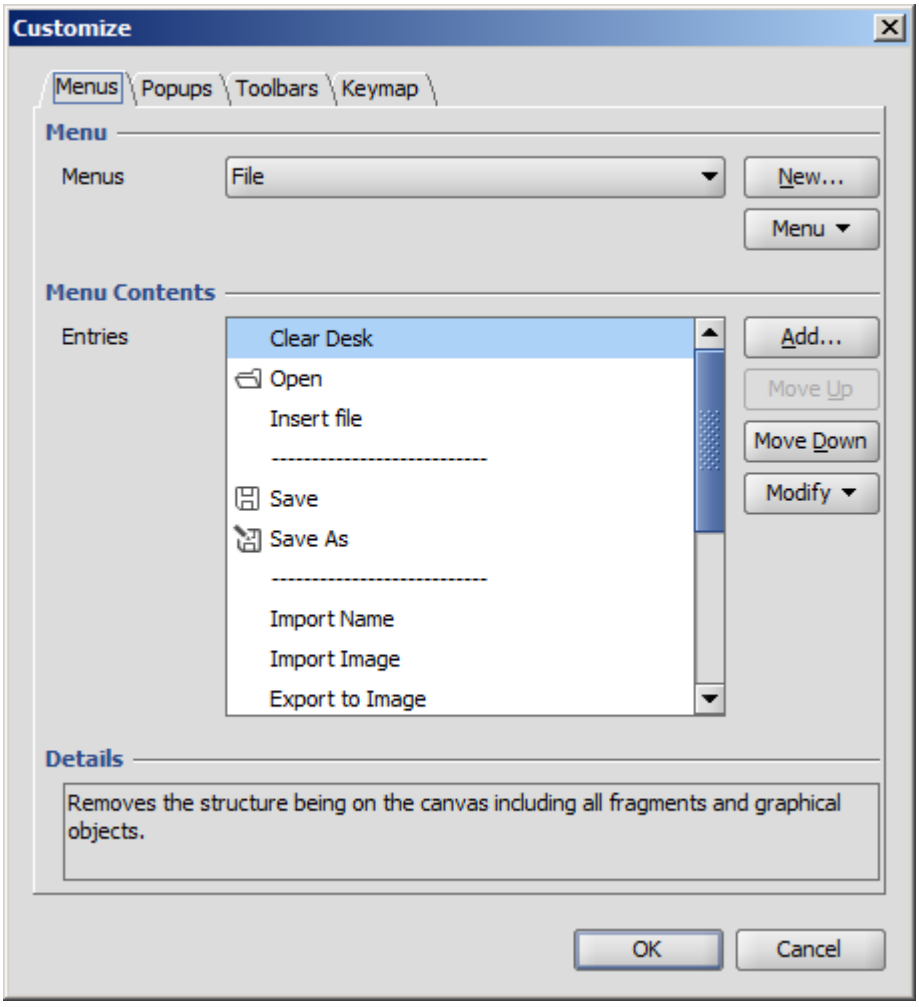
1. **Dimension Button**
   Switches between 2D and 3D modes. If the current structure is represented in 3D, then switching to 2D mode performs a 2D cleaning upon confirmation.
2. **File Status Indicator**
   This sign appears dynamically if there are unsaved modifications on the current structure, and disappears upon a Save command.
3. **Structure Checker Status**
   By default it is disabled as seen on the first image. To enable manual checking double-click on it. Right-click enables automatic checking. The status bar displays different images when there is no problem, if checking is in progress or if problems were found.
4. **Navigation Buttons**
   The Navigation Buttons appearing on the Status Bar dynamically using multipage molecular documents provide a quick way to navigate between pages.
   For information about how to enable multipage molecular documents please visit this link.

Dialogs of MarvinSketch

Contents

Customize

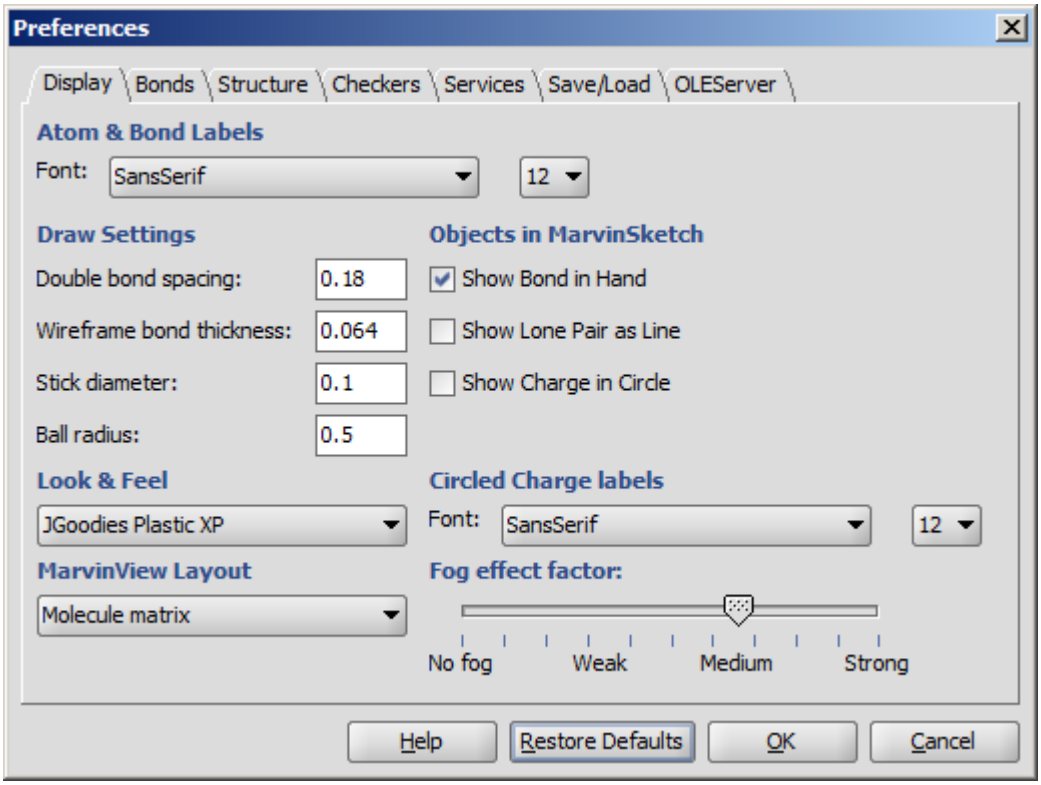
The Customize dialog window, located in the **View > Editor style** menu, provides options for altering the user interface by adding, removing, or reorganizing its elements. For a detailed description, please consult this page.



Preferences

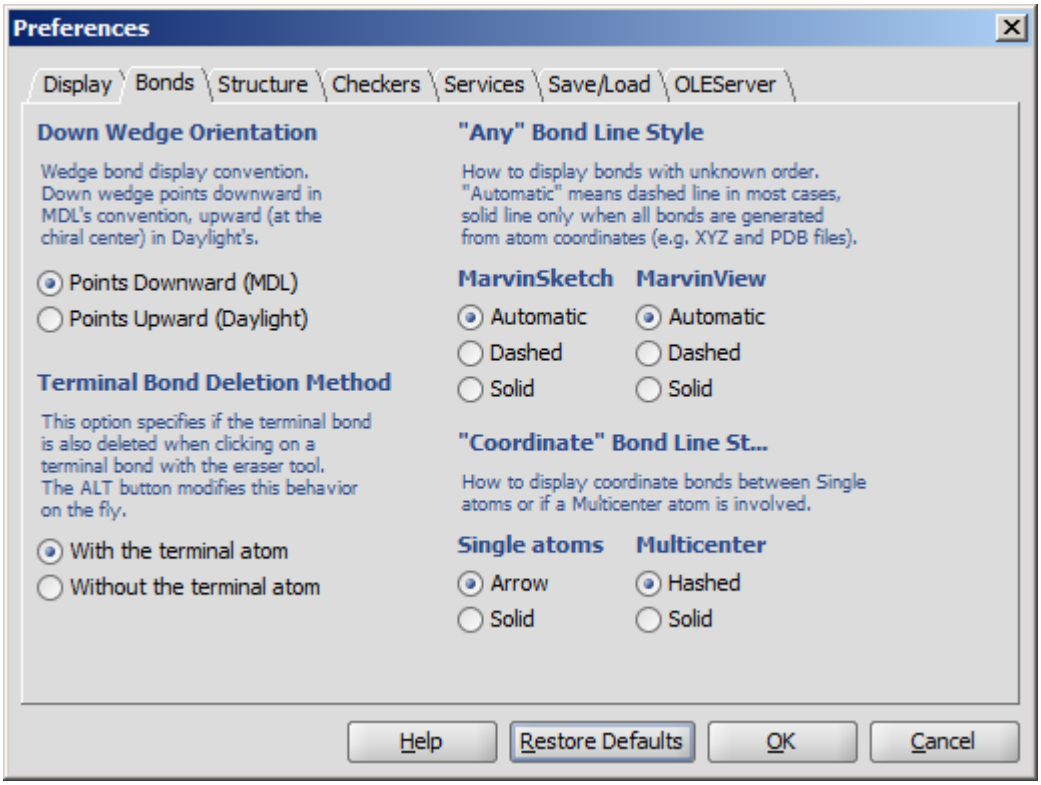
The Preferences dialog window is located at the **Edit** menu. It allows you to change many of the MarvinSketch display settings, including look & feel, error highlighting, and object visibility.
All settings are saved and used when the application is restarted.

Display



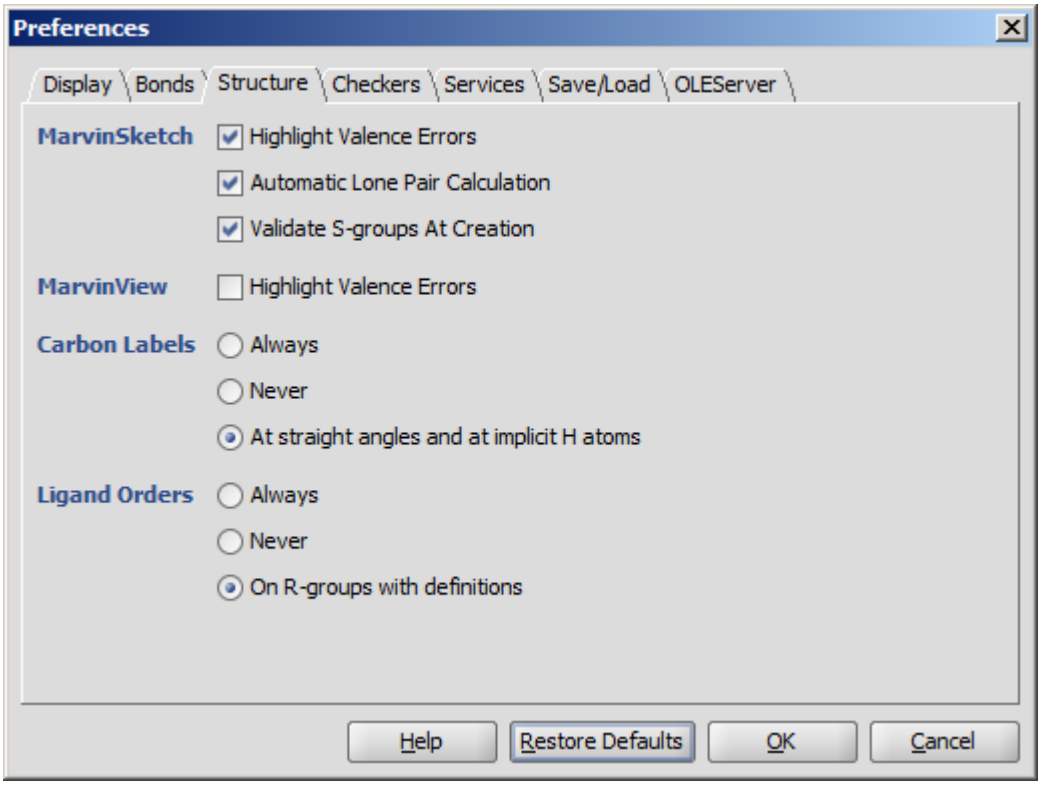
- **Atom & Bond labels** are used as the default font type and size to labels such as C/T label of bonds, atom query property labels of atoms, etc.
- **Double bond spacing** is a gap between two lines/sticks representing a double or triple bond measured in Angstroms.
- **Wireframe bond thickness** is the width of bonds in wireframe mode. It is measured in Angstroms.
- **Stick diameter** is the width of bonds in stick mode in Angstroms.
- **Ball radius** is the size of atom spheres in Ball draw type, measured in Angstroms.
- **Look & Feel** allows changing the visual appearance of GUI components. The available options are: Java Metal, Motif, JGoodies Plastic, JGoodies Plastic XP, and the native Look & Feels (Windows, Aqua) based on the underlying operating system.
- **MarvinView Layout** sets the default layout to Automatic, Molecule matrix or Spreadsheet.
- **Show Bond in Hand** when checked, bond types are shown under the mouse cursor like template structures.
- **Show Lone Pair as Line** when checked, lone pairs on the canvas are shown as lines.
- **Show Charge in Circle** when checked, a circle is displayed around the charge.
- **Circled Charge labels** are used as the font type and size of the circled charge symbols.
- **Fog effect factor:** manual setting of the fading strength. No fog: all regions of the structure is displayed with the same line strength and color. Strong effect: the fading is at its maximum (molecule is only slightly visible at the far end).

Bonds



- **Down Wedge Orientation** allows changing the wedge bond display convention. Down wedge points downward in MDL's convention, upward (at the chiral center) in Daylight's.
- **Any Bond Line Style** offers three different modes to display bonds of unknown types: Automatic, Dashed and Solid. This option can be separately set to be used in MarvinSketch and MarvinView.
- **Terminal Bond Deletion Method** offers 2 ways to delete the terminal bond of a molecule: only the bond is deleted or the terminal atom disappears with the bond.
- **"Coordinate" Bond Line Style** allows changing the type of coordinate bonds from the default ones (arrow for single atom and hashed for multicenter) to solid.

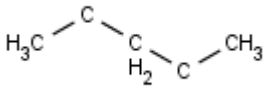
Structure



- **Highlighting Valence Errors** highlights atoms having wrong valences with red underline when it is

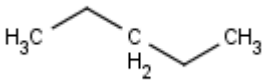
checked.

- **Automatic Lone Pair Calculation** calculates lone pairs automatically. Make sure **View** > **Misc** > **Lone Pairs** is checked to see the result.
- **Validate S-groups At Creation** disables the S-group types in the drop-down list which would not yield a chemically correct structure. Usage in MarvinSketch.
- **Carbon Labels** options determine the condition of displaying C labels on Carbon atoms.



Always

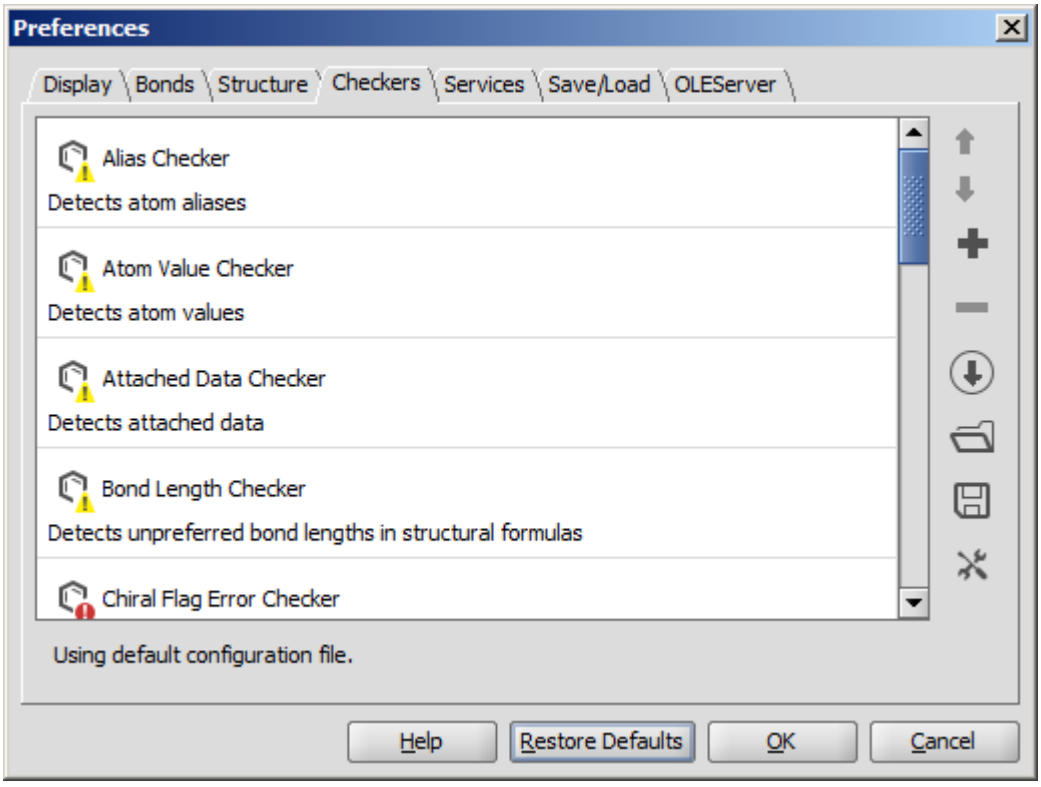
Never



At straight angles and implicit H atoms

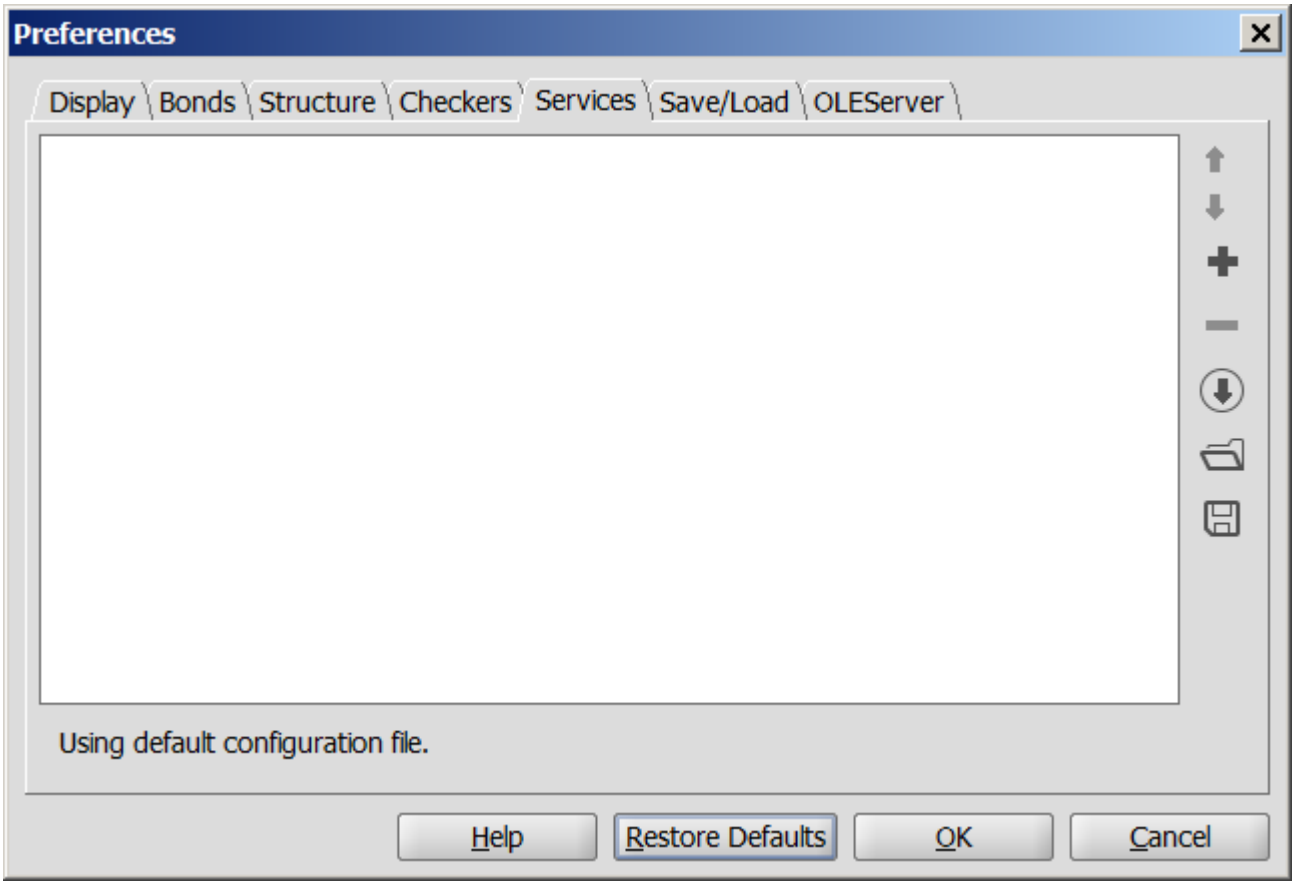
- **Ligand Orders**
  - Always
  - Never
  - On R-groups with definitions

Checkers



- **Move up/down the checker items:** the fixing process may depend on the sequence of the checkers. Checking order can be set using the Up/Down buttons on selected checkers.
- **Add checkers to the list:** the default list can be modified by adding other checkers.
- **Remove checkers from the list:** the default list can be modified by removing checkers not needed.
- **Open checker configuration from URL** open a checker configuration from URL.
- **Open checker configuration:** open your custom checker configuration from file.
- **Save checker configuration:** save your custom checker configuration to file.
- **Configure external checkers/fixers:** add external checkers/fixers; save or load external checker/fixer configuration.

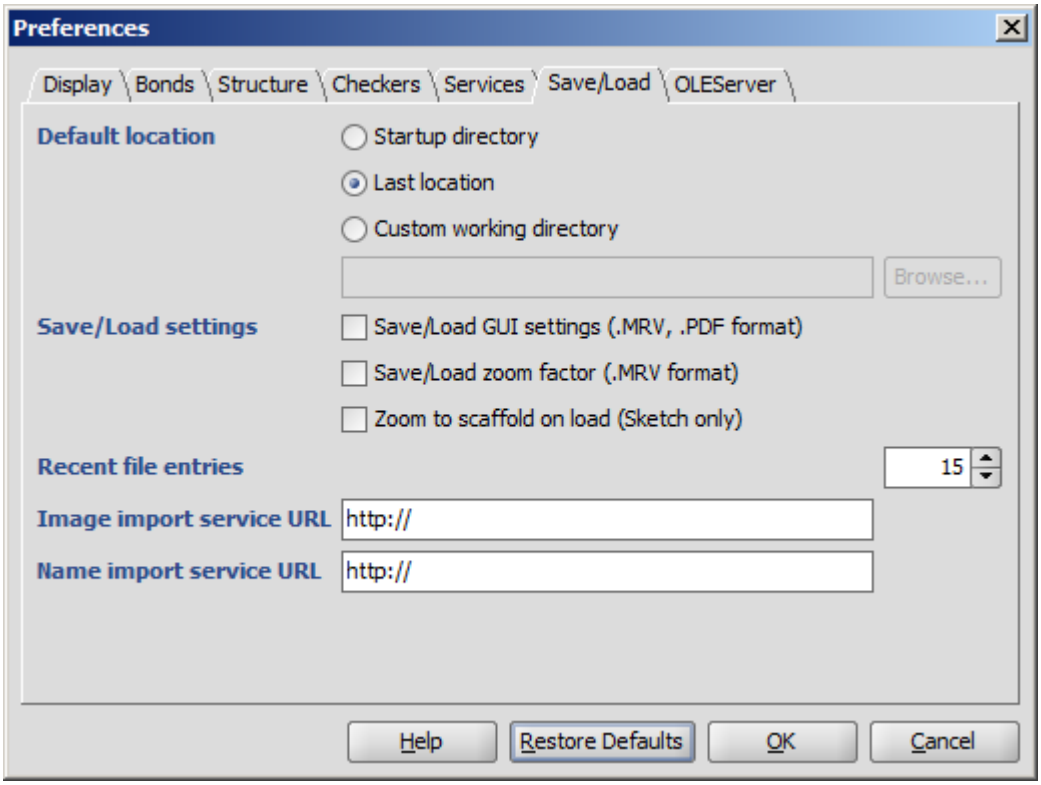
Services



The Services module provides seamless integration of third-party calculations into Marvin Sketch. You can add and configure the desired calculations in the *Services* tab. The set service(s) can be used from the Tools > Services menu afterwards.

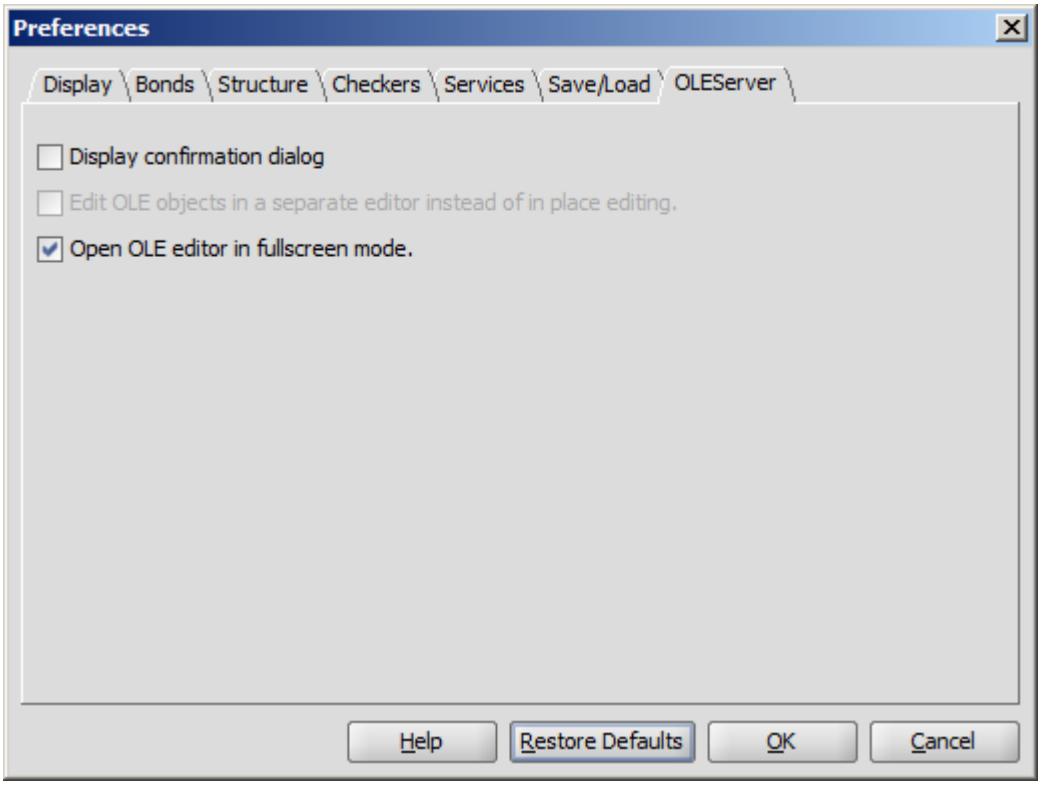
- **Set the order** of services by moving them up and down using the Up/Down buttons.
- **Add a new service** to the list by the add button. The preference window of the new service will pop up. Read more about setting different services.
- **Remove the selected service** from the list by the remove button.
- **Open** Service Configuration from URL. Specify a previously set configuration of services with its URL.
- **Import** Service Configuration from file. Import a previously set configuration XML file.
- **Export** Service Configuration to file. You can export the set services to a configuration XML file.

Save/Load



- **Default location:** the folder from which to load or to save molecules may be set by the user.
  - Startup directory: the folder where the command to start the application was given.
  - Last location: the last folder used for opening or saving a structure.
  - Custom working directory: a user-defined folder. If a molecule is loaded from another folder, then the file's location will be offered for saving.
- **Default file format** determines which type is offered by default when structures are saved to file.
- **Save/Load settings**
  - **Save/Load GUI settings (.MRV, .PDF format)** allows storing and loading of display options like background color, font type, stereo labels, atom indices *etc.* in addition to the chemical structure itself. This option can only be used with MRV and PDF formats.
  - **Save/Load zoom factor (.MRV format)** stores and loads the zooming scale of the structures. This option can only be used with the MRV format.
  - **Zoom to scaffold on load (Sketch only)** sets the zooming scale to 'Scaffold' if the loaded file contains defined R-groups, so the R-group definitions might not be seen on the canvas without scrolling. The 'Zoom level' dropdown list on the General Toolbar is supplemented with 'Scaffold' and 'R1, R2, R3...' only when there are defined R-group(s). Without R-group definitions the zooming scale for the loaded structure(s) will not be modified, the last zooming scale will be used.
    When this option is switched off in the 'Preferences' menu then MSketch opens the new file with the last zoom level.
- **Recent file entries** defines the number of files in the Recent files list in the File menu, with values between 1 and 10.
- **Image import service URL** URL of a server on which a chemical structure recognition program runs can be given.
- **Name import service URL** URL of a server on which a chemical name recognition program runs can be given.

OLEServer



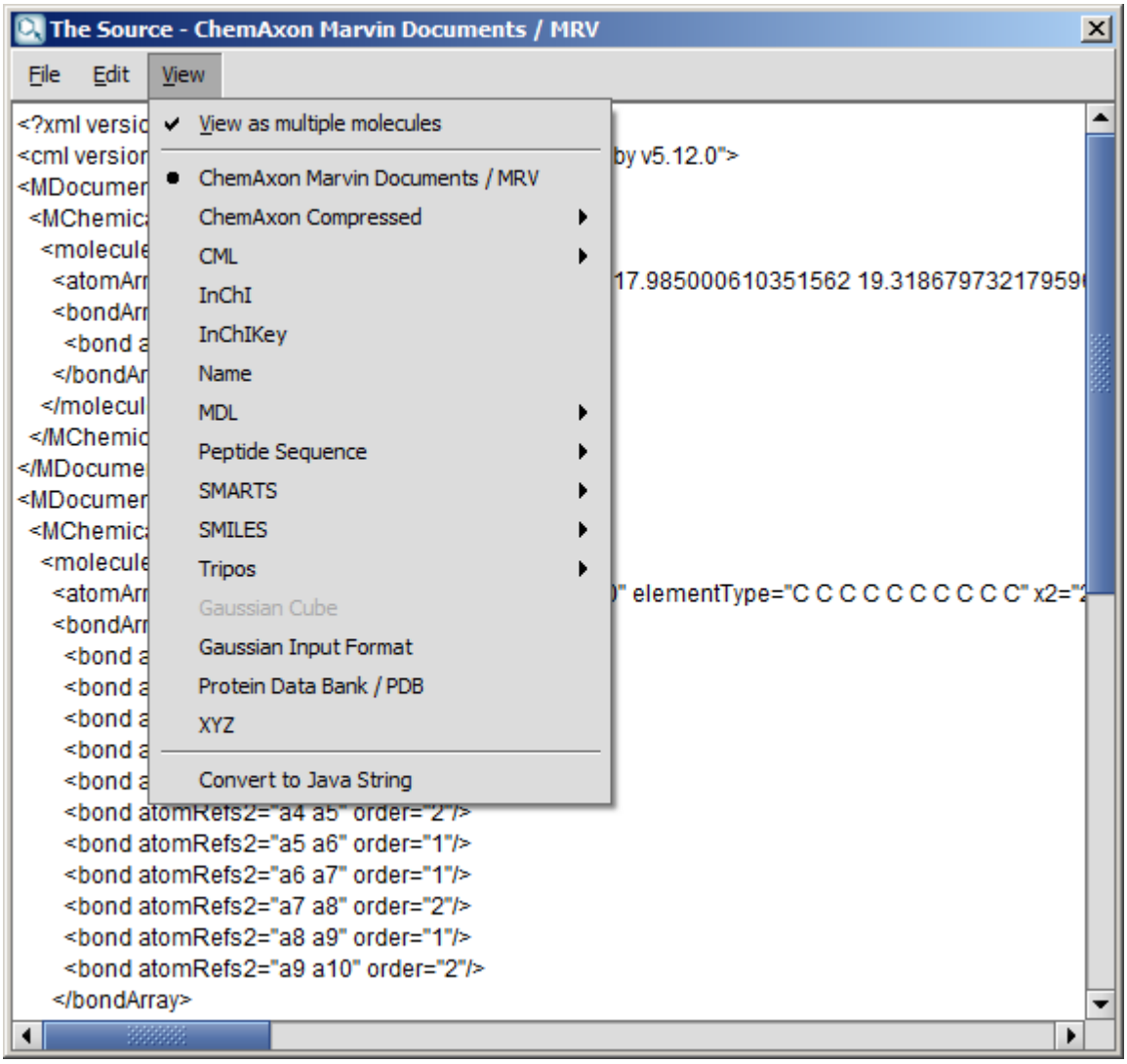
Edit Source

You can alter a molecule by directly editing its source in the Edit Source dialog window.

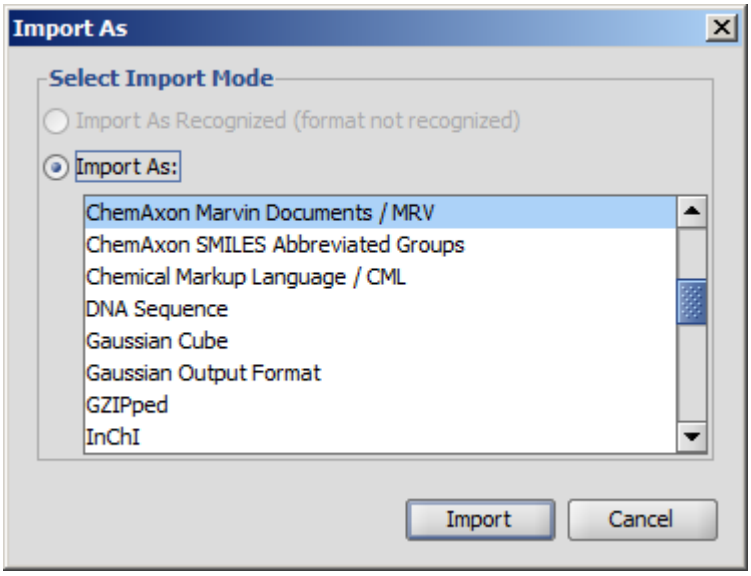
The dialog window provides standard clipboard operations and it is also possible to send the source text to the console.

You can view and edit the source in any of the supported file formats. You can also convert it to Java String which allows easy integration of the structure to a custom Java application code.

To change the format of the source, simply select one from the **View** Menu. If there are more than one molecule on the canvas, setting **View as multiple molecules** in the **View** Menu causes each molecule to appear in a separate block in the source. This feature works only in those cases where the selected format is able to handle multiple fragments.



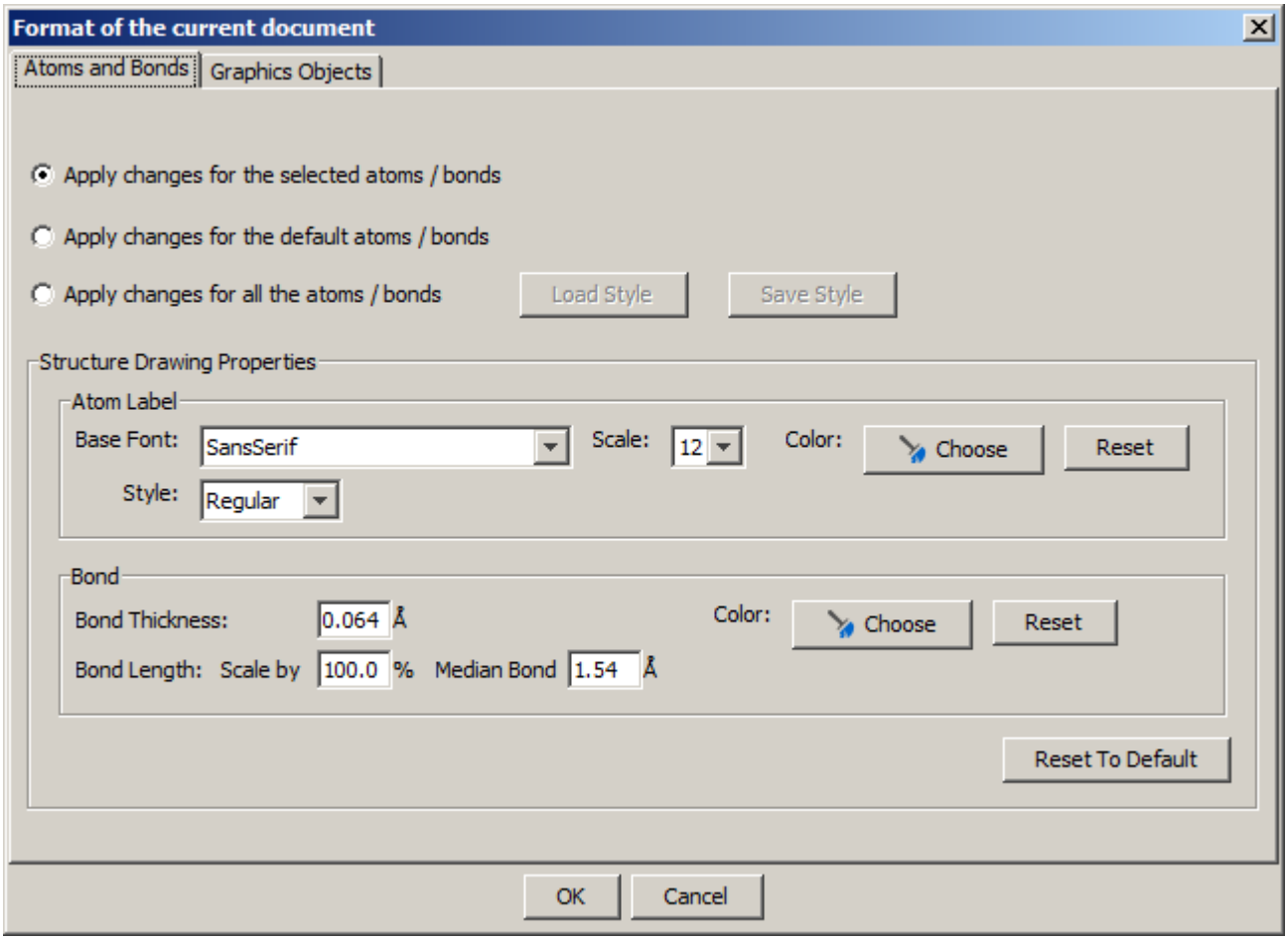
After editing the source text, you can send the structure back to the MarvinSketch canvas by invoking **File > Import As**, and pressing **Import** on the appearing dialog window. This will close the Edit Source dialog window.



Format

Atoms and Bonds

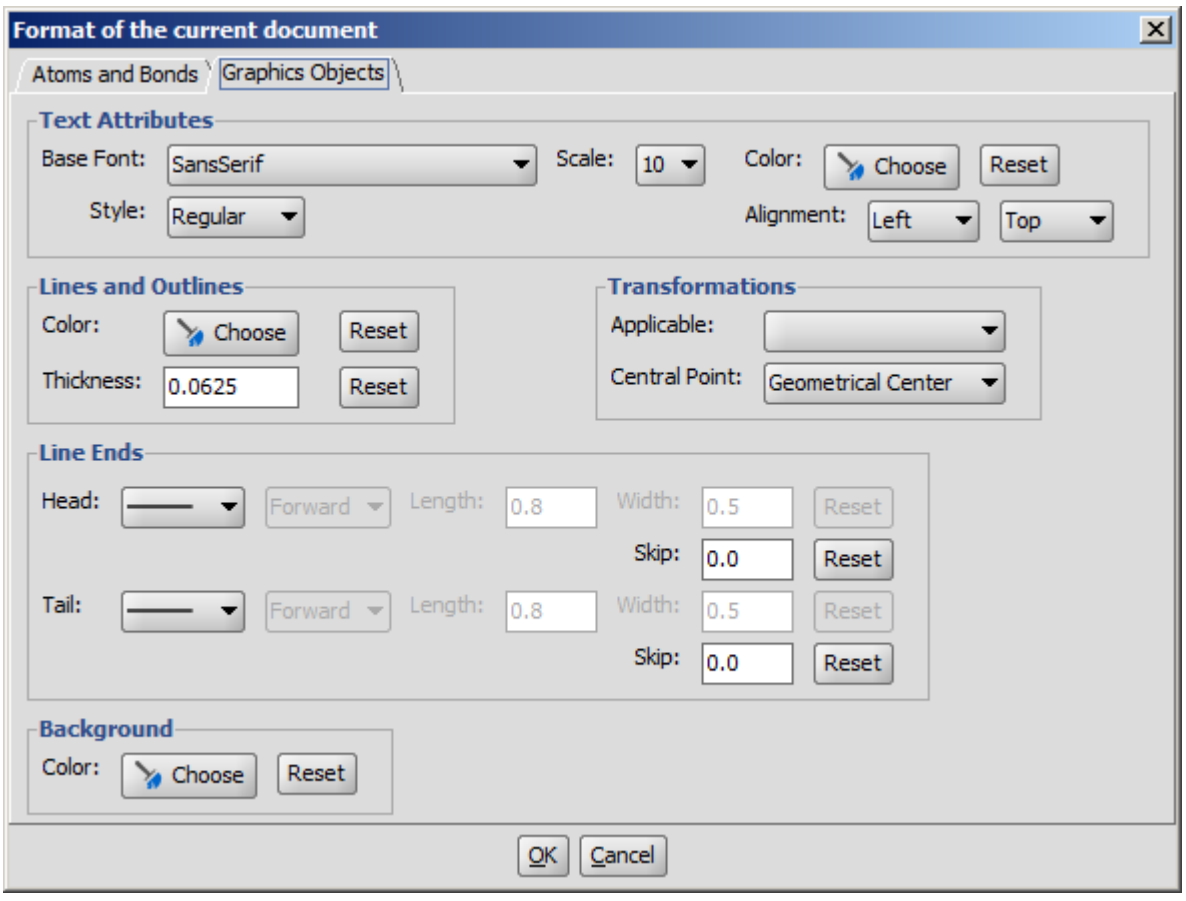
On this panel there are many options to change the drawing properties of atoms and bonds.



For more information about using structure drawing styles, please visit this link.

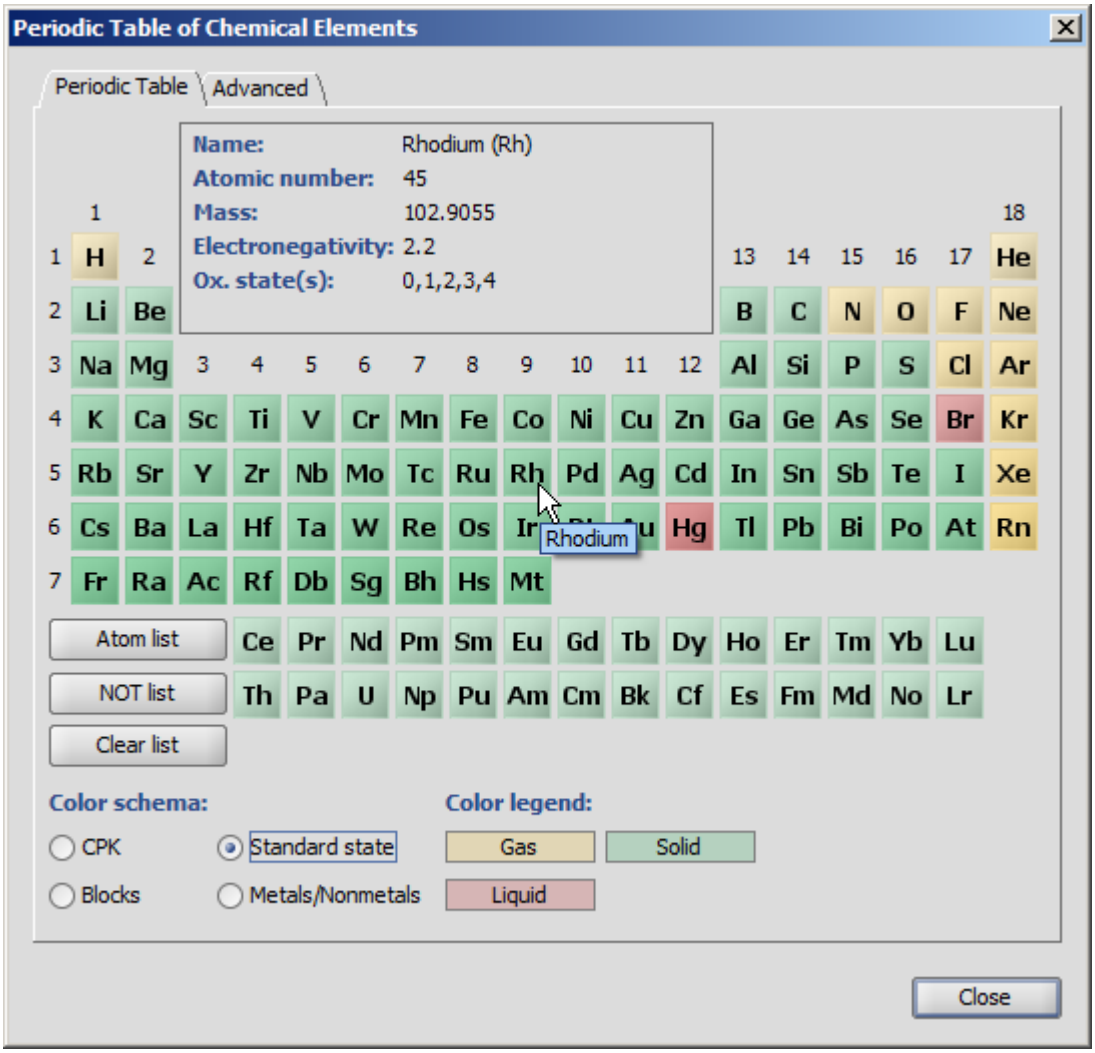
Graphics Objects

The drawing properties of graphics objects (text boxes, brackets, lines, etc.) can be changed on this panel.



Periodic Table of Chemical Elements

Periodic Table



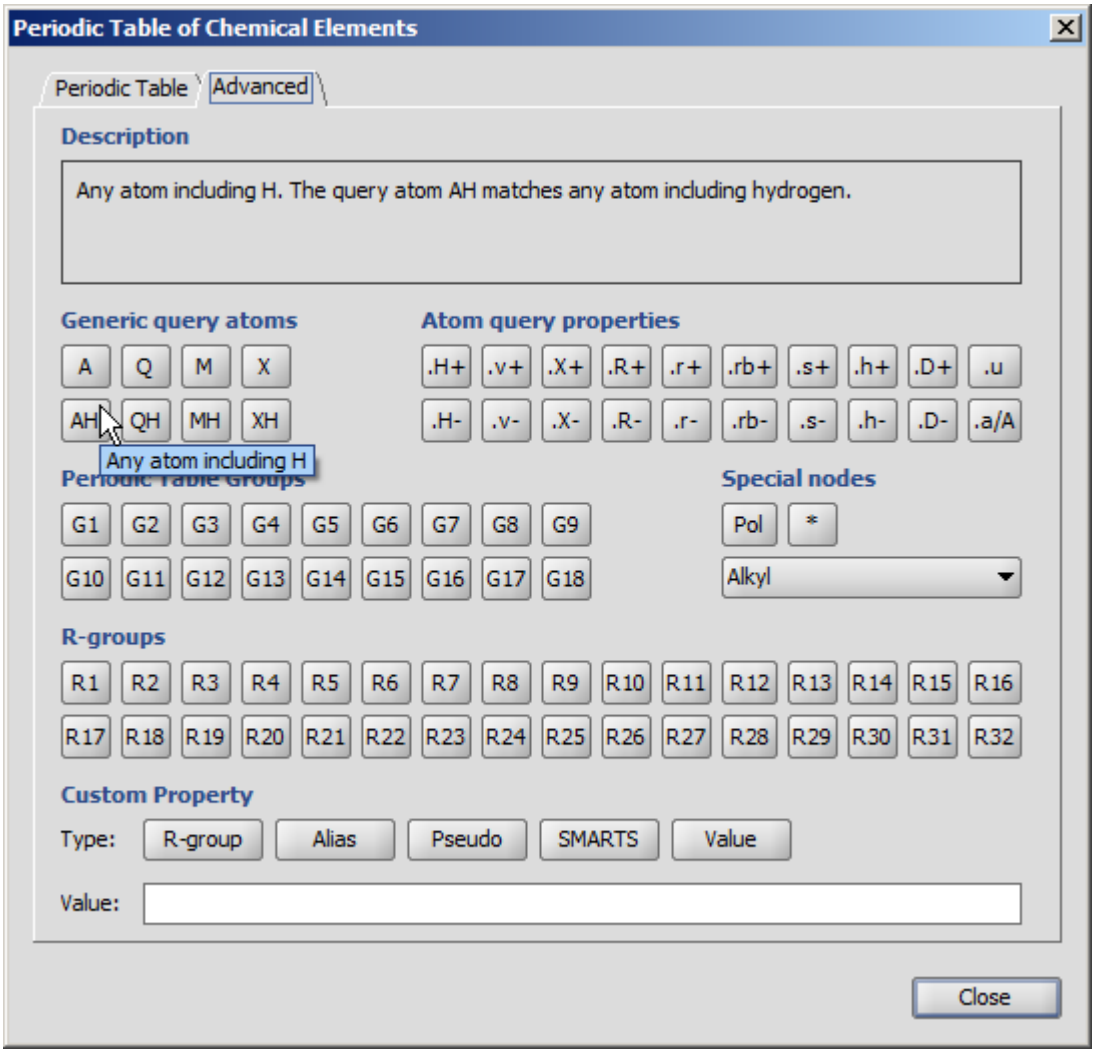
Chemical elements are available as buttons on the Periodic Table panel of MarvinSketch.
Atom buttons are arranged according to the standard periodic table layout.
When the mouse cursor is over a specific atom button, the information panel displays the name of the atom, the atomic number, mass, electronegativity and the oxidation states.
When one of the atom buttons is pressed, the corresponding atom can be placed on the canvas. The atom symbol appears under the mouse cursor, while the button is highlighted in this case.

The **Atom List** and **NOT List** buttons can be used to create special atom lists that can be used in queries. When one of these buttons is pressed, atoms can be added to the list by pressing atom buttons one after the other. The lists are not cleared when the list buttons become unselected. The atoms of the list are also shown under the mouse cursor above the canvas. See Query Guide for more details about *atom lists* and *not lists*.

Four different **coloring schemas** can be chosen:

1. CPK: colors the atoms according to the Corey-Pauling-Kultun coloring scheme
2. Standard state: colors according to the standard state of the element (gas, liquid, solid)
3. Blocks: colors elements according to the highest-energy electron's orbital (s-, p-, d- or f-block)
4. Metals/Nonmetals: colors according to the metallic character of the elements (alkali, alkaline earth, metalloid, transition metal, other metal, nonmetal)

Advanced



For the meanings of the buttons on the Advanced tab please refer to the Query Guide.
When the mouse cursor is over a button, a short description appears on the information panel.

Generic query atoms

Name	Description
A	Any (any atom except hydrogen)
AH	Any atom, including hydrogen
Q	Hetero (any atom except hydrogen and carbon)
QH	Hetero atom or hydrogen (any atom except carbon)
M	Metal (contains alkali metals, alkaline earth metals, transition metals, actinides, lanthanides, poor(basic) metals, Ge, Sb and Po)
MH	Metal or hydrogen
X	Halogen (F,Cl,Br or I)
XH	Halogen or hydrogen

Atom query properties

Adding query properties to structures.

Name	Description
.H+	Increase number of *total hydrogens* (total number of hydrogen substituents)
.H-	Decrease number of *total hydrogens* (total number of hydrogen substituents)

.v+	Increase number of *valence* (total bond order)
.v-	Decrease number of *valence* (total bond order)
.X+	Increase number of *connections* (number of substituents including hydrogens)
.X-	Decrease number of *connections* (number of substituents including hydrogens)
.R-	Increase number of*rings* (number of rings the atom is a member of)
.R+	Decrease number of *rings* (number of rings the atom is a member of)
.r+	Increase *smallest ring size* (size of the smallest ring the atom is a member of)
.r-	Decrease*smallest ring size* (size of the smallest ring the atom is a member of)
.rb+	Increase *ring bond count* (number of ring bonds next to the atom)
.rb-	Decrease *ring bond count* (number of ring bonds next to the atom)
.s+	Increase *substitution count* (number of non-H substituents)
.s-	Decrease *substitution count* (number of non-H substituents)
.h+	Increase number of *implicit hydrogens* (number of implicit hydrogen substituents)
.h-	Decrease number of *implicit hydrogens* (number of implicit hydrogen substituents)
.D+	Increase *degree* (number of explicit connections; default for "n" is one)
.D-	Decrease *degree* (number of explicit connections; default for "n" is one)
.u	Mark as *unsaturated atom* (atom has double, triple or aromatic bond)
.a/A	Mark as *aromatic/aliphatic* (has aromatic bond)

Periodic Table Groups

Name	Description
Group 1 (IA,IA)	the alkali metals or hydrogen family/lithium family
Group 2 (IIA,IIA)	the alkaline earth metals or beryllium family
Group 3 (IIIA,IIIB)	the scandium family
Group 4 (IVA,IVB)	the titanium family
Group 5 (VA,VB)	the vanadium family
Group 6 (VIA,VIB)	the chromium family
Group 7 (VIIA,VIIB)	the manganese family
Group 8 (VIII)	the iron family
Group 9 (VIII)	the cobalt family
Group 10 (VIII)	the nickel family
Group 11 (IB,IB)	the coinage metals or copper family
Group 12 (IIB,IIB)	the zinc family
Group 13 (IIIB,IIIA)	the boron family
Group 14 (IVB,IVA)	the carbon family
Group 15 (VB,VA)	the pnictogens or nitrogen family
Group 16 (VIB,VIA)	the chalcogens or oxygen family
Group 17 (VIIB,VIIA)	the halogens or fluorine family
Group 18 (Group 0)	the noble gases or helium family/neon family

Special nodes

Name	Description
Pol	Pseudo atom 'Pol'. This button changes the selected atom to a pseudo atom labelled Pol (polymer).
*	This button creates a '*' atom, which indicates an unspecified end group in polymers.
homology groups	The drop-down list contains the default homology groups. Detailed list.

R-groups

These atoms can be used to describe unknown or unspecified molecule parts or to draw R-group queries or Markush structures.

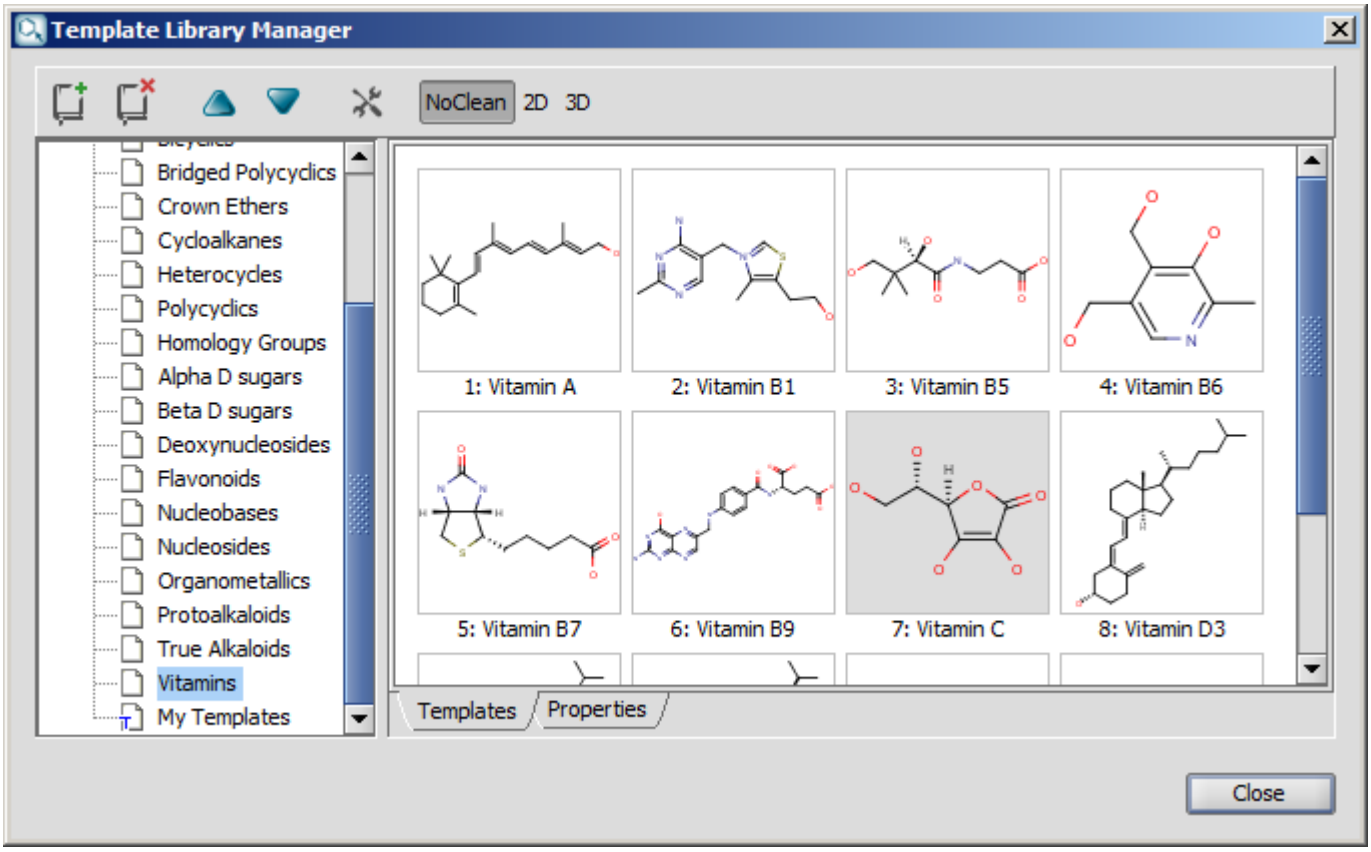
Custom Property

Name	Description
R-group	Converts the atom to an R-group with the given number (only numerical characters are allowed). Maximum index is 32767. This atom can be used to describe an unknown or unspecified molecule part or to draw an R-group query or Markush structure.
Alias	The given value is shown as atom label but the atom itself does not change.
Pseudo	The given value is shown as atom label and the type of the atom is changed to 'Any'.
SMARTS	Converts the given value to a complex SMARTS query molecule or atom. If the cursor is kept over the canvas during typing, the conversion can be seen on-the-fly.
Value	Adds the given value to an atom as a custom property ("Atom value").

Template Library Manager

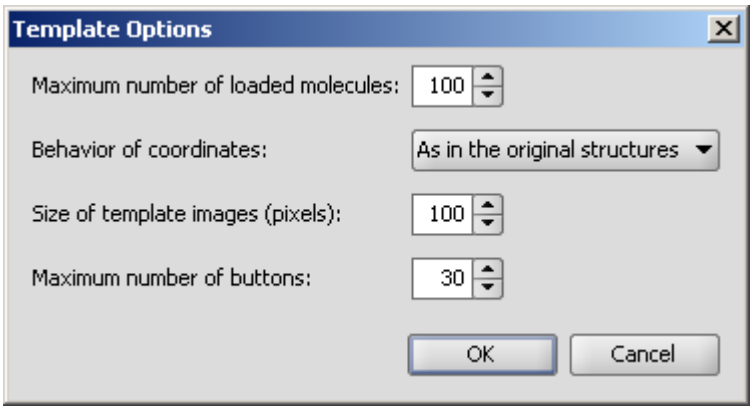
The Template Library is a hierarchic display of template sets.

It contains several template sets by default (such as Generic, Rings, Amino Acids, etc), and a special set called My Templates.



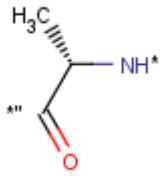
The dialog has buttons to customize template handling. With the help of these buttons you can add and remove template sets to/from the template library, can change order of a given template set, or open the "Options" dialog. The cleaning options of the templates can be set using the last three buttons on the toolbar. With these buttons you can specify how the template will be placed onto the canvas (NoClean, 2D, or 3D). These options can be set separately for each template category. Note, that the buttons are synchronized with the "Template Options" dialog settings.

Template Options

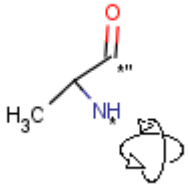


- **Maximum number of molecules:** template sets can contain large number of molecules. This option maximizes the number of structures being loaded from a template set when it is selected in the Template Library. For example if the option is set to 100, only 100 structures will be loaded to memory and displayed in the library, even if the underlying molecule file contained 25000 structures.
- **Coordinates:** this option is to specify an operation affecting the coordinates when the templates are placed on the canvas.
  For example result of placing L-Alanine to the canvas with different options:

As in the original structures



Always perform Clean2D

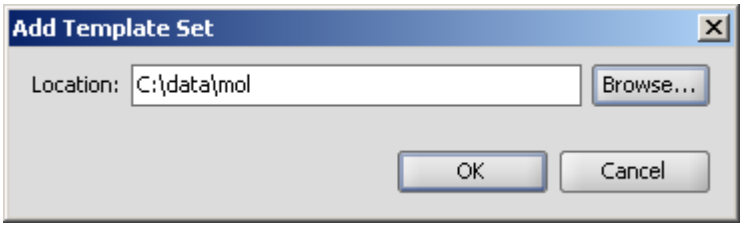


Always perform Clean3D

- **Size of templates:** the size with which each template is displayed in the library, measured in pixels.
- **Maximum number of buttons:** this determines the maximum number of buttons allowed on the Advanced Templates Toolbar

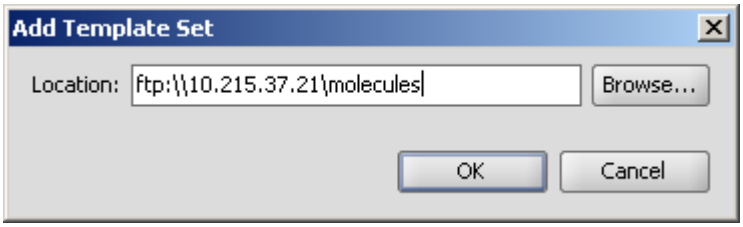
Adding a new template set to the library

It is possible to add new template sets to the library using the Add Template Set button on the tool bar. Using the Browse button you can select a directory or a file of the file system. Specifying a directory will create a hierarchic template set containing all subdirectories and files.



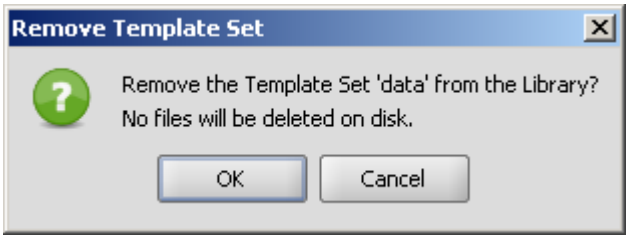
It is also possible to specify a location with ftp protocol. The underlying subdirectories and files will be displayed as with the local file system.

Please note that protocols other than file and ftp are not supported. However remote file systems can help to overcome this restriction.



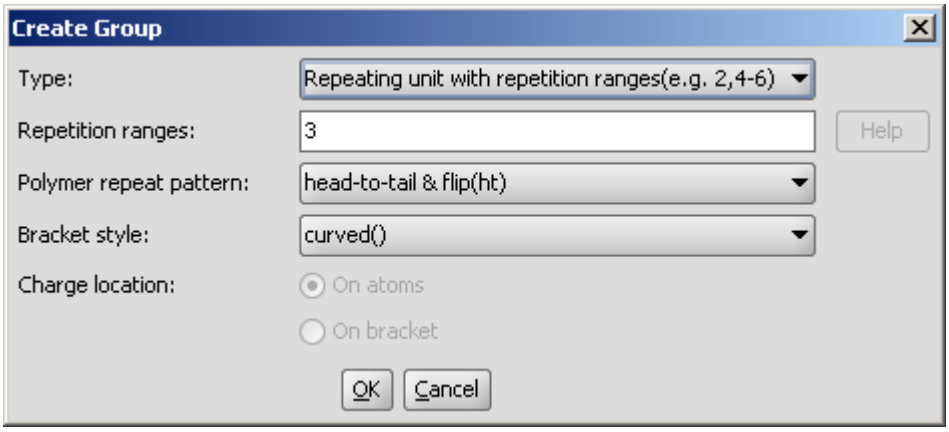
Removing a template set from the library

You can remove template sets from the library using the Remove Template Set button on the tool bar. The template set will only be removed from the library, without modifying files on the file system.



Create Group

This dialog makes it possible to create a number of groups along with setting their properties. Group drawing in MarvinSketch.



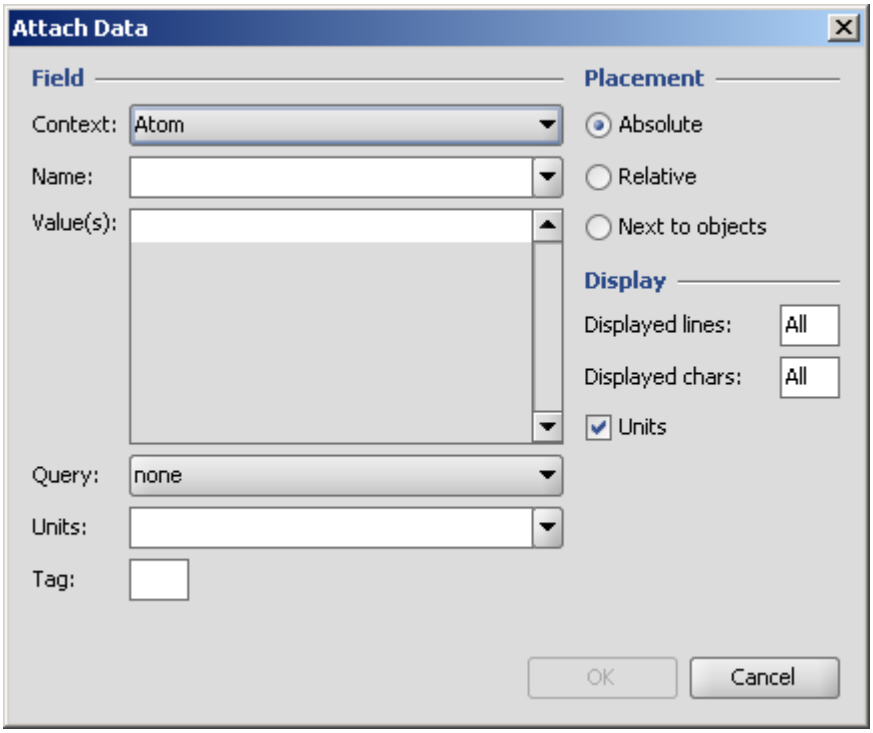
The available groups and their detailed description are available by clicking on the links below:

- Anypolymer (anyp)
- Component (c)
- Copolymers
- Crosslink (xl)
- Generic ()
- Graft
- Mer (mer)
- Modification (mod)
- Monomer (mon)
- Multiple group
- Ordered mixture (f)
- Repeating units with repetition ranges
- R-group
- SRU polymer(n)
- Superatom (abbreviation)
- Unordered mixture (mix)

Displaying charges on groups is described here.

Attach data

Attached data is a custom field assigned to atoms or brackets. It has an identifier string (name) and a value. Furthermore, a query operator can describe different restrictions in queries.
The dialog provides interface to set the properties of such a field.



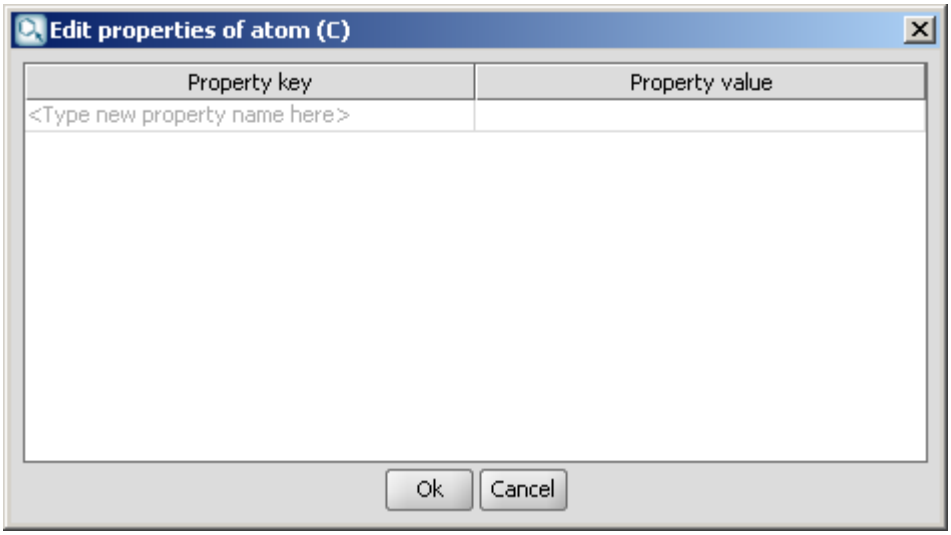
Further details of attached data can be found in the Query guide.

Attaching data in MarvinSketch is described here.

The Attach Data dialog is customizable; configuration options and a small example can be found here.

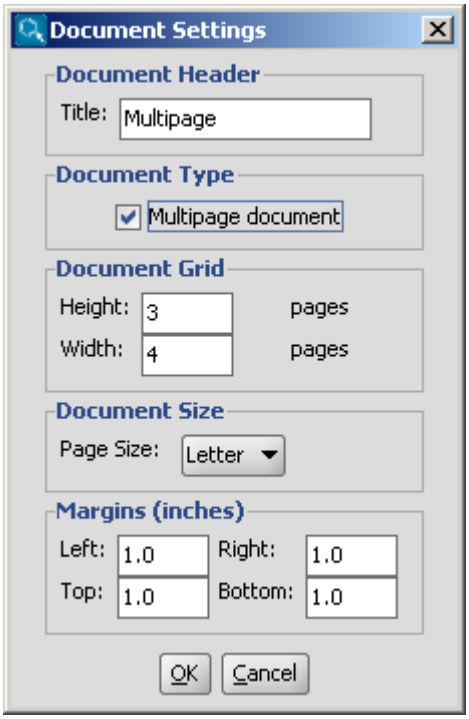
Edit properties

Properties may be added and viewed in MarvinSketch. Various properties can be added, but the value is displayed only on the canvas. Detailed description



Document Settings

You can set the number of horizontal and vertical pages in the Document Grid part, and you can also define the title, the page size and the margins in the corresponding sections of this dialog window. Henceforward, the given title will specify the "molecule title" property.


Document Settings
Document Header
Title:
Multipage
Document Type
Multipage document
Document Grid
Height:
3
pages
Width:
4
pages
Document Size
Page Size:
Letter
Margins (inches)
Left:
1.0
Right:
1.0
Top:
1.0
Bottom:
1.0
OK
Cancel

Shortcuts of MarvinSketch

The table below contains a list of the available shortcuts in MarvinSketch.

The way of changing the default shortcuts is described in the Customization section.

Keyboard shortcut	Function
Mouse Wheel	Scrolls canvas vertically.
Shift+Mouse Wheel	Scrolls canvas horizontally.
Ctrl+Mouse Wheel	Zooms canvas in and out.
Arrow Keys, Ctrl+Arrow Keys	Scrolls canvas in the proper direction if no object is selected on the canvas.
Arrow Keys	Moves the seleted object if an item is selected on the canvas. (You can scroll the canvas with Ctrl+Arrow Keys in this case.)
Shift+Arrow Keys	Move the selected object on the canvas in greater units.
Delete	Removes the selected element.
Ctrl+A	Select All
Ctrl+C, Ctrl+Insert	Copy
Ctrl+K	Copy As
Ctrl+L	Copy As Smiles
Ctrl+X, Ctrl+Shift+Delete	Cut
Ctrl+V, Ctrl+Shift+Insert	Paste
Ctrl+Y	Redo
Ctrl+Z, Alt+Backspace	Undo
Ctrl+L	Copy as SMILES
Ctrl+O	File open (if available)
Ctrl+S	Save to file (if available)
Ctrl+Shift+S	Save as... (if available)
Ctrl+P	Print (if available)
Ctrl+M	Display Periodic Table dialog (More window)
Ctrl+N	Create a new window
Ctrl+Delete	Clear Desk
Ctrl+W	Close current window
Ctrl+Q	Exit from the application
Ctrl+G	Create Group
Ctrl+2	Clean in 2D
Ctrl+B	Clean Wedge Bonds
Ctrl+3	Clean in 3D
Ctrl+F	Select conformer
Ctrl+T	Opens the Template Library
Ctrl+R	Checks and corrects chemical structures.
Ctrl+Shift+N	You can view the name of the current structure, and enter a new name to be

	imported.
Ctrl+Shift+M	Open MarvinSpace
F5	Exit transformation mode and return to *Sketching* mode.
F6	Switch on the *Zoom* mode.
F7	Enter into the *Rotate in 3D* mode.
F11	Sets the visibility of the main menubar.
Space	Changes transformation mode from Drag to Rotate in 2D, Rotate in 2D to Rotate in 3D, while Rotate in 3D to Drag.
-	Negative charge
+	Positive charge
1	Single bond
2	Double bond
3	Triple bond
4	Aromatic bond
5	Single up bond
6	Single down bond
7	Single up or down bond
12	Single or double bond
14	Single or aromatic bond
24	Double or aromatic bond
0	Any bond
*	Any atom
Q	Hetero atom
C, N, H, ...	carbon, nitrogen or hydrogen atom. For the other elements, type the mark of the element, e.g.: **Cl** for Chlorine. (Also works in lower case: **n**, **cl** etc.)
Au,Ag,Pt,...	Atom List can be defined by typing chemical symbols separated by commas. (Also works in lower case: **au**,**ag**,**pt**,...)
!Au,Ag,Pt,...	Not List can be defined by starting the atom list with an exclamation mark. (Also works in lower case: !**au**,**ag**,**pt**,...)
R1, R2, ..., R32767	R-group label with specified number. To define a set of fragments as R-group, select the fragments before the shortcut. To create an attachment point in the R-group, select an atom in the R-group and type the name of the R-group (e.g.: R5) (Also works in lower case.) To define a set of fragments as R-group 5, select the fragments then type **R5**. After then, you can choose an attachment point on R-group 4, just type **R5** and click on the atom.
M1, M2, ...	Atom maps for reactions. (Also in lower case.)
M0	Unmap
M= or M+	Unique atom map labels. Assigns unique atom map numbers to individual atoms picked by the mouse or to selected atoms in selection mode.
11, 22, ..., 77	Select a template. Select first, second, ..., or 7th element from the actual template list from the toolbar (if the referred index is not out of range).
abs, or1, or2, and1, and2	Stereochemical groups: **abs** (ABSOLUTE),\ **or1**,**or2**,...,**or10**,... (OR *n*), **and1**,**and2**,...,**and10**,...,**&1**,**&2**,..., **&10**,... (AND *n*)
AcAc, Acm, Ade, ...	The abbreviated group denoted by the abbreviation. You can ungroup the abbreviated group if you press the SHIFT button when you place it to the canvas.

	(Also in lower case.) To complete a longer name, press **ENTER** or **END** after typing the first few characters.
.a,.A,.u,.H0,H1	Special atom properties: **.a** (aromatic), **.A** (aliphatic), **.u** (unsaturated), **.H0**, **.H1**, ... (number of hydrogens), **.h0**, **.h1**, ... (implicit hydrogens), **.X0**, **.X1**, ... (connectivity), **.D0**, **.D1**, ... (degree), **.R0**, **.R1**, ... (rings), **.r3**, **.r4**, ... (smallest ring size), **.s***, **.s0**, **.s1**, ... (substitution count), **.v0**, **.v1**, ... (valence), **.rb***, **.rb0**, **.rb1**, ... (ring bond count).

Customizing MarvinSketch GUI

You can personalize the user interface to better suit your needs or style.
For example, you can reorganize the menu bar, you can create, delete or modify toolbars, and many more.
Any changes you make will become your personal default environment, though you can restore the default settings any time.

Basic Changes

Moving Toolbars

To move a toolbar, drag it by its separator bar, which is located at the left edge of horizontal toolbars or at the top of vertical toolbars.
(Note, that depending on the Look&Feel you currently use, the separator bar might be harder to notice and drag.)
While dragging the toolbar, you can see a colored border around it, indicating the place and direction the toolbar will have if you finish dragging. Depending on the current Look&Feel the colors of the border are different. For example, using JGoodies SkyBluer Look&Feel theme, light-blue border means that the toolbar will float, while dark-blue shows that the toolbar will be docked. If you set a toolbar to be floating, you can dock it back by closing it.

Hide/Show Toolbars

You can change the visibility of toolbars in the **View > Toolbars** menu.

Hide/Show Menu Bar

To hide the Menubar, choose **View > Menubar**. To show it, press F11 after clicking on the canvas.

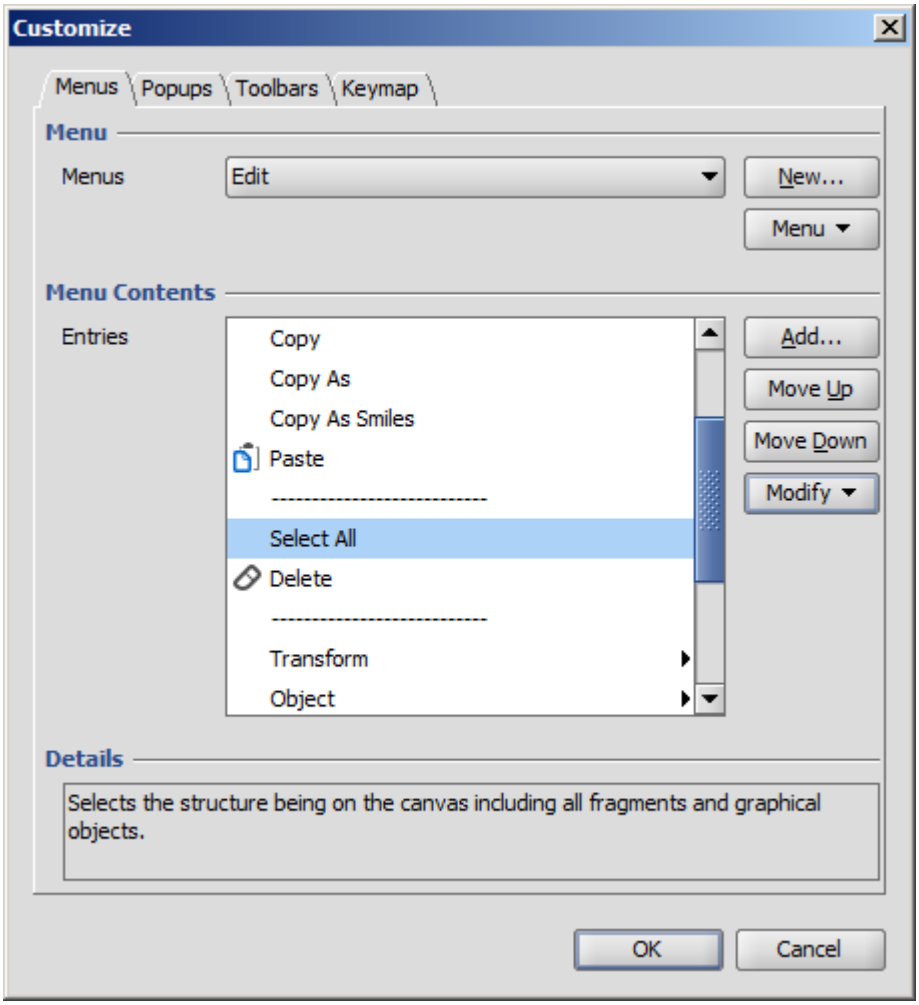
Hide/Show Status Bar

View > Status Bar turns the Status Bar on or off.

Advanced Changes

The graphical user interface of MarvinSketch can interactively be personalized using the **View > Editor Style > Customize...** dialog.
Note that the customization related functions usually do not ask for confirmation before taking action to make the procedure faster. The original interface can be restored any time by choosing **View > Editor Style > Reset current configuration**.

Menus

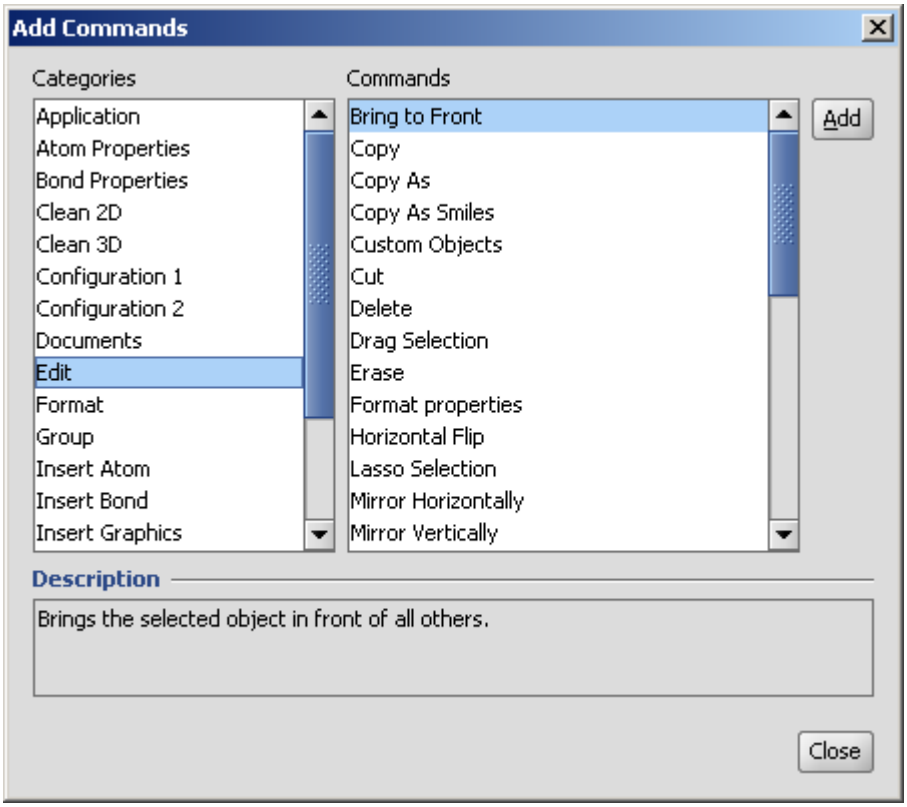


By choosing a menu from the Menus list, the contents of the selected menu will be listed in the Menu Contents. With selecting a menu entry, its detailed help text will appear in the Details field. If a black triangle is visible on the right side of a menu entry, it means that this entry is a Submenu. To list the contents of the submenu, select it from the Menus list.

List of the available Menu commands

New	Creates a new menu and places it at the end of the Menu Bar.
Menu > Move	Allows altering the position of main menus.
Menu > Rename	Renaming a menu in an appearing dialog.
Menu > Delete	Removes a menu with all of its contents.

List of the available Menu Contents commands

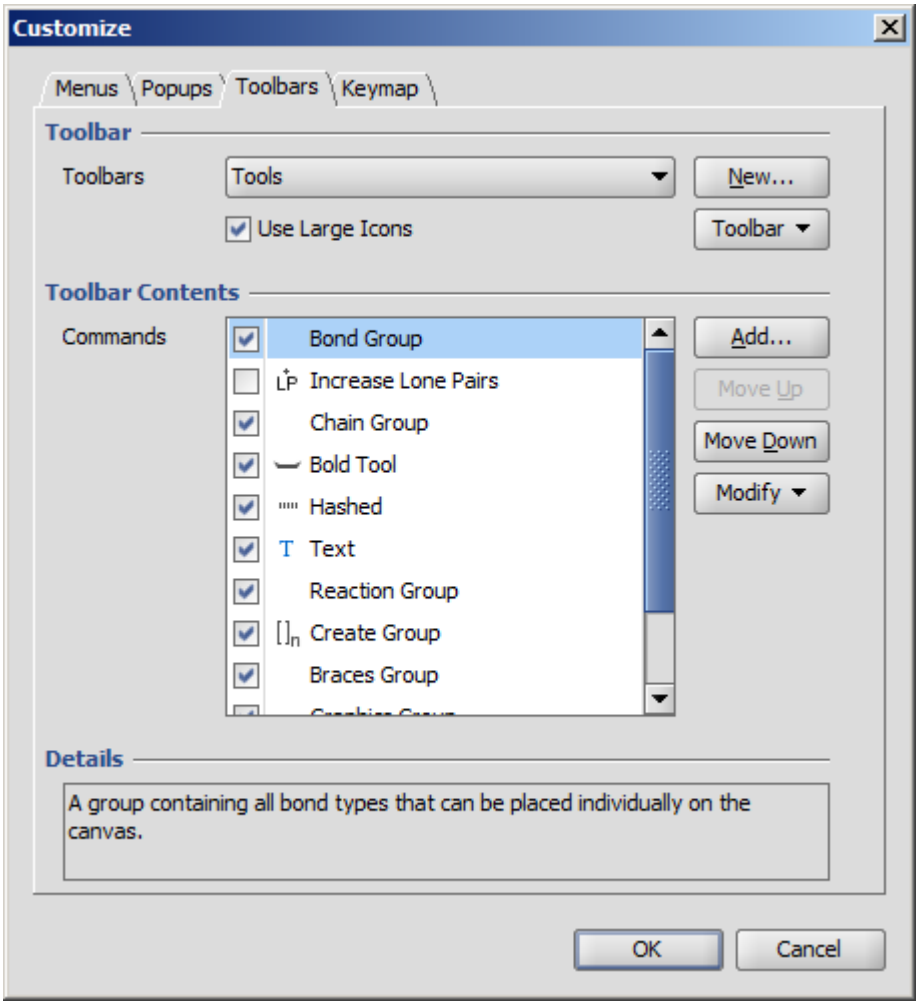


Add	Makes the above **Add Commands** dialog visible, where you can browse all available commands of MarvinSketch. The commands are organized to Categories, and are listed in alphabetical order.
Move Up/Down	Moves a menu element by one position in the container menu.
Modify > Add Submenu	Adds a new submenu after the currently selected element.
Modify > Begin a Group	Adds a menu separator after the currently selected element.
Modify > Rename	Renames a sumbenu or menu element. You can also change the mnemonics by replacing the & sign in the name.
Modify > Delete	Removes the menu element or submenu.

Popups

The customization of Pop-up menus are similar to normal menus. However it is not possible to remove, rename or create a new Pop-up menu, you can only change the contents of the available Pop-up menus. The reason for this is that these menus are context-sensitive, and their name and existence are bound to the underlying contexts.

Toolbars



Note, that the Advanced Templates Toolbar is not possible to be customized.

List of the available Toolbar commands

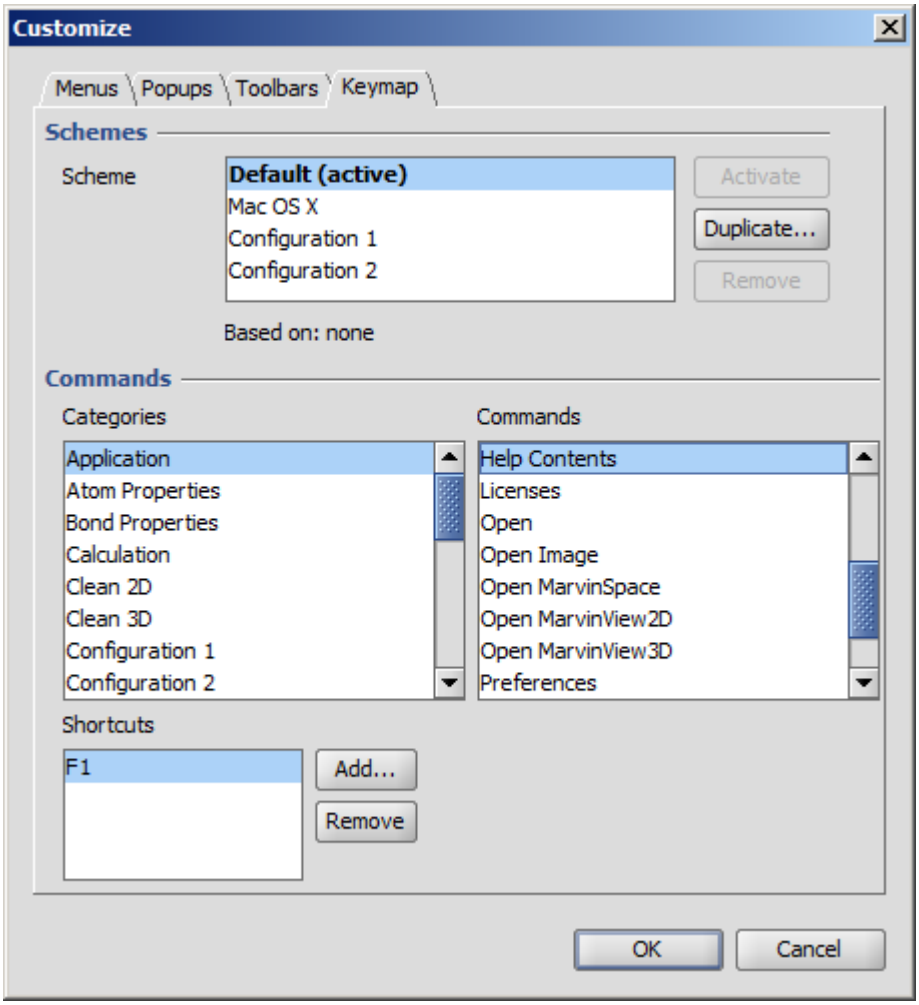
Use Large Icons	When checked, all toolbar buttons have 24x24 pixel sized icons, otherwise the 16x16 pixel versions. By default the large icons are used.
New	Creates a new toolbar and places it north to the first row having some space on the right-hand side.
Toolbar > Rename	Renaming a toolbar in an appearing dialog.
Toolbar > Delete	Removes a toolbar with all of its contents.
Toolbar > Icons Only	The buttons contained by this toolbar will be shown by icon only. Those commands that does not have a corresponding icon defined will be shown by text in this case too.
Toolbar > Text Only	The buttons contained by this toolbar will be shown by text only.
Toolbar > Icons & Text	Icon and text will also be shown for the buttons contained by this toolbar. The text is appearing below the icon.

List of the available Toolbar Contents commands

Add	Makes the **Add Commands** dialog visible, where you can browse all available commands of MarvinSketch. The commands are organized to Categories, and are listed in alphabetical order.
Move Up/Down	Moves a toolbar element by one position in the container toolbar.
Modify > Rename	Renames an element. You can also change the mnemonics by replacing the & sign in the name.
Modify > Delete	Removes the element or separator.
Modify > Begin a Group	Adds a toolbar separator after the currently selected element.

Keymap

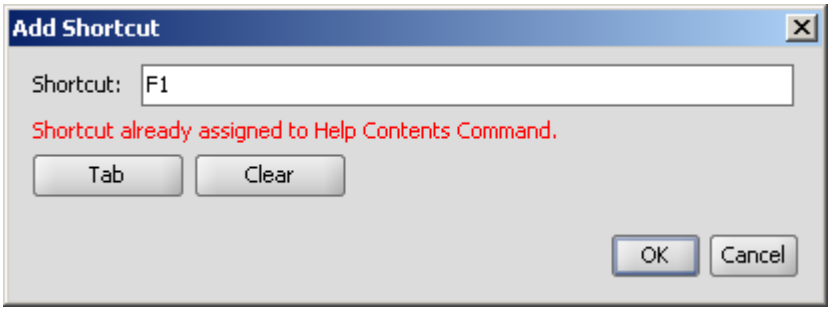
It is possible to define and switch between Keymap Shemes, where all Sheme is a different shortcut-set.
On the Keymap tab, you can browse all available commands of MarvinSketch to define shortcuts to any of the commands you would like to.



Only one scheme can be active at a time. A scheme can be made active by selecting and pressing the **Activate** button. If a scheme is based on another it means that all of the shortcuts are inherited from the base scheme, though they can be overwritten one-by-one. **Duplicating** a scheme will create and activate a new scheme which will be based upon the previously selected one. Shemes - except the default one - can also be **Removed**.

Adding shortcuts

A shortcut can be added by focusing the Shortcut field, and pressing the desired shortcut combination, for example F1. If the shortcut already exists, a warning message appears, and shows which command has the activated shortcut.



The **Tab** button is required if you would like to use the Tab key for a shortcut, because if you press Tab in the Shortcut field, it will loose the focus instead of defining the shortcut.
The **Clear** button helps you to remove the shortcut from the field, because pressing the Backspace button defines a new shortcut instead of removing it.

This document described the interactive way of customizing the user interface using the user interface itself.

Another way of personalization is shown in the Configurations document.

The same method can be used on server side as well.

Special commands

There are a few elements which are not part of the default configuration of MarvinSketch but you can add it via the customization dialog. These are:

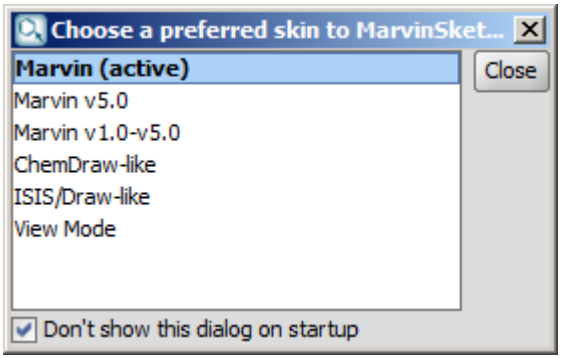
- **Lone Pair Group**
  The toolbar and the menu can be customized to contain the "Lone Pair Group" tool. You have to disable "Automatic Lone Pair" calculation (Preferences dialog, Structure tab) to be able to set the lone pairs manually. Then choose View > Customize..., Menu or Toolbars tab. The Lone Pair Group can be added in the menu contents section. Choose Tools from the Toolbars list, then click Add at the Toolbar contents section. Choose Lone Pair Group from the Insert Lone Pair category, click Add then click Close. The Lone Pair Group tool is now visible on the toolbar on the left of the canvas.
- **Radical Group**
  You can add the "Radical Group" toolbar to your MarvinSketch configuration. This group contains a "Radical switch" button, a "Monovalent radical" button and a "Radical off" button.
- **Free Radical Group**
   You can add the "Free Radical Group" to your MarvinSketch configuration. This group contains a  "0 radical",  "1 radical",  "2 radicals",  "3 radicals",  "4 radicals" and "Increase Radical" buttons. The last one increases the number of radical electrons on the atom by one. In case the number of radicals on the atom is 4, it will be set to zero instead of increasing.
- **Manual Atom Map**
   "Manual Atom Map" can be added from "Structure" category. Selecting the "Manual Atom Map" tool, hold down the left mouse button on an atom of the first molecule, then drag it to the corresponding atom of the second molecule. The same map number will be added to both atoms.
- **Manual Atom Map-Unmap Group**
  A group containing actions: "Manual Atom Map" and "Unmap Atoms".
- **Reaxys Generics**
   "Reaxys generics" can be added from the "Insert Template" category. This template library contains the generic abbreviation commonly used in the Reaxys database.
- **Substitution Count**
  Extension of the menu with the "Substitution Count": create a new entry recommendably in the "Atom" menu. Select the new submenu in the Menus dropdown list. Select the new entry and click Add.. Choose the commands from Atom Properties category (Substitution Count off, Substitution Count as Drawn, 0 substituent, 1 substituent, etc.), click Add, then click Close.

Configurations of MarvinSketch

The whole collection of Menubar, Toolbar, Pop-up menu and Shortcut definitions is called **Configuration**.

In the **Customization** section we describe the way of personalizing the Graphical User Interface (GUI) of MarvinSketch. This includes adding, removing and modifying elements of the interface.

At the first launch of MarvinSketch a dialog asks the user to select the desired skin for the GUI configuration:

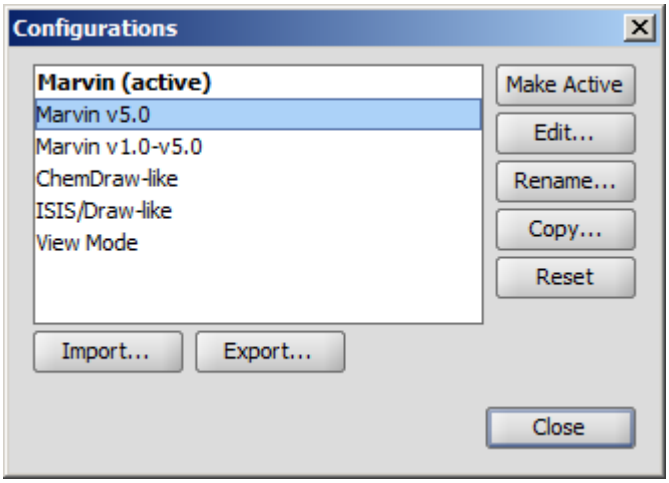


The default configuration is called **Marvin** Configuration, and it has the **(active)** suffix. This selection can be changed any time from the **View** menu.

These configurations can be modified, exported and imported, or reset to the default settings from the **Configuration Settings** submenu. As soon as any changes are made, the configuration becomes modified, but a new configuration is not created yet, the modifications are only stored. If the **Configuration Settings** are **Reset**, the modifications will be lost, and it is not possible to restore them. To prevent this, a new configuration can be made which stores the personalized GUI settings.

Six predefined configurations are available by default: **Marvin, Marvin v5.0, Marvin v1.0-5.0, ChemDraw-like*, ISIS/Draw-like***, and the **View Mode**. Each one has its own menubars, toolbars, etc.
A configuration can inherit the definitions from others. For example the **Marvin v5.0** configuration inherits the default menubar, pop-up menu and shortcuts definitions from the **Marvin v1.0-v5.0**, only the toolbars are redefined.
Note: configuration settings will not change the behavior of the application, it only applies to the GUI.

The configuration-related commands can be found in the **View > Editor Style** (or **View > Configurations**) menu.



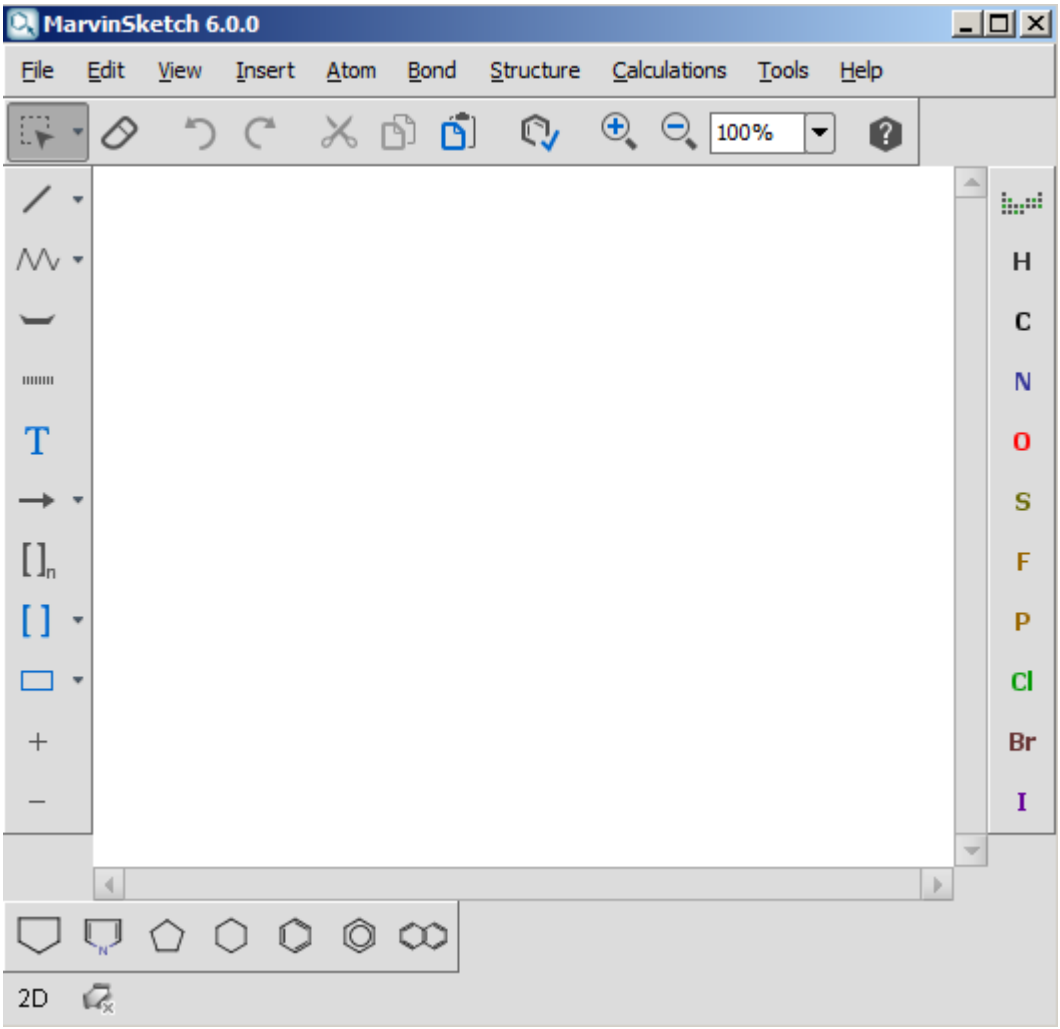
The available functions are described in the following table:

Make Active	Activates a configuration which will not cause the loss of modifications when the current configuration is modified.
Edit	Opens the **Customize** dialog with the selected configuration definitions loaded.

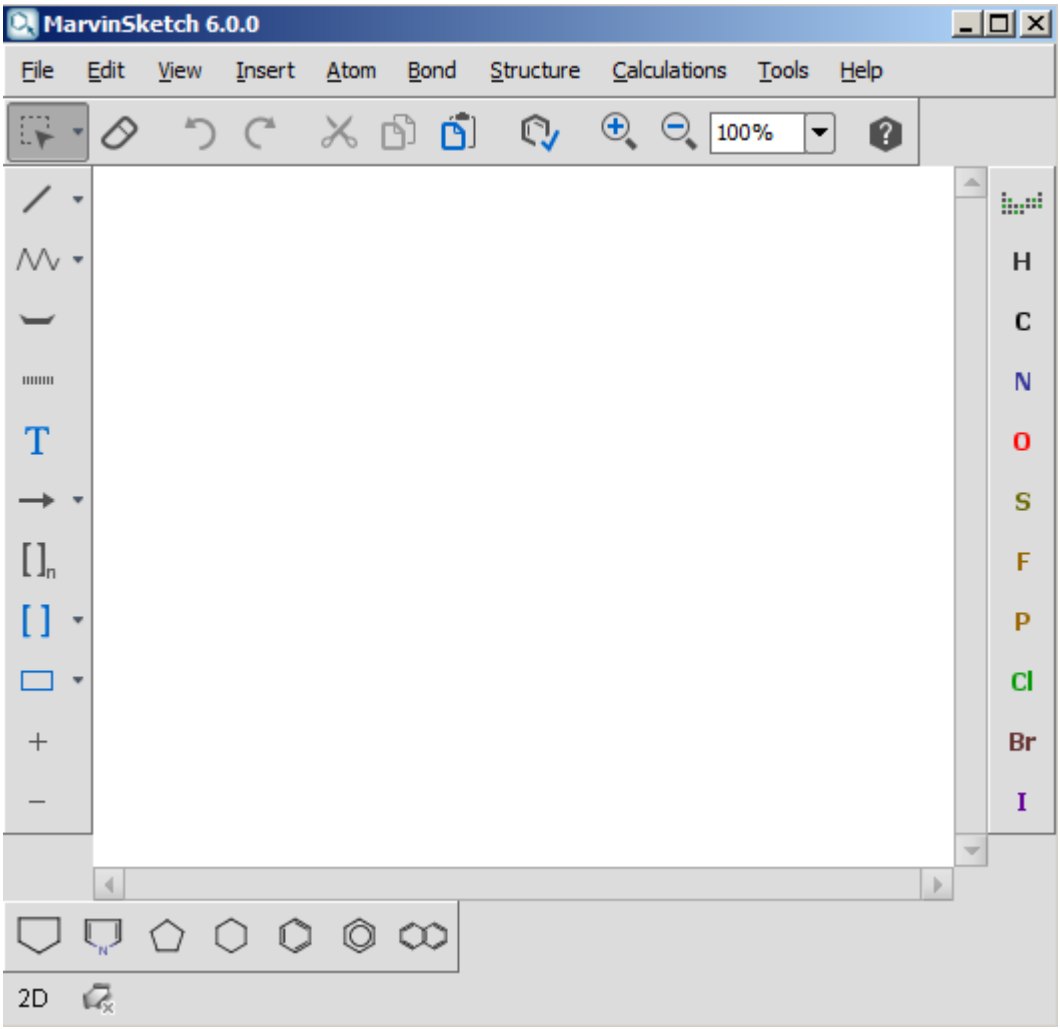
Rename	Simply changes the name of a configuration.
Copy	Creates a new configuration based on the selected one inheriting all GUI definitions.
Reset	Returns to the default configuration settings by dismissing all modifications. **This operation cannot be undone.**
Import	Imports an XML or a serialized (.ser) configuration file.
Export	Exports the active configuration to an XML or a serialized (.ser) file.

Screenshots of the six available configurations:

1. Marvin Configuration

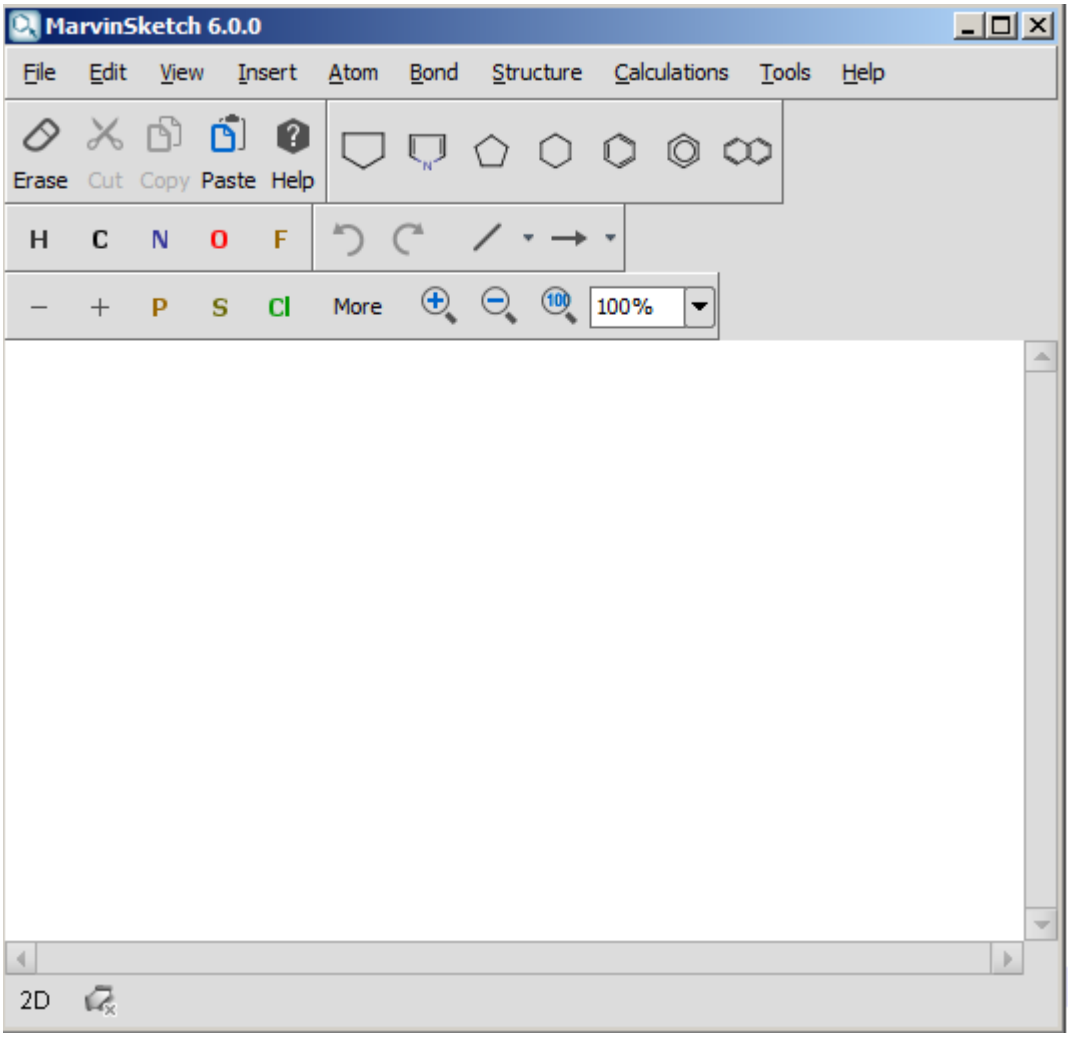


2. Marvin v5.0 Configuration

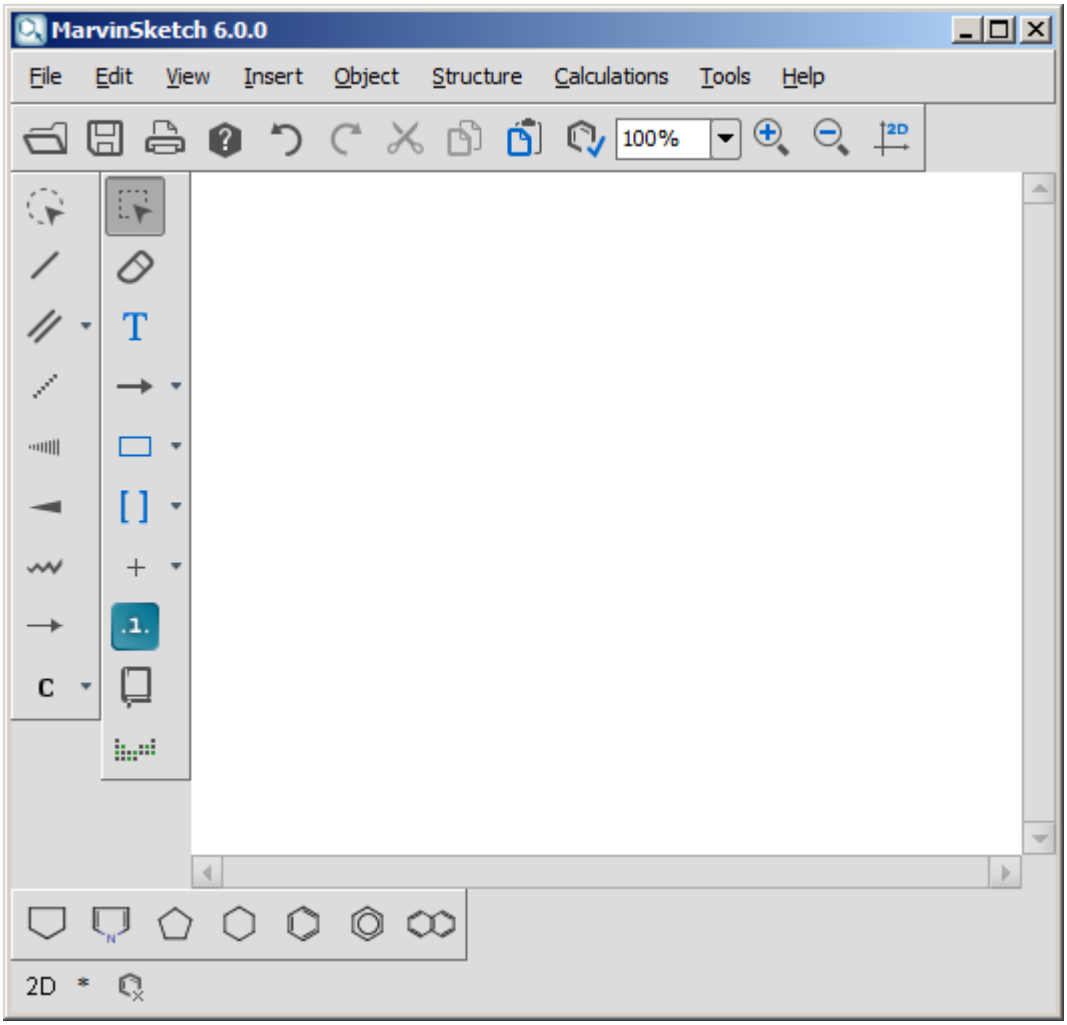


Note: only menu items are different from the ones in "Marvin Configuration".

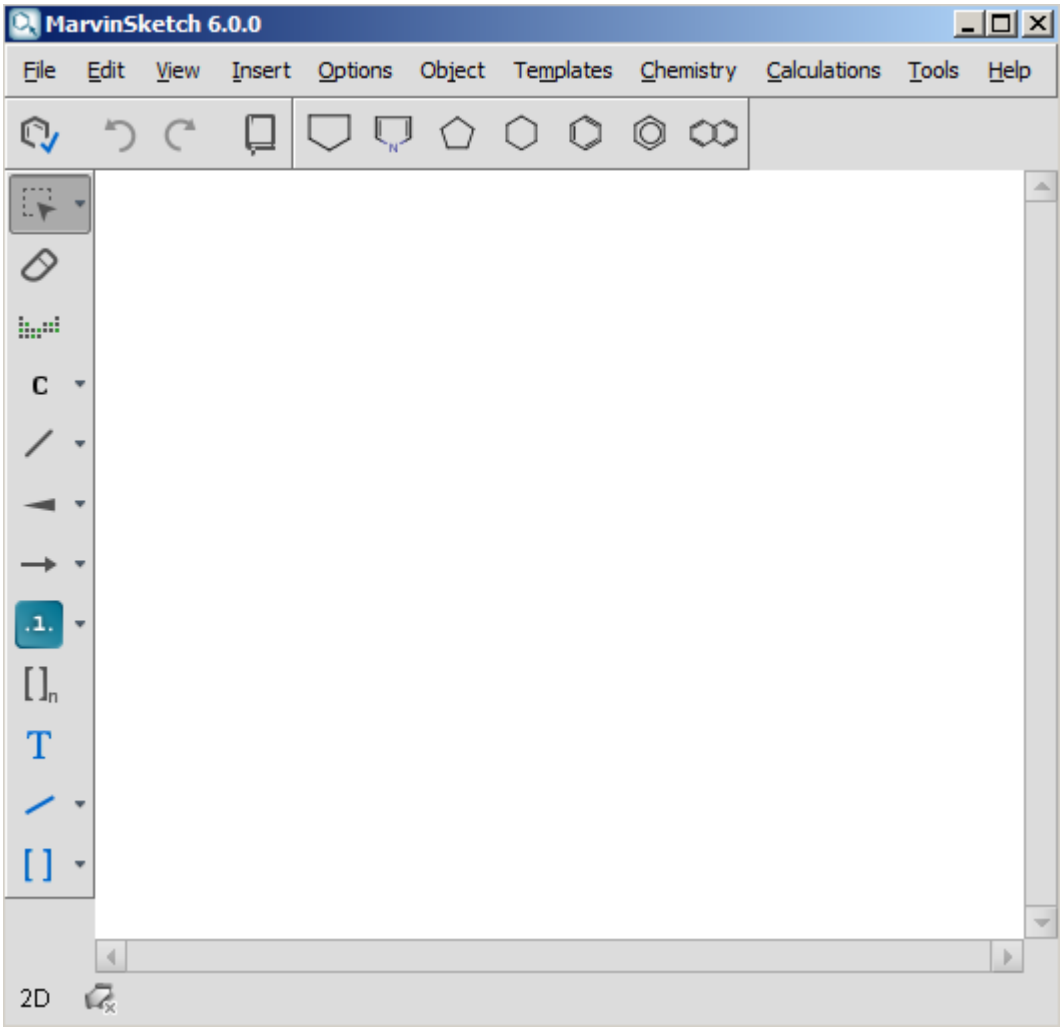
3. Marvin v0.1-0.5 Configuration



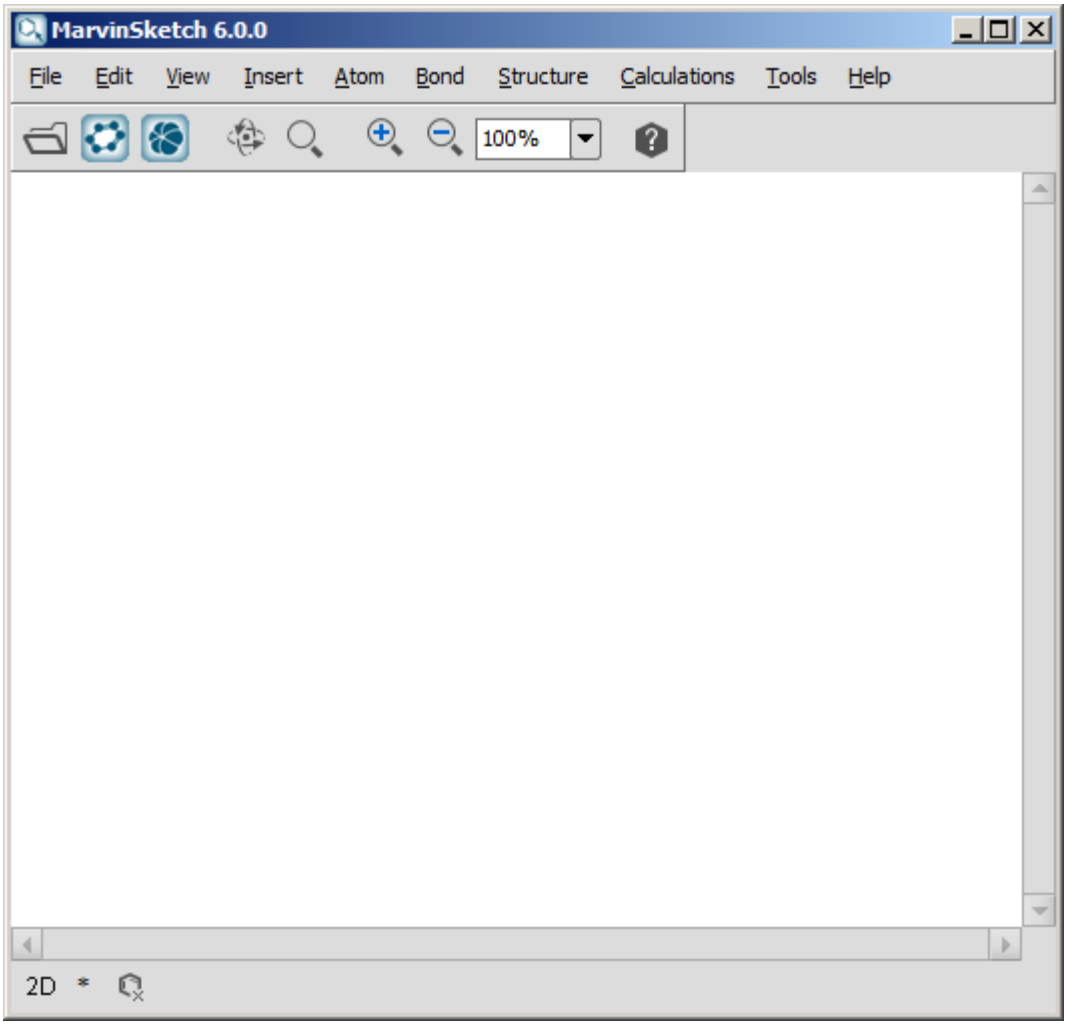
4. ChemDraw-like* Configuration



5. ISIS/Draw-like* Configuration


MarvinSketch 6.0.0
File
Edit
View
Insert
Options
Object
Templates
Chemistry
Calculations
Tools
Help
2D

6. View Mode



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* Please see the Trademarks document for details.

Customizing MarvinSketch GUI - Server side

The Customization document demonstrates an easy, interactive way of GUI personalization.

This document shows how to use the same interactive method to customize the GUI if MarvinSketch is used as an **applet** being on a server or as a **JavaBean**.

Note, that API and XSD will also be available very soon.

The configuration file

MarvinSketch stores all changes made on the GUI in a **configuration file**.
This file is located at `USER_HOME/CHEMAXON_DIR/VERSION/customization.xml`, where

- `USER_HOME` is `C:\Documents and Settings\USERNAME` on Windows, `/home/USERNAME` on Unix
- `CHEMAXON_DIR` is `chemaxon` (Windows) or `.chemaxon` (Unix)
- `VERSION` is the actual version number of MarvinSketch, with which the customization is made

Example location:
Windows: `C:\Documents and Settings\USERNAME\chemaxon\6.0.0\customization.xml`
Unix/Linux: `/home/USERNAME/.chemaxon/6.0.0/customization.xml`

Applet customization step-by-step

1. Remove the the configuration file from your local file system (make sure to create a backup)
2. Launch MarvinSketch on the client side
3. Personalize the GUI using the methods described in the Customization document
4. Upload the newly created configuration file to be beside the MarvinSketch applet on the server, *e.g.*, http://example-server.org/marvin/customization.xml
5. Set the "menuconfig" applet parameter to the URL of the configuration file, *e.g.*,
   ```
   msketch_param("menuconfig", "http://example-server.org/marvin/configuration.xml");
   ```
   or
   ```
   msketch_param("menuconfig", "files/marvin/configuration.xml");
   ```

JavaBean customization step-by-step

1. Remove the the configuration file from your local file system (make sure to create a backup)
2. Launch MarvinSketch on the client side
3. Personalize the GUI using the methods described in the Customization document
4. Copy the newly created configuration file to a path which is included in the classpath of the application
5. Use UserSettings to instantiate the bean:

```
UserSettings userSettings=new UserSettings();
userSettings.put("menuconfig", "org/example/configuration.xml");
MSketchPane sketchPane=new MSketchPane(userSettings);
```

Example 1 : Make ISIS/Draw-like configuration to be the default

The Configurations document describes built-in alternative schemas for personalized GUIs.
To make a configuration schema to be the default, the identifier of the desired configuration has to be set in a simple xml file.

The identifiers of the available configurations are below:

Configuration	Identifier
Marvin	default
Classic Marvin	classic
ISIS/Draw-like	config1
ChemDraw-like	config2

The contents of the configuration file:

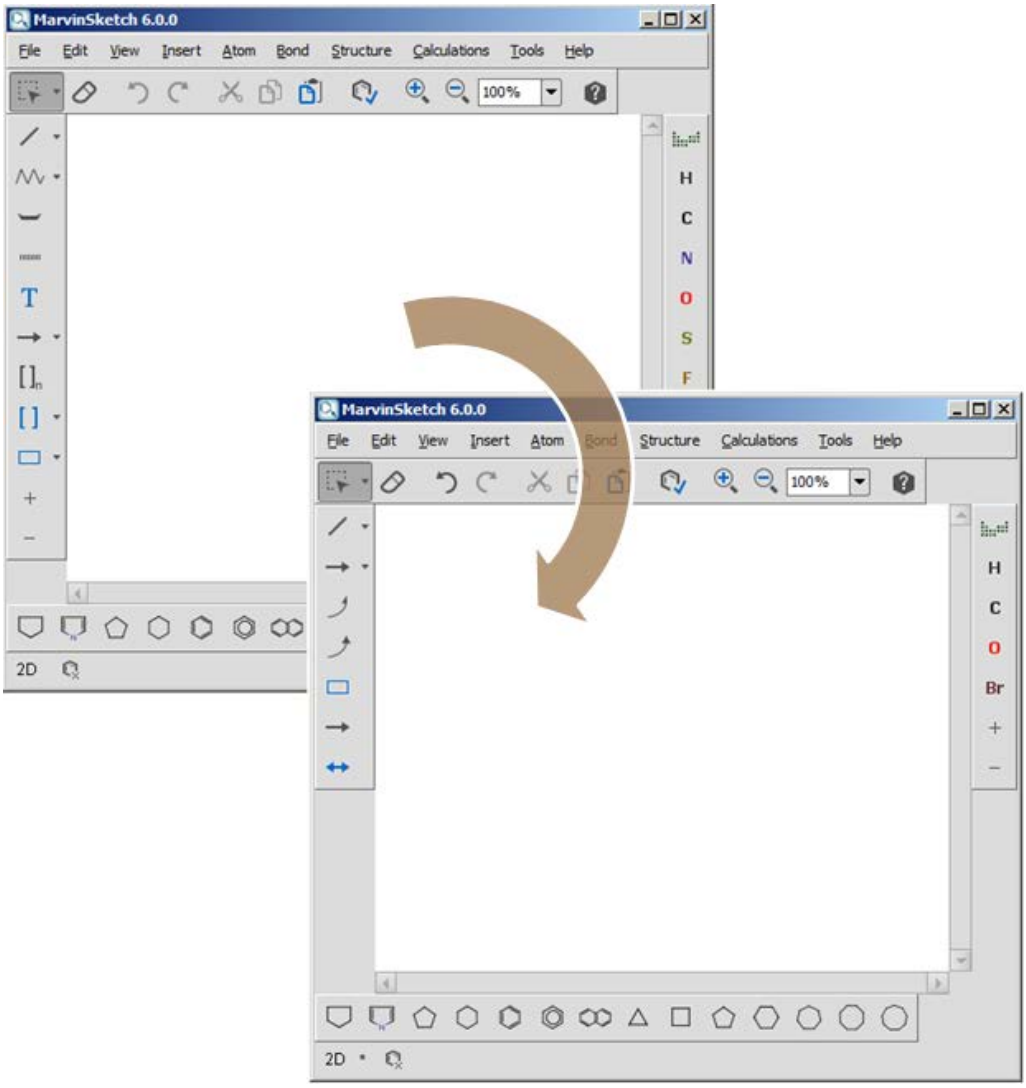
```
<?xml version="1.0" encoding="UTF-8"?>
<customization active="config1">
</customization>
```

Example 2: Creating a custom Tools palette

This example shows a configuration file which performs the following changes:

- the Tools toolbar on the left hand side is hidden
- a new toolbar is defined in its place with some custom actions
- the Atoms toolbar on the right hand side is changed

The result is shown in the picture below:



The content of the *default* scheme of the configuration file is as follows:

```
       <scheme id="default">
        <modify path="toolbar/atoms/atom.N" visible="false"/>
        <modify path="toolbar/atoms/atom.S" visible="false"/>
        <modify path="toolbar/atoms/atom.F" visible="false"/>
        <modify path="toolbar/atoms/atom.P" visible="false"/>
        <modify path="toolbar/atoms/atom.Cl" visible="false"/>
        <modify path="toolbar/atoms/atom.I" visible="false"/>
        <add path="toolbar/atoms">
          <item id="increaseCharge"/>
          <item id="decreaseCharge"/>
        </add>
        <order
itemorder="periodicSystem/atom.H/atom.C/atom.N/atom.O/atom.S/atom.F/atom.P/atom.Cl/atom.Br/atom.I/increaseCharge/decreaseCharge"
 path="toolbar/atoms"/>
        <modify index="1" path="toolbar/tools" row="0" visible="false"/>
        <toolbar anchor="west" id="CustomToolbar-0" index="0" name="Custom-Tools-Palette" row="0">
          <item id="bondGroup"/>
          <item id="insertElectronFlow"/>
          <item id="insertElectronFlow2"/>
          <item id="insertRectangle"/>
          <item id="insertArrow"/>
          <item id="insertTwoHeadedArrow"/>
```

```
    </toolbar>
  </scheme>
```

Currently using a configuration file is the only way to change the GUI of applets or beans. The possibility of using the API will be available soon.

Note that the graphical user interface of MarvinView and MarvinSpace can not be customized yet.

Configure the Attach Data Dialog in MarvinSketch

The Schema definition

The XML Schema Definition file of the configuration xml can be downloaded from this link.

With the help of the XSD file, you can validate your configuration before applying it to the MarvinSketch application. You can also find information about the usable elements, and attributes in the documentation sections of the definition file.

The default AttachData dialog configuration

The default configuration becomes active when no user configuration is found. If a user configuration file is in the [.]chemaxon directory inside the home directory of the user with the name "AttachDataDialog.xml" can be found, then the configuration defined in the file will be used, and the default configuration will not take effect.

Contents of the default configuration:

```
<?xml version="1.0" encoding="UTF-8"?>
<AttachDataDialogConfig
    xmlns="AttachDataDialogConfig"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="AttachDataDialogConfig AttachDataDialogConfig.xsd ">
<context name="Atom"></context>
<context name="Bond"></context>
<context name="Single Bond"></context>
<context name="Double Bond"></context>
<context name="Fragment"></context>
<context name="Group" displayName="Group (Selection)">
    <dataname textRepresentation="COEFF"/>
    <dataname textRepresentation="Stoichiometry"/>
    <dataname textRepresentation="[DUP]"/>
    <dataname textRepresentation="REAGENT"/>
</context>
</AttachDataDialogConfig>
```

A complex example configuration file

```
<?xml version="1.0" encoding="UTF-8"?>
<AttachDataDialogConfig
    xmlns="AttachDataDialogConfig"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="AttachDataDialogConfig AttachDataDialogConfig.xsd ">
<context name="Atom">
    <dataname textRepresentation="foo" defaultTag="f" multipleValuesEnabled="false"
valueFieldEditable="false">
        <value>bar1</value>
        <value>bar2</value>
        <value>bar3</value>
        <unit>u1</unit>
        <unit>u2</unit>
    </dataname>
    <dataname textRepresentation="foo2" multipleValuesEnabled="true">
        <value>bar2</value>
        <value>bar4</value>
        <unit>u1</unit>
        <unit>u3</unit>
```

```
    </dataname>
</context>
<context name="Group" displayName="Group (Selection)" nameFieldEditable="false">
    <dataname textRepresentation="foo">
        <value>bar3</value>
        <value>bar4</value>
        <value>bar5</value>
        <unit>u1</unit>
        <unit>u3</unit>
        <unit>u4</unit>
    </dataname>
</context>
<context name="Bond"/>
<context name="Single Bond">
    <dataname textRepresentation="foooo"/>
</context>
</AttachDataDialogConfig>
```

The result of this configuration can be seen in the dialog.
With this file the following have been configured:

- The context field will have four values: the Atom, Group, Bond, Single Bond
- When the Atom context is selected, the Name combo box will have the following values set: editable empty field, foo, foo2
- When the Atom context is selected, and the value foo is selected in the Name combo box, the Value field will not be editable
- When the Group context is selected, the Name combo box will have the following value set: foo
- When the Group context is selected, the Name combo box will not be editable
- When the Bond context is selected, the Name combo box will only contain the editable empty field
- When the Single Bond context is selected, the Name combo box will have the editable empty field, and the foooo name set
- In one session if the user enters something into the editable empty field, then that value will be added to the list of names belonging to the context. These values will be missing after restarting the application.
- Same names in the name field are independent from each other, if they are in a different context. Same names inside the same context will cause confusion, and maybe malfunction.
- After selecting the name, the Value field will load the defined values in the given Context for the specified name, if there are any.
- If the multipleValuesEnabled attribute of the namedata element is set to true, then the user can select more than one value in the Values field, otherwise only one value can be selected.
- If the defaultTag attribute is set for the dataname element, and the name is selected, then the Tag field will be filled with its defaultTag. (Tag can be of a single character length, this is only checked by the GUI.)
- The Values field also has an empty editable field, newly entered values work the same as by the Name field.
- The Unit field also has an empty editable field, newly entered values work the same as by the Name field.

Configuring copy/paste operations in applets.

Using this configuration the copy/paste operations available in the applet can be controlled: the formats available for copy or paste can be manipulated, or the corresponding resources can be preloaded.
For example, the copy or paste of specific file formats can be forced to be immediately available after the start of the applet, so instead of loading the underlying architecture on demand, the required resources are loaded during the applet initialization time.
In addition, the formats available on the clipboard after a simple copy operation can be configured, as well as the list of formats available in the Copy As dialog.

The configuration is available through a Java properties file which has to be placed to the APPLET_CODEBASE/chemaxon/marvin/datatransfer.properties file. If this file is available in the applet codebase, the configuration will take effect.

This properties file contains settings for format keys. The property name format is as follows: `formatkey.configuration.setting.id`, so for example, if somebody wants to disable the png format on the copy as dialog, then the `png.use.dialog` key has to be set to false.

Available format keys in the property file, and the corresponding formats:

Format key	The corresponding format
mrv	Marvin Document Format
skc	IsisDraw Sketch file format
cdx	ChemDraw Sketch file format
mol	MDL MOLfile format
rxn	MDL RXNfile format
smiles	Daylight SMILES format
smarts	Daylight SMARTS format
cxsmiles	Chemaxon extended SMILES format
cxsmarts	Chemaxon extended SMARTS format
name	IUPAC name format
trad_name	Traditional name format
inchi	IUPAC InChI format
inchikey	IUPAC InChIKey format
string	Molecule source, containing the actual file format of the molecule object
emf	Enchanced Metafile picture format (available only on windows platforms)
jpg	JPG image format
png	PNG image format

Available configurable properties for all formats and their meanings:

Parameter name	Valid values	Meaning
name	can be any String	This will be displayed in the Copy As dialog to represent the format.
disabled	true/false	If set to false, then the format won't be available at all.
preload.copy	true/false	If set to true, then the classes needed for copying in the specified format will be preloaded at applet initialization.
preload.paste	true/false	If set to true, then the classes needed for pasting in the specified format will be preloaded at applet initialization.
preload	true/false	If set to true, then the classes needed for copying or pasting in the specified format will be preloaded at applet initialization.

use.default	true/false	If set to true, then the molecule will be placed to the clipboard by a simple copy operation in the specified format.
use.dialog	true/false	If set to false, then the specified format won't be available in the Copy As dialog.

By default, none of the formats are preloaded, all of them are configured as they worked before.

Other available options:

The following keys are not related to the formats, and should be used as they are:

Property name	Valid values	Meaning
ole.enabled	true/false	If Microsoft OLE object copy should be disabled then set to false.
ole.name	can be any String	This will be displayed in the Copy as dialog to represent the Microsoft OLE object format.
separator	a comma separated list of format keys.	After the enumerated formats a separator will be placed in the copy as dialog.

The default configuration file

```
#define where to place separator in the copy as dialog.
#comma separated list, separators will be placed after the listed formats
separator = string

#OLE related settings. Note: OLE is usable only on Windows platforms.
ole.name = Marvin Object (OLE)
ole.enabled = true

#structure formats
mrv.name = Marvin Document (MRV)
mrv.disabled = false
mrv.preload.copy = false
mrv.preload.paste = false
mrv.use.default = true
mrv.use.dialog = true

skc.name = ISIS (Symyx) file (SKC)
skc.disabled = false
skc.preload = false
skc.use.default = true
skc.use.dialog = true

cdx.name = ChemDraw file (CDX)
cdx.disabled = false
cdx.preload = false
cdx.use.default = true
cdx.use.dialog = true

mol.name = MDL MOLfile
mol.disabled = false
mol.preload.copy = false
mol.preload.paste = false
mol.use.default = true
mol.use.dialog = true

rxn.name = MDL RXNfile
```

Configuring copy/paste operations in applets.

```
rxn.disabled = false
rxn.preload.copy = false
rxn.preload.paste = false
rxn.use.default = true
rxn.use.dialog = true

smiles.name = Daylight SMILES
smiles.disabled = false
smiles.preload.copy = false
smiles.preload.paste = false
smiles.use.default = false
smiles.use.dialog = true

smarts.name = Daylight SMARTS
smarts.disabled = false
smarts.preload.copy = false
smarts.preload.paste = false
smarts.use.default = false
smarts.use.dialog = true

cxsmiles.name = ChemAxon SMILES (CXSMILES)
cxsmiles.disabled = false
cxsmiles.preload.copy = false
cxsmiles.preload.paste = false
cxsmiles.use.default = false
cxsmiles.use.dialog = true

cxsmarts.name = ChemAxon SMARTS (CXSMILES)
cxsmarts.disabled = false
cxsmarts.preload.copy = false
cxsmarts.preload.paste = false
cxsmarts.use.default = false
cxsmarts.use.dialog = true

name.name = Name
name.disabled = false
name.preload.copy = false
name.preload.paste = false
name.use.default = false
name.use.dialog = true

inchi.name = InChI
inchi.disabled = false
inchi.preload = false
inchi.use.default = false
inchi.use.dialog = true

inchikey.name = InChIKey
inchikey.disabled = false
inchikey.preload = false
inchikey.use.default = false
inchikey.use.dialog = true

string.name = Molecule Source (Plain Text)
string.disabled = false
```

```
string.preload = false
string.use.default = true
string.use.dialog = true

#image formats
#emf supported only on Windows platforms
emf.name = EMF Image
emf.disabled = false
emf.preload = false
emf.use.default = true
emf.use.dialog = true

#default copy contains these formats because Java Image Flavor is used in default copy.
jpg.name = JPG Image
jpg.disabled = false
jpg.preload = false
jpg.use.default = false
jpg.use.dialog = true

png.name = PNG Image
png.disabled = false
png.preload = false
png.use.default = false
png.use.dialog = true
```

Further format couplings

Please consider this information also while changing the configuration.

- If OLE is enabled, then the OLE data will contain the mrv, the mol or rxn file, and the emf image also.
- Default copy places image data to the clipboard, in java image format. If you want to disable this behaviour you have to set the `jimage.use.default` property to true.

How to Use Basic MarvinSketch Functions

Table of Contents

Creating a New Molecule

A new, blank molecule is created when you first launch MarvinSketch. You can immediately begin working with this molecule. A MarvinSketch window can hold only one molecule at a time, so all work you do within the canvas is considered part of the same molecule. You can create a new, blank molecule at any time during your session by choosing **File > New > Clear Desk** from the menu bar. This will clear the desk and discard any unsaved changes to the molecule you were previously working with (but you can get it back using the Undo option).

The application allows you to work with multiple molecules in multiple windows by choosing **File > New > New Window**.

Opening and Saving a Molecule File

To Open an Existing Molecule File

You can open existing molecule files (from supported file formats) by choosing **File > Open...** on the menu bar. It will load the content of the molecule file into Marvin and discard any unsaved changes.

Tick the **Show preview** checkbox to see the contents of the file (molecules, reactions, queries). A single item is displayed in the preview window; the text field at the bottom shows the index of the current structure and the number of structures in the file. When a multiple structure file is selected (*e.g.*, mrv, sdf), the navigation buttons become active. Their functions are: go to first, go to previous, go to next, go to last. Note that the preview window allows you only to check the contents of a file, but not to select the structures you would like to open. For this purpose the **Select** textbox has to be used, where you can write the serial numbers of the molecules to open. The numbers have to be separated either by commas or by a dash. (Clicking on the **Info** button in this row will present tips for specifying the desired molecules.) Leaving this textbox empty means that every molecule in the file will be loaded onto the canvas. Currently this is the default behavior of file loading in MarvinSketch.
In order to open a pdf file containing chemical names in MarvinSketch, you need to apply Document to Structure (d2s) conversion. If your pdf file conatins images of compounds, you need OSRA to be installed on your computer in order to import the structures into Marvin (possible since version 5.3.0). Please consult this page for details.

The **File > Insert file** menu option has to be chosen if you want to open a file, but, at the same time, you do not want to lose the molecule(s) currently on the canvas. The **Insert** dialog window works in the same way as the **Open** dialog.

You can also Paste existing structures from other windows, as well as Drag & Drop a chemical structure into the MarvinSketch window. Both actions will add the new structure to the currently loaded ones without overwriting the contents of the canvas.

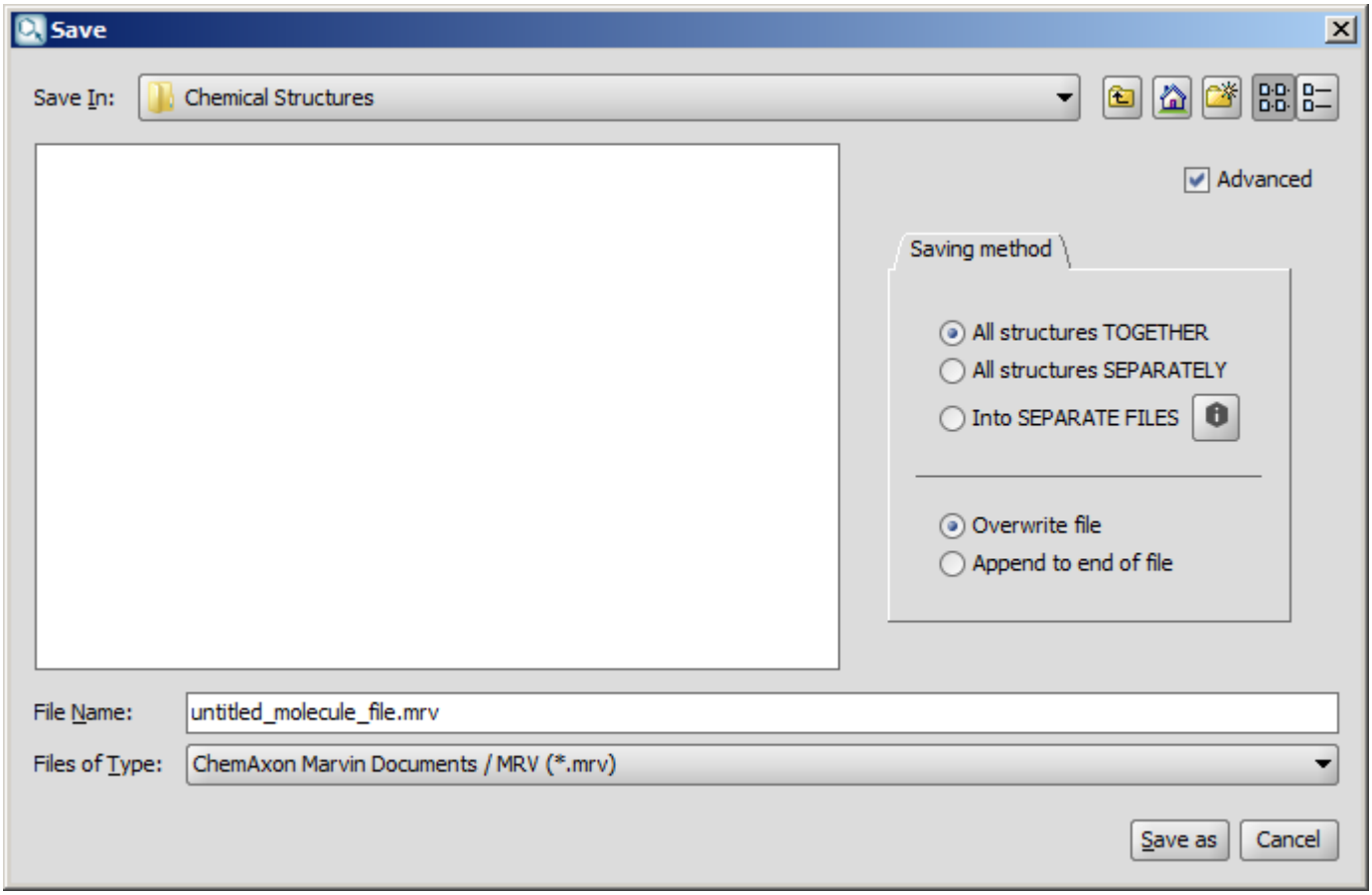
Importing structures from image files or pasting them from the clipboard with the help of OSRA is also possible (since version 5.3.0). Select **File > Import Image** if you want to open an image file. The supported formats are: bmp, png, jpg, gif, svg, and tif. Alternatively, the **File > Open...** menu option can also be used for opening an image file. In this case you should select **All Files** from the list of **Files of Type**.

To Save a Molecule File

You can save the molecule in any of the supported file formats. This will allow you to open and work with this molecule later. In case of a single structure, the default behavior of the **Save** menu is to save the molecule to the same file as it was opened from, in the same format. If you want to change the filename or format, choose **Save As**. If you are working with a new molecule, **Save** will function the same way as **Save As**. If you are working with a multistructure file, both **Save** and **Save As** will open a dialog window where you have to define

the parameters for saving.
On the dialog window used for saving files, a **Saving method** tab can be opened with the help of the **Advanced** checkbox. The first half of the tab offers the following choices:

- **All structures TOGETHER:** Saves all structures together in a single file.
  This is the default behavior of saving. If you do not open the **Saving method** tab, this option will be applied.
- **All structures SEPARATELY:** Saves all structures separately in a single file.
- **Into SEPARATE FILES:** Saves each structure into a separate file.
  In this last option, the numbering of molecule files begins with the molecule in the upper left corner.



The second option remains inactive unless the chosen file type supports multimolecule files (such as mrv or sdf). Similarly, for one molecule only files, only the first option is enabled. The same applies to reactions and structures containing R-group definitions: in these cases only the "All structures TOGETHER" option is available as well.
When the given parameters for saving (filename, format, and route) are the same as for an already existing file, the outcome will be determined by the other two radio buttons of the dialog window. If you select the **Overwrite file** option, the original contents of the file will be replaced. However, selecting the **Append to end of file** radio button will add the new structures to the original file, so its content will be preserved. In the first case, a new dialog window will be displayed, where you can reinforce or change your decision about overwriting the file. If the chosen file format does not support multiple structures, the **Overwrite** option is applied automatically.

To Edit and Save atom, bond, and molecule properties

You can add, edit, and save properties of atoms, bonds, and molecule; just select the relevant part and choose "Edit properties..." option from the contextual menu. The added properties will be saved in the file which supports properties such as MRV or SDF (in case of the molecule property only). You can display atomic properties, setting **Menu>View>Misc>Atom Properties**; bond and molecule properties cannot be displayed on the canvas currently.

To Save as an Image File

The **Export to Image** choice in the **File** menu allows you to save an image of the molecule in the sketcher. Marvin supports the following image formats: JPG, PNG, PPM, SVG, BMP, and SVG. Please note that the saved image cannot be edited in Marvin.

Printing

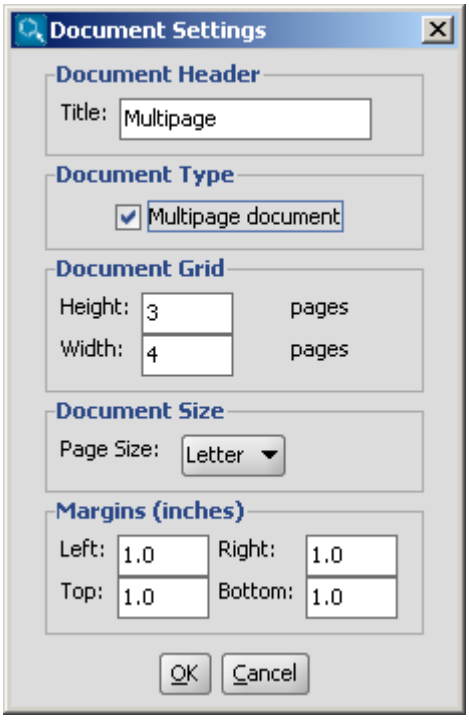
You can print an image of the current molecule by choosing **File > Print**. If you print from a single page document, if the size of your molecule(s) is bigger then the paper size, it will be shrunked to one page.

If you want to print your molecule(s) to multiple pages, you have to change the document type to Multipage Document in **File > Document Settings...**, and arrange the structures on the pages.

Working with Multipage Molecular Documents

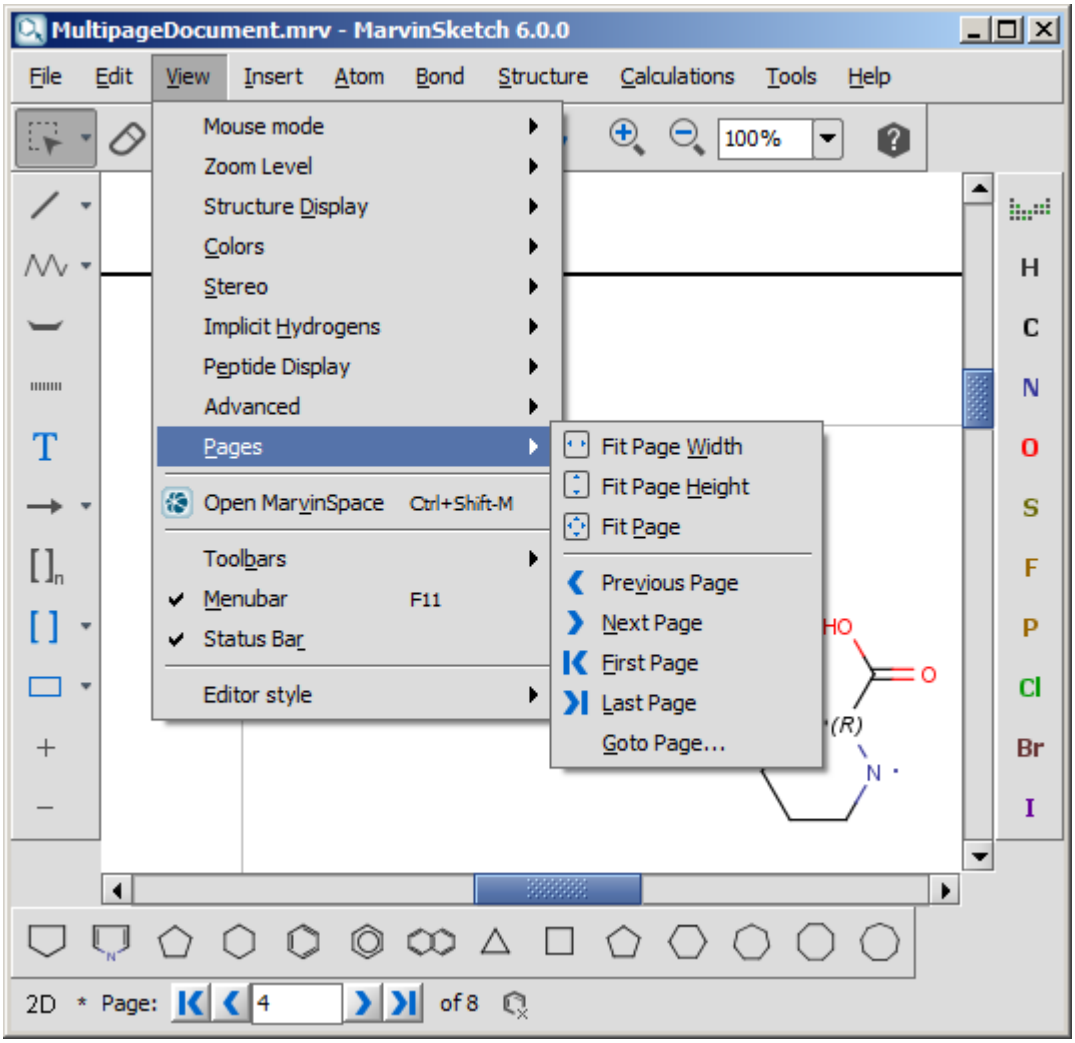
How to create a multipage molecular document

Multipage molecular documents help to work with large drawings by dividing them into pages. You can create a multipage molecular document by choosing **File > Document Settings...**, then checking in the **Multipage document** checkbox.



You can set the number of horizontal and vertical pages in the **Document Grid** part, and you can also define the title, the page size and the margins in the corresponding sections of this dialog window. After pushing the OK button, the following controls become automatically available:

- The items in the **View > Pages** menu are enabled
- A navigation status bar appears on the bottom of the window
- The frame of the pages appear on the canvas, while the title, the margins and the page numbers are displayed on each page



How to navigate in multipage molecular documents

The navigation status bar and the items in the **View > Pages** menu are available only if the **Multipage document** checkbox is set. The status bar contains information about the current page number in a text field and the number of all pages on a label. It also contains a collection of buttons to aid your quick navigation in the document. You can go the first, previous, next, and last page using them. Alternatively, you can go directly to a specific page by entering a number in the current page field and pressing enter.

All the navigation possibilities: go to first, previous, next, last, specific pages are available from the **View > Pages** menu as well. In addition, some automatic page zooming functions are also available in this menu, such as:

- **View > Pages > Fit page height** adjusts the height of the current page to the height of the canvas.
- **View > Pages > Fit page width** adjusts the width of the current page to the width of the canvas.
- **View > Pages > Fit page** adjusts the height and/or the width of the current page to see the whole page, and places it centralized within the canvas.

Drawing Structures

You can create structures using atoms, bonds, and templates.

How to Draw Atoms

- Select an atom from the Atoms Toolbar, the Periodic Table dialog window, or by shortcut.
- Move the mouse into the molecule canvas. You will see the symbol of the selected item at the tip of your cursor. It can be placed in the molecule by left-clicking on the desired location.
    - Marvin is chemically intelligent. It will account for implicit hydrogens and set the charge according to valence rules.

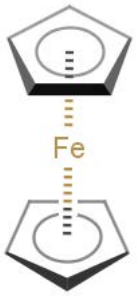
In case of metals, the following rules apply: metallic elements from the 1st and 14-16th groups are added hydrogens, other appear as simple elements as default.

- You can replace any atom in the molecule by placing a new atom on top of it.
- You can represent atoms in a molecule with practically any arbitrary symbol instead of standard atomic symbols by using Atom Aliases. An alias can be defined on the Advanced tab of the **Periodic Table**, among the Custom Properties.

How to Draw Bonds

- Select a bond type using the **Bond** toolbar button or by shortcut.
- To link two existing atoms, click on one then drag the cursor to the other.
  - Marvin will allow you to draw a bond between any two atoms in the molecule. Valence errors will be highlighted (if that option is enabled).
- To draw a bond from a single atom, simply click the atom. A carbon atom will be added at the other end of the bond.
- If you add a bond to empty canvas space, a carbon atom will be added to each end of the bond.
- You can replace any bond in the molecule by placing a new bond type on top of it.
- Bond types can also be changed using the Bond pop-up menu. Single bonds can be changed to Double or Triple by left-clicking on them.
- Bold Tool, , is intended to be used for graphical presentations of molecules. Activate the tool, click on a bond and it will be changed to bold. In case of single, double, or aromatic bond the tool keeps the type of the bond during multiple clicking. In case of aromatic bond, Bold Tool has four positions: bold single, bold aromatic up, reversed bold aromatic up, and single. Note: your mouse must point to the same position of the bond. In case of other bond types (e.g., triple, wedges) multiple clicking has a different result; it does not retain the original bond type, but undoing the action does. Bold Tool is located in the Bond Menu, Tools toolbar, and bond PopUp menu by default.

  Example



- You can make the selected bond hashed: Choose the icon from the "Tools" toolbar or the **Bond** >**Hashed** menu. It only retains single original bond type.

How to Draw Chains

You can draw carbon chains easily selecting the **Insert** > **Chain** menu or clicking on the "Draw Chain" ( ) icon of the "Tools" toolbar. For curved chains click on the icon. The direction of the chain growth follows the mouse path. The number of carbon atoms can be increased or decreased by dragging the mouse. The chain drawing direction is mirrored based on the direction of the mouse movements.

Templates

MarvinSketch provides several predefined chemical structures, called **templates** or **structure templates.** They are categorized into template groups, like Amino Acids, Polycyclics e.t.c.
The following template groups are available in MarvinSketch by default:

- Generic

Rings
- Amino Acids
- Aromatics
- Bicyclics
- Bridged Polycyclics
- Crown Ethers
- Cycloalkanes
- Heterocycles
- Polycyclics
- Homology Groups
- Alpha D sugars
- Beta D sugars
- Deoxynucleosides
- Flavonoids
- Nucleobases
- Nucleosides
- Organometallics
- Protoalkaloids
- True Alkaloids
- Vitamins
- My Templates

The templates can be accessed via the Advanced Templates Toolbar or through the **Insert > Template** menu item.

How to use Templates:

- Select a template using the Template Library or the Advanced Templates Toolbar area.
- In case the template structure contains any S-groups, the group(s) can be optionally expanded or contracted by pressing the Shift button.
- Place the template structure by left-clicking on the desired location.

The **Template Library Manager** dialog contains buttons that customize template handling.

New substituent (fragment) editing

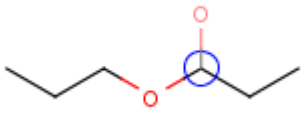
In some cases, you will find it difficult to add new fragments to your molecule file, for example if you already have structures cleaned in 3D. To add a new fragment to the canvas, follow these steps:

1. Choose the  New substituent from the Insert menu.
2. Draw the structure in the new canvas. If you would like to transfer and match it to your original 3D molecule, do a 3D clean on the new fragment (Structure/Clean 3D).
3. Click the  Transfer button in the top left corner to return to the original canvas and place the new fragment.

Sprouting

Atom sprouting:

- Click an atom symbol on the toolbar or in the Periodic Table.
- Place the cursor over the atom where you would like to add the atom.
- Press the Shift key on the keyboard then click the atom. The new atom will be attached to that atom.



Template sprouting: you can add the template connected by a bond formed between the selected non-primary atom and the attachment point of the template. This way adding a substituent will only replace a hydrogen atom on the selected atom, not the atom itself. This feature is limited to the use of symmetrical templates where attaching the template has only one possibility (e.g. as for phenyl).

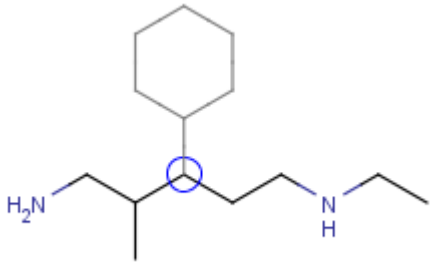
- Select a template from the toolbar or from the Template Library
- Moving the cursor over an atom, a grey colored image will show you the positioning of the template.
- Left-click on the atom will place the template.

To change the connection type (no sprouting):

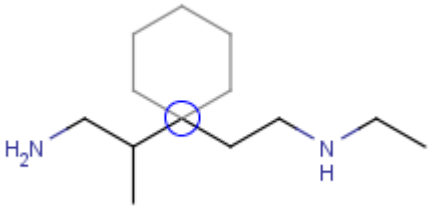
- Select a template from the toolbar or the template library.
- Move the cursor to the canvas and hover over an atom.
- Press the Shift key and while holding it down, click the atom.

In both cases, you can change the bond angle by rotating the template: holding down the left mouse button, move the mouse to rotate the molecule, and release it when desired position is reached.

Adding a cyclohexane template to a secondary carbon atom:



Adding a cyclohexane template to a secondary carbon atom while holding down the Shift key:



Notes:

1. Abbreviated groups will be extended when holding down the Shift key, its attachment is not affected in terms of sprouting.
2. The grey outlined template will not be shown if the creation of a new bond would lead to the valence error of the atom but will be added if you click the atom.

Merging structures

If you would like to form a new structure by combining two already drawn molecules, you have the possibility to merge them in few steps. This starts with defining the merging points in both the template and the substituent molecules (1, 2 or 3 pairs of them). The template molecule' coordinates are not changed, only the substituent is resized, rotated (in three dimensions) and moved to fit the template.

1. Select Assign Atoms from the Structure menu, Directed Merge submenu.
2. Click and drag the arrow from the atom of the substituent to the template molecule. The arrow will be

numbered.

3. Repeat the assigning (the Assign Atoms action is still active, no need to re-select the command) once ore twice to define more merging points.
4. Merge the molecules by selecting the Merge command from the Structure menu, Directed Merge submenu.
5. In case of assigning 1 or 2 atom pairs, the subsituent is selected after the merge and the Rotate in 3D mode is active, and you can rotate the substituent around an axis:

   1 atompair
   - In case of one bond, this bond is the axis;
   - In case two bonds, the axis is the bisector of the angle of these bonds;
   - In case of 3 bonds have to choose the x,y, or z axis, or define the axis by selecting two atoms.

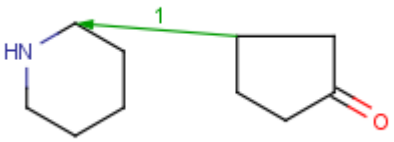
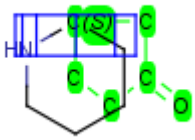
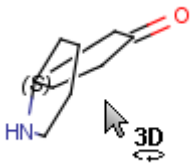
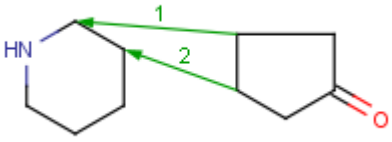
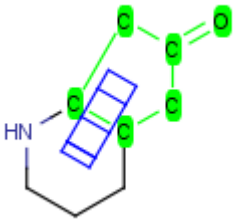
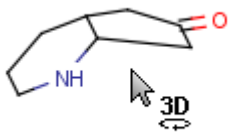
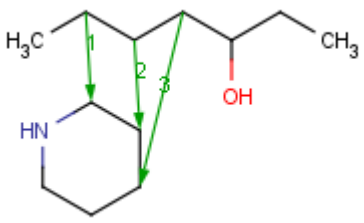
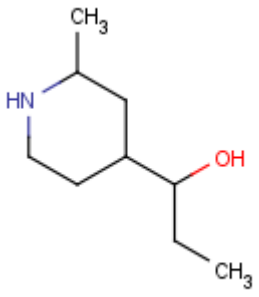
   2 atompairs
   - The rotation axis is defined by the two connection points of the template and the substituent. Now the user can rotate the substituent, and if any atom pairs fall in the merging range after the 3D rotation, they will be merged.

   After the 3D rotation, any atom pair that falls in the merging range are merged. If this second merge happens only on one atom pair, the substituent remains selected, and is subject to a second 3D rotation action, where the rotation axis is defined by the original and the new connection points. Now rotate the substituent around this new axis, and again, if any atom pairs fall in the merging range after the 3D rotation, they will be merged.

   Note: pressing the Shift key on your keyboard offers an alternative rotation axis

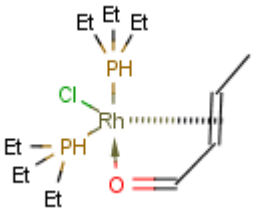
6. To finish merging, click anywhere on the blank canvas.

How to merge structures

	Assigned atoms	Selected for rotation	Merge product
1 atom pair			
2 atom pairs			
3 atom pairs			

Coordination compounds

You can use coordinate bond to represent coordination compounds (ferrocenes, metallocenes). For example:



The coordinate bond type can represent the connection between an atom and a group of atoms. The coordinate bond has two kinds of appearance according to IUPAC recommendation:

- arrow between two atoms,
- dashed line between an atom and a group of atoms.

In the **Edit >Preferences >Bonds** menu item you can change the default line type of coordinate bonds to solid. To draw a bond between two atoms just choose the coordinate bond from the bond list and draw the bond by specifying the required direction. To draw a bond between an atom and a group of atoms you need to create a multi-center attachment point to represent the group of atoms.

To draw a coordinate bond between an atom and a group of atoms

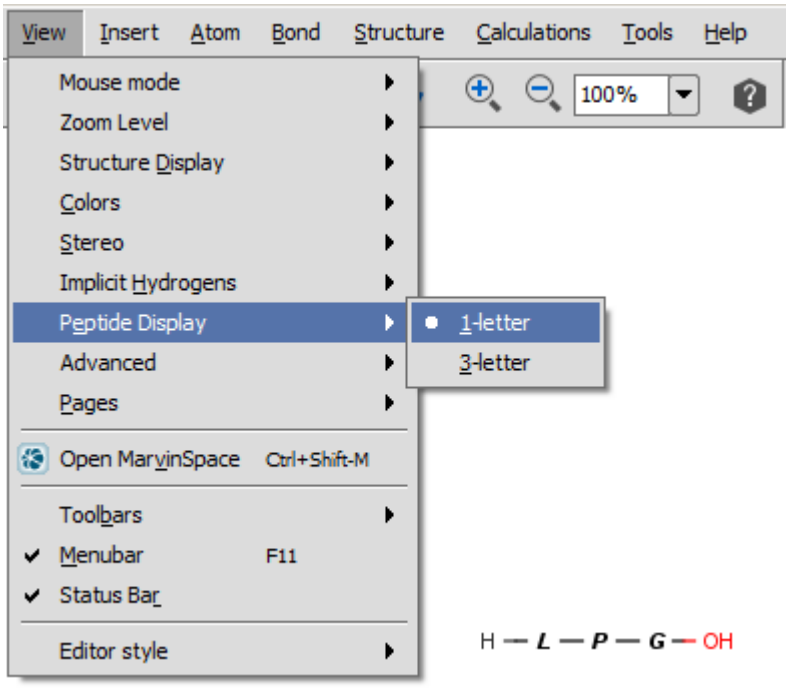
- Select the atoms to be represented at one end of the coordinate bond by a multi-center.
- Choose "Structure>Add>Multi-center" from the main menu or "Add/Multi-center" from the contextual menu. A multi-center represented by a "*" will be added. If you move the cursor to the multi-center the represented atoms are highlighted (blue circle around the atom labels).
- Draw a coordinate bond from the multi-center and edit the other end of the bond if required. The "*" representing the multi-center disappears after bond drawing.
- Repeat steps 2-4 to draw further multi-centers and coordinate bonds if required.

Importing and displaying biomolecules

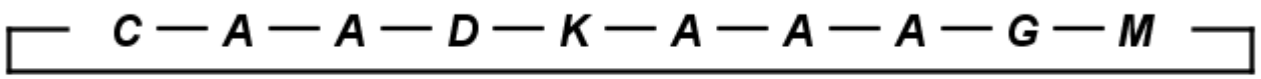
You can import RNA, DNA and peptide sequences from the menu choosing **File > Import As** or through the **Edit > Source** panel.

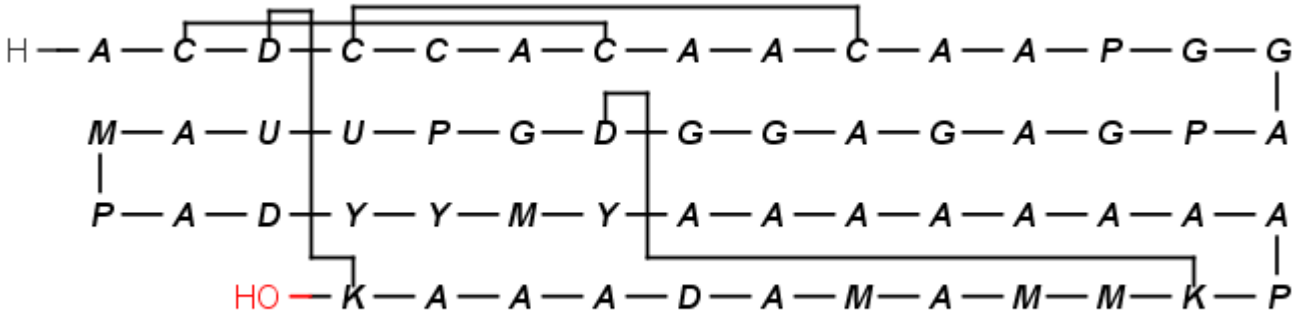
In the second case you have to select the import mode ('Peptide Sequence', 'DNA Sequence', or 'RNA sequence') if it is not possible to decide whether the sequence belongs to a peptide or to a nucleic acid. Peptides can be entered using their 1- or 3-letter amino acid codes (see documentation on peptide import). DNA nucleic acid sequences can be imported in four different formats: ACGT, A-C-G-T, dAdCdGdT or dA-dC-dG-dT. RNA nucleic acid import accepts sequences in two formats: ACGU and A-C-G-U. DNA/RNA sequences are displayed with their 1-letter code on the canvas.

For peptides/proteins MarvinSkecth offers you the possibility to display them as their 1-letter or 3-letter codes selecting the **View > Peptide Display** menu item.

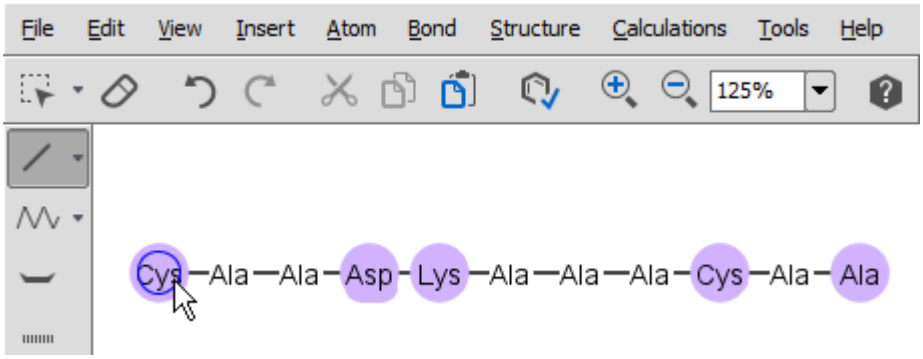


You can easily draw peptide bridges and cycles in MarvinSketch. This way, you can better visualize disulphide bridges, cyclic peptides, and lactame or lactone structures occuring frequently in peptides and proteins.

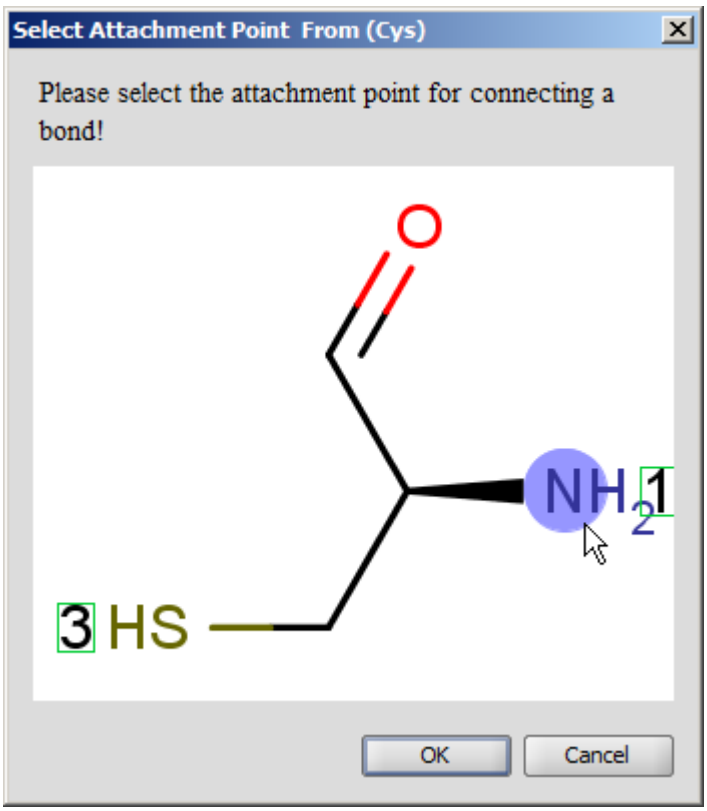




Select single bond tool and start to drag a bond from an amino acid: when you do this, the amino acids which have free attachment point(s) get highlighted. Please do not forget to delete the "H" and "OH" from the terminal amino acid chain if you would like to draw a cycle. Note, you cannot start a bond from an amino acid which does not have at least one free attachement point.



When you release the mouse, the new bond is established. If there is more than one free attachment point on the starting and/or ending amino acid, you have to select the appropriate one from the pop-up dialog.



You can expand an amino acid group selecting 'Expand Groups' from the contextual menu over the group. To expand all groups of the peptide you should select 'Expand Groups' from the contextual menu over the canvas. Nucleotides of a DNA/RNA sequence can also be expanded in the same way.

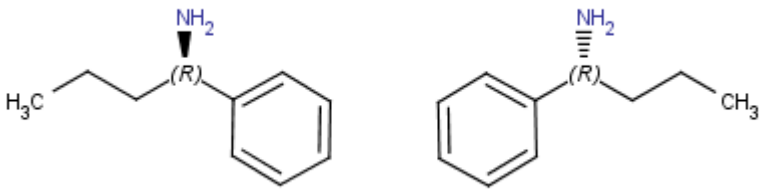
Geometric Transformations of Structures

Geometric transformation functions (**Flip**, **Mirror**, **Invert**) can be used from the **'Edit > Transformation'** main menu on the whole molecule or only on the selected part of the structure.

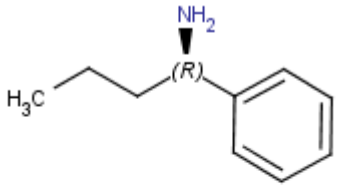
Flip a molecule

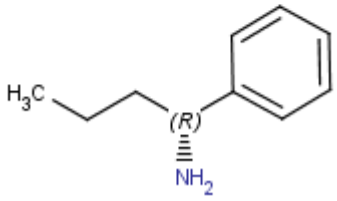
You might need to flip the whole or parts of the structures. These operations are located in the **Edit > Transformation menu**. If no selection is made, the operation will be executed on the whole structure (except for Group Flip). The flip operation is equal to a rotation of 180° around a horizontal or vertical axis in the plane of the drawing.
All flips result in stereocenter retention.

Horizontal flip
(around *y* axis)

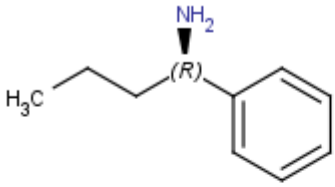


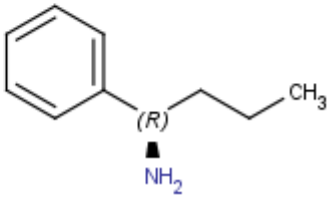
Vertical flip
(around *x* axis)





Rotate 180°
(in canvas plane, around *z* axis)





Horizontal Flip, Vertical Flip, Rotate 180°

Flip a selection:

1. Select part of the structure.
2. Right-click on the structure or go to **Edit > Transformation menu.**
3. Click on the command.

Flip the whole structure without selection:

1. Go to the **Edit > Transformation menu.**
2. Click on the command.

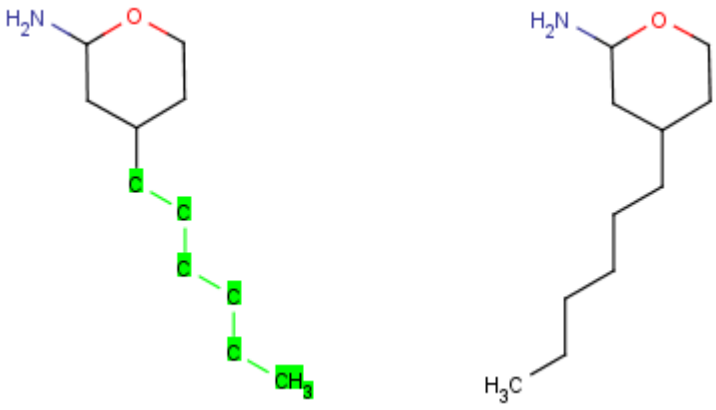
Note: If no structure is selected, the right-click on the canvas will not offer the flip command.

Group Flip

The Group Flip operation can be executed only on a selected structure connected to the rest of the molecule by only one bond (of any type): the selection can not be in the 'middle' of a molecule. The selection is not permitted for disjunctive structures either.

This operation rotates the selected group by 180° around an axis set on the bond connecting the selection to the rest of the molecule. Stereocenters in the molecules are retained, the wedge bond styles change to keep the stereo information.

Group flip

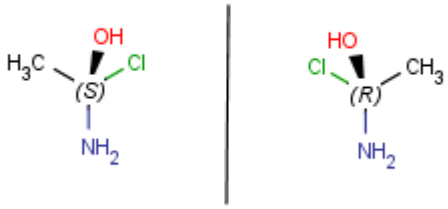


1. Select part of the molecule.
2. Right-click on the canvas and select **Transformation > Group Flip**; or go to the **Edit > Transformation menu.**
3. Select **Flip > Group.**

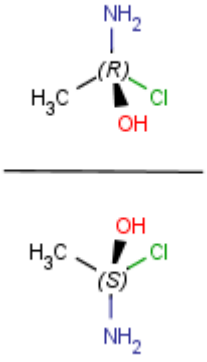
Mirror a molecule

Apart from flipping Marvin is able to produce mirror images of the molecules or parts of. These operations can be found in the **Edit > Transformation menu**. If no selection is made, the operation will be executed on all the structures present in the canvas. Stereocenters will be inversed. Mirroring horizontally means that the theoretical mirror is horizontal and placed perpendicular to the canvas (left-to-right mirroring); the vertical mirroring means the mirror is vertical and perpendicular to the canvas (upside-down mirroring).

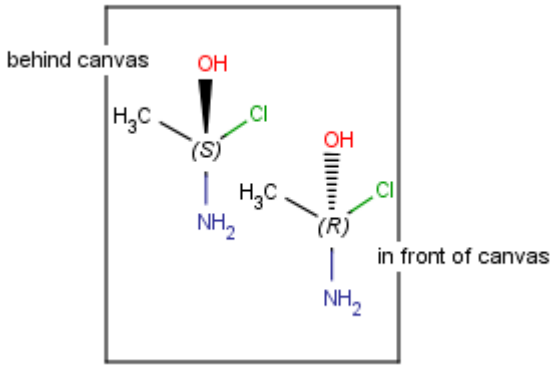
Horizontal mirroring (to *yz* plane)



Vertical mirroring (to *xz* plane)



Mirroring to canvas plane (to *xy* plane)



Mirror a selection:

1. Select part the molecule.
2. Right-click on the canvas or go to the **Edit > Transformation menu.**
3. Click the command.

Mirror the whole structure without selection:

1. Go to the **Edit > Transformation menu.**
2. Click on the command.

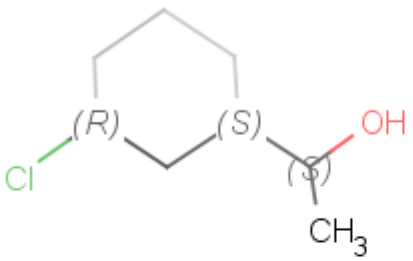
Group Mirror

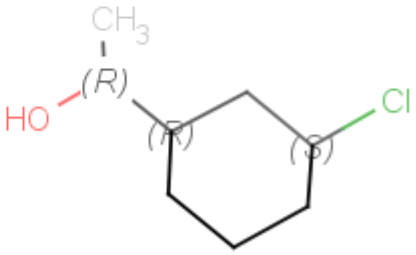
In case of only one connecting bond between the selected and unselected parts of the structure, the Group mirror command is available. The group is mirrored to the plane perpendicular to the plane defined by the two atoms of the above mentioned connecting bond plus a neighboring atom (in the group) that is not collinear with the connecting bond.

Central inversion of a molecule

This feature mirrors all compounds on the canvas or selected fragments in 3D to a selected inversion center. The chirality is changed, all R is inversed to S, and vica versa.

- The inversion center is the geometric center of the selected atoms: if there are more than one selected fragment, then all fragments are inversed separately to their geometric center.
- The inversion center is a selected atom: all fragments are mirrored to the selected atom.





Reactions

How to Draw Reactions

You can place a reaction arrow on the canvas at any time, even on a blank canvas. Only one reaction is allowed per molecule.

1. Select the Insert Reaction Arrow button. You will see the reaction arrow on the tip of the cursor when you move the mouse into the canvas area.
2. Click the location of the tail of the arrow.
3. Drag the mouse and release at the location of the head.

Once you have placed a reaction arrow on the canvas, MarvinSketch considers each part of the molecule in relation to the reaction. All parts of the molecule that are before the arrow are considered reactants. Every molecule after the arrow is a product, and the ones placed along the arrow are considered agents. You can align and/or distribute the objects of the reaction scheme by selecting the relevant option in **Edit** > **Object** menu. The centers of the objects will be considered during the alignment/distribution of objects. **Note** Selected agent fragments and texts are moved together with the arrow while keeping the distance between them.

How to Map Reactions

The arrow tool provides the easiest manual way to map corresponding reactant and product atoms. Select the arrow tool, hold down the left mouse button on a reactant atom, and drag it to the corresponding product atom. The same map number is added to both atoms marking, that they represent the same atom on the two sides of the reaction scheme. Similar tool "Manual Atom Map" can be added by customization. There are also keyboard shortcuts for mapping. Type m8, for example, and click on an atom. Atom map 8 is assigned to that atom.

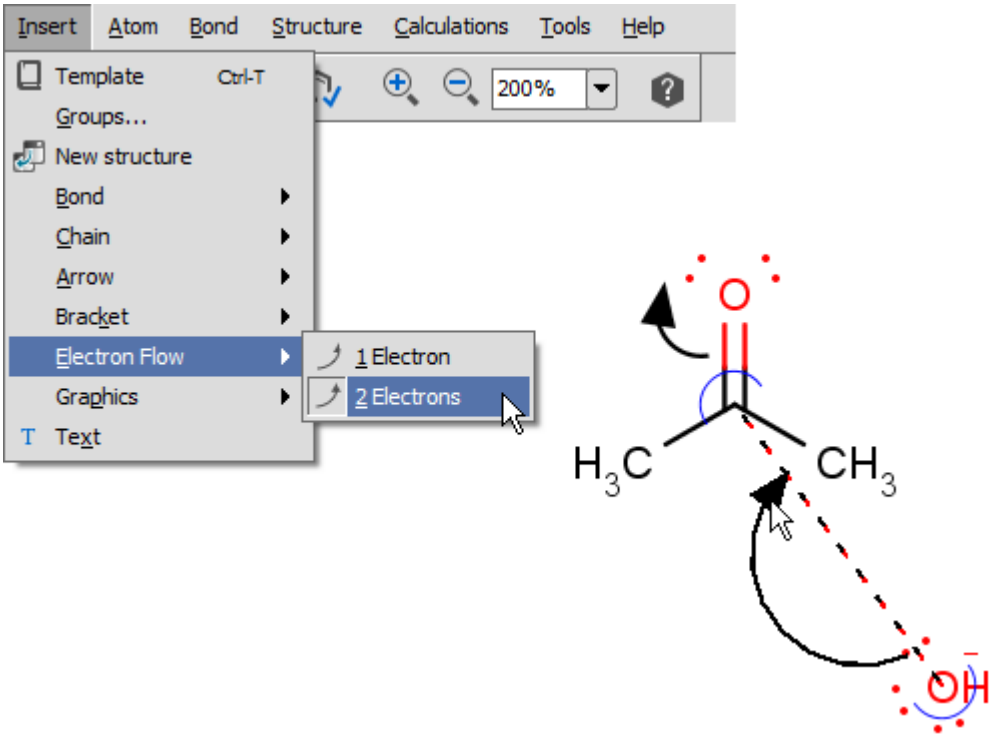
Marvin contains an automapper tool as well (available as Structure > Mapping > Map Atoms) assigning map numbers to all selected atoms of a reaction automatically.

Map numbers of the selected atoms can be removed by the Structure > Mapping > Unmap Atoms menu item, or by typing m0 for the selected atoms.

How to Draw Electron Flow Arrows

Electron flow arrows show the actual direction of motion of the electrons. They can point from an electron or lone pair of an atom or from a bond to another atom or bond or even to an incipient bond (formed after the electron transition).

1. Select the arrow type (single electron flow or electron pair flow). (Menu: **Insert** > **Electron Flow**)
2. Move the cursor over a bond, electron, or lone pair (or over the atom itself if the valence electrons are not displayed around it) of the structure on the canvas, and push the mouse button. (It will be the source of the electron flow.)
3. Select the destination: drag the arrow while holding down the mouse button and release the button over the destination to finalize the electron flow arrow.



See detailes of handling and displaying endpoints here.

Query Structures

There are molecules that cannot be represented by a single structure. Although it is possible to run multiple structure searches in cascade, it is much more efficient to run a search only once using a well designed query structure. This structure often contains query features, possibly including complex conditional expressions for atoms and bonds. For a more detailed description of this please see the Query Guide.

The easiest way to use Query Atoms, different Query Groups and Query Atom Properties is to find them on the Periodic Table's Advanced tab.

Atom Lists and NOT Lists

It is possible to define the type of an atom in a custom atom list. If the type of the corresponding atom in the target molecular structure is a member of the list, it is considered a matching atom. NOT lists can be used to specify atoms to be excluded in the search.

"Atom List" and "NOT List" can be reached from the Periodic Table's Periodic Table dialog.

Custom Properties

Values can be added to the following "Custom Property" types from the Periodic Table's Advanced tab.:

R-group Converts the atom to an R-group with an index of the input "Value". (Only numerical values are allowed, with a maximum number of 32767.) This atom can be used to describe an unknown or unspecified molecule part or to draw an R-group query or a Markush structure.

Alias Converts the Alias value to the atom label. The input of the textbox is displayed as the atom label, but the atom itself does not change.

Pseudo Converts the input of the textbox "Value" to Pseudo atom type. The input of the textbox is displayed as the atom label, but the atom is replaced by an *"Any"* type Query atom.

SMARTS Converts the input of the textbox "Value" to a complex SMARTS query molecule or atom. If the cursor is kept over the canvas during typing, the conversion can be seen on-the-fly.

Value Adds the input of the textbox "Value" to the atom as its "Atom Value" property.

Homology Groups

'Built-in' Homology groups can be found in the 'Special Nodes' section of the Periodic Table's Advanced tab, as a dropdown list, starting with "Alkyl".

More deatils of some other Query features and Homology groups are in the Query Guide.

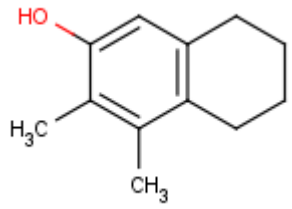
R-group Query

An R-group query describes a set of derivatives in one query structure (substitution variation). It can be drawn the following way: First draw the root structure and place some R atoms either from the Periodic Table dialog window, from the popup menu or by typing a corresponding label such as "R1" on the keyboard. Then draw the variable R-group ligands and select those substituting the R1 atom. If you type "R1" now, the selected groups will be marked with "R1". Additional R-group conditions (Occurrence, RestH, If-then) can be set in the R-logic dialog window available from the **Structure > Attributes** menu.

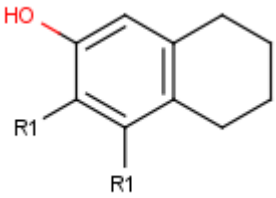
To draw the attachment points for the R-definitions, you can use menu "*Atom > R-group Attachment*" from the menu (or *R-group Attachment* from the popup menu), or alternatively, when you draw the R-definitions and the mouse cursor still shows "R1", clicking on an atom of the definition will toggle the attachment point on that atom. (Please note that divalent R-groups must have two attachment points defined.)

How to draw R-group queries -- Step by step example

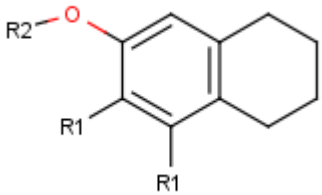
1. Draw the root structure first.



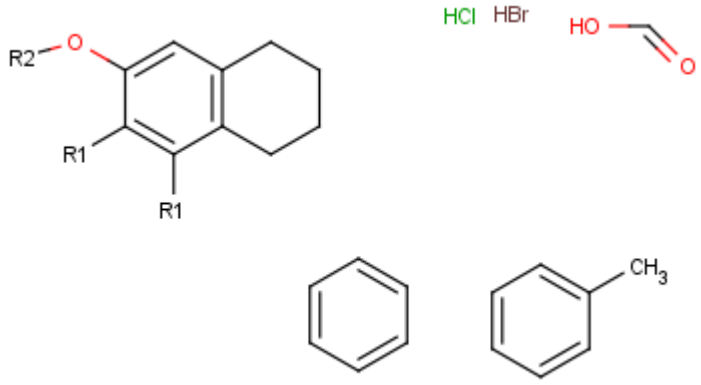
2. Move the cursor to the atom where you would like to place the R-group. (In this example, we place R-groups in place of the terminal carbon atoms.) When the atom is highlighted (blue circle around the atom label), type the shortcut of the required R-group ID (e.g. R1). Alternative solution is selecting the ID from *R-group* sub-menu of the popup menu by pressing right mouse button over the atom.



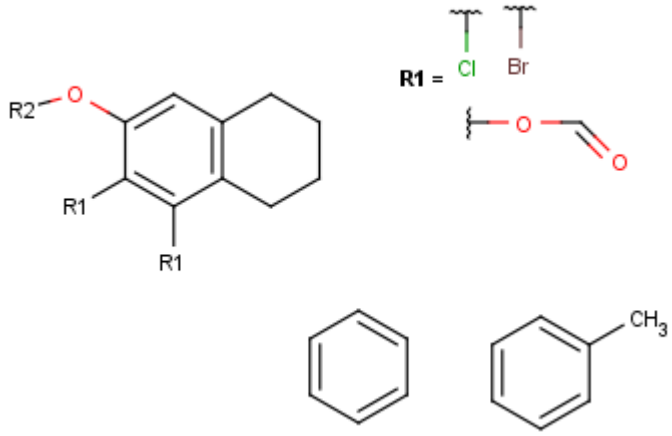
3. Draw an alternative ligand with an R-group connection: Move the cursor to an empty place on the canvas (take care that nothing is selected) then press the shortcut of the next R-group (R2). The "in hand" object changes to the ID of the R-group (R2). (In this example, we add a ligand to terminal oxygen atom.) Click the terminal oxygen, then drag the mouse. You will see that the new bond is displayed and its orientation follows the cursor. Release the mouse button when the bond stands in the right direction.



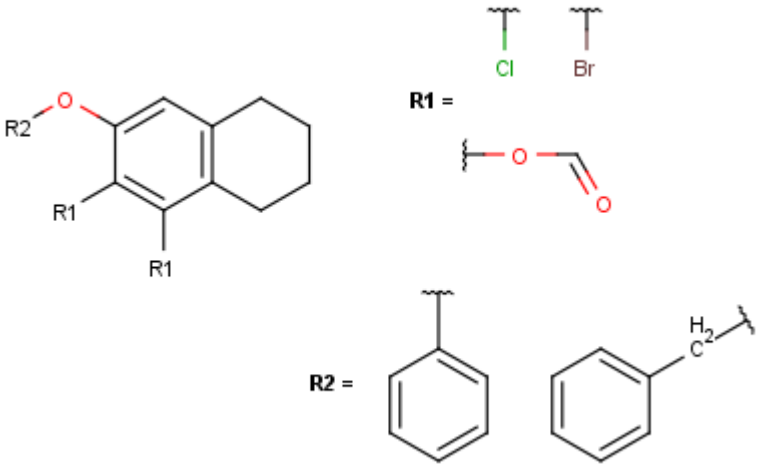
4. Draw new fragments to the canvas (separately from the root structure), which will be the R-group definitions. (In this example, we draw the fragments for the first R-group definition to the right side and the second R-group definition will be placed below the root structure.)



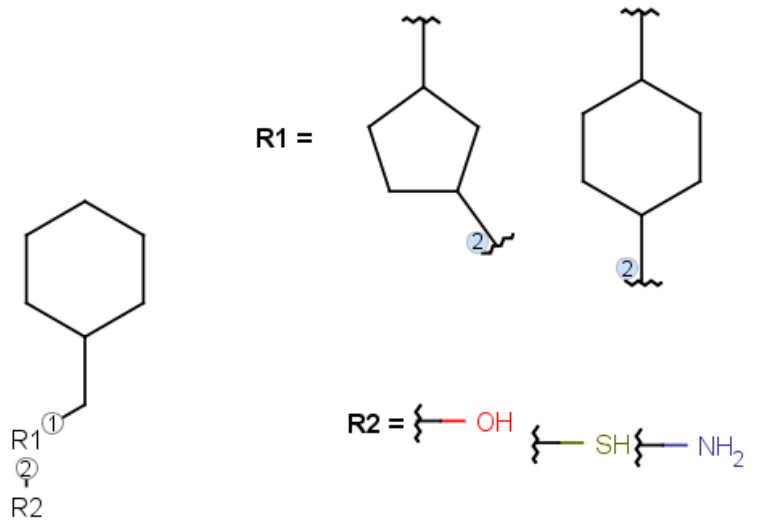
5. Next, define the R-group definitions. To do this, select those fragments that the first R-group should contain (on the right side). After the selection, press the shortcut of the R-group ID (R1). The ID and equal sign (R1=) will display beside the selected set and the "in hand" object will be the R-group ID.
6. Define attachment point to R-group members: Click the left mouse button on atoms where you would like place the attachment points. Repeat this operation on the other definitions of the R-group. (In this example, at the third definition, we select the left oxygen atom for attachment.) Alternatively, you can define R-group attachment points via the popup menu (by selecting *R-group Attachment* option on an atom of an R-group definition).



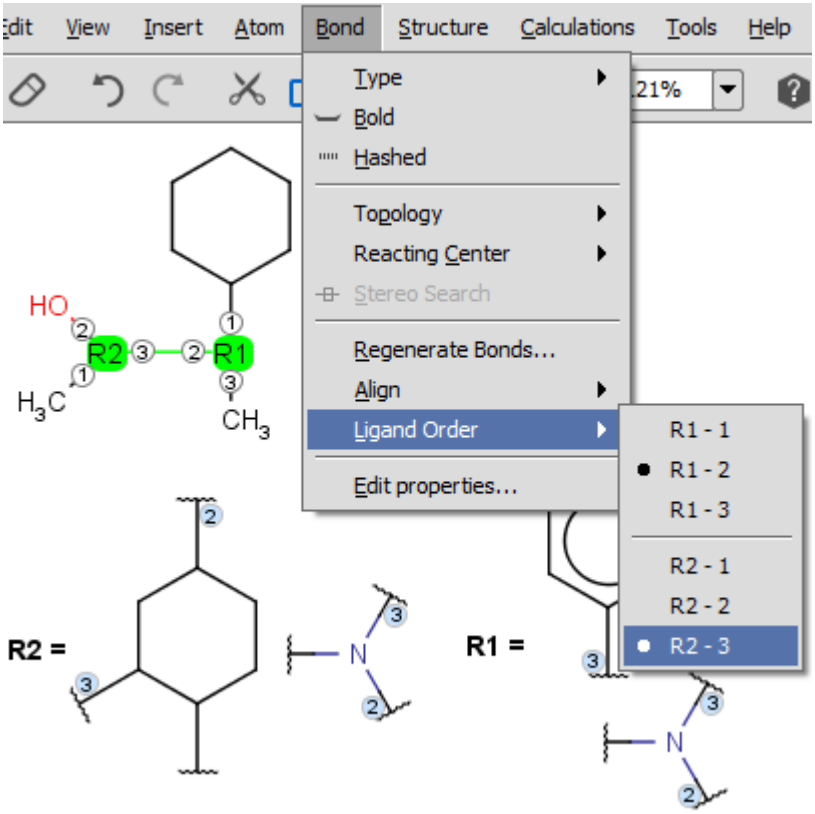
7. Create the second R-group by repeating the last two steps on the two remaining fragments.



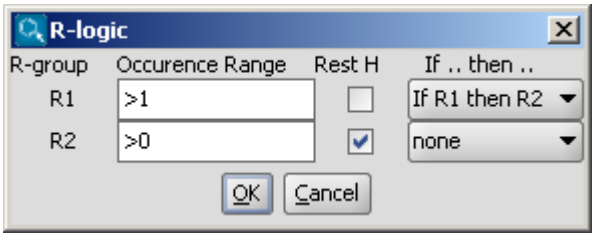
8. In case of one attachment point, the connections are not numbered, only marked by a wavy line on the substituent side.
   In case of more than 1 attachment point, the connections are marked by numbers on the scaffold. Connection points on the substituents are marked with a wavy line, and the order is indicated by numbers (except for the 1st).



If two R-groups are connected by a bond, the ligand order may be changed simply by the Bond > Ligand order command. Simply select the bond in question and select the combination in the menu (also available upon mouseover in the context menu).



9. You can define additional conditions, such as occurrence, rest H and if-then expressions to R-groups in the R-logic dialog window. To do this, select menu option **Structure > Attributes > R-logic**. After setting the conditions in the *R-logic* dialog window, press the *OK* button to apply the changes. R-logic can be visualized by switching on the Display > Misc > R-logic option.



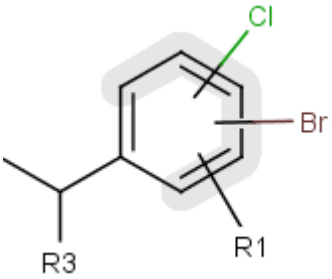
Markush structures

A Markush structure is a description of compound classes by generic notations. They are often used for patent claims and for combinatorial libraries. Link R-groups, link nodes, atom lists, position variation and repeating units

with repetition ranges are commonly used features in the representation of Markush structures.

Position Variation (variable point of attachment)

You can create a variable point of attachment to represent a variable connection point to a group of atoms. The representation is similar to the above mentioned multi-center bonds. For example:

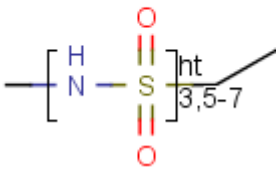


The alternative attachment points are displayed with grey shadow. If you move the cursor to the center (the bond ending in the ring) the represented atoms are highlighted (blue circle around the atom labels). **How to draw Position Variation:**

- Draw the structure that will include the position variation.
- Select the alternative connection point atoms.
- Choose "Structure/Add/Multi-center" from the main menu or "Add/Multi-center" from the contextual menu. A multi-center represented by a "*" will be added. If you move the cursor to the multi-center the represented atoms are highlighted (blue circle around the atom labels).
- Draw a bond from the center and edit the bond if required. The represented atoms are displayed with grey shadow after this step. The "*" representing the multi-center disappears after bond drawing.
- Repeat step 2-4 to draw further variable points if required.

Frequency variation (Repeating unit with repetition ranges)

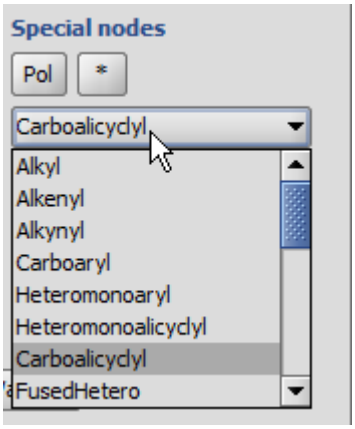
A sequence of ranges to specify the repetition can also be used in a special group called repeating unit with repetition ranges. For example:



Here the repetition range is "3,5-7". The repetition count for the included structure (enclosed by the brackets) can be: 3,5,6 or 7. See Repeating units with repetition ranges for further information on drawing this feature.

Homology groups in a Markush structure

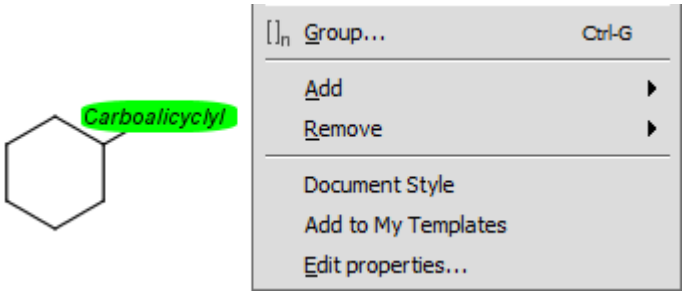
The simplest way is to insert homology groups from the Periodic Table's Advanced tab.



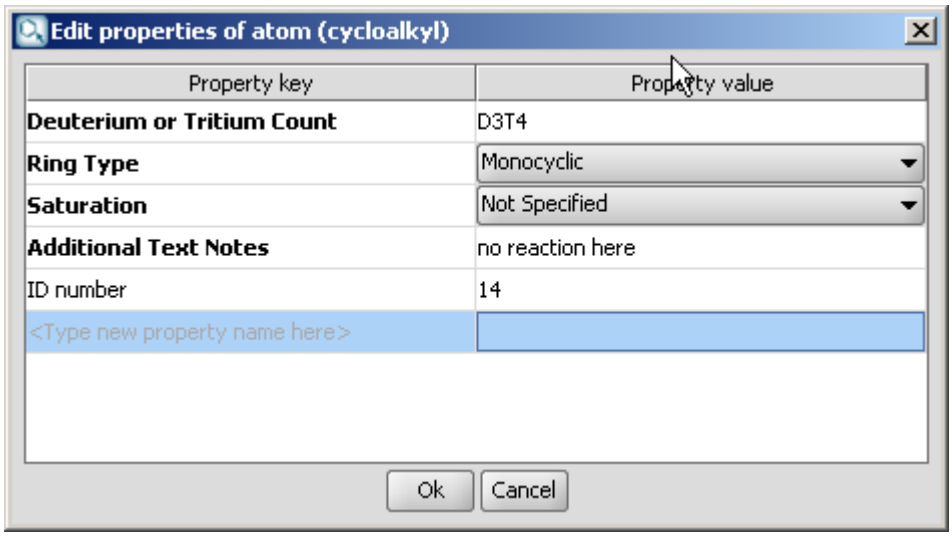
1. Open the Periodic Table (toolbar or from the Atom menu), choose the Advanced tab.
2. In the Special nodes section, choose the homology group from the dropdown list.
3. The homology group stays at the mouse pointer, you can click the atom(s) on the canvas. You don't need to close the Periodic Table to continue drawing.

Editing the homology group properties in MarvinSketch

Select the homology group and right-click. Choose Edit Properties... Set the group properties in the dialog box.



Here is an example of the property dialog window for a cycloalkyl group:



By default, the atom and homology group properties are not shown. You can switch it on by checking the View > Advanced > Atom Properties menu.

How to Create Groups

You can create a group easily from a structure. There are two possibilities:

- Select the molecule or part of the molecule. Click the Create Group button in the toolbar and edit the group properties in the dialog window.
- Click the Create Group button in the toolbar then select parts of the group. Upon releasing the mouse button, the Group dialog pops up.

Command shortcut: Ctrl-G

Edit groups: (since version 5.3) right-click on the group, select Edit group from the contextual menu and the group dialog opens.
Alternatively, select the group atoms and select Edit Group from the structure menu, Group submenu.

Group types: In the dropdown list of the group type only those types are allowed which are enabled for the actual selection in the molecule (to enable all types: go to Edit > Preferences > Structure tab and uncheck the 'Validate S-groups at creation' box.)
Enabling/disabling a group type depends on:

- The number of crossing bonds it would have.

The embedding of groups into each other: several conditions are checked here for the group to be created
- whether it can be embedded into the groups which would contain it,
  e.g. polymer S-groups can not be embedded into multiple S-groups
- whether it can embed all the groups which would be contained by it,
  e.g. structural repeating unit S-groups (SRU) can not embed monomers
- whether it can be embedded directly into the group which would be its direct embedder,
  e.g. component S-groups can be directly embedded only into ordered or unordered mixtures
- whether it can directly embed the groups which would be embedded by it directly,
  e.g. mixtures can directly embed only components.

- Expandable S-groups are not allowed to be embedded into each other.

Since those group types which are allowed only for whole fragments (mixtures, components and monomers) are always extended to whole fragments, thus these types are allowed even if only fragment parts where selected, if they are correct when extended to the whole fragment.
Extension to whole fragment is not allowed if the group type is changed by editing an existing group: in this case mixtures (etc.) are not allowed for fragment parts.

Abbreviated (superatom) groups

Abbreviated groups are used to represent a part of a structure with a text abbreviation.

- **Insert an abbreviated group** into your sketch: type the name of the abbreviation, to complete a longer name, press ENTER or END after typing the first few characters. Typing group abbreviations is case sensitive: *e.g.*, typing either "NO" or "no" both lead to the nitrosyl (NO) functional group, while typing "No" results in the atom symbol of nobelium. If the cursor was placed over an atom, it will be automatically changed to the abbreviated group. If no atom was selected, the abbreviation is placed on the cursor. Click on the canvas to place it. If you would like to ungroup an S-group before placing it to the canvas, press the *SHIFT* button before you release the mouse on the desired location.
- **Create an abbreviated group**: Click the Create Group button in the toolbar then select the group atoms and bonds. Upon releasing the mouse button, the Group dialog window pops up (this dialog window may be opened from the Structure > Group submenu as well). Name the group in the dialog window.

You can retrieve the hidden structure from the text abbreviation with the "Expand" function and hide the structure with the "Contract" function. Manipulation with abbreviated groups is possible with "Expand", "Contract", "Ungroup", and "Remove" from the Group submenu.

A short animation about abbreviated groups: Expand and ungroup abbreviated groups.

Add attachment points to abbreviated groups

After creating the abbreviated group (see previous section), right-click the corresponding atom and choose "Add S-group attachment", or select the atom and use the same option in the Atom menu. The attachment point is marked by a number in a green rectangle. This way, you defined a connection point of this group. (Please note that attachment points can be added only to abbreviated groups, so it is important to define the group first.)
There is no limit to how many attachment points can be added to an abbreviated group; they will be numbered in the order of their creation. Crossing bonds will connect to group atoms through their first free attachment point. Only attachment points not occupied by crossing bonds are marked by numbers in the expanded abbreviated group. Similarly, crossing bonds connect to a contracted abbreviated group through the first free attachment point of the whole group.
Removal of an attachment point works the following way: Select the "Remove S-group attachment" option either from the pop-up menu or from the Atom menu to erase the attachment point with the highest number on the atom in question.
When you defined an abbreviated group, you can add it to the templates. Select the group, right-click and press "Add to My Templates". The template can be inserted by typing its name and clicking on the canvas.

Syntax of the abbreviated group name

Numbers are automatically subscripted unless "\n" is used or at the start of string. Charges (+, -, ++, --, 3+ etc.) are automatically superscripted at end of string or if the following character is a closing parenthesis.

Allowed control sequences in the abbreviated group name:

- \s - subscript
- \S - superscript
- \n - normal mode.

Example: \S13CH4

User-defined abbreviated groups

Besides the default abbreviated groups you can also set up your own user-defined groups or redefine the default ones. Marvin stores its default groups in a formatted .txt file named **default.abbrevgroup** and by adding your own group file you can complement the default. To assemble your own **.abbrevgroup** file you should strictly follow abbreviated groups file format. The newly defined file must be named **user.abbrevgroup** and should be stored in the chemaxon folder of your home directory in your file system. Note that Marvin gives priority to the user-defined abbreviated groups and overrides the default after redefinition.

Multiple groups

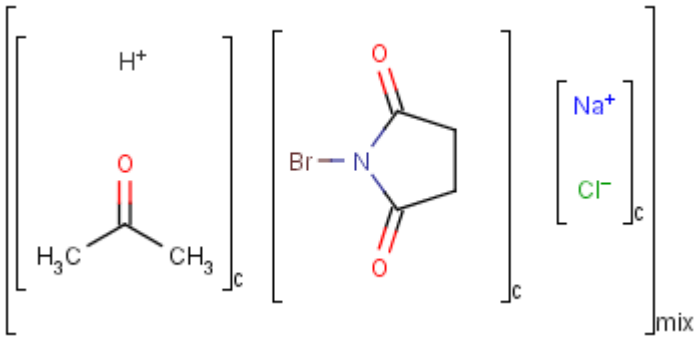
Multiple groups are used to represent a repeating part in a structure with a shorter form. To create a multiple group, click the Group tool on the toolbar, then select the structure involved. Here you can specify a positive repeating count depending on how many times you want the structure to be repeated. You can retrieve the whole structure from the condensed form with the "Expand" function and shorten the structure with the "Contract" function. Manipulation with multiple groups is possible with "Expand", "Contract", "Ungroup", "Edit Group", and "Remove" from the Group submenu.

Components, Unordered Mixtures and Ordered Mixtures

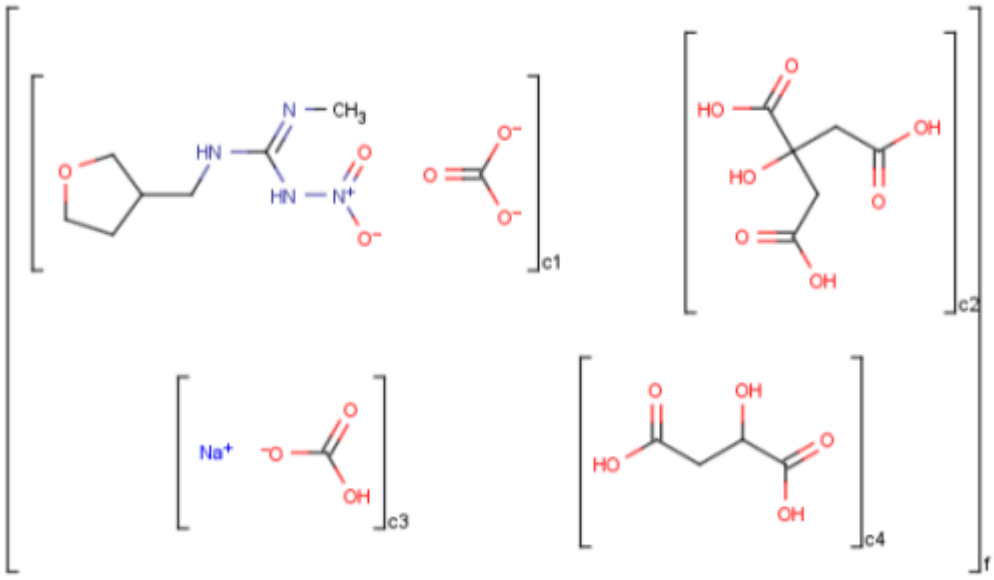
These features can be expressed by brackets (groups) of type component, unordered mixture (also called mixture) and ordered mixture (also called formulation). A component here is a set of atoms contained by a component bracket.

Ordered and unordered mixtures

An unordered mixture (denoted by "mix" at the bottom of the right bracket) consists of several unordered components (denoted by "c" at the bottom of the right bracket). For these types of mixtures, the order of addition during the preparation is not important. Example:



Ordered mixtures, on the other hand contain ordered components, which define the order of addition. Example:



To draw an unordered component

1. Draw the structures that form the mixture.
2. To define a structure as a component in a mixture, click the Group tool on the toolbar, then select the structure.
3. In the "Create Group" dialog window choose "Component (c)" from the "Type" list.
4. The "Order" field should be empty or should contain "none". If the "Order" field already contains a number, just delete it (you can type in "none" as well).
5. Click OK.

To draw an ordered component

1. Draw the structures that form the mixture.
2. To define a structure as a component in a mixture, click the Group tool on the toolbar, then select the structure.
3. In the "Create Group" dialog window choose "Component (c)" from the "Type" list.
4. If this is the first component of the mixture, click the "Order" field and enter "1" in place of "none". If the "Order" field already contains a number Marvin will automatically increment the "Order" field for subsequent components.
5. Click OK.

To draw a mixture

1. Create the components to form the mixture.
2. Click the Group tool on the toolbar, then select the structures.
3. In the "Create Group" dialog window choose the type ("Ordered mixture(f)" or "Unordered mixture(for)") from the "Type" combobox.
4. Click OK.

To change the type of a mixture

1. Hover the mouse over the group.
2. Choose "Edit Group" from the contextual menu (right mouse click on the selected mixture).
3. Change the type of the mixture.
4. Click OK.

To add a new component to a mixture

1. Draw the new component.
2. Drag one part of the bracket and move it to enclose the new component.

To delete a component from a mixture

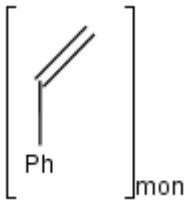
1. Select the component.
2. Press the Delete button on your keyboard or select the Erase tool.

Polymers

The polymer structure consists of structural fragments. These fragments are enclosed by polymer brackets. The meaning of a polymer bracket is that the fragment within the brackets can repeat with itself. The fragment within the bracket is called repeating unit. Polymers can be represented as structure-based or source-based polymers depending on how much structural detail is known.

Source-based representation of polymers

You can use the monomer (mon) or mer (mer) repeating unit types to draw a polymer where only the source-based representation is known. For example:

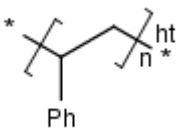


To draw a repeating unit, click the Group tool on the tooolbar, then select the atoms you want to be included.

Structure-based representation of polymers

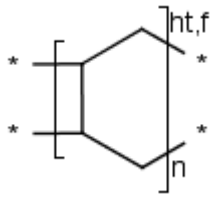
You can use the structural repeating unit type (SRU) to draw a polymer where the structure-based representation is known. Each SRU S-group has two or more dedicated bonds, called crossing bonds, which cross the brackets. The crossing bonds of an SRU show how the repeating units may connect in several ways to each other within the polymer. Depending on the number of crossing bonds and brackets we differentiate the following polymers and connectivities within the polymer:

- Polymers with two crossing bonds. If the polymer has one crossing bond on each bracket of the SRU there are three possibilities for the repeating pattern:
  - head-to-tail
  - head-to-head
  - either/unknown



- Ladder-Type Polymers. Polymers with paired brackets and with two crossing bonds on each bracket are called ladder-type polymers. Here it must be specified how the two crossing bonds on each bracket connect to the corresponding bonds of the adjoining repeating units. Additionally to the head-to-tail, head-to-head connectivity information there is flip information to specify whether the repeating unit flips around the polymer backbone when it connects to the adjoining SRU. These types of information are handled only in case of brackets with exactly two crossing bonds on both side (head and tail side). We differentiate the following polymer connectivities:
  - head-to-tail with no flip
  - head-to-tail with flip
  - head-to-head with no flip
  - head-to-head with flip

- either/unknown



- Polymers with three or more brackets. If the polymer has three or more bonds with a separated bracket on each bond, the polymer always has the either/unknown repeating pattern.

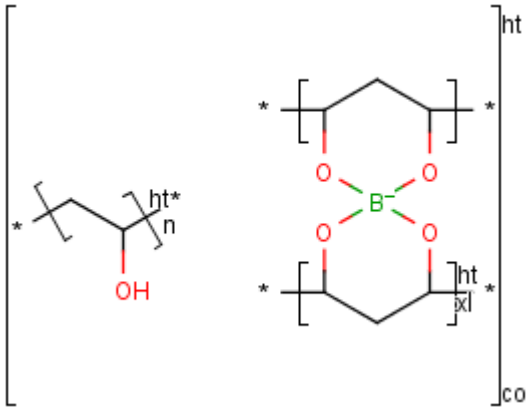
The end groups of polymers are often unknown or unspecified which are represented by star atoms (*). The modified (mod), grafted (grf) and crosslinked (xl) form of a structural repeating unit can be drawn as well.

Copolymers

If the structure consists of more than one repeating unit (mon, mer) or structural repeating unit, Copolymer (co) brackets/groups can be used to represent the structure. Copolymers might contain crossing bonds and star atoms. The following copolymers can be drawn:

- random(ran)
- alternating(alt)
- block with or without junction unit (blk)
- copolymer to represent modified polymers (mod)
- copolymer to represent grafted polymers (grf)
- copolymer to represent cross-linked polymers (xl)

For example:



To draw a simple polymer

1. Draw the structure that forms the polymer.
2. Click the Group tool on the toolbar, and select the structure. Leave out the atoms that should be replaced by "*" (star atoms).
3. In the "Create Group" dialog window choose the appropriate type from the "Type" list.
4. Set the polymer repeat pattern if necessary.
5. Click OK. The star atoms ("*") will be added automatically.

To draw a ladder-type polymer

1. Draw the structure that forms the polymer.
2. Click the Group tool on the toolbar, and select the structure. Leave out the atoms that should be replaced by "*" (star atoms).
3. In the "Create Group" dialog window choose the "SRU polymer" type from the "Type" list.
4. Set the polymer repeat pattern if necessary.
5. Click OK. The star atoms ("*") will be added automatically.
6. To create a bracket that crosses two bonds select the two brackets each crossing a bond and click **Merge**

Brackets in the contextual menu.

To draw a copolymer

1. Create the components to form the copolymer.
2. Click the Group tool on the toolbar then select the components to be included.
3. In the "Create Group" dialog window choose the type ("Copolymer (co)", "Copolymer, alternating (alt)", "Copolymer, block (blk)" or "Copolymer, statistical (stat)") from the "Type" list.
4. Click OK.

To change the type of a polymer

1. Hover the mouse over the group.
2. Choose "Edit Group" from the contextual menu (right mouse click on the selected mixture).
3. Change the type of the polymer.
4. Click OK.

To add a new subpolymer to a copolymer

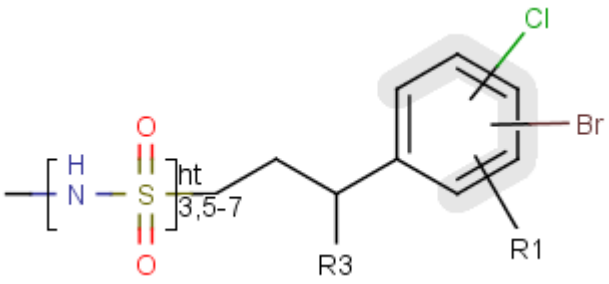
1. Draw the subpolymer to add outside of the bracket.
2. Drag one part of the bracket to include the new subpolymer. The new molecule should be marked with blue circles when you hover the mouse cursor over it.

To delete a subgroup from a copolymer

1. Select the subpolymer to delete.
2. Press the Delete button on your keyboard or with the Erase tool.

Repeating units with repetition ranges

A sequence of ranges to specify the repetition can also be used in a special group called **repeating unit with repetition ranges**. For example:



Here the repetition range is "3,5-7". The repetition count for the included structure can be: 3,5,6 or 7.

Syntax of the repetition ranges

The **repetition ranges** consist of ranges separated by commas. A range can be either a simple non-negative number (e.g. 3) or two non-negative numbers separated by "-" (e.g. 5-7).

To draw a repeating unit with repetition ranges

1. Draw the structure that forms or contains the repeating unit.
2. Click the Group tool on the toolbar, and select the structure.
3. In the "Create Group" dialog window choose the type "Repeating unit with repetition ranges" from the "Type" list.
4. Set the repetition ranges.
5. Click OK.

Charge of the group

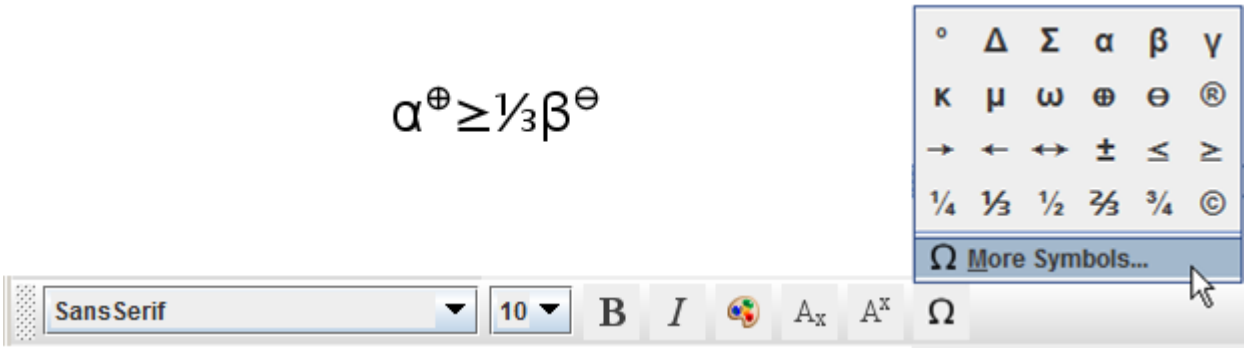
Four types of groups can be assigned a charge sign: generic, component, monomer and mer groups. During group creation, you have the option to display the charge on the charged atom itself or the whole group. In the latter case, the charge will be displayed outside of the bracket on the right. If any additional charges are added (negative or positive) the net charge will be calculated and displayed. The charge-bearing atom can be revealed by pointing the cursor over the group (in select mode). To replace the charge, select the group and go to the Structure menu, Group submenu and click Edit Group (or right-click the selected group, and select Edit Group).

How to Draw Graphic Objects and Text Boxes

To draw a (poly)line, rectangle or text box, use the **Insert** menu or the toolbar (if visible). These objects are depicted in blue color outlines to indicate that any object here does not bear any chemical meaning like reaction arrows or S-group brackets (in black). Point the mouse to the desired position on the canvas, click and hold the left button, move the mouse and release the button. To create a small rectangle or text box click again.

The shape of an object is changeable or resizable by dragging one of its points to do it.

After placing a text box, you can immediately use the keyboard to type a text. Symbols can be inserted directly through the Insert symbol tool, Ω. The tool contains the list of the most commonly used symbols by default. This list will be updated according to your latest selections. Click on the relevant symbol and it will appear in the textbox. If the desired symbol is not on the list, click on More Symbols for the full character list.



To change the contents of a text box, choose **Select** mode, click on the box, then use the keyboard.

You can place a text box with the IUPAC name(s) from the **Structure > Structure to Name > Place IUPAC Name** menu command and it will be automatically inserted under the structure. The name will be updated in real-time.

How to Draw a Link atom

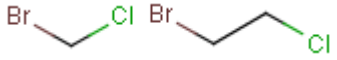
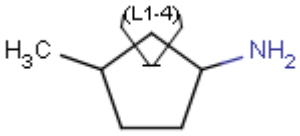
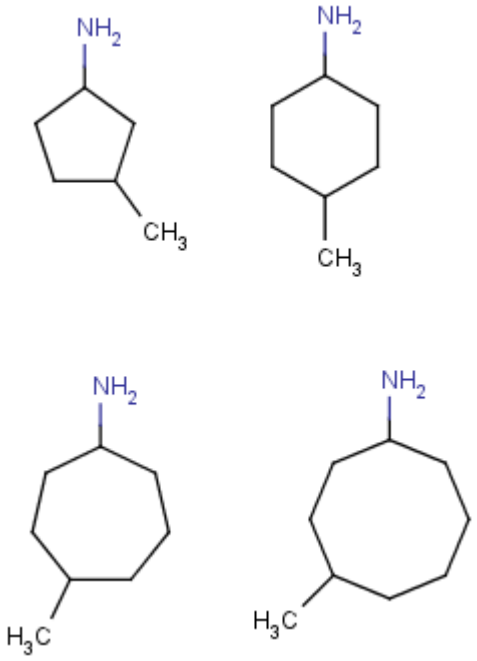
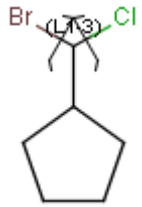
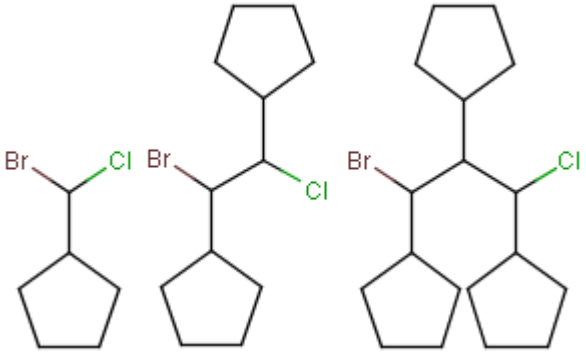
You can draw link atoms using the popup menu in two ways:

1. Right-click on the atom to bring up the popup menu. Select the required repetition number from the "Link node" submenu. Marvin will find out the outer (non-repeating) bonds for you.
2. Select the atom you would like to be the link node and two neighboring bonds for outer (non-repeating) bonds. Right-click anywhere on the canvas to bring up the popup menu. Select the required repetition number from the "Link node" submenu.

Marvin will advise you if it is not possible to create a link node for the specified configuration (for example at ring fusions).

Outer (non-repeating) bonds will be denoted by brackets crossing them, and the repetition numbers will be put on the atom. All portion of the molecule connected to the link atom through non-outer bonds are supposed to

repeat together with the atom. See examples below.

Molecule with link node	Meaning
	
	
	

To edit a link node repetition number or change outer bonds, repeat the drawing steps above. To make a link atom ordinary atom again, select "Off" from the "Link node" submenu.

How to Select a Structure

1. Set Selection mode on by clicking one of the three available Selection buttons.
    1. To select a single atom, click on it.
    2. To select two joined atoms, click on the bond that links them.
    3. To select a rectangular region, choose Rectangle Selection, click at one corner of the desired region and drag the mouse to the opposite corner. While the mouse button is pressed down, a guide will be displayed to aid you.
    4. To select a non-rectangular region, choose Lasso Selection, press the left mouse button to start selecting, and draw the region with your mouse without releasing the mouse button. A blue guide line appears along the selection region. A pink line will connect the start and end points.
    5. To select a fragment
        - double-click on an atom or bond using Rectangle or Lasso selection,
        - or use the Structure Selection button and single-click on an atom or bond.

You can unselect all by clicking an empty area of the canvas.

How to Delete a Structure

Using the Erase button:

1. Set Erase mode on by clicking the **Erase** button.
    1. To erase a single atom or bond, click on it. The deletion of the terminal bond deletes the terminal atom by default. Pressing the Alt button while deleting the bond, the terminal atom is not deleted. To change the default behaviour, go to Edit > Preferences > Bonds tab and choose the desired Terminal Bond Deletion Method.
    2. To erase a rectangular region, click at one corner of the desired region and drag the mouse to the opposite corner. While the mouse button is pressed down, a guide will be displayed to aid you.
    3. To select a non-rectangular region, use the lasso selection function first, then press the Erase button.

Using Selection mode:

1. Select a portion of the structure.
2. Click the **Cut** button or use the DELETE button on your keyboard.

Using pop-up menus:

1. Right click on an atom or bond.
2. Select **Remove** from the pop-up menu.

How to Work with Structures

Visually Editing the Structure

You can edit a molecule using the methods described in How to Draw Structures and How to Delete a Structure.

Editing the Source

You can alter a molecule by directly editing its source in the Edit Source Window. You can view and edit the source in any of the supported file formats. To change format, simply select the desired one from the **View** Menu. If there are multiple molecules on the canvas, checking **View as multiple molecules** in the **View** Menu leads to each molecule appearing in a separate block in the source. This feature works only, if the selected format is able to handle multiple structures.

To reload the molecule described by the text in this window into the MarvinSketch canvas (including any changes you may have made), select **File > Import As**. If the automatic format recognition detects a file format (checking it by a priority list), it will be offered in the Select Import Mode field (Import as Recognized, indicating the file type in brackets). If the structure is associated to a file type of higher priority than your choice, choose the Import As option to set the file format.
For example, you want to create the seryl-asparagine dipeptide: write "SN" in the Source, then select Import. The automatic option detects it as SMILES, but if you select the Import As option, and then the "Peptide Sequence" from the list, it will be imported correctly.
In addition, there are some cases when the automatic recognition cannot detect the file format, even though the entered text is correct (although it is very rare). In this case the Import As Recognized option is disabled and you have to choose the format from the list of the Import As option.

Cleaning

Marvin allows you to clean your molecule in either 2D or 3D. Cleaning will calculate new coordinates for the atoms. Generating conformers and choosing the favored one is also supported. You can initiate cleaning via the **Structure > Clean2D/3D** submenu. For more information on molecule cleaning, please visit this link.

Submenus

- Clean 2D
  - Clean in 2D: cleans the molecule(s) in 2D
  - Hydrogenize Chiral Cneter: adds an explicit hydrogen with a wedge bond to chiral centers which have no terminal atoms as substituents
  - Clean Wedge Bonds: changes wedge bonds for convention display
- Clean 3D
  - Clean in 3D: cleans the molecule(s) in 3D
  - Cleaning Method: choosing from various methods
  - Display Stored Conformers: works only if conformers of the sketched molecule had been generated with the help of the Conformer plugin, choosing the 'Store conformer information in property field' option. See details in the plugin's documentation.

Aromatic Rings

You can toggle the display of rings as aromatic using the **Structure > Aromatization** submenu.

Structure Display Options

There is a wide range of functions related to the display of the molecules. These settings can be found in the View menu and the Preferences dialog window. Additionally, you can move, rotate, and zoom in/out on the structure.

Moving and Rotating

You can move or rotate a selected structure.

First, select the part of the structure you wish to move.

1. **Moving the selection:**
   1. Move the mouse pointer toward the center of the selected structure until a blue rectangle appears. (You can also use the Space key to change between transformation modes.)
   2. Translate the selection by dragging the mouse.
2. **Rotating the selection:**
   1. Move the mouse pointer toward the outline of the molecule until a blue gear appears. (You can also use the Space key to change between transformation modes.)
   2. Rotate the selection by dragging the mouse.
3. **Rotating the selection in 3D:**
   Rotation in 3D of the following structural parts is possible:
   - all compounds on the canvas,
   - selected fragments,
   - selected groups.

   Rotation of all compunds on the canvas in 3D can be accomplished by the View > Mouse mode > Rotate in 3D menu option.
   The axis of the 3D rotation for selected objects can be determined in the Edit > Transform > Rotate in 3D menu (or from the contextual menu) by choosing from the following list:
   - Around an arbitrary axis defined by two atoms: in this case you are asked to select the atoms prior to the rotation.
   - Around x axis: horizontal axis in the plane of the canvas
   - Around y axis: vertical axis in the plane of the canvas
   - Around z axis: axis perpendicular to the plane of the canvas
   - Free 3D rotation: the rotation follows the movement of the mouse (click&drag).
     (Note: 3D rotation mode until version 5.3.x: pressing the Space key 3 times initiates the free 3D rotation.)

Group Rotate: available only for a selected group in a molecule. The connecting bond(s) is recognized between the selected and unselected parts of the structure and selects the rotation axis accordingly.

The rotations are visualized by the fog effect: parts of the molecule behind the canvas are of lighter colour than the parts on the canvas. To see best the 3D view, use white background (View > Colors > White Background).

4. **Customized tool: 3D plane:**
    1. Select 3 atoms in the molecule.
    2. Click the 3D Plane button or select Edit > Transformation > 3D Plane. 

The selected 3 atoms will lie in the plane of the canvas. The coordinates are changed, not only the view of the structure.

- Note: currently 3D coordinates of brackets (e.g. monomer, component type groups) are not correctly updated when rotating the molecule in 3D mode. Avoid when possible.

Scaling

Set the magnification of the molecule on the canvas by the Zoom buttons. If you have a mouse with a wheel, hold down the Ctrl key, and then scroll the wheel to zoom in or out. When a molecule is loaded into the sketcher, it is scaled automatically to fit the window.

Individual objects (bonds, reaction arrows, graphical objects, text boxes) or sets of objects can be scaled, too. Selecting these objects, corners of a bounding rectangle will appear. Dragging one of these corners, the selection will be scaled proportionally. In case of bond scaling, the percentage of the current bond length relative to the default value will be visible. The same result can be achieved by opening the **Format...** dialog either through the **File > Document Style** option or from the pop-up menu.

Molecule Format

You can set the display format for the molecule and screen resolution using the **View > Structure Display** submenu. Available molecule formats are **Wireframe, Wireframe with Knobs, Sticks, Ball and Stick,** and **Spacefill**. You can set the resolution to low or high via the **Quality** submenu.

Colors

The **View >Colors** submenu allows you to specify the color scheme of the molecules. The available options are:

- Monochrome
- CPK
- Shapely - based on RasMol's shapely color scheme for nucleic and amino acids
- Group - based on PDB residue numbers
- Atom Set

Implicit/Explicit Hydrogens

Marvin has a number of options for the display of implicit and explicit hydrogens. Because Marvin is chemically intelligent, it will automatically add hydrogens as necessary within the structure. Generally, these will be implicit and displayed based on the options set in the **View** menu.

To view all hydrogens explicitly, displayed as atoms with bonds to neighbors, chose **Structure > Add > Add Explicit Hydrogens**. The **Structure > Remove > Remove Explicit Hydrogens** will return to the previous display mode.

To view implicit hydrogens by symbol, use the **View > Implicit Hydrogens** menu group. This option is disabled in Spacefill and Ball & Stick display modes.

Displaying the label of carbon atoms

Displaying the label of carbon atoms in structures is possible the following way:

- Always - Always show the atom labels of carbon atoms.
- Never - Never show the atom labels of carbon atoms.
- At straight angles and at impl. Hs - Show the atom labels of carbon atoms at straight angles and at implicit Hydrogens.

This option can be set in the **Display** tab of the **Edit > Preferences** box.

Error Highlighting

Marvin can not automatically correct all valence errors or any reaction errors. Instead, these errors are highlighted and you may make the appropriate corrections yourself. This option can be enabled and disabled through the **Edit > Preferences** box.

Saving Display Options

Many of the display settings in Marvin are saved and reloaded the next time you start the program. Background color, molecule color scheme, and hydrogen visibility can be set from the **View menu** and will be saved automatically when you exit the program. Other options, including look & feel, error highlighting, and object visibility can be set using the **Preferences** dialog window from the **Edit menu**.

Launching Other Windows

2D and 3D Viewer Windows

Choosing **View >Open 2D Viewer** or **Open 3D Viewer** launches a MarvinView window containing the current molecule of MarvinSketch.

How to customize structure drawing styles

More advanced display format can be obtained for the molecule by applying format styles. Format styles in Marvin include the setting of the following attributes:

- type of atom font,
- size of atom font,
- color of atoms,
- thickness of bonds,
- color of bonds,
- length of bonds.

All these options can be collectively set using styles. To load or define styles use the **File > Document Style** menu. This menu brings up the "Format of the current document" dialog in which atom and bond format options can be specified. The original attributes for atoms and bonds can be restored by using the **Reset** functions of the dialog at any time.

When loading a molecule all atoms/bonds belong to the default atom/bond set if no styles were applied previously. After selecting an atom/bond set and applying a style for it, the selected atoms/bonds are removed from the default atom/bond set and a new set is created from the atoms/bonds with new style. All the atoms/bonds, whose style were not yet modified by selection and applying a style on them, still belong to the default atom/bond set.

Your changes might be applied for a set of atoms/bonds:

- for the selected atom/bond set,

- for the default atom/bond set,
- for all the atoms/bonds.

The top three radio buttons specify the target of the format settings being edited in the dialog. The "Apply changes for all the atoms/bonds" option allows loading of predefined styles or creation of custom styles using the **Load Style** and **Save Style** buttons.

Loading a style

After pressing the **Load Style** button, you can load a style from a combo box or browse amongst the previously defined style files. The chosen style will be loaded into the "Structure Drawing Properties" in the "Format of the current document" dialog.

Saving a style

Set the "Structure Drawing Properties" you wish to save and press the **Save Style** button to get to the "Save" dialog where you can enter the name of the style file and save the style. All your own saved files will be stored under the chemaxon/styles/ directory of your home directory and will be added to the combobox items. A new style file can be added to the chemaxon/marvin/styles directory under the Marvin installation directory. This new style file has to be listed in file chemaxon/marvin/styles/styleFileList.properties. The new style file will be copied to the chemaxon/styles/ library in your home directory and appear in the combobox of the "Loading of a journal style" dialog. (Existing style files will not be overwritten.)

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http://www.chemaxon.com/marvin

File Formats in Marvin

Molecule file conversion with the MolConverter program

Cut/Copy/Paste and Drag & Drop Functionality

The cut, copy, and paste operations work in the bean and application versions of Marvin, and also in the applets. However, because of security reasons, the untrusted (unsigned) applets perform these operations using a local clipboard inside the JVM process. The non-applet versions of Marvin and the signed Marvin applets are allowed to use the system clipboard.

Where available?

	Marvin unsigned applets	Marvin signed applets[1]	Marvin Beans and applications
Cut/Copy/Paste	inside Marvin	yes	yes
Drag & Drop	no	yes[2]	yes

1: You can find more info about signed Marvin applets in the following documents: Browser compatibility of Marvin Applets, Signed applets

2: Drag & Drop works only when the sketcher is in its own window. When the applet is in the browser window, drop events are received by the browser instead of the applet.

Copy, Copy As..., Copy as Smiles

Marvin has three commands to place objects on the clipboard: `Copy`, `Copy As...` and `Copy as Smiles`.

- Using the **Copy** command, the structure is copied to the clipboard in a couple of formats. The molecule always will be there in **mrv**, **MDL Molfile** and **DayLight SMILES** formats. The other formats (like *Plain Text* or *Bitmap Image*) are optional. See the table in the Clipboard formats section about supported options and default settings.
- Using the **Copy As...** command, a dialog will display to select in which format you would like to place the molecule to the clipboard.
- Using the **Copy as Smiles** command, the Smiles string of the structure is copied to the clipboard in `String` and `Plain Text` formats.

  *Note:*Any file format of Marvin can be copied to the clipboard as a `string` or as `plain text`. From the `Edit` menu choose `Source` then `Edit/Copy` to place the desired format on the clipboard as plain text.?

Clipboard formats

Marvin can place more than one clipboard object on the clipboard, each represents the same molecule in different format. Copy from Marvin supports the following representations:

- **Marvin Document (mrv)**: Marvin's own format. Only Marvin can paste it.
- **MDL Molfile**: a popular molecule description format. A lot of chemical drawing tool can paste it like Marvin, ChemDraw, etc.
- **Daylight SMILES**: wide range molecule format. Several chemical editor can paste it. In a few editor, SMILES can not be pasted directly. E.g. ChemDraw uses the "Paste Special/SMILES" option to copy SMILES from the clipboard.
- **Daylight SMARTS**: a chemical format for specifying substructural patterns in molecules. Compared to SMILES, SMARTS is a more general notation thanks to its use of extended sets of atomic and bond symbols and logical operators, which make SMARTS a useful tool in substructure searching.
- **Plain Text (molecule source)**: To be able to copy the molecule source into text editors or into other application that do not support chemical formats.
- **Bitmap Image**: To paste molecule image into presentations or into documents.
- **Vector Graphical Image (EMF)**: The vector graphics is scalable unlike bitmap image. It can be pasted into MS-Office documents or into other applications that support Enhanced MetaFile format.

OLE object: To copy a Marvin OLE object into MS-Office. This format is available under Windows. To be able to paste it into an MS-Office document, marvinOLEServer.exe registration is required. (Marvin installer does it automatically or you can register it manually in Marvin applications through the *Edit/Preferences/OLEServer* menu.) You can read more about OLE support in Marvin OLE User's Guide.

- **Portable document format (PDF)** which contains vector graphical image. It is the default format in MacOSX.

A couple of formats are not available on a few platforms.

Setting copy format options

You can also apply or deny the accessibility of one or more copy formats. You can set it by the following ways:

- On the **Copy** panel of the **Preferences** dialog in the **Edit** menu.
- As an applet parameter: copyOpts
- From the Marvin Beans API: UserSettings.setCopyOpts(String)

Format	Windows	Mac OS X	Linux
Marvin Document (mrv)	+D	-	+D
MDL Molfile	+D	-	+D
Daylight SMILES	+D	-	+D
Plain Text (molecule source)	+	+	+D
Bitmap Image	+	+	+D
Vector Graphical Image (EMF)	+D	-	-
OLE object	+D	-	-

+ supported
- not supported
D selected as default

When the **content of the clipboard** is pasted into an application (and it is available in more than one format), the application retrieves data in the most descriptive format. Most versions of Microsoft Office prefer pasting **image** instead of **text** if the content of the clipboard is available in both formats. But there are a few ones that paste text as default. In that case, you should use "Paste As Special" option in MS-Office to paste it as image but it can be unconfortable to someone. The workaround can be the restriction of the text copy from Marvin. That is the reason why text copy is disabled in the default settings of Marvin (on a couple of platforms).
In that case, we recommend **Copy As...** or **Copy as SMILES** to paste text into MS-Word and in other editors. Another solution can be to change the default options of the **Copy** command (see above how to do it).

If we compare **Bitmap** and **Vector Graphical Image** formats, the situation is the same as in the previous case (text vs. image). Most of the applications prefer bitmap image although they can accept vector graphical images as an Enhanced MetaFile (EMF), like MS-Word. Since vector graphics are scalable unlike bitmap images, we have chosen EMF as default from image formats (where it is supported).

Data transfer between Marvin and other chemical drawing tools

	Windows[1]	Macintosh OS X[4]
ISISDraw[2]	Copy & Paste	Copy & Paste
ChemDraw	Copy & Paste	Copy & Paste
ChemDraw Plugin	Copy & Paste	Paste

Copy: copy a structure from the application into Marvin
Paste: copy a structure from Marvin into the application

1: On windows in Java 1.2-1.3.1, the <Java home directory>/jre/lib/flavormap.properties file must be edited: `MDLCT=chemical/x-mdl-Molfile`

2: In case of ISISDraw the following option must be checked: *Option -> Settings -> General -> Copy Mol/Rxnfile to the Clipboard*

3: *Copy as SMILES* works

4: In OS X, since Java 1.4, data transfer in chemical formats does not work. In that case, molecule can be pasted only as image or text into chemical drawing tools. Copy from an application to Marvin works if the application can place data as Plain Text to the clipboard.

Data transfer between Marvin and other applications

Marvin can paste SMILES strings, MDL MolFiles, etc. from a text editor as molecules.

X Window System: most text editors (xedit, emacs, gvim, etc.) do not transfer data to the X clipboard, so Marvin is unable to communicate with them. Copy & Paste works with the following editors and other programs:

- **GNOME programs**: gedit, gnotepad+ (gnp), gxedit, etc.
- **Motif programs**: asWedit, nedit, Netscape, etc.

Note: With the xclipboard program, you can test whether your favorite editor uses the X clipboard or not.

Chemical Features of MarvinSketch

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Valence Check

MarvinSketch does not automatically correct valence errors. Instead, they are highlighted by a red underline and you may make the appropriate corrections. This option can be turned on or off using the **Edit> Preferences** box.

Structure Checker

MarvinSketch offers a structure checking addon that gives warning for specific features or errors in the molecule. Single molecules can be checked in MarvinSketch, batch usage is available via command line or API (with license). Read more about Structure Checker.

Charges

In MarvinSketch, the charge of an atom is initially set to be neutral. As bonds are added or removed, MarvinSketch adjusts the number of implicit hydrogens to let the charge remain neutral. You may change the charge of any atom using the 'Atom' popup menu. The number of implicit hydrogens will be adjusted, if possible, to accommodate the new charge. MarvinSketch will then perform a valence check and highlight the atom if an error is found. Optionally, it is possible to display the charge symbols in circles. To set this option, go to the Display tab of the **Preferences** dialog located in the **Edit** menu. Here, you can also change the font type/size of the circled charge symbols.

Working with Radicals

MarvinSketch allows you to specify that an atom in the molecule is a radical. This functionality is available via the 'Atom' popup menu.

To change an atom into a radical, right-click on it to access the 'Atom' popup menu. Select the type of radical from the **Radicals** submenu. A radical symbol will appear next to the atom and a valence check will be run with errors highlighted.

Isotopes

MarvinSketch allows you to change an atom into one of its isotopes using the 'Atom' popup menu or selecting the atom and choosing **Atom>Isotope** from the Menu Bar.

There is the possibility to extend the isotope list with custom items. Technical details.

Stereochemistry

MarvinSketch provides enhanced stereochemical representations. Using the 'Atom' menu or 'Atom' popup menu, you can set the configuration of each chirality center in a molecule. The absolute configuration of a chiral molecule can also be defined by using Structure Menu. To see R/S labels in the structure, set the Stereo options in 'View' menu.

You can find more info about the scientific background of stereochemistry in MarvinSketch.

E/Z Feature

By choosing **View > Stereo > E/Z Labels** , you can toggle the display of absolute double bond stereoconfiguration labels. Bonds known to have an (E) or (Z) configuration will be marked as such.

Reactions

MarvinSketch allows you to draw reactions in your molecule by placing a reaction arrow. You can place the reaction arrow in any position, pointing in any direction. The structures before the arrow will be considered Reactants, structures along the arrow Agents, and structures after the arrow as Products.

Mapping

MarvinSketch allows you to set a map label on any atom in the molecule. Map labels are useful because they remain constant, unlike atom indexes, which can change as the molecule is altered. Atom mapping can be very useful when drawing reactions. It allows you to specify that specific reactant atoms will become specific product atoms. You can assign the same free map number to both of these atoms by pressing the 'Reaction' Button on the toolbar then drawing the arrow from the first atom to the second one. You can also select a map number for an atom from the 'Atom' popup menu or use the shortcuts M1, M2, ... to assign map labels, M0 to remove map labels, and M= or M+ to assign unique map numbers.
Alternatively, you can use the built-in automapper tool of Marvin, available from the **Structure >Mapping > Map Atoms** menu or from the 'Selection' popup menu, to assign map numbers to atoms in a reaction automatically.

Abbreviated groups (Superatom group)

MarvinSketch has a rich collection of features related to abbreviated groups.

Predefined Abbreviated Groups

A number of predefined abbreviated groups are available in MarvinSketch. The complete set is listed in the **Groups** menu. These groups are also available as shortcuts.
Their usage is described in the Basic MarvinSketch page.
The rotation of the molecule might change the groups' writing order, thus retaining the chemically correct connectivity. Read a detailed description of this feature.

User-Defined Abbreviated Groups

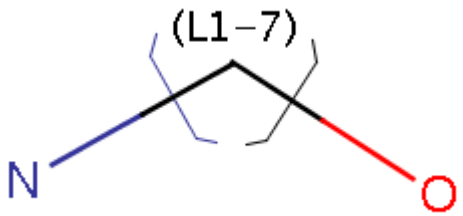
You can easily create new groups that you often use. Select the structure and give it a name (*Superatom (abbreviation)* in **Structure > Groups > Create Group**) and if needed, define an attachment point. Details.

S-groups as My Templates

User-defined groups are, by default, session-only. To retain an abbreviated group for future use, add it to **My Templates**. This will also make the group available in the **Groups** menu or as a shortcut.

Link Nodes

Link nodes enable specifying query structures containing rings or chains of variable size. In the following example, the number of carbons can be between 1 and 7:



Working with Groups

Group manipulation functions are available through the **Structure > Group** submenu and by right-clicking on an existing group.
Choosing **Contract** from the context menu or **Structure > Group > Contract Group** from the main menu contracts one group to its abbreviation if there is one group selected, otherwise contracts all groups in the molecule.
Choosing **Expand Group** from the context menu or **Structure > Group > Expand Group** from the main menu displays the full structure instead of a contracted group if there is one group selected, otherwise expands all

groups in the molecule.
Selecting **Ungroup** will remove all abbreviated groups from the molecule. The structures will remain, but will no longer be associated with their abbreviations. You will be unable to Expand/Contract these structures.
To add or remove an Attachment Point, right-click on an atom within the group and select the **S-group attachment** icon.

Query features

The JChem Query Guide provides more detailed information on how to use JChem's query functionality. The following are some of the query building features available in MarvinSketch.

R-groups

MarvinSketch allows you to specify R-groups within your molecule. An R-group is a variable representing a user-defined list of structures. These R-group definitions can be applied in R-group queries.
Using R-groups in a query structure can allow you to quickly search for a wide range of substructure hits using only a single query.

You can set or change the R-group label of a molecule node from the 'Atom' popup menu or by typing the corresponding R-group label on the keyboard.
To define the set of structures that are represented by an R-group label, select the structures you wish to include. Then, select the corresponding label from the **Periodic Table** or use one of type the R-group label on the keyboard. Set additional Occurrence, RestH and If-then conditions for the query in the R-logic dialog available from the Edit/Attributes menu.

Atom List

MarvinSketch allows you to add Atom List query atoms to your molecule. An Atom List is a user-defined list of elements included in a query structure, any of which will produce a hit if found in the target.

You can add Atom Lists to your molecule through the **Periodic Table**. To add an Atom List to the molecule, select the **Atom List** button, then select the elements you wish to include in the list. Move the mouse into the canvas and click to add a Query atom representing this atom list.

You can create the preferred Atom List without opening the **Periodic Table**. Move your mouse over the canvas and start typing the chemical symbols you wish to add to the Atom List. The entries of the Atom List must be separated by commas (e.g., au,pt,ag). You can use Backspace to delete errors. The items of the Atom List appear on the upper left corner of the canvas and concurrently at the tip of the pointer (e.g., L[Au,Pt,Ag]). Click on the query atom you want to add this Atom List.

You can move your mouse over the appropriate atom of a molecule or make selections on one or multiple atoms of the molecule before creating the Atom List as a different manner. When you start typing chemical symbols separated by commas, the Atom List adds directly to the selected atoms.

NOT List

A NOT List is a query atom that allows you to define a list of elements that should not be included in the target structure. If an atom within the query structure is set as a NOT List, then the atom in the same position within the target structure can be any atom that is not on the list to produce a hit.
To add a NOT List to the molecule, select the **Not List** button in the **Periodic Table**, then select the elements you wish to include in the list. Move the mouse into the canvas and click to add a query atom representing this Not List.

You can create Not Lists without opening the **Periodic Table**. Move your mouse over an empty space of the canvas and type an exclamation mark first, then start typing the chemical symbols you wish to add to the Not List. The entries of the Not List must be separated by commas (e.g., !au,pt,ag). You can use Backspace to delete errors. The items of the Not List appear on the upper left corner of the canvas and concurrently at the tip of the

pointer (e.g., ~L![Au,Pt,Ag]). Click on the query atom you want to add this Not List.

You can move your mouse over the appropriate atom of a molecule or make selections on one or multiple atoms of the molecule before creating the Not List as a different manner. Start with an exclamation mark and then type the chemical symbols separated by commas. The Not List adds directly to the selected atoms.

Generic Query Atoms

MarvinSketch supports the following types of Generic Query Atoms:

Name	Description
A	Any (any atom except hydrogen)
AH	Any atom, including hydrogen
Q	Hetero (any atom except hydrogen and carbon)
QH	Hetero atom or hydrogen (any atom except carbon)
M	Metal (contains alkali metals, alkaline earth metals, transition metals, actinides, lanthanides, poor(basic) metals, Ge, Sb and Po)
MH	Metal or hydrogen
X	Halogen (F,Cl,Br or I)
XH	Halogen or hydrogen

Generic Query Atoms can be added to a query structure to include a wide range of elements. For a more detailed description of this please see the Query Guide.

To add a Generic Query Atom to the molecule, select one of the Generic Query Atom types from the **Periodic Table** and place it on the canvas with the mouse.

Atom Properties

Atom properties: various atom properties can be added to an atom in the drawing. The property key and the value is free to set by the user in the Edit properties dialog. First select an atom in the molecule, right-click and choose Edit properties... In the dialog box double-click the blue text field and type the property key then the value. Press Enter after each entry. The visibility of the atom properties can be switched on and off: go to View > Advanced > Atom properties.

Query properties: You can define the chemical neighborhood for an atom within a query structure. MarvinSketch allows you to set properties, such as hydrogen count, valence count, ring size, and aromaticity, which must be matched by the corresponding atom in the target structure to produce a hit.

- First select one or more atoms then go to the Advanced tab of Periodic Table to add the propertiy to every selected atom.
- First go to the Periodic Table then click individual atoms to increase/decrease property value.
- Each query property can be drawn typing .<query property name> (e.g., .H2) while the mouse pointer is over the relevant atom or there is active selection containing atoms.

The list of available query properties can be found here.

Attached data

Information may be attached to atoms and brackets. This data may include search restrictions in queries. Find details of query usage in JChem's Query Guide.

Adding data

Select an atom or group bracket, right-click and choose **Add > Data...** or **Data...**, respectively, from the context menu. Fill the appropriate fields in the dialog and click OK. The attached data can be edited any time: right-click the atom, the bracket or the data label and choose Edit Data... from the context menu.

Context field

- Atom - the data will be attached independently to all atoms in the selection.
- Bond - the data will be attached independently to all bonds in the selection.
- Single Bond - the data will be attached independently to all single bonds in the selection.
- Double Bond - the data will be attached independently to all double bonds in the selection.
- Fragment - the data will be attached independently to all disconnected fragments that are completely or partially contained by the selection.
- Selection - the data will be attached to the whole selection.

The number and name of the selectable contexts may vary in different configurations.

URLs as attached data

Values starting with www and including at least 2 full stops are handled as web page links (no spaces allowed). The format <scheme>://<authority><path>?<query>#<fragment> is also recognized. Double-click or Ctrl-click on the link will open the webpage. Links are currently not underlined.

Customizability

The elements of the 'Name' and the 'Value' editable combo boxes can be customized by the administrator. The corresponding elements of the 'Value' combo box can be defined for each element in the 'Name' combo box list, just as the corresponding 'Name' combo box contents for each element in the context combo box.
Details on the customization process.

Label placement

The labels can be positioned in 3 ways: absolute, relative or next to objects. Absolute means a stationary label, which can be moved independently from the structure. If the structure is moved, the label does not change its place. Relative labels always move with the same xy coordinates as the object. Labels next to objects can not be moved separately.

Mouseover highlights all details of the attached data.

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Stereochemistry

Scientific Background

Tetrahedral Stereocenters

The dimension of a molecule can be interpreted topologically, based on the connections of the consisting atoms, or spatially, based on the Cartesian coordinates of them. In this section the notion of dimension is used in spatial sense.

Molecules with same connectivity but different spatial arrangement are called stereoisomers.

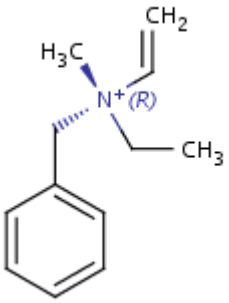
Stereoisomer types:

- Enantiomers: Molecules that are non-superimposable, complete mirror images of each other.

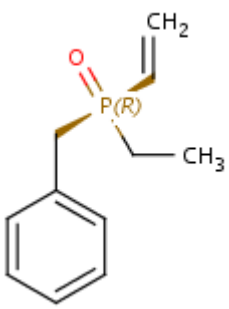
- Diastereomers: Stereoisomers that are not enantiomers.

Special cases

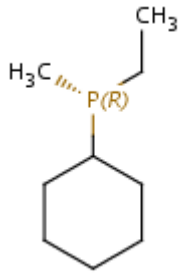
- Non-carbon tetrahedral stereocenters
  - Ammonium and phosphonium salts



  - Amine oxides and phosphanones

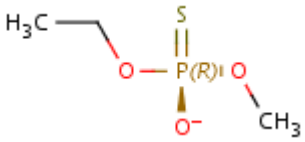


  - Phosphanes

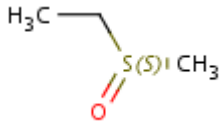


In this case the lone pair of phosphorus atom is considered as the fourth ligand.

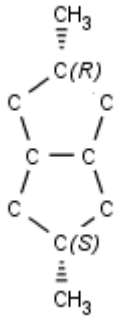
- Phosphates and phosphonates



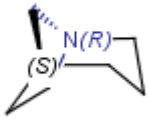
- Sulfoxides



- An atom *in a ring* is a tetrahedral center, if
  - the central atom has 2 different kinds of ligands outside the ring, and
  - the graph invariant of the ring is *not* the same in the two sides of the central atom, or
  - the graph invariant of the ring *is the same* in the two sides of the central atom, but
    - the ring contains even numbers of atoms (including the parity central atom), or
    - there is an atom with nonzero parity in the opposite side of the ring:



- Nitrogen atoms in a ring is tetrahedral stereo center, if
  - they are bridgehead atoms.



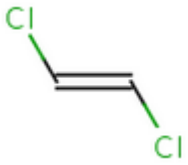
- N is a tetrahedral stereo center in a 3 membered ring,
  - if the graph invariant of the ring is *not* the same in the two sides of the nitrogen atom.

Representation in 0D, 2D and 3D

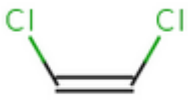
- **0D:** Stereoinformation is defined in 0 dimension by parity.
- **2D:** Stereoinformation in 2 dimension is defined by wedge, hatch or wiggly bond types.
- **3D:** Stereoinformation in 3 dimension is defined by the coordinates.

Cis-Trans stereoisomerism

In general, single bonds are rotatable, but double bonds are not. If the substituents on each side of the double bond are different, then two diastereomers of the molecule can be distinguished based on the orientation of the ligands. Two substituents located on the same side of the double bond are referred to as *cis* isomer, otherwise, if the two substituents are located on the opposite side it is referred to as *trans* isomer.

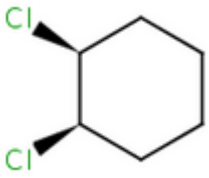


trans-1,2-dichloroethene

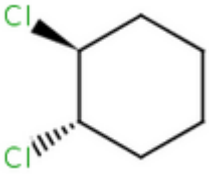


cis-1,2-dichloroethene

Alicyclic compounds can also display cis-trans isomerism. In this case a single bond becomes non rotatable due to constrain of a cycle. However, in these cases we use tetrahedral stereochemistry.



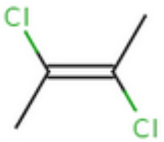
(1*R*,2*S*)-1,2-dichlorocyclohexane



(1*S*,2*S*)-1,2-dichlorocyclohexane

E/*Z* notation

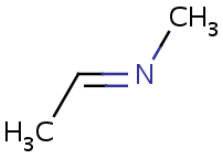
The cis/trans system for naming isomers is not effective if more than two different substituents are attached to the double bond. In this case, following the Cahn-Ingold-Prelog priority rules, a priority is assigned to each substituent on a double bond. If the two groups of higher priority are on opposite sides of the double bond (*trans* arrangement), then the *E* configuration is assigned to the bond. If the two groups of higher priority are on the same side of the double bond (*cis* arrangement), than the *Z* configuration is assigned to it.



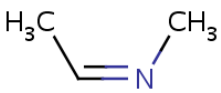
2*E*-2,3-dichlorobut-2-ene

2*Z*-2,3-dichlorobut-2-ene

E/*Z* stereochemistry of the nitrogen atom is also supported:



(*E*)-ethylidene(methyl)amine

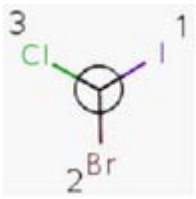


(*Z*)-ethylidene(methyl)amine

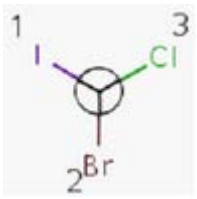
Chirality

An atom in the molecule around which the ligands are arranged so that interchange of two ligands leads to stereoisomer is called *stereocenter* or *stereogenic center*. Chirality appears in stereoisomerism which is due to tetrahedral stereogenic centers. These centers can have point chirality. The ligands of the chiral center are

assigned a priority based on the Cahn-Ingold-Prelog priority rules. Each chiral center is then labeled by R or S based on the orientation of the assigned numbers. The center is oriented so that the lowest-priority is pointed away from the viewer. If the priority of the remaining three substituents decreases clockwise, it is labeled *R*, otherwise, if it decreases counter clockwise, it is *S*.



R-bromo(chloro)iodomethane



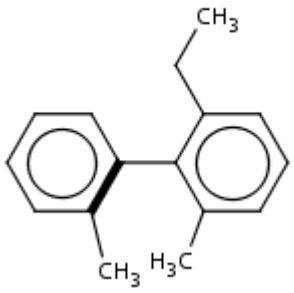
S-bromo(chloro)iodomethane

Cahn-Ingold-Prelog priority rules

Explained in Wikipedia: Cahn-Ingold-Prelog priority rules.

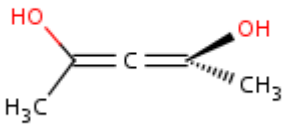
Atrop stereocenters

Hindered rotation around single bonds where the steric strain barrier to rotation is high enough to allow the isolation of the conformers resulting in atrop stereoisomerism.



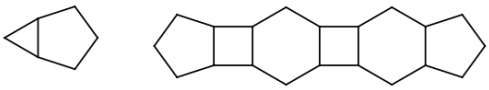
Axial stereocenters

If two stereoactive atoms (atoms with at least three different ligands) are connected by an even numbered chain of rigid parts then axial stereo information can be defined on the ligands of the stereactive atoms. These ligands are the ones which are not in the chain of the rigid part.



The following substructures are considered as rigid parts:

- double bonds,
- four- or six-membered ring,
- odd membered rings having lower than eight members, connected to each other directly or connected by intermediate four or six membered rings. Connection of two rings means that they share exactly one common bond (all rings are fused). The intermediate even membered rings have to connect to other rings by bonds on the opposite sides.



You may find more information concerning stereochemistry in the query guide or in the developer guide.

Stereo Specification

Basic stereo specification

- **Chirality**

  The relative position of ligands on a chiral atom is marked with wedge bonds: *up (solid)*, *down (hatched)*, *up or down (wiggly)*. Having wedge bonds at chiral atoms with the *chiral flag* on the entire structure implies that a single isomer is present. The absolute configuration (R or S) is known for all chiral centers that are marked with wedge bonds.

  Non-stereo bond to atom at stereogenic centers implies that no information is known about the configuration of a stereogenic center. It could be either of two stereoisomers, or a mixture of the two.

  The existence of wedge bonds at chiral atoms *without chiral flag* on the entire structure has two meanings depending on the file format used.
  MDL file types (mol, sdf ...): The structure is a racemic mixture of the two enantiomers.
  Daylight file types (smiles, smarts): Wedges mean absolute stereo configuration, the structure represents a single enantiomer.

- **Cis-Trans isomerism**

  The positions of the double bond ligands already define the stereo configuration of the double bond (*cis* or *trans*). Special query double bond types allow us to specify *cis or trans*, *not trans* or *not cis* isomers.

Enhanced stereo specification

Works in MDL molecule formats: mol, rgf, sdf, rxn etc... and in ChemAxon Extended SMILES format: cxsmiles.

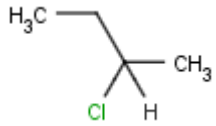
Enhanced stereochemical representation introduces three types of identifiers that can be attached to a stereogenic center. A stereochemical group label is composed from an identifier and a group number. Each stereogenic center marked with wedge bonds belongs to one (and only one) stereochemical group. Grouping allows us to specify relative relationships among stereogenic centers.

Stereochemical group types:

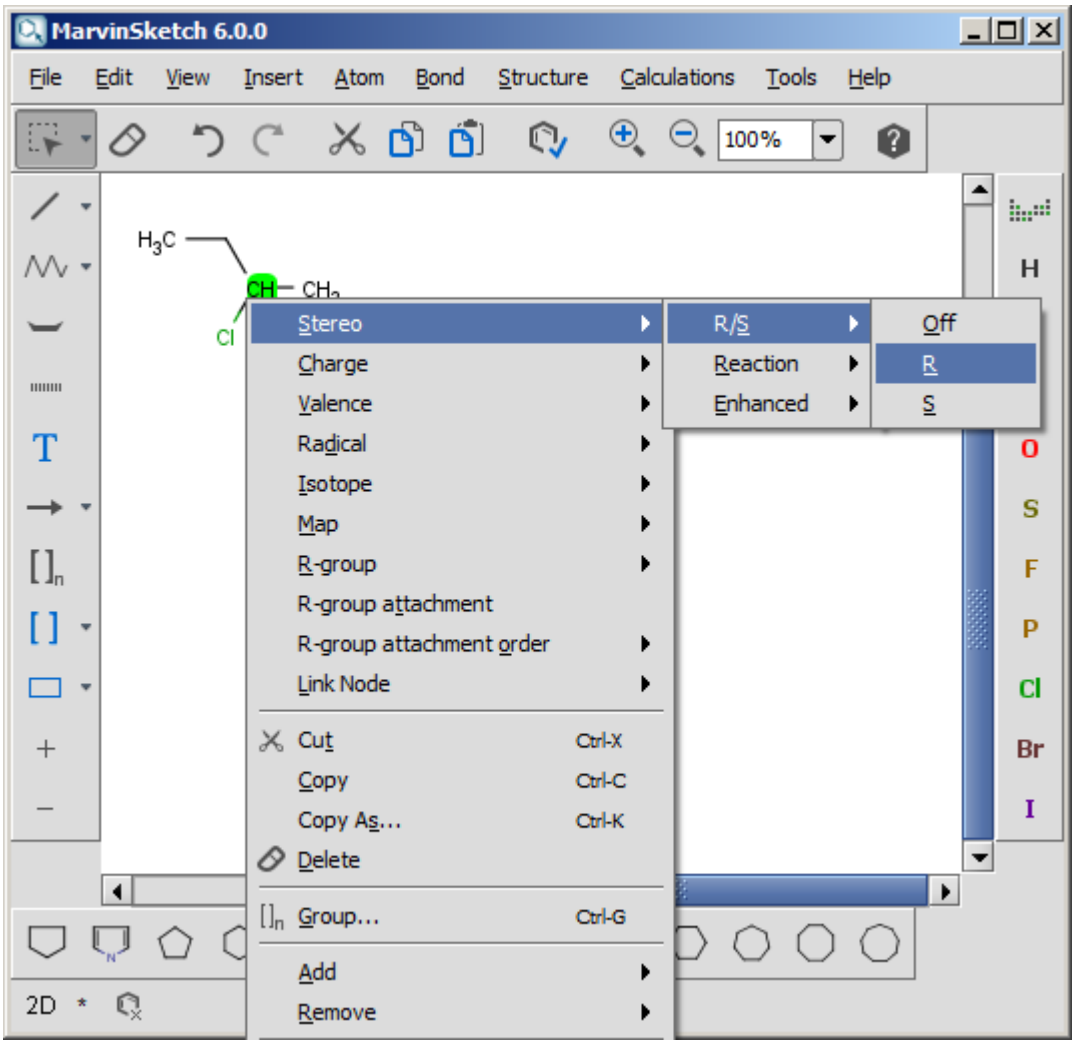
- ABS
  Stereogenic center where the absolute configuration is known.
- OR
  Stereogenic center where the relative configuration is known, but the absolute configuration is not known. The structure represents one stereoisomer that is either the structure as drawn (R,S) OR the epimer in which the stereogenic centers have the opposite configuration (S,R).
- AND
  Mixture of stereoisomers. It can be a pair of enantiomers or all the diastereomers.

How to specify and view R/S configuration

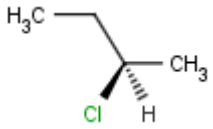
1. Draw a chiral molecule.



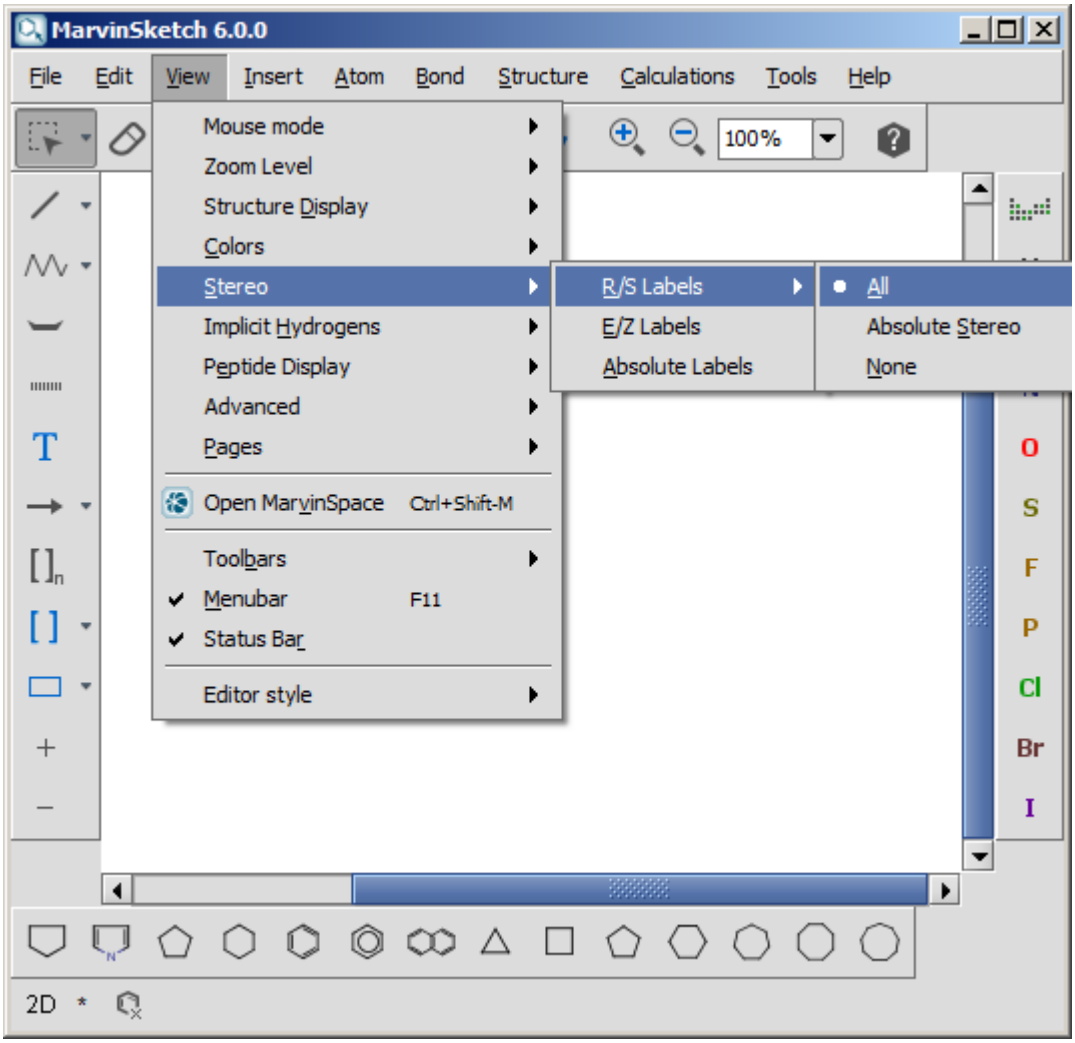
2. Click on (select) the asymmetric carbon atom that you want to configure as *S* or *R*. Right-click onto the carbon atom pops up the **Atom menu**. Choose **Stereo > R/S** and the appropriate configuration.



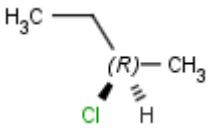
3. The relevant bonds will change automatically according to the proper R or S configuration.



4. To display the stereo label on the asymmetric carbon atom, select **View menu** > **Stereo** > **R/S Labels** > **All**.



5. The configuration of the asymmetric carbon atom presents in parentheses as follows.



6. If you want to remove the stereo label from the the asymmetric carbon atom, choose **View menu** > **Stereo > R/S Labels > None**.
7. If you want to delete stereo representation, right-click on the asymmetric carbon atom and choose **Atom menu** > **Stereo > R/S > Off**.

References

[1] http://accelrys.com/products/informatics/cheminformatics/ctfile-formats/no-fee.php

Calculator Plugins

Introduction

Calculator Plugins are modules of ChemAxon's Marvin and JChem cheminformatics platforms which calculate physico-chemical properties from chemical structures. Calculator Plugins currently cover a wide range of life-science-related properties.

Short usage guide

They are available directly from Marvin, Instant JChem and Reactor applications, and also from command line, API, or via ChemAxon's Chemical Terms language. The calculations can be performed in single or batch mode.

- The available calculator plugins are located in the **Calculations** menu in the graphical user interface of **MarvinSketch**, and in the **Tools** menu in **MarvinView**.
- **`cxcalc`** is the command line tool of the Calculator Plugin. Batch processing is available using `cxcalc` (see the list of calculations accessible from `cxcalc`).
- Calculators are used in the **Chemical Terms** language to calculate combinations of properties (like Lipinski's rule of 5) in an easy way. Learn more about it in the Chemical Terms section.
- Plugin calculations can be used for filtering results of database searches in **JChem Base**, **Instant JChem** and **JChem Cartridge**.
- Define smart reaction rules using plugin calculations in **Reactor** (ChemAxon's virtual reaction processing tool).
- Plugin calculations can be integrated easily into any **Java application.** For more information on using calculator plugin Java API, please see our chemaxon.marvin.calculation package.
- Some of the calculators (such as log*P*, pK_a and Predictor) can be trained with the user's data **via cxtrain**.
- **Third-party calculations** can be integrated easily into **MarvinSketch** via the Services module of the graphical user interface. For more information on integrating third-party calculations, see our Setting Services page.

List of Calculator Plugins

- Elemental Analysis Plugin
- Naming Plugin
- Protonation
  - pK_a Plugin [training]
  - Major Microspecies Plugin
  - Isoelectric Point Plugin
- Partitioning
  - log*P* Plugin [training]
  - log*D* Plugin [training]
- Charge
  - Charge Plugin
  - Polarizability Plugin
  - Orbital Electronegativity Plugin
  - Dipole Moment Calculation Plugin
- NMR
  - CNMR Prediction
  - HNMR Prediction
  - NMR Spectrum Viewer

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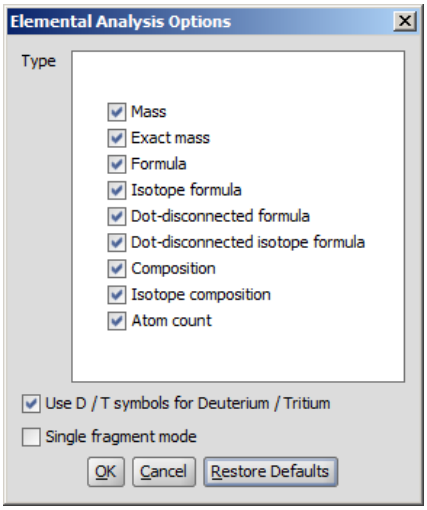
http://www.chemaxon.com/marvin

Elemental Analysis Plugin

Basic molecular values related to the elemental composition of the molecule are calculated by the Elemental Analysis plugin.

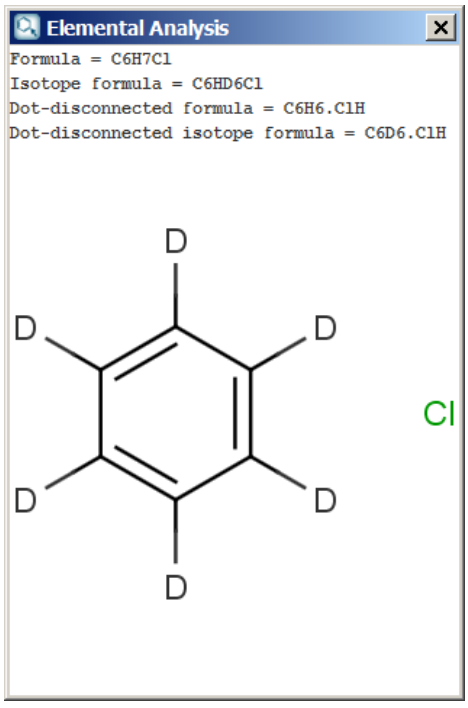
In the **Elemental Analysis Options** panel you can check different properties:



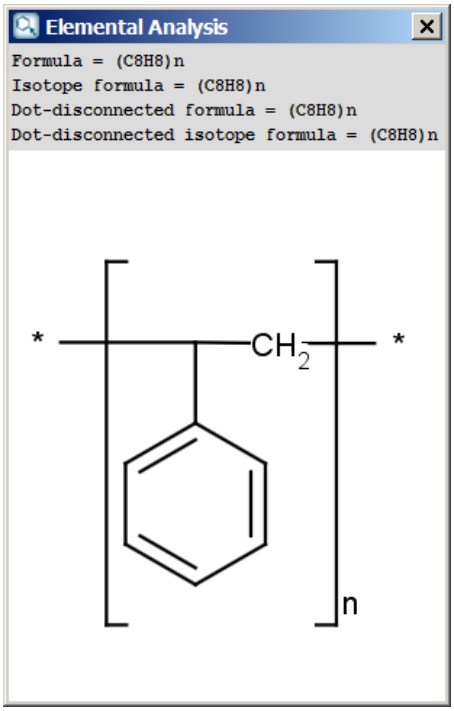
- **Type**
  - **Mass:** average molecular mass calculated from the standard atomic weights [1].
  - **Exact mass:** monoisotopic mass calculated from the weights [2] of the most abundant natural isotopes of the elements.
  - **Formula:** chemical formula of the molecule according to the Hill system [3]: the number of carbon atoms is indicated first, the number of hydrogen atoms next, and then the number of all other chemical elements subsequently, in alphabetical order. Isotopes (like Deuterium and Tritium) are not listed separately but counted together (e.g., deuterium and tritium atoms are counted as hydrogens). When the formula contains no carbon, all the elements, including hydrogen, are listed alphabetically. If the molecule contains an SRU or Repeating Unit S-group, it will be taken into account and Polymer Formula will be generated.
    Note: For polymer structures, mass, composition, and atom count calculations are not available and will return NaN, N/A, and -1, respectively.
  - **Isotope formula:** chemical formula of the molecule listing isotopes separately according to the Hill system.
  - **Dot-disconnected formula:** chemical formula of the molecule(s) separating fragment formulas by dots (e.g. salts, counterions, solvent molecules etc. are present).
  - **Dot-disconnected isotope formula:** chemical formula of the molecule separating fragment formulas by dots and listing isotopes separately.
  - **Composition:** elemental composition given in weight percentage (w/w %) calculated from the atomic masses.
  - **Isotope composition:** elemental composition listing isotopes separately (w/w %).
  - **Atom count:** number of all atoms in the molecule.

The examples shown below illustrating the difference between formula types:

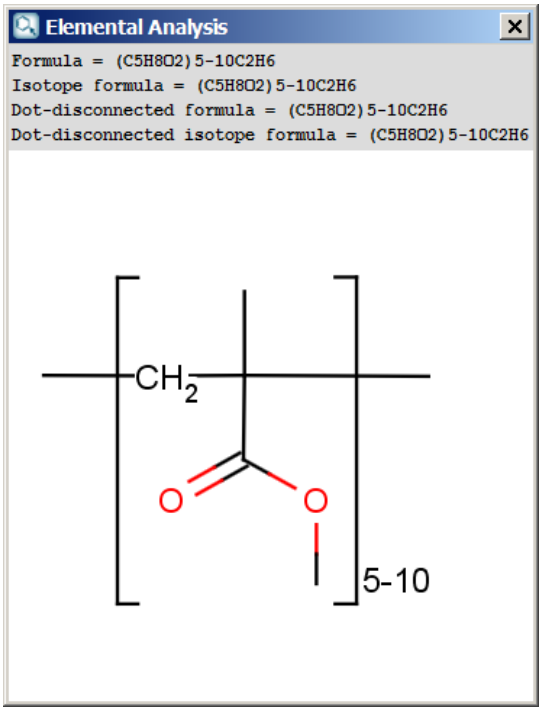
Multifragment Molecule with isotopes



SRU Polymer S-group



Polymer defined as Repeating units S-group

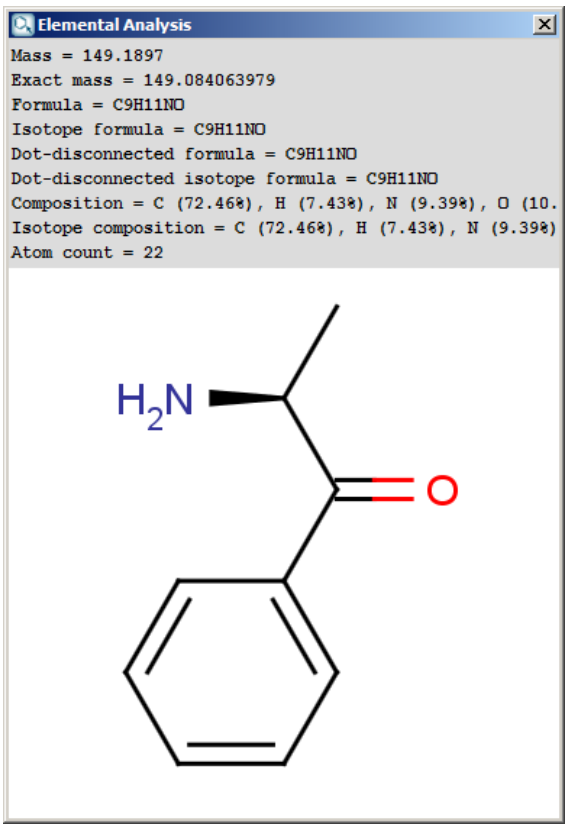


- **Use D / T symbols for deuterium / Tritium:** if unchecked (default), isotopes of hydrogen are displayed in formulas as 2H and 3H, if checked, D and T

symbols are used.

- **Single fragment mode:** if unchecked (default), the calculation handles unlinked molecules together (e.g. salt molecules), summing up the masses of each component, if checked, the results are displayed in a scroll window.

The results are shown in a new window:



The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu from MarvinView.

References

- Atom weights: M. E. Wieser, "Atomic weights of the elements 2005 (IUPAC Technical Report)" Pure Appl. Chem., Vol. 78, No. 11, pp. 2051-2066, 2006; doi
- Isotope weights: G.Audi and A.H.Wapstra, "The 1995 update to the atomic mass evaluation" Nuclear Physics A595 vol. 4, pp. 409-480, 1995; doi
- The Hill system: E. A. Hill, "On A System Of Indexing Chemical Literature; Adopted By The Classification Division Of The U. S. Patent Office". J. Am. Chem. Soc., 22(8), pp. 478-494, 1900; doi

Name generator

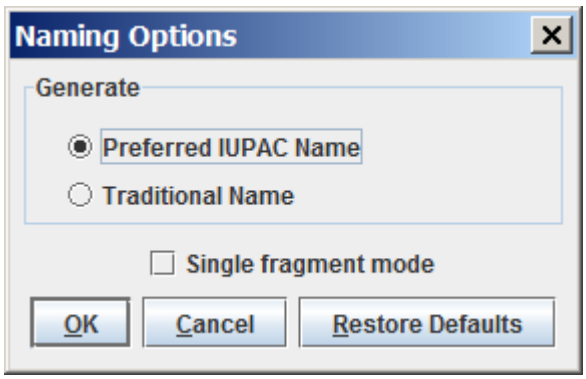
Since version 4.1.7, Marvin contains a name generator for the evaluation of the IUPAC name or traditional name of any compound.

When possible, the generated name conforms to the IUPAC Provisional Recommendations for the Nomenclature of Organic Chemistry published in 2004. However, we do not claim full conformance with that document. Our current goal is to generate chemically correct names for as many cases as possible.

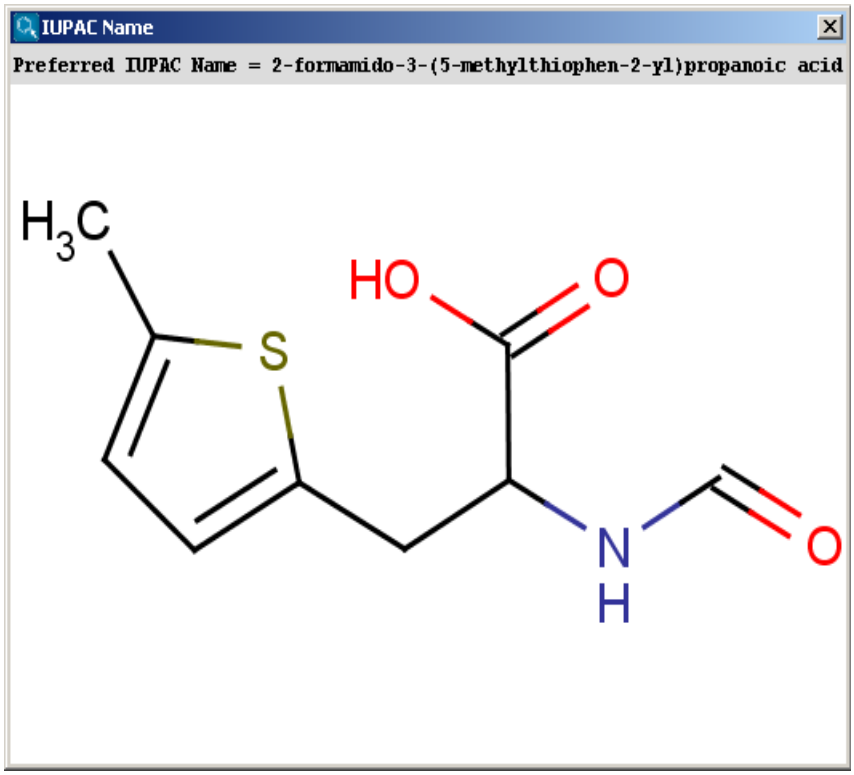
Importing IUPAC names is available from version 5.1.

You can generate either the "Traditional Name" or the "Preferred IUPAC Name" of the molecules; you can change between these options in the **Naming Options** panel. By default, the "Preferred IUPAC Name" option is set. If the traditional name is requested but cannot be generated, the preferred IUPAC Name will be generated instead.

By default, molecules are handled separately if more than one molecule are drawn in the sketcher. However, sometimes a single molecule consists of more fragments (e.g. salt molecules), where the fragments should be treated as one molecule. This can be reached by switching off the "Single fragment mode" option in the **Naming Options** panel.

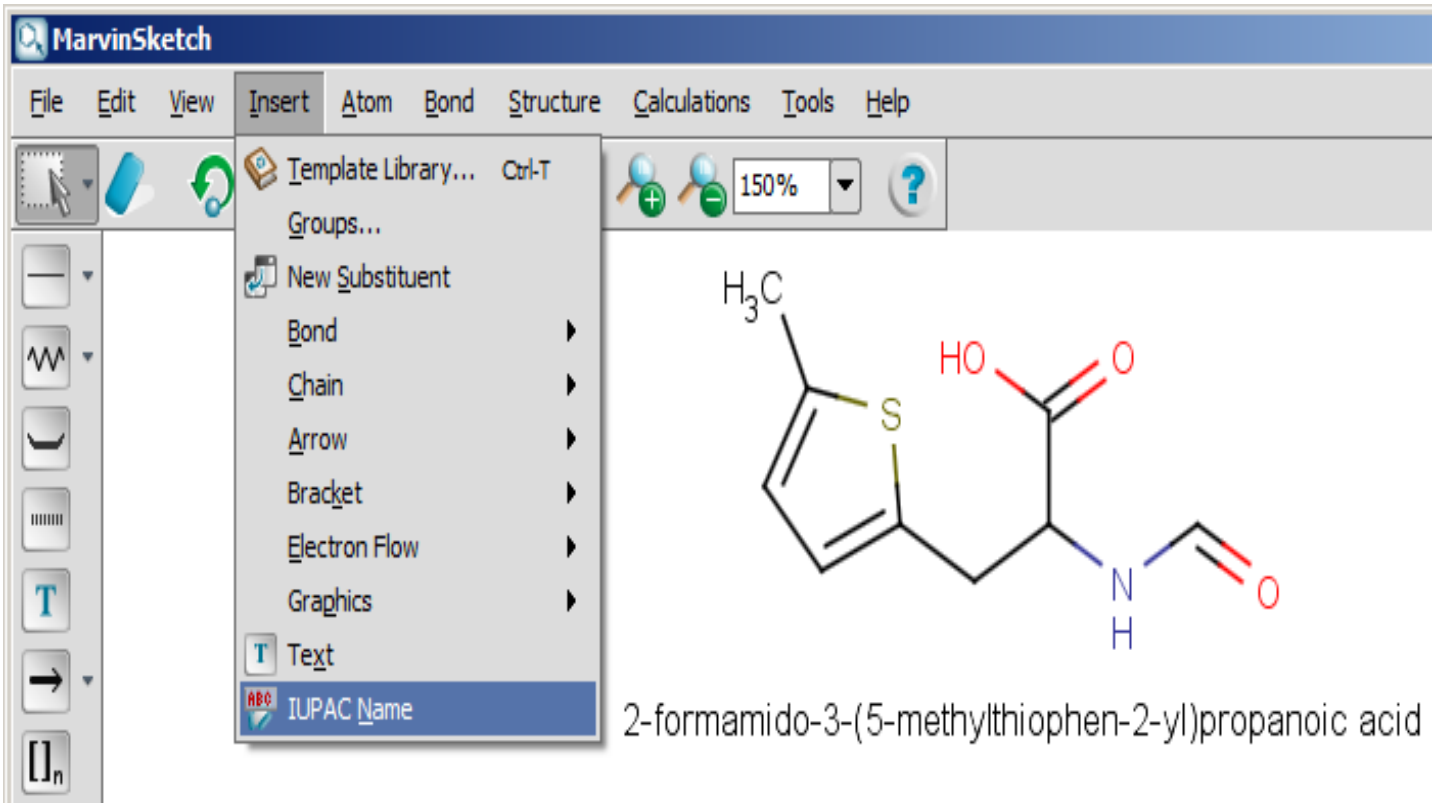


The snapshot below shows a molecule taken from the IUPAC specification, with its name computed by Marvin.



The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu when right-clicking on it.

The next snapshot below shows a functionality that is available from version 5.0: the IUPAC name can be inserted into the sketch, and it changes with the structure dynamically. This functionality is available from the **Structure** menu by selecting the **Structure to Name** > **Place IUPAC Name** option.



Features

Supported nomenclatures include:

- Chains, Monocycles
- Retained/traditional names for ring systems with and without heteroatoms
- Spiro ring systems
- All cases of von Baeyer nomenclature for bridged ring systems
- Fused ring systems (linear fused ring systems are named using the fused nomenclature, others using von Baeyer nomenclature)
- Ethers
- Common characteristic groups
- Ionic compounds
- Compounds with one radical
- Unlimited number of atoms and rings
- All atom types
- Substitutive nomenclature
- Isotopes
- Stereochemistry

Current limitations

- Molecules containing multiple radicals (e.g. `ethane-1,2-diyl`) are not supported yet.
- Amino-acids and peptides are supported only when the amino-acids are represented as groups.
- Molecules containing coordinate bond are not supported.
- Some aspects of nomenclature are only partially implemented, in particular complex cases of fused systems and multiplicative nomenclature. In those cases, a less straightforward but chemically correct name will be generated.

Usage

Individual molecules

You can name molecules by using the **Naming** menu entry of **Tools** menu in MarvinView, or **Structure** > **Structure to Name** > **Generate Name** in MarvinSketch.

In MarvinSketch, the name can be added to the canvas by using the **Structure to Name** > **Place IUPAC Name** entry in the **Structure** menu. The name will be displayed below the molecule, and updated in real-time when the molecule is modified.

Batch naming

Naming of a large number of molecules contained in a file can be achieved in two ways: with MarvinView, and on the command line, with molconvert. In both cases, all formats supported by Marvin are acceptable as input.

With MarvinView, open the file containing the structures to be names. Then select the menu File/Save As, and choose "IUPAC Name files" in the "Files of type" drop-down box. Choose a name for the file, and click on the Save button. The file will contain the names of the structures, one per line.

Alternatively, on the command line, you can use the following command:

```
molconvert name inputs.mol -o names.txt
```

The file `names.txt` will contain the names of the molecules in the input file, with one name per line.

It is possible to use a format option to chose a nomenclature style:

- `i` (default) uses the IUPAC rules for preferred names;
- `t` uses a more traditional style.

For instance, to generate traditional names, use the following:

```
molconvert name:t inputs.mol -o names.txt
```

Generate all common names for a structure:

```
molconvert "name:common,all" -s tylenol
```

Generate the most popular common name for a structure (It fails if none is known.):

```
molconvert name:common -s viagra
```

Adding names as an additional field to a SDfile can be achieved with the cxcalc tool.

```
cxcalc -S name input.sdf -o named.sdf
```

API

For information about how names can be generated from Java programs, see the developer documentation.

References

- IUPAC Provisional Recommendations for the Nomenclature of Organic Chemistry

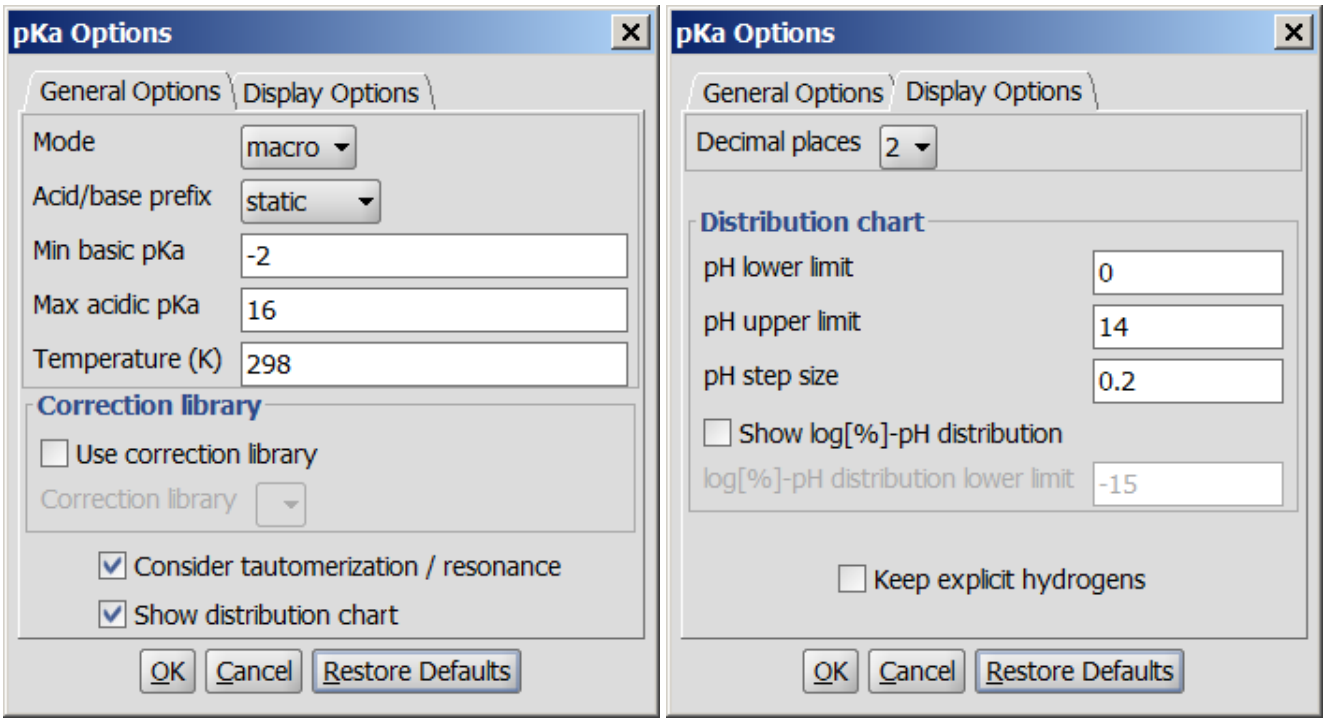
Protonation

pK_a Plugin

Most molecules contain some specific functional groups likely to lose or gain proton under specific circumstances. Each ionization equilibrium between the protonated and deprotonated forms of the molecule can be described with a constant value called pK_a. The pK_a plugin calculates the pK_a values of all proton gaining or losing atoms on the basis of the partial charge distribution.
Learn more about how the plugin calculates pK_a.

We introduced the trainable pK_a calculation from version 5.2! You can define a file with experimental data, and use its values for the correction of calculations.

The **pK_a options** panel offers different parameters to set:



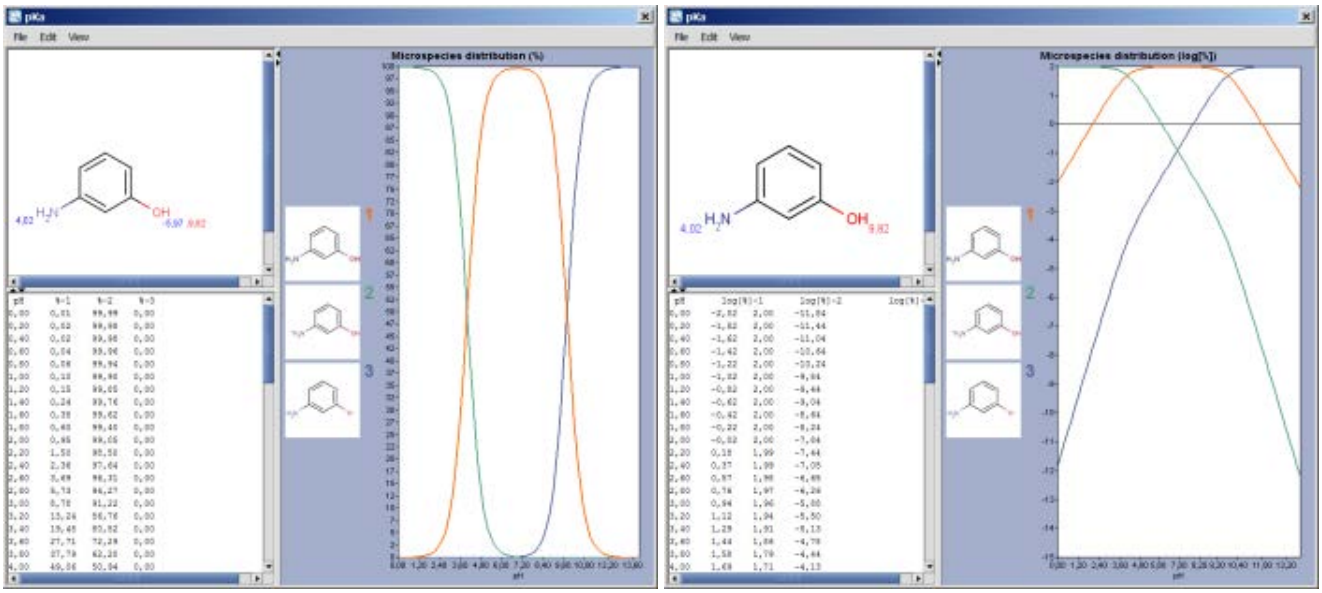
General Options

- **Mode:** micro, macro: micro and macro acidic dissociation constants. Read details.
- **Acid / base prefix:**
  - **static:** submitted ionic forms are converted to their neutral forms (adding or removing protons) and their pK_a is calculated.
  - **dynamic:** the pK_a of ionic forms are calculated, not their conjugated acids or bases.
- **Min basic pK_a:** widens the calculation range because weak bases will have lower pK_a values than the default -10.
- **Max acidic pK_a:** widens the calculation range because weak acids will have higher pK_a values than the default 20.
- **Temperature:** setting the temperature in Kelvin.
- **Correction library**
  - **Use correction library:** check this box to use a file with experimental data for the calculation. See the detailed guide for training data setup.
- **Consider tautomerization:** checking this option, the most feasible tautomer and resonance structures are considered as subject of the pKa calculation.
- **Show distribution chart:** checking this box, you will have microspecies/macrospecies distribution as function of pH calculated and displayed. Go to Display Options tab for further settings of the distribution chart. Unchecking this box, only the pK_a of the drawn molecule will be calculated.

Display Options

- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Distribution chart:** you can set the range of displaying the microspecies distribution diagram.
  - **pH lower limit**
  - **pH upper limit**
  - **pH step size**
- **Show log[%] - pH distribution:** checking this box, the common logarithm of microspecies/macrospecies distribution is calculated and displayed as function of pH.
  - **log[%] - pH distribution lower limit:** you can set the lower value of the Y axis ranging from -35 to zero.

Results are shown in a separate window. When checking the Show microspecies distribution box, this window appears (for the explanation about the **red&blue color representation** of the pK_a values next to the protonable groups read this document):



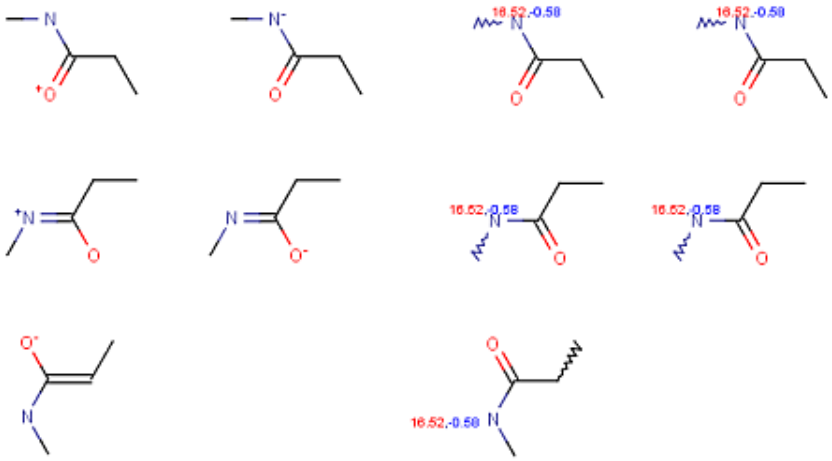
The chart shows the microspecies distribution, or the common logarithm of microspecies distribution curves vs. pH. The microspecies images are shown in the legend. When clicking on an image, the corresponding microspecies molecule is displayed in the upper-left viewer. (The viewer can be detached from the chart panel by double clicking in it, or else by selecting **Open Viewer** from the **View** menu.) The original molecule with the pK_a values is shown when clicking on the chart outside of the legend image areas, or else when selecting **pKa Values** from the **View** menu.

Note: If there are 8 or less ionizable atoms in the molecule, then microspecies distribution is displayed on the chart, otherwise macrospecies distribution is shown. Images of microspecies are displayed only on the microspecies distribution chart; on macrospecies distribution chart the formal charges of the macrospecies are shown.

The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu from MarvinView.

When moving the mouse over one of the microspecies images, the corresponding (pH : % of the microspecies) coordinates appear on the curves.

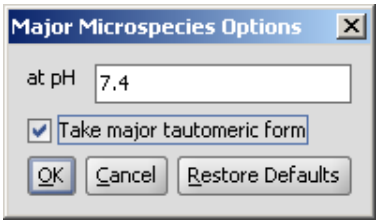
Calculation with the option 'Take major tautomeric form' gives same values for different tautomers.



Major Microspecies Plugin

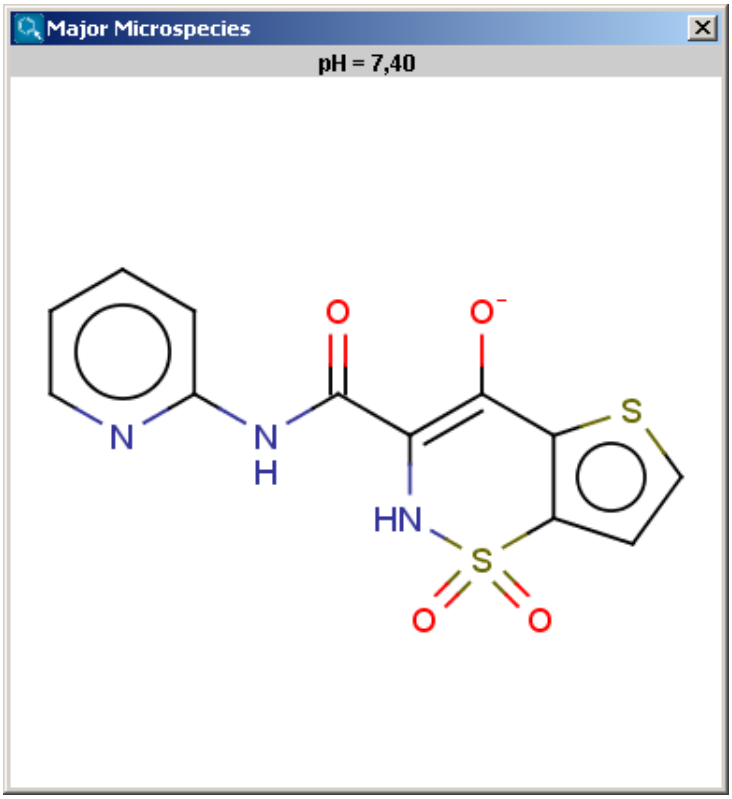
Determines the major protonation form at a specified pH.

The pH can be set in the **Major Microspecies Options** panel, the default pH is 7.4.



- **Take major tautomeric form:** if tautomeric forms are more likely to occur, tha major tautomer is used to calculate the major microspecies.

The result is shown in a separate window, indicated the pH value and the structure in a MarvinView field.

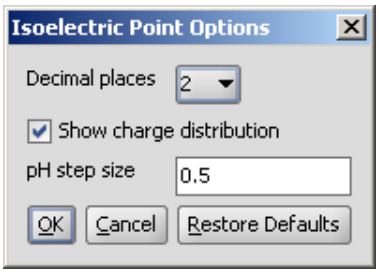


The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu from MarvinView.

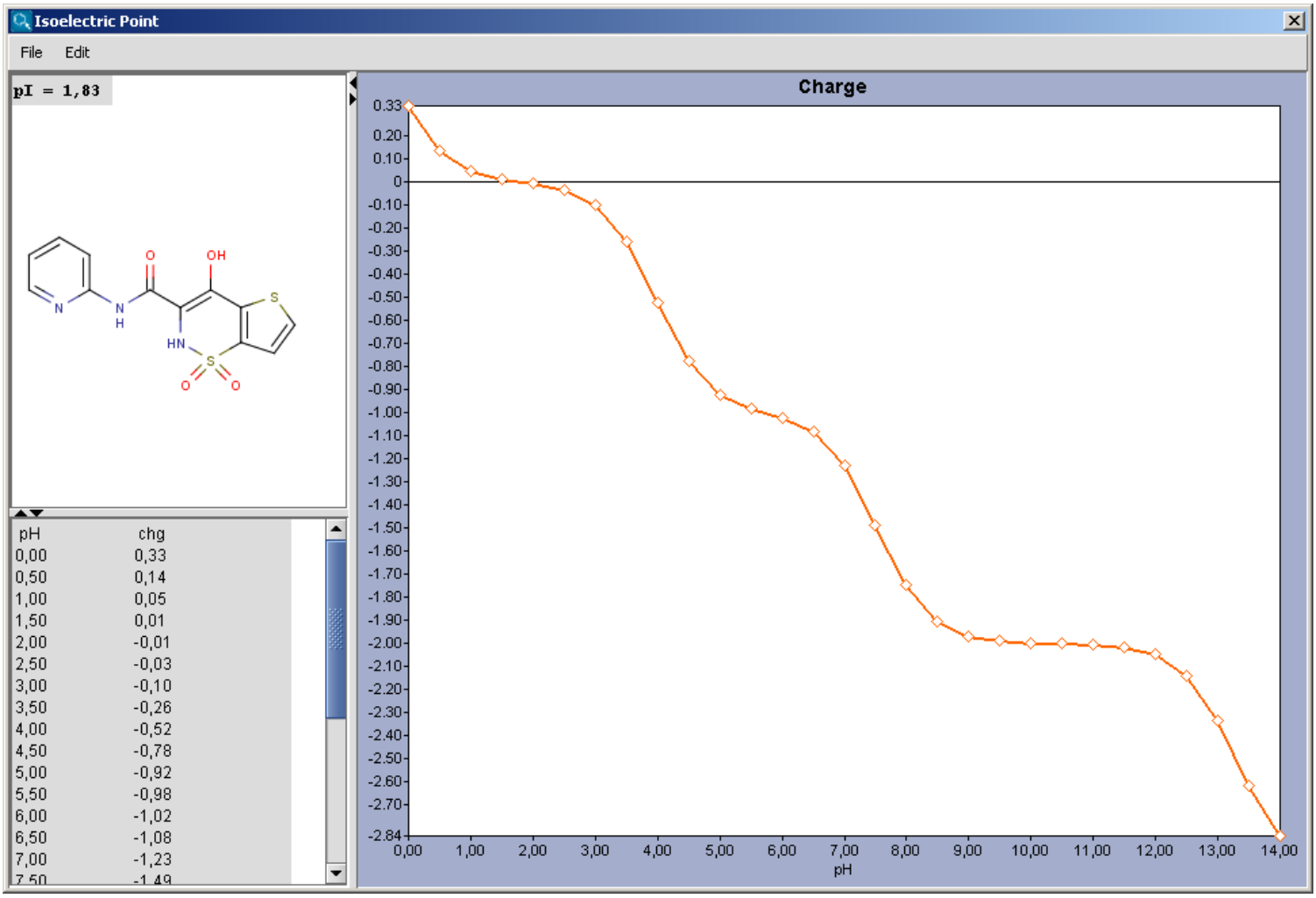
Isoelectric Point Plugin

Net charge of an ionizable molecule is zero at a certain pH. This pH is called the isoelectric point, also referred to as pI. Isoelectric point plugin calculates gross charge distribution of a molecule as function of pH.

The **Isoelectric Point Options** panel contains the pH, and the option to switch off the charge distribution chart of the charge of the molecule vs. pH:



The result is shown in a separate window, containing the molecule structure at the pI and the value of pI. If the Show charge distribution checkbox was checked, the charge vs. pH curve is displayed. When moving the mouse over the dots in the curve, the coordinates (pH : charge) appear.



The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu from MarvinView.

Partitioning

log*P* Plugin

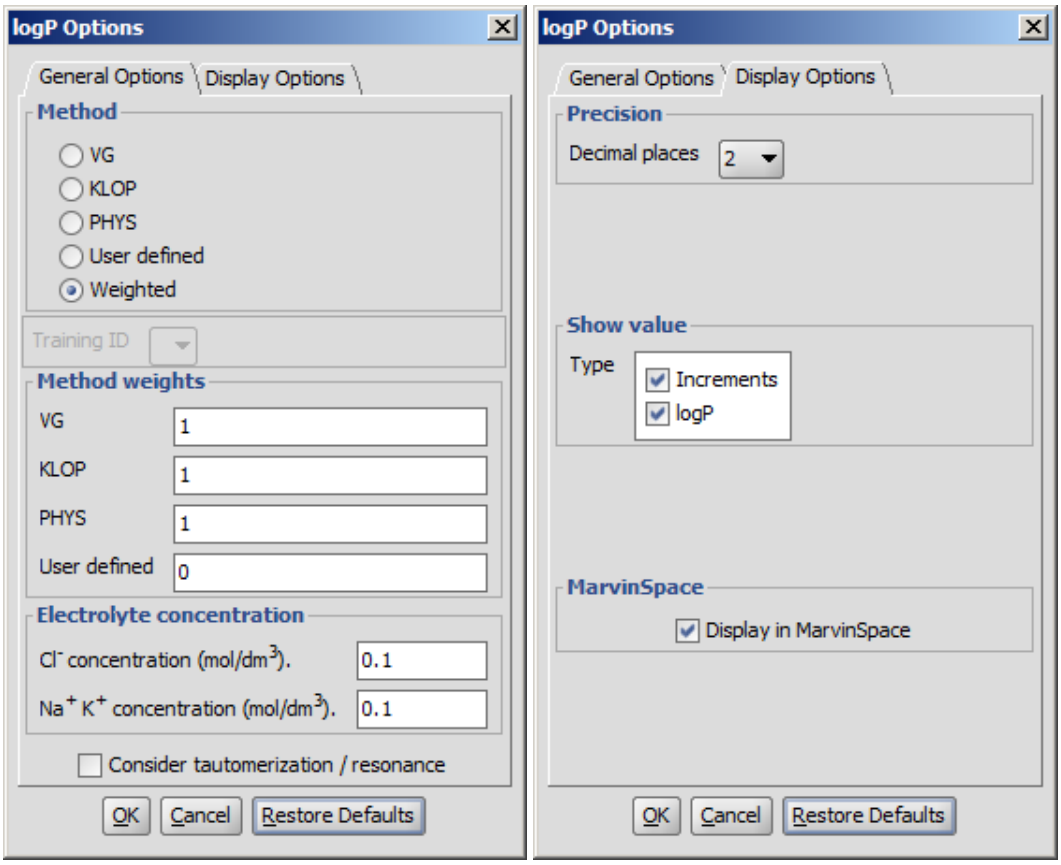
The log*P* plugin calculates the octanol/water partition coefficient, which is used in QSAR analysis and rational drug design as a measure of molecular hydrophobicity. The calculation method is based on the publication of Viswanadhan et al. (see Ref.1.) The log*P* value of a molecule is composed of the increment values of its atoms. The algorithm described in the paper was modified at several points. Many atomic types were redefined to accommodate electron delocalization. Contributions of ionic forms were added. The log*P* value of zwitterions are calculated from the log*D* value at the isoelectric point. The effect of hydrogen bonds on log*P* is considered if there is a chance to form a six membered ring between suitable donor and acceptor atoms. New atom types were introduced especially for sulfur, carbon, nitrogen, and metal atoms.

Learn more about how the plugin calculates log*P* and how a user defined set is used in the calculations.

We introduced the trainable log*P* calculation in version 5.1.3.
What does trainability mean? With this new feature you can teach our program, how it should calculate the log*P* values of structures in your compound library. Experimental data and the molecules are saved into a file which is used in the calculation if user defined method is selected.

Read how you can benefit from the user defined method used in the calculations. Technical details about setting up.

Different calculation parameters can be set in the **log*P* Options** panel:



General Options

- **Method**
  - **VG:** the calculation method derived from Reference 1. is applied (VG stands for Viswanadhan and Ghose, first authors of the cited paper).
  - **KLOP:** log*P* data from Klopman's paper is applied.
  - **PHYSPROP:** log*P* data from PHYSPROP© database is used.
  - **User defined:** if a training set of structures and corresponding experimental log*P* values is created by the user, and stored in the appropriate format, it can be used as a database for related molecules' log*P* calculations. See this document about creating such sets.

Weighted: default setting. The use of methods can be melted by the user, selecting this method turns the Method weights section active.

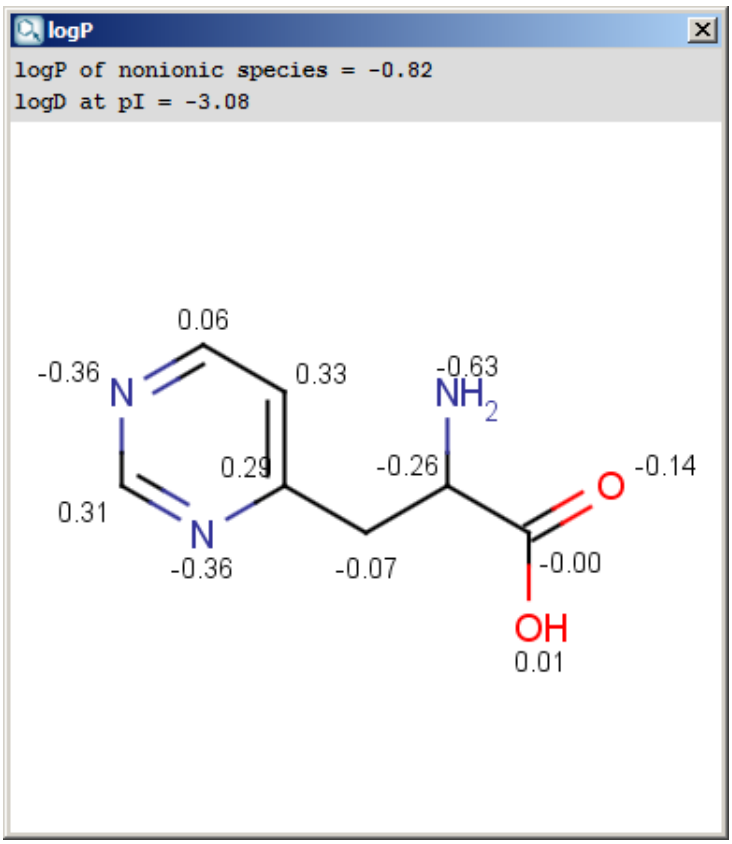
- **Training ID:** if the **User defined** or the **Weighted** method is selected, this dropdown list becomes active. All created training sets are listed here. Choose the one to apply for the calculation. Read more on creating a training set.
- **Method weights:** you can set the proportion of the methods used in the calculations. Acitve only in Weighted method.
- **Electrolyte concentration**
  - **Cl^- concentration:** can be set between 0.1 and 0.25 mol/L.
  - **Na^+ K^+ concentration:** can be set between 0.1 and 0.25 mol/L.
- **Take major tautomeric form:** the log*P* of the major tautomer will be calcutated.

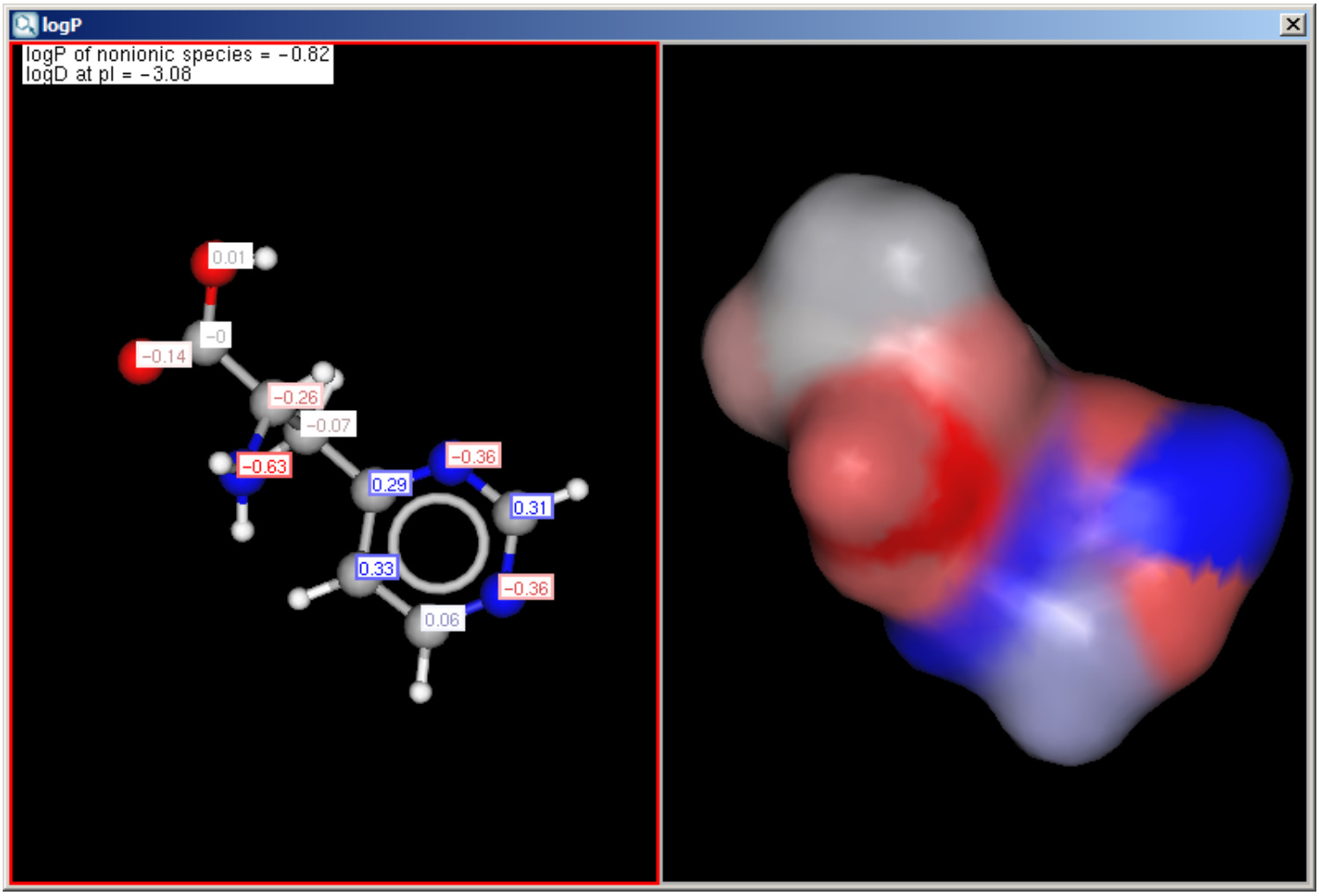
Display Options

- **Precision:** setting the number of decimal places with which the result value is given.
- **Show value**
  - **increments:** calculates the increments given by the atoms.
  - **log*P*:** calculates the value of log*P*
  - **Increments of hydrogens:** displays the increments given by hydrogens (in brackets).
- **Display in MarvinSpace:** the result window opens as 3D MarvinSpace viewer. If unchecked, the results will be shown on a 2D picture.

Notes to Method and Method Weights: These log*P* methods were developed by us based partly on the atom types given in Reference 1.. The three abbrevations only refer to the appropiate training log*P* data set according to the references 1, 2 and 3. Weighted method is a combination of the above three log*P* calclulations. The three methods are equally weighted (1/3) by the default setting. The calculated log*P* in this way will be the arithmetic average of the three methods. The weighted method usually provides more reliable log*P* value than any one of the three separate methods.

The result of the calculation appears in a new window, either in a MarvinView (2D) window or a MarvinSpace (3D) window:



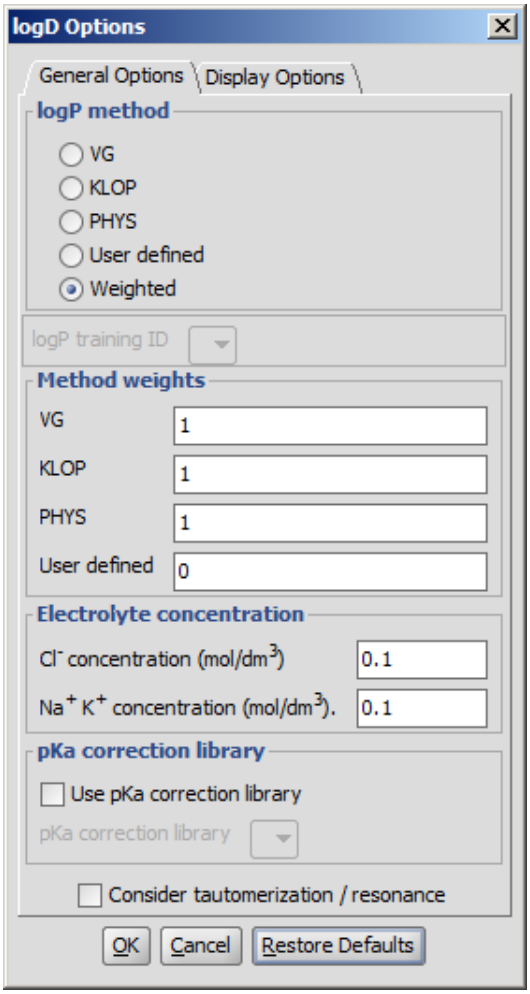


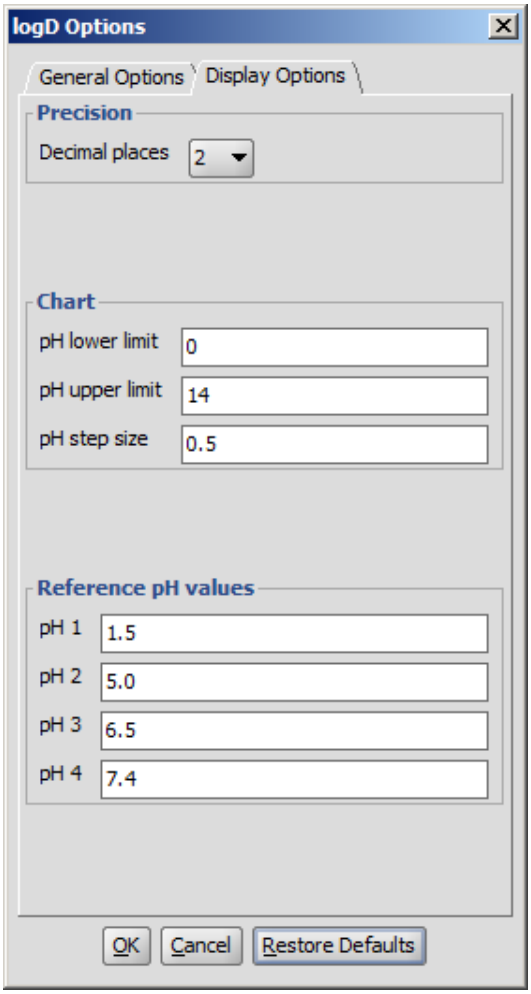
The result window shows the log*P* increments for each atom. The numbers in brackets refer to the log*P* increment sums of implicit H atoms, and displayed only if the "Increment of Hs" option is switched on in the **log*P* Options** panel.

log*D* Plugin

Compounds having ionizable groups exist in solution as a mixture of different ionic forms. The ionization of those groups, thus the ratio of the ionic forms depends on the pH. Since log*P* describes the hydrophobicity of one form only, the apparent log*P* value can be different. The octanol-water distribution coefficient, log*D* represents the compounds at any pH value (see Ref. 3.).
Learn more about how the plugin calculates log*D*.

Different calculation parameters can be set in the **log*D* Options** panel:





General Options

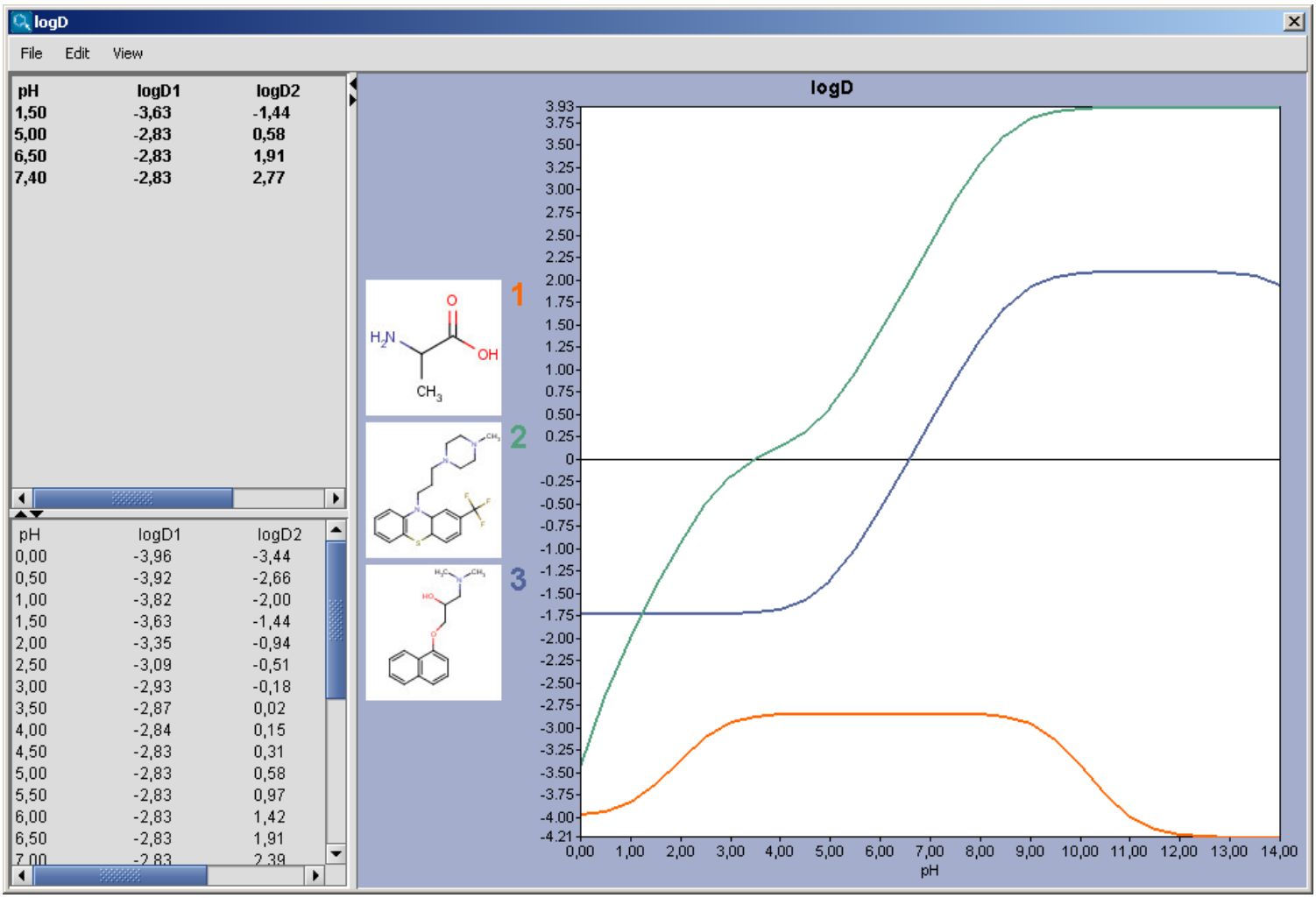
- **log*P* Method**
  - **VG:** the calculation method derived from Reference 1. is applied (VG stands for Viswanadhan and Ghose, first authors of the cited paper).
  - **KLOP:** log*P* data from Klopman's paper is applied.
  - **PHYSPROP:** log*P* data from PHYSPROP© database is used.
  - **User defined:** if a training set of structures and corresponding experimental log*P* values is created by the user, and stored in the appropriate format, it can be used as a database for related molecules' log*P* calculations. See this document about creating such sets.
  - **Weighted:** default setting. The use of methods can be melted by the user, selecting this method turns the Method weights section active.
- **Log*P* Training ID:** if the **User defined** or the **Weighted** method is selected, this dropdown list becomes active. All created training sets are listed here. Choose the one to apply for the calculation. Read more on creating a training set.
- **Method weights:** you can set the proportion of the methods used in the calculations. Acitve only in Weighted method.
- **Electrolyte concentration**
  - **Cl^- concentration:** can be set between 0.1 and 0.25 mol/L.
  - **Na^+ K^+ concentration:** can be set between 0.1 and 0.25 mol/L.
- **pKa correction library:** the custom pKa training for the compounds may be used. First, create a training set for your compunds, which then will appear in the dropdown list. If the option is checked, this list becomes active. Read more on creating a training set.
- **Consider tautomerization:** in case of tautomer structures, all dominant tautomers at given pH are taken into account during the log*D* calculation.

Display Options

- **Precision:** setting the number of decimal places with which the result value is given.
- **Chart: pH limits, pH step size:** defines the pH window in which the log*D* is calculated, with pH values starting

from the lower limit incremented by the step size, the results given in table format and a chart.

- **Reference pH values:** the log*D* at the given reference pH values are calculated, both pH and log*D* values with an accuracy of the decimal places value set.



The chart shows the log*D*(pH) curves for each molecule drawn in the sketcher. The molecule images are shown in the legend. When clicking on an image, the corresponding molecule is displayed in the upper-left viewer. The viewer can be detached from the chart panel by double clicking in it, or else by selecting **Open Viewer** from the **View** menu. The reference log*D* values originally shown can be restored by either clicking on the chart outside of the legend image areas, or else by selecting **log*D* at reference pHs** from the **View** menu.

References

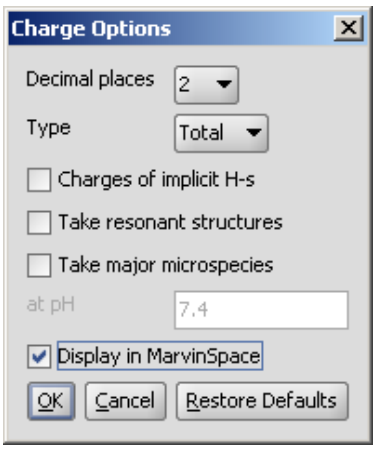
1. Viswanadhan, V. N.; Ghose, A. K.; Revankar, G. R.; Robins, R. K., *J. Chem. Inf. Comput. Sci.*, **1989**, *29*, 163-172; doi
2. Klopman, G.; Li, Ju-Yun.; Wang, S.; Dimayuga, M.: *J.Chem.Inf.Comput.Sci.*, **1994**, *34*, 752; doi
3. PHYSPROP© database
4. Csizmadia, F; Tsantili-Kakoulidou, A.; Pander, I.; Darvas, F., *J. Pharm. Sci.*, **1997**, *86*, 865-871; doi

Charge

Charge Plugin

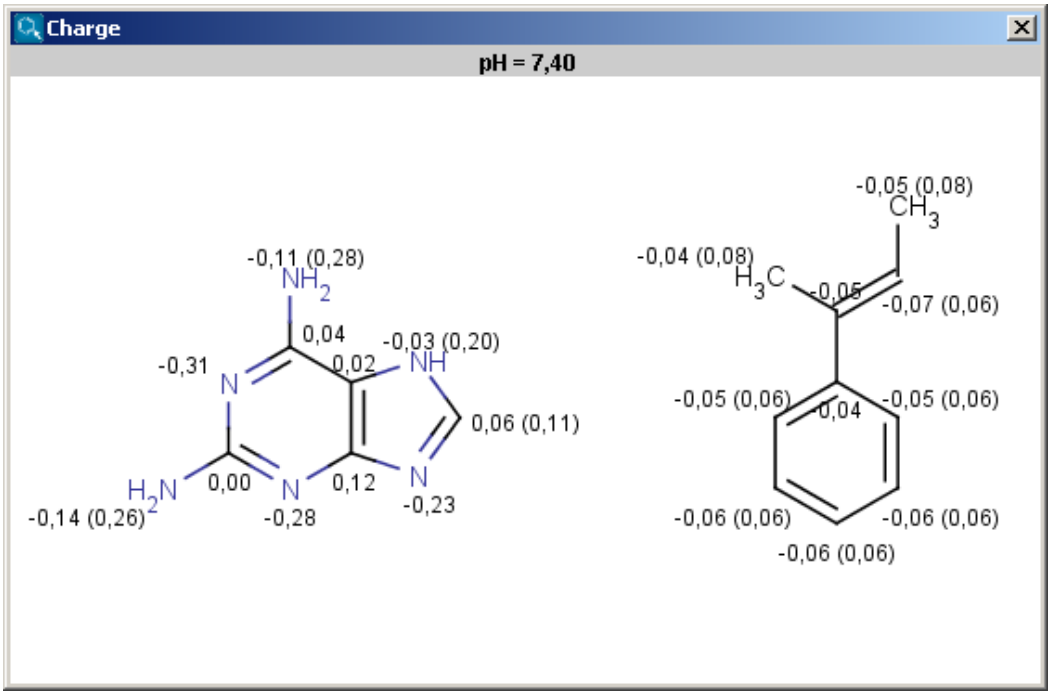
The partial charge distribution determines many physico-chemical properties of a molecule, such as ionization constants, reactivity and pharmacophore pattern. Use Charge plugin to compute the partial charge value of each atom. Total charge is calculated from sigma and pi charge components, and any of these three charge values can be displayed. Learn more about how the plugin calculates the partial charge.

In the **Charge Options** panel you can set the following:



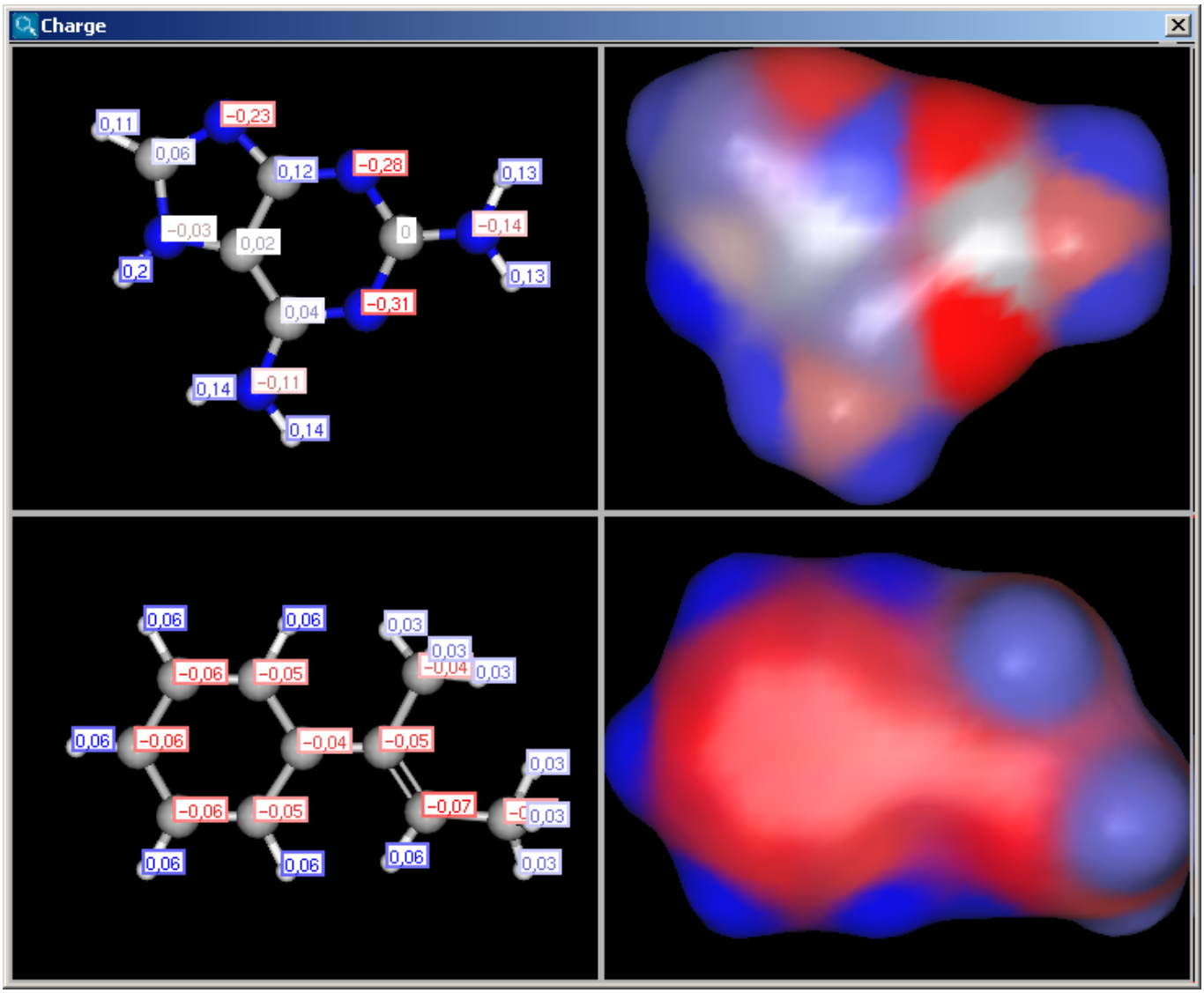
- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Type:** setting type of the calculus: total charge, sigma charge or pi charge components.
- **Charges of implicit hydrogens:** gives you in detail the increments of the charge by the implicit hydrogens.
- **Take resonant structures:** the average of the charge of the resonant srtuctures will be calculated.
- **Take major microspecies/ at pH:** the charge of the major microspecies present at the given pH.
- **Display in MarvinSpace**: the result window opens as 3D MarvinSpace viewer. If unchecked, the results will be shown on a 2D picture.

The results are shown in a new window, if more molecules present on the sketching canvas (in MarvinSketch) then all molecules appear in one single field in 2D:



Charge is expressed in atomic unit [e].The numbers in brackets refer to the charge sums of implicit hydrogen atoms, and displayed only if the "Increment of Hs" option is switched on in the **Charge Options** panel.

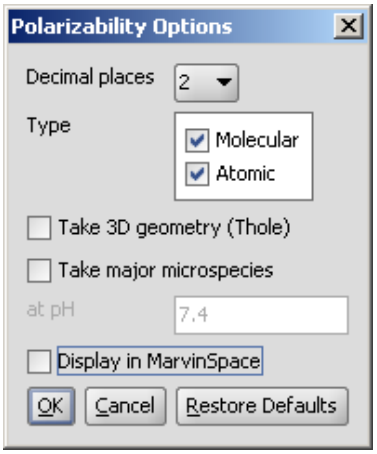
If the Display in MarvinSpace checkbox was checked, the results appear in seperate fields, but operations (zooming, rotating etc.) are linked:



Polarization Plugin

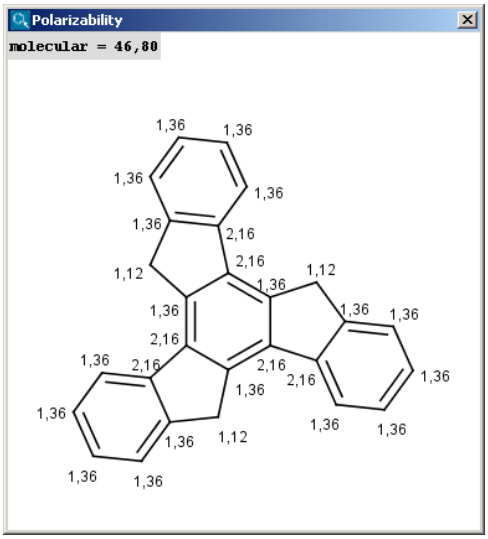
The electric field generated by partial charges of a molecule spread through intermolecular cavities and the solvent. The induced partial charge (induced dipole) has a tendency to diminish the external electric field. This phenomenon is called polarizability. The more stable the ionized site is the more its vicinity is polarizable. This is why atomic polarizability is an important factor in the determination of pK_a and why it is considered in our pK_a calculation plugin. Atomic polarizability is altered by partial charges of atoms. We use two methods to calculate polarizability: one of the calculations is based on Miller's and Savchik's atomic parameters, while the other method is based on Thole's parameters.

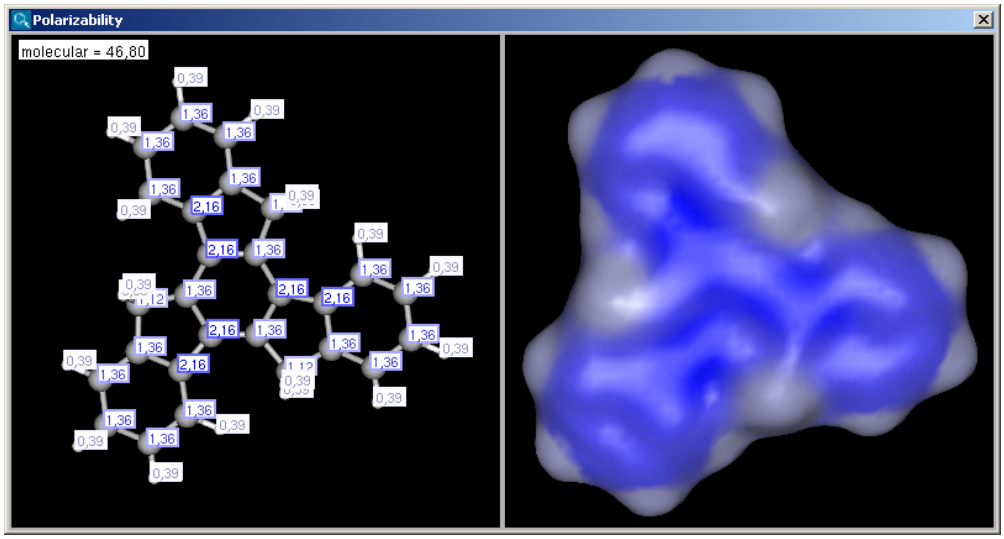
In the **Polarizability Options** panel you can set the following:



- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Type:** setting type of the calculus: molecular or atomic polarizability components.
- **Take 3D geometry (Thole):** calculates the polarization tensor values.
- **Take major microspecies:** the polarizability of major microspecies at the given pH is calculated.

The result appears in a new window, displaying on each atom its polarizability value (dimension: $Å^3$) (2D view and 3D view):



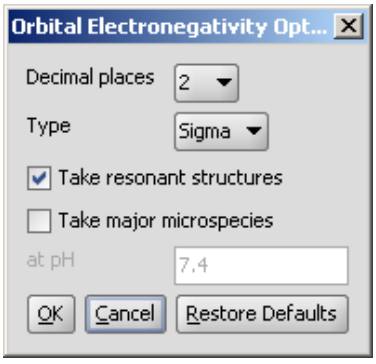


The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu from MarvinView.

Orbital Electronegativity Plugin

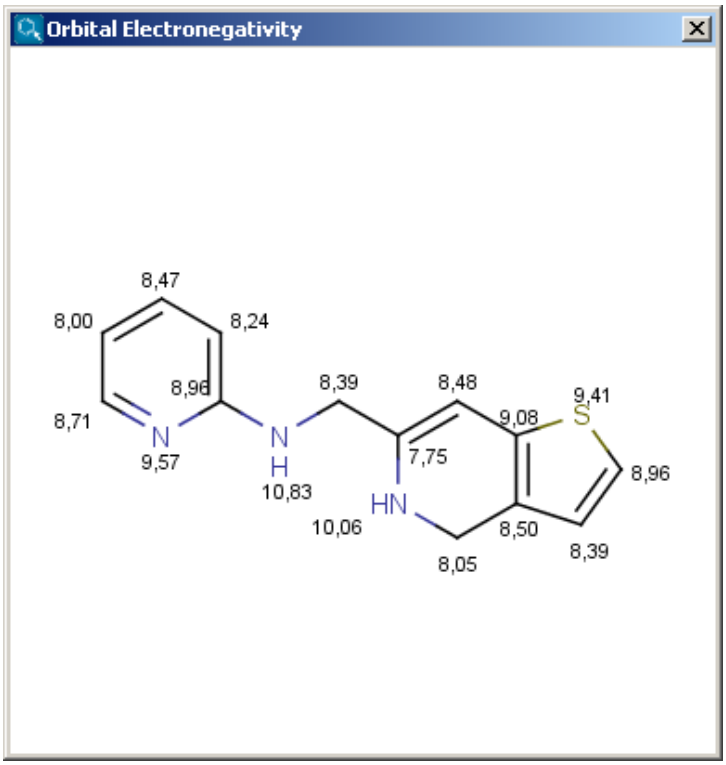
Partial charge distribution of the molecule is governed by the orbital electronegativity of the atoms contained in the molecule.
Learn more about how the plugin calculates orbital electronegativity.

In the **Orbital Electronegativity Options** panel you can set the following:



- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Type:** setting type of the calculus: sigma charge or pi electronegativity components.
- **Take resonant structures:** the average of the charge of the resonant srtuctures will be calculated.
- **Take major microspecies:** the electronegativity of major microspecies at the given pH is calculated.

The result appears in a new window, displaying on each atom (except of hydrogens) its EN value:

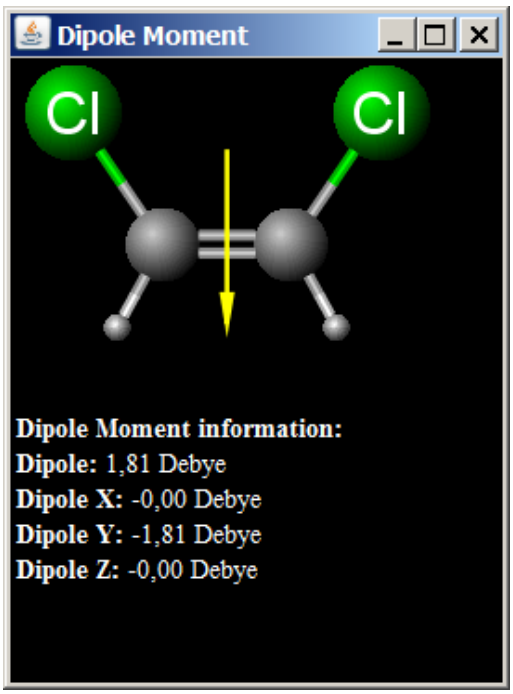


The structure field offers a context menu from MarvinView.

Dipole Moment Calculation Plugin

Dipole moment (μ) is the measure of net molecular polarity, and describes the charge separation in a molecule, where electron density is shared unequally between atoms.

Dipole Moment Calculation presents the overall dipole moment of a molecule as a vector expressed in the principal axis frame. The dipole moment information is deduced about the molecular geometry and partial charges. The unit of the dipole moment is Debye (D).



References

- Miller, K. J.; Savchik, J. A., *J. Am. Chem. Soc.*, **1979**, *101*, 7206-7213; doi
- Jensen, L.; Åstrand, P.-O.; Osted, A.; Kongsted, J.; Mikkelsen, K.V. *J. Chem. Phys.*, **2002**, *116*, 4001-4010; doi

Prediction of nuclear magnetic resonance (NMR) spectra

Version 6.1.7

Fast and accurate prediction of ^{13}C and ^{1}H NMR spectra from the molecular structure plays an important role in structure validation and elucidation of molecules. The NMR predictor application is able to predict NMR spectra for standard organic molecules containing the most frequent atoms (H, C, N, O, F, Cl, Br, I, P, S, Si, Se, B, Sn, Ge, Te, As).
Chemical shifts are estimated by a mixed HOSE and linear model based on a topological description scheme and are in relation to the chemical shift of tetramethylsilane (δ(TMS)=0 ppm). ^{13}C and ^{1}H chemical shift training data were retrieved from the NMRShift Database. Read more about NMR chemical shift model description.

Basic features

- Prediction of **^{13}C** and **^{1}H** **NMR** chemical shifts;
- **Spin-spin couplings** are taken into account according to the first order approximation;
- **H-H, H-F and C-F couplings** are considered during NMR spectrum calculation;
- **Diastereotopic protons** are differentiated;
- NMR Spectrum Viewer is able to display NMR spectra in JCAMP-DX format.

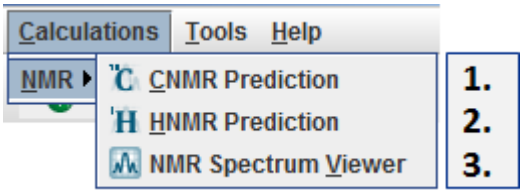
The NMR Predictor graphical user interface incorporates the following features:

- **Export** predicted spectrum to **molfile**;
- **Export** predicted spectrum to JCAMP-DX file and/or **import JCAMP-DX** (*.jdx) reference spectrum;
- Create **PDF file as report** of your prediction, containing molecule structure, predicted spectrum, and related tables;
- Detached **Copy to clipboard** action for all predictor panels and tables is available;
- **Update** molecule from MarvinSketch;
- Toggle between decoupled and **coupled NMR spectrum**;
-  Toggle between explicit and **implicit hydrogen display**;
- Select NMR **prediction frequency** from a predetermined list;
- **Add** common organic **solvent peaks** to predicted spectrum;
- **Add tautomer peaks** to predicted spectrum;
- **Restore** default NMR predictor **settings**, e.g., prediction frequency, display, and view options;
- Display **realistic** or **line** NMR spectra;
- **Add** atom indices or chemical shift values to signals as **spectrum labels**;
- Display spectrum scale in **ppm** or **Hz** units;
- Show **integral curve** to assign value to NMR spectrum signals;
- Display **legend** on spectrum display panel.
- Show local maximum values of reference spectrum;
- Personalize the **color management** of NMR Predictor;
- **Set** chart **color** uniquely;
- When you click on a peak on spectrum display panel or on an atom on molecule preview panel, selection will move to and zoom in on the selected signal;
- Choose multiplet selection mode: **individual selection** in case of overlapping multiplets is available;
- Use **various modes of zoom in** on spectrum.
- Find spectrum and molecule structure related information in **Atom**, **Multiplet**, and **Coupling** tables.
- Show atom indices on molecule structure corresponding to the different multiplets;

Atoms of the input molecule and multiplets of the NMR spectrum are linked together: upon selection of an atom the corresponding multiplet is highlighted and vice versa.

A single NMR prediction is allowed to contain more molecules.

NMR predictor is integrated into **MarvinSketch**'s **Calculations** menu, and contains the following three components to discover NMR spectra of molecules:



1. **CNMR Prediction** and
2. **HNMR Prediction**;
3. **NMR Spectrum Viewer**.

NMR Prediction is accessible via **cxcalc** as well (`cxcalc nmr -h`).

To improve our product, please send feedback to calculators-support@chemaxon.com.

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NMR Prediction - Tool to predict ^{13}C and ^{1}H Nuclear Magnetic Resonance spectra

Contents

NMR Prediction - ^{13}C and ^{1}H NMR predictor

NMR Prediction is integrated into MarvinSketch and is able to predict carbon-13 and hydrogen-1 nuclear magnetic resonance (^{13}C NMR and ^{1}H NMR) spectra for standard organic molecules drawn in MarvinSketch. Chemical shifts are estimated by a mixed HOSE and linear model based on a topological description scheme, and they are relative to the chemical shift of tetramethylsilane (δ(TMS)=0 ppm). NMR Prediction provides the details of the predicted spectrum for browsing in separate panels.

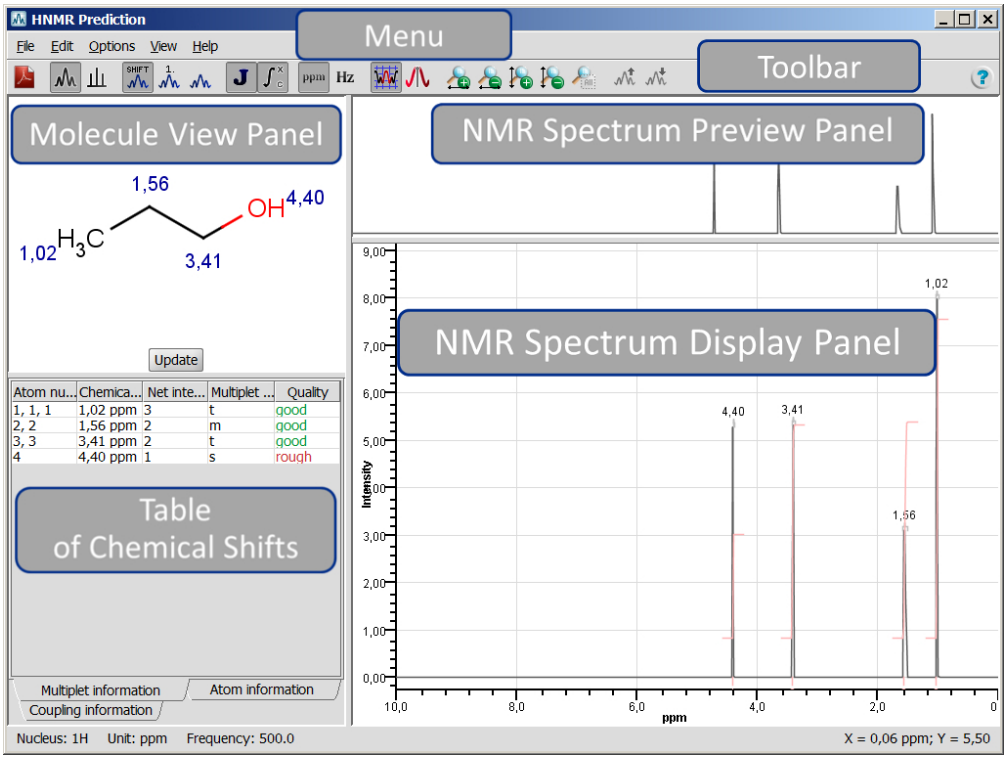
NMR Prediction - Usage

You can predict ^{13}C NMR and ^{1}H NMR spectra of organic molecules drawn in MarvinSketch using the relevant prediction in **Calculations** menu.

1. Draw molecule in MarvinSketch.
2. Go to *Calculations* > *NMR* >
   - *CNMR Prediction* to discover the predicted ^{13}C NMR spectrum of the molecule, or
   - *HNMR Prediction* to discover the predicted ^{1}H NMR spectrum of the molecule.
3. The predicted spectrum will open in **CNMR Prediction** window if you chose *CNMR Prediction*, and in **HNMR Prediction** window if you chose *HNMR Prediction*, respectively.

Note: You can predict both spectra of the molecule in question which will open in separate windows.

NMR Prediction Window



Both NMR Prediction windows consist of a menu, toolbar, and four panels. The name of the window is displayed at the top left corner. At the bottom left corner of the status bar general information on the NMR prediction is shown, i.e., nucleus, measurement unit, and prediction frequency; while at the bottom right corner the coordinates of mouse cursor position on the NMR Spectrum Display Panel are shown. We will discuss the menu elements and panels of both ^{13}C and ^{1}H NMR Prediction windows together. Differences will be marked by the appropriate icon (: **CNMR Prediction**, : **HNMR Prediction**).

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NMR Prediction Menu

The menu contains **File**, **Edit**, **Options**, **View**, and **Help** elements.

File menu

is to export spectra to various molfiles or JCAMP-DX file format, to import spectrum of JCAMP-DX file format and superimpose it on predicted NMR spectrum, to remove the imported spectrum, and to close NMR Prediction.

- File > **Export to PDF...**: Exports the molecule structure, predicted spectrum (full), and related tables to PDF file. You can select *Keep view settings* option on the export dialog panel to keep the actual view of spectrum during export to PDF.
- File > **Export to JCAMP-DX...**: Exports predicted spectrum to JCAMP-DX (jdx) file format.
- File > **Export to Molfile...**: Exports predicted spectrum to molfile. You can export the predicted spectrum data to SDF file format. The SDF file will contain *structure* and *NMR Spectrum* fields. The *NMR Spectrum* field contains the relevant atom number (AN), value of chemical shift (vδ), unit of chemical shift (uδ), and multiplicity of the signal (M) in the following format:

  vδ1;uδ1,M1;AN1|vδ2;uδ2,M2;AN2|...|vδi;uδi,Mi;ANi.

- File > **Import from JCAMP-DX**: Imports a spectrum in JCAMP-DX format. The imported spectrum will be superimposed on the predicted NMR spectrum.
- File > **Remove Imported Spectrum**: Removes previously imported JCAMP-DX spectrum from *NMR Spectrum Display Panel.*
- File > **Exit**: Closes NMR prediction window.

Edit menu

is to copy specific panel to clipboard and to update the molecule from MarvinSketch. You can also apply the right-click of your mouse on the proper panel to copy it to the clipboard.

- Edit > **Copy Spectrum**: Copies the actual view of Spectrum Display Panel to the clipboard.
- Edit > **Copy Spectrum Preview**: Copies the actual view of Spectrum Preview Panel to the clipboard.
- Edit > **Copy Molecule**: Copies the actual view of Molecule View Panel to the clipboard.
- Edit > **Copy Multiplet Table**: Copies Multiple Table to the clipboard.
- Edit > **Copy Atom Table**: Copies Atom Table to the clipboard.
- Edit > **Copy Coupling Table**: Copies Coupling Table to the clipboard.
- Edit > **Update Molecule**: Updates molecule on Molecule View Panel and the whole prediction at the same time. You can switch back to MarvinSketch window without closing NMR predictor window; modify the molecule or draw a new molecule of which NMR spectrum you wish to predict. Switch back to NMR predictor window and either select Update Molecule or click on the Update button on Molecule View Panel to refresh NMR prediction.

Options menu

is to select optional NMR prediction settings:

- Options > **Spin-Spin Coupling**: Prediction considers spin-spin coupling; the result is splitting of signals into multiplets according to the interaction between two nuclei.
- Options > **Implicit Hydrogen Mode**: Hydrogens are displayed only on hetero and terminal atoms.
  Note If you switch off this mode:
  - all hydrogens will be visible on Molecule Panel;
  - atoms will be re-numbered on all corresponding panels;
  - coupling table will be filled in with relevant data.
- Options > **NMR Prediction Frequency**: Sets the frequency of the NMR prediction. Select prediction frequency from the predetermined list. Prediction frequency influences the fine structure of the spectrum.
- Options > **Add Solvent Peaks...**: Adds NMR signal(s) of selected common organic solvent(s) to the predicted spectrum. Select solvents from the predetermined list and click OK. The signal(s) of selected solvent(s) will be added to the predicted spectrum. When spectrum labels are displayed, you can see the name of the solvent attached to the corresponding signal. We used the NMR shift data of common organic solvents in $CDCl_3$ collected by Gottlieb et al.
- Options > **Select Tautomers...**: Opens a dialog where tautomers of the relevant molecule are displayed. The major tautomer is automatically selected. The values of tautomer distributions are obtained from MarvinSketch's Dominant tautomer distribution calculation. You can select altogether 8 tautomers to add their signal(s) to the predicted spectrum. Check the upper right check box of the appropriate tautomer. The distribution of each tautomer has to be set before proceeding. When spectrum labels are displayed, the corresponding signals of the active tautomer can be seen on Spectrum Display Panel, while the tautomer peaks are signed according to their symbols.
- Options > **Clear Tautomers**: Removes all selected tautomer peaks from predicted spectrum.
- Options > **Reset Default Settings**: Resets zoom and the default Options, Color, and View settings of NMR predictor.
  - CNMR Predictor:
    - NMR Prediction Frequency: 500 [125] MHz
    - Spectrum Display: Realistic Spectrum
    - Spectrum Labels: Chemical Shifts
    - Measurement Unit: ppm
    - Zoom Follows Selection: On
  - HNMR Predictor:
    - Spin-Spin Coupling: On
    - Implicit Hydrogen Mode: On

NMR Prediction Frequency: 500 MHz
- Spectrum Display: Realistic Spectrum
- Spectrum Labels: Chemical Shifts
- Measurement Unit: ppm
- Integral Curve: On
- Zoom Follows Selection: On

View menu

is to select different display options related to the predicted spectrum and the molecule structure:

- View > **Spectrum Display**:
  - **Realistic Spectrum**: Displays predicted spectrum in a realistic way.
  - **Line Spectrum**: Predicted chemical shifts are presented by distinct lines with proper intensity.
- View > **Spectrum Labels**: In order to assign signals and relevant atoms more easily, you can display the atom numbers or the chemical shift values of each signal on the NMR Spectrum Display an Molecule View Panels. Select:
  - **Atom Numbers** to see atoms assigned to each signal and to display atom numbers on **Molecule View Panel** as well.
  - **Chemical Shifts** to see the exact chemical shift value of NMR signals on **NMR Spectrum Display Panel**.
  - **None** to remove spectrum labels.

  Note that you can display only one type of label at a time.
- View > **Measurement Unit**: The chemical shift of tetramethylsilane (TMS) is set to zero, and all other chemical shifts are predicted relative to it. Display unit can be:
  - **Hz** or
  - **ppm**.
- View > **Integral Curve**: Displays integral curve on spectrum. Default setting is: on.
- View > **Display Legend**: Displays legend on Spectrum Display Panel. The legend contains information on different functions of Spectrum Display Panel.
- View > **Reference Spectrum**: It is an imported JCAMP-DX NMR spectrum that can be superimposed on the predicted NMR spectrum.
  - **Display Shifts**: If the imported JCAMP-DX file has "PEAKTABLE" property, the chemical shifts of the imported spectrum can be displayed.
  - **None**: Remove chemical shift labels of the reference spectrum.
- View > **Set Colors...**: You can customize the color of the predicted spectrum, reference spectrum, and selection.
- View > **Zoom Follows Selection**: If you select an exact atom on Molecule View Panel, or a signal on NMR Spectrum Display Panel, the appropriate signal is centered and zoomed in on **NMR Spectrum Display Panel**.
- View > **Select Individual Multiplets**: In case of overlapping multiplets, this option enables highlighting individual multiplets.
- View > **Horizontal Zoom In**: Zooms in on spectrum in X-axis direction.
- View > **Horizontal Zoom Out**: Zooms out of spectrum in X-axis direction.
- View > **Vertical Zoom In**: Zooms in on spectrum in Y-axis direction. **Note**: the bottom of the selection window is fixed.
- View > **Vertical Zoom Out**: Zooms out of spectrum in Y-axis direction. **Note**: the bottom of the selection window is fixed.
- View > **Reset Zoom**: Displays the whole spectrum in both directions.
- View > **Scale Up Reference**: Increases intensity of imported reference spectrum. Active when reference spectrum is imported.
- View > **Scale Down Reference**: Decreases intensity of imported reference spectrum. Active when

reference spectrum is imported.

Help menu

- Help > Quick Help
- Help > **Help Contents**

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NMR Prediction Toolbar

You can use toolbar elements to access selected NMR Predictor menu items.

	Export to PDF...
	Spectrum Display
	Spectrum Labels
	Spin-Spin Coupling
	Integral Curve
	Measurement Unit
	Zoom Follows Selection
	Select Individual Multiplets
	Horizontal Zoom In
	Horizontal Zoom Out
	Vertical Zoom In
	Vertical Zoom Out
	Reset Zoom
	Scale Up Reference
	Scale Down Reference
	Quick Help

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NMR Prediction Panels

NMR Prediction window contains **Molecule View Panel**, **Table of Chemical Shifts**, **NMR Spectrum Preview Panel**, and **NMR Spectrum Display Panel** to present the predicted spectrum and to display selected features. Panels can be copied separately as images by right-clicking on the appropriate panel and selecting **Copy to clipboard** action.

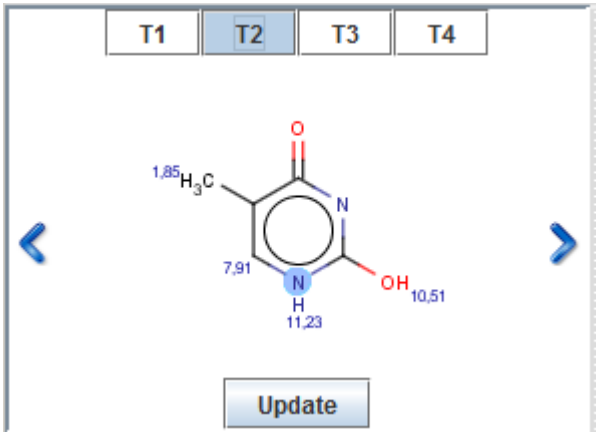
Molecule View Panel

displays the molecule of prediction. Molecule has to be drawn in MarvinSketch. Using the Ctrl button while the cursor is located in this panel, the view of molecule can be controlled:

- Ctrl+Mouse scroll button: Zooms in/out the molecule
- Ctrl+Mouse dragging: moves the molecule

If you select *View* > *Spectrum Labels* > *Atom Numbers*, atom numbers will appear on both **Molecule View Panel** and **NMR Spectrum Display Panel**.

If you select *View* > *Spectrum Labels* > *Chemical Shifts*, chemical shift values of predicted multiplets will appear on both **Molecule View Panel** and **NMR Spectrum Display Panel**
If you have added tautomers to the predicted spectrum via "Select Tautomers..." option, the layout of Molecule View Panel will change: the active tautomer is displayed on the panel. To go to the next/previous tautomer, click on the arrows next to the molecule. Above the displayed molecule, symbols T1, T2, ..., T_n, mark the selected tautomers. Hover over to see tautomer structure in a pop-up window. Click on the symbol to make it active.



Click on **Update** button after you have made any modifications on molecular structure in MarvinSketch and you want to predict the NMR spectrum of the new molecule. Effect of **Update** button on **Molecule View Panel** is equal to *Edit* > *Update Molecule* action.

Table of Chemical Shifts

The following tabs are available on this panel: **Multiplet information**, **Atom information**, and **Coupling information** tabs. Table on all tabs contains data of the predicted spectrum in Multiplet or Atom point of view. Coupling table contains the calculated coupling constants when Spin-Spin coupling option is selected.

Multiplet information Table has six columns, namely: Atom numbers, Chemical shift, Net intensity, Intensity pattern, Multiplet information, and Quality. You can sort data according to these columns.

- **Atom numbers** are the numbers displayed on the molecule structure and are assigned automatically.
- **Chemical shift** values are displayed in the selected Measurement Unit.
- **Net intensity** is the integration value of the relevant signal.
- **Intensity pattern** describes the relative intensity of the multiplet elements.
- **Multiplet information** is the conventional one letter abbreviation of multiplicity, e.g.: **s** - singlet; **d** - doublet; **t** - triplet; ...
- **Quality** defines the prediction quality according to our validation method. Definitions: good, medium, rough.

Atom information Table has five columns, namely: Atom number, Chemical shift, Net intensity, Multiplet information, and Quality.

- **Atom numbers** are the numbers displayed on the molecule structure and are assigned automatically.
- **Chemical shift** values are displayed in the selected Measurement Unit.
- **Net intensity** is the integration value of the relevant signal.
- **Multiplet information** is the conventional one letter abbreviation of multiplicity, e.g.: **s** - singlet; **d** - doublet; **t** - triplet; ...
- **Quality** defines the prediction quality according to our validation method. Definitions: good, medium, rough.

Coupling information Table has four columns, namely: Atom 1, Atom 2, Value, and Quality.

- **Atom 1** and **Atom 2** are the number of atoms that the coupling constant is connected to.
- **The value** of the coupling constant is displayed in Hz.

- **Quality** defines the prediction quality according to our validation method. Definitions: good, medium, rough.

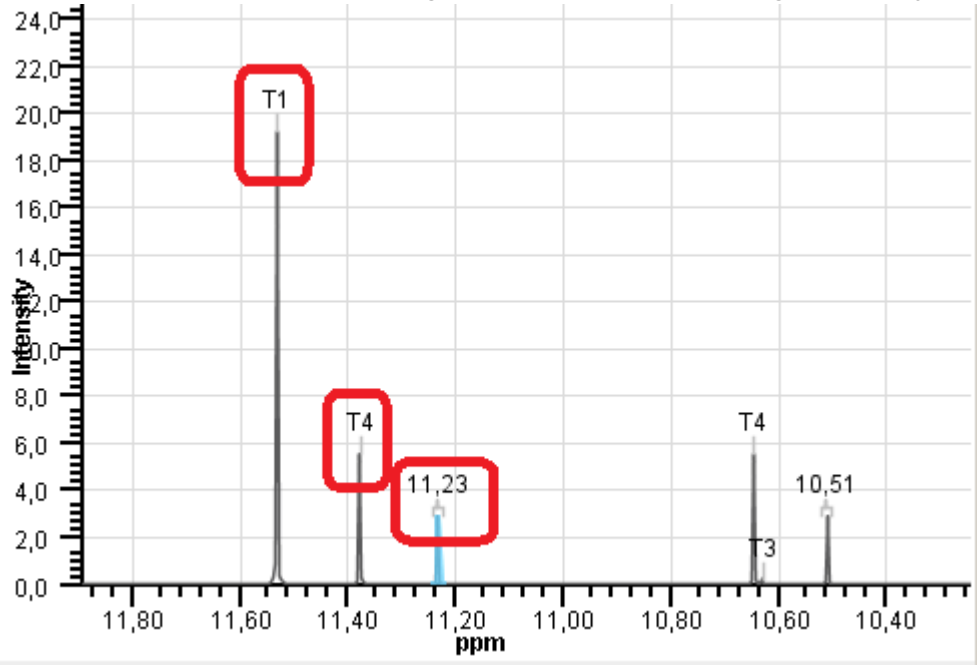
NMR Spectrum Preview Panel

displays the whole predicted spectrum. You can zoom in and out on spectrum by using your mouse, toolbar zoom items, or menu items.

- If you want to zoom in on specific region of the spectrum, use *left-click and drag* on **NMR Spectrum Preview Panel**. The background of the selected region will turn to white, while unselected region of the spectrum will turn to grey.
- You can move the selection window by left-clicking into the middle of the selection window; hold mouse button while moving the selection, and release button to place it.
- You can resize the selection window if you grab-and-drag its yellow side frames (except bottom frame).

NMR Spectrum Display Panel

displays the appropriate zoom region of the spectrum of the molecule presented on Molecule View Panel.
Move your mouse pointer over the **NMR Spectrum Display Panel** and use mouse-wheel to zoom in and out on NMR spectrum along the X-axis. Using Ctrl+mouse-wheel will zoom in and out on NMR spectrum along the Y-axis.
If you have added tautomers to the predicted spectrum via "Select Tautomers..." option and *Spectrum Labels* are on, the inactive tautomer signals are marked according to their symbols (T1, T2, ...).



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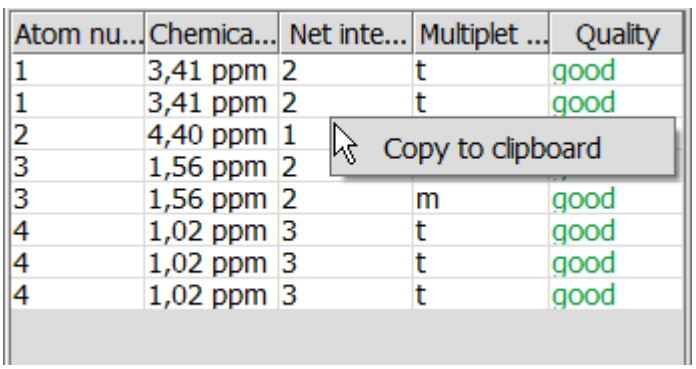
NMR Prediction Pop-up Menu



Right-clicking on any panel pops up a menu with the following element:

- **Copy to clipboard**: The panel in question will be copied to the clipboard.

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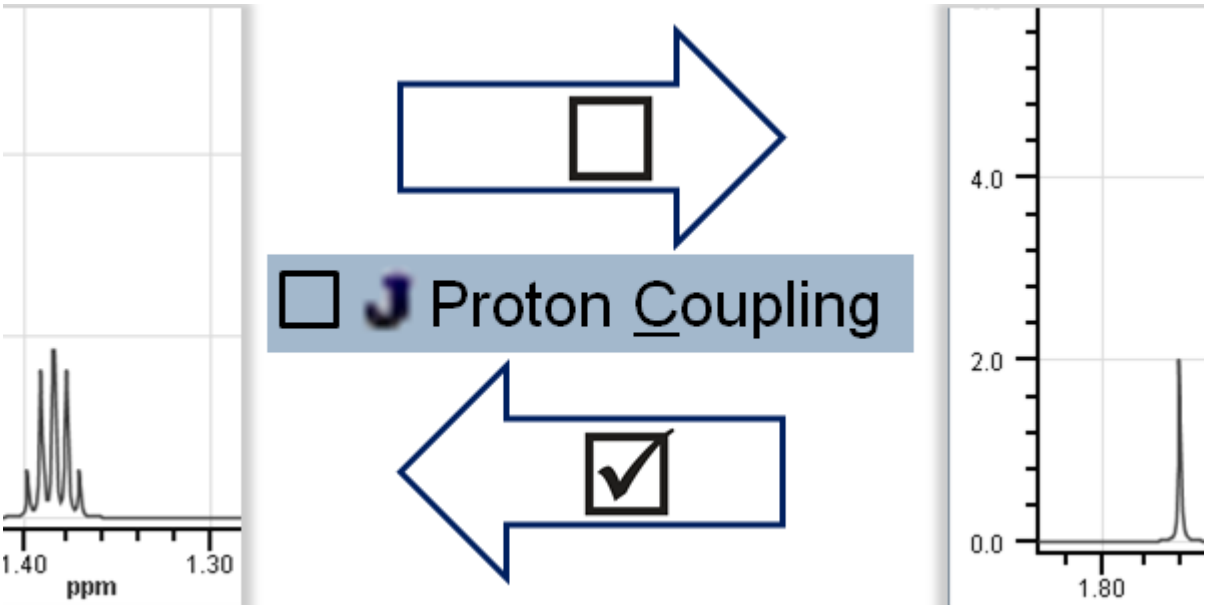
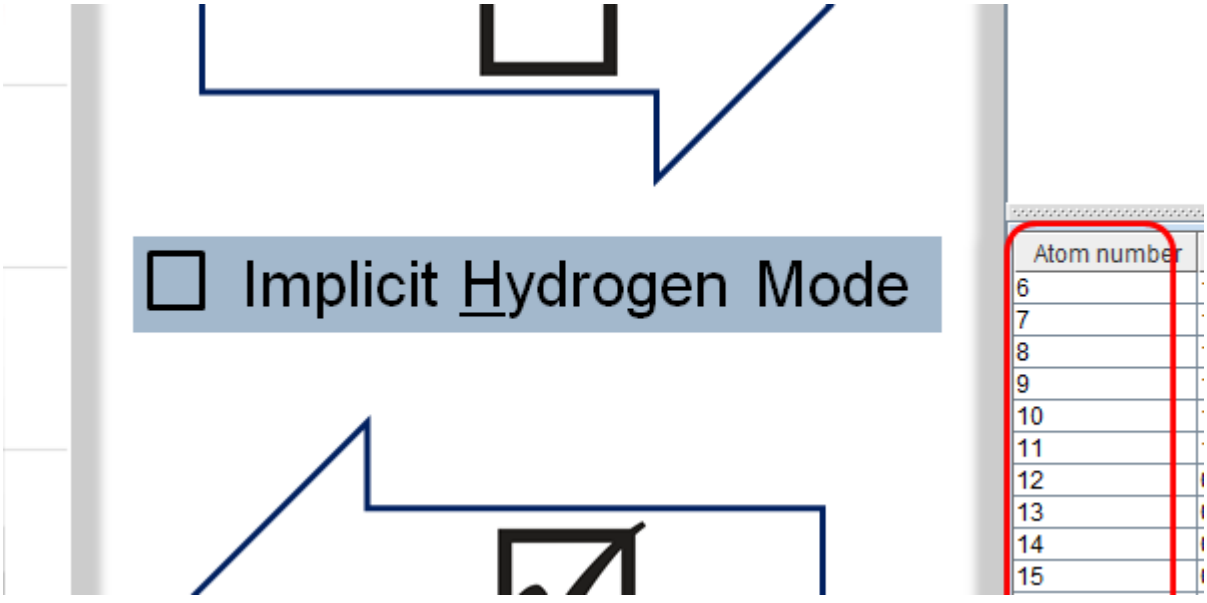
Examples

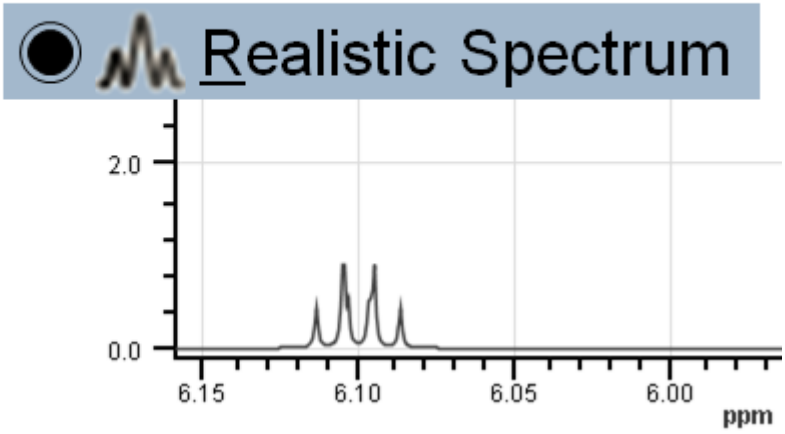
Toggle **Spin-Spin Coupling**: Options > Spin-Spin Coupling



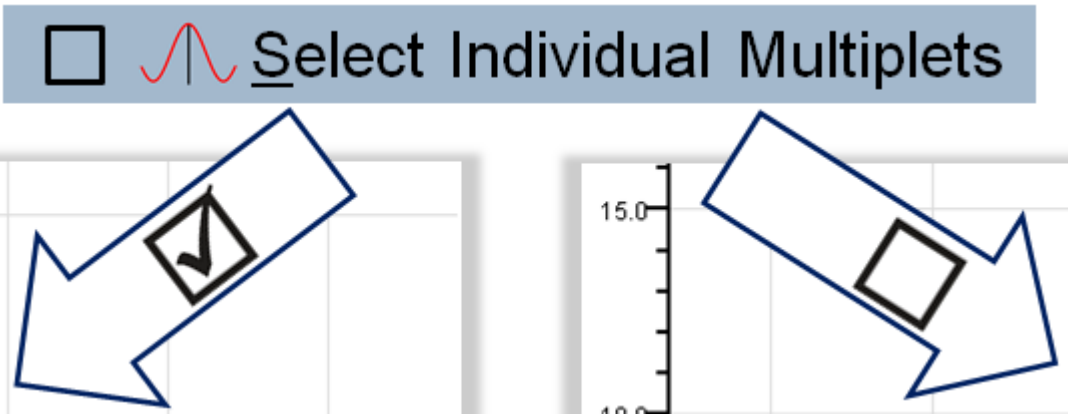
Toggle **Implicit Hydrogen Mode**: Options > Implicit Hydrogen Mode
Change default setting to: **View** > **Spectrum Labels** > **Atom Numbers**; Zoom in on the certain spectrum region.



Switch between **Realistic** and **Line Spectrum** display: View > Spectrum Display >



Select Individual Multiplets:



References

Gottlieb, H.E.; Kotlyar, V.; Nudelman, A. *J. Org. Chem.*, **1997**, *62*, 7612-7515; doi

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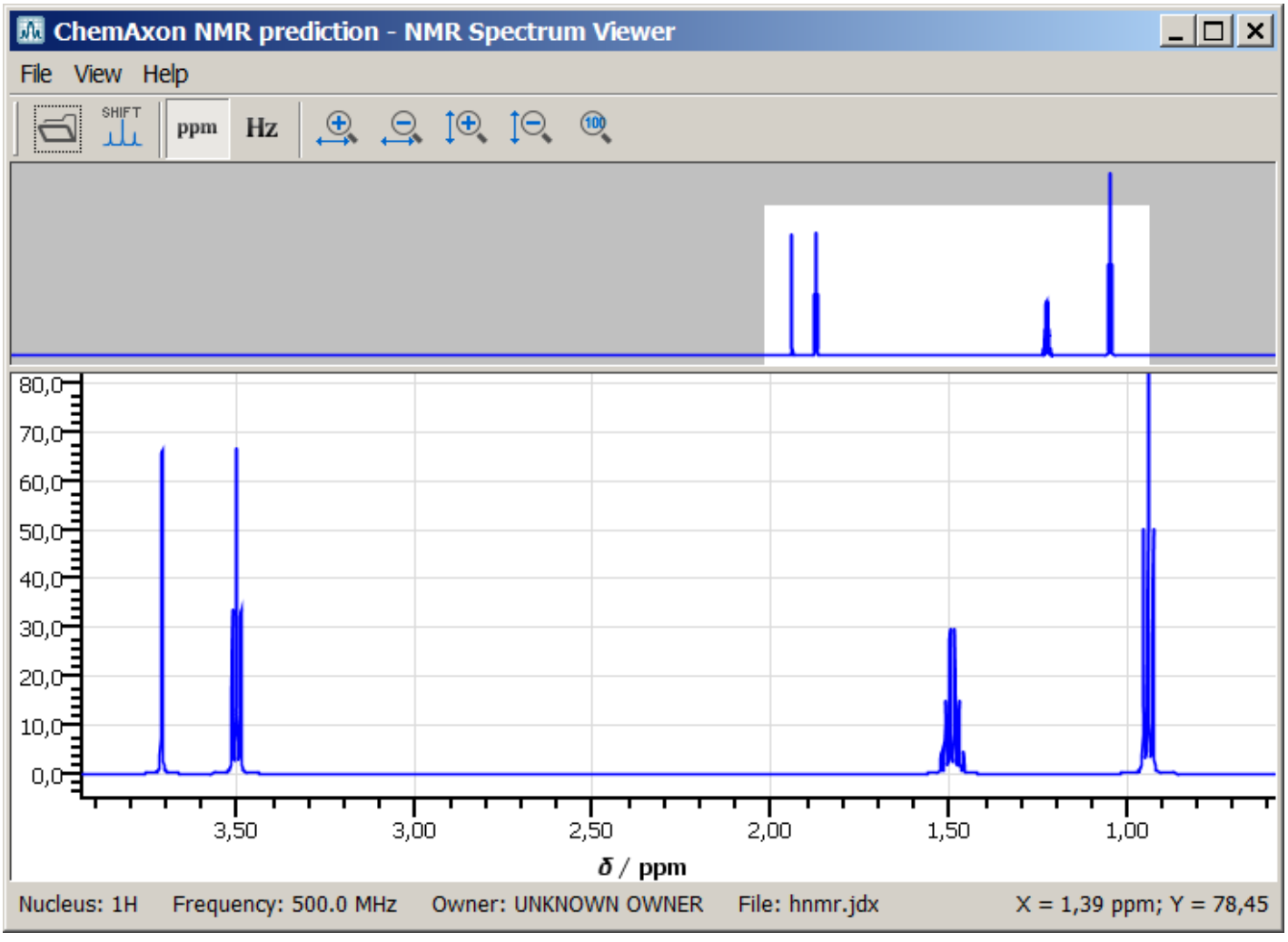
NMR Spectrum Viewer - ChemAxon's tool to view Nuclear Magnetic Resonance spectra

Version 6.1.7

Contents

NMR Spectrum Viewer

NMR Spectrum Viewer is part of the NMR Calculation group. It is able to display Nuclear Magnetic Resonance spectra saved in JCAMP-DX format (*.jdx). The opened spectrum can be zoomed in, exported to PDF files, or simply copy-pasted as image.



The **NMR Spectrum Viewer** window consists of a menu, toolbar, two panels, and a status bar.

NMR Spectrum Viewer Menu

The menu contains **File**, **View**, and **Help** elements.

File menu

- File > **Import from JCAMP-DX...**: Open an NMR Spectrum in JCAMP-DX format to display it in NMR Spectrum Viewer. Clicking on this menu item will launch the **Open** dialog window. Select an NMR spectrum in JCAMP-DX format and click on **Open**.
- File > **Exit**: Close application.

View menu

- View > **Measurement Unit**: Display NMR spectrum in one of the following units:
  - Hz **Hz** or;
  - ppm **ppm**.
- View > **Display Local Maximum Places**: NMR Spectrum Viewer can display local maximum places as spectrum labels when the JCAMP-DX file contains PEAKTABLE information.
- View > **Horizontal Zoom In**: Zoom in on NMR Spectrum along the X-axis.
- View > **Horizontal Zoom Out**: Zoom out on NMR Spectrum along the X-axis.
- View > **Vertical Zoom In**: Zoom in on NMR Spectrum along the Y-axis.
- View > **Vertical Zoom Out**: Zoom out on NMR Spectrum along the Y-axis.
- View > **Reset Zoom**: Restore spectrum zooming to full spectrum view.

Help

- Help > **Help Contents**: Open this help page in your browser.

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NMR Spectrum Viewer Toolbar

You can use toolbar elements to access selected NMR Spectrum Viewer menu items.

- Import from JCAMP-DX...
- Display Local Maximum Places
- Measurement Unit
- Horizontal Zoom In
- Horizontal Zoom Out
- Vertical Zoom In
- Vertical Zoom Out
- Reset Zoom

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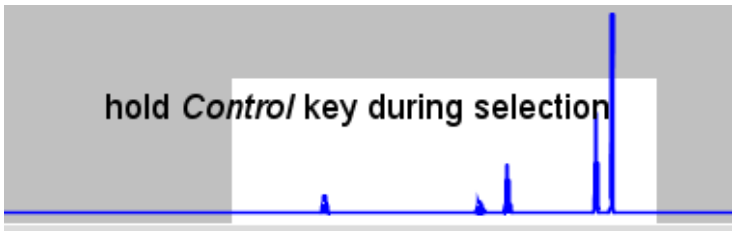
NMR Spectrum Viewer Panels

Panels can be copied separately as images by right-clicking on the appropriate panel and selecting **Copy to clipboard** action.

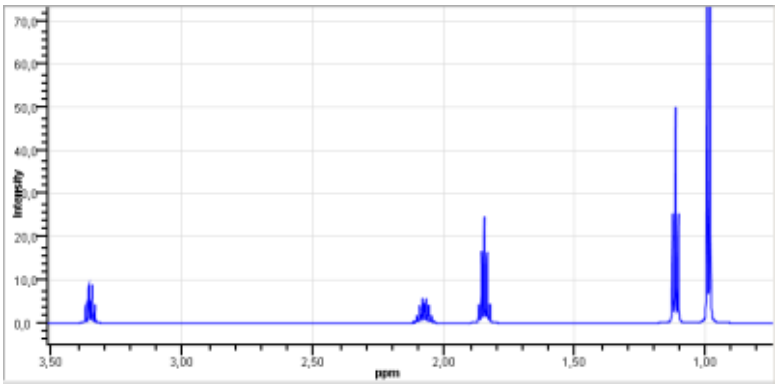
Spectrum View Panel



Displays the whole imported spectrum.

- If you want to zoom in on specific region of the spectrum, use *left-click and drag* or *ctrl + left-click and drag* on **NMR Spectrum Preview Panel**. The background of the selected region will be highlighted in white, while unselected region of the spectrum will turn to grey.
- You can move the selection window by left-clicking into the middle of the selection; hold mouse button while moving the selection, and release button to place it.
- You can resize the selection window if you grab-and-drag the yellow side frame around the highlighted area.

Spectrum Display Panel



Displays the appropriate zoom region of the spectrum. Move your mouse pointer over the **NMR Spectrum Display Panel** and use mouse-wheel to zoom in and out horizontally, ctrl+mouse-wheel to zoom in and out verically on the NMR spectrum.

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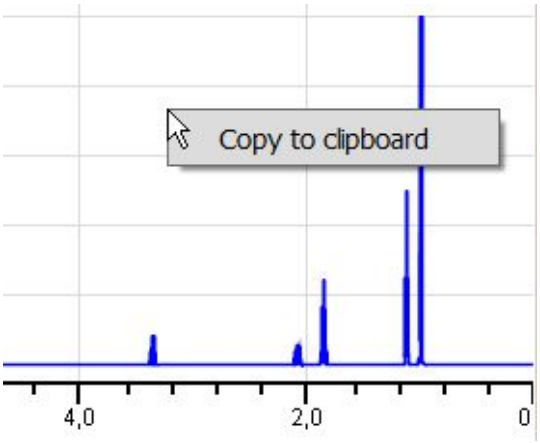
NMR Spectrum Viewer Pop-up Menu



Right-clicking on any panel pops up a menu with the following element:

- **Copy to clipboard**: The panel in question will be copied to the clipboard.

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NMR Spectrum Viewer Status Bar

The status bar of NMR Spectrum Viewer displays the X and Y coordinates of mouse cursor position, and the following data stored in the opened JCAMP-DX file:

- Nucleus;
- Frequency,
- Owner;
- File.

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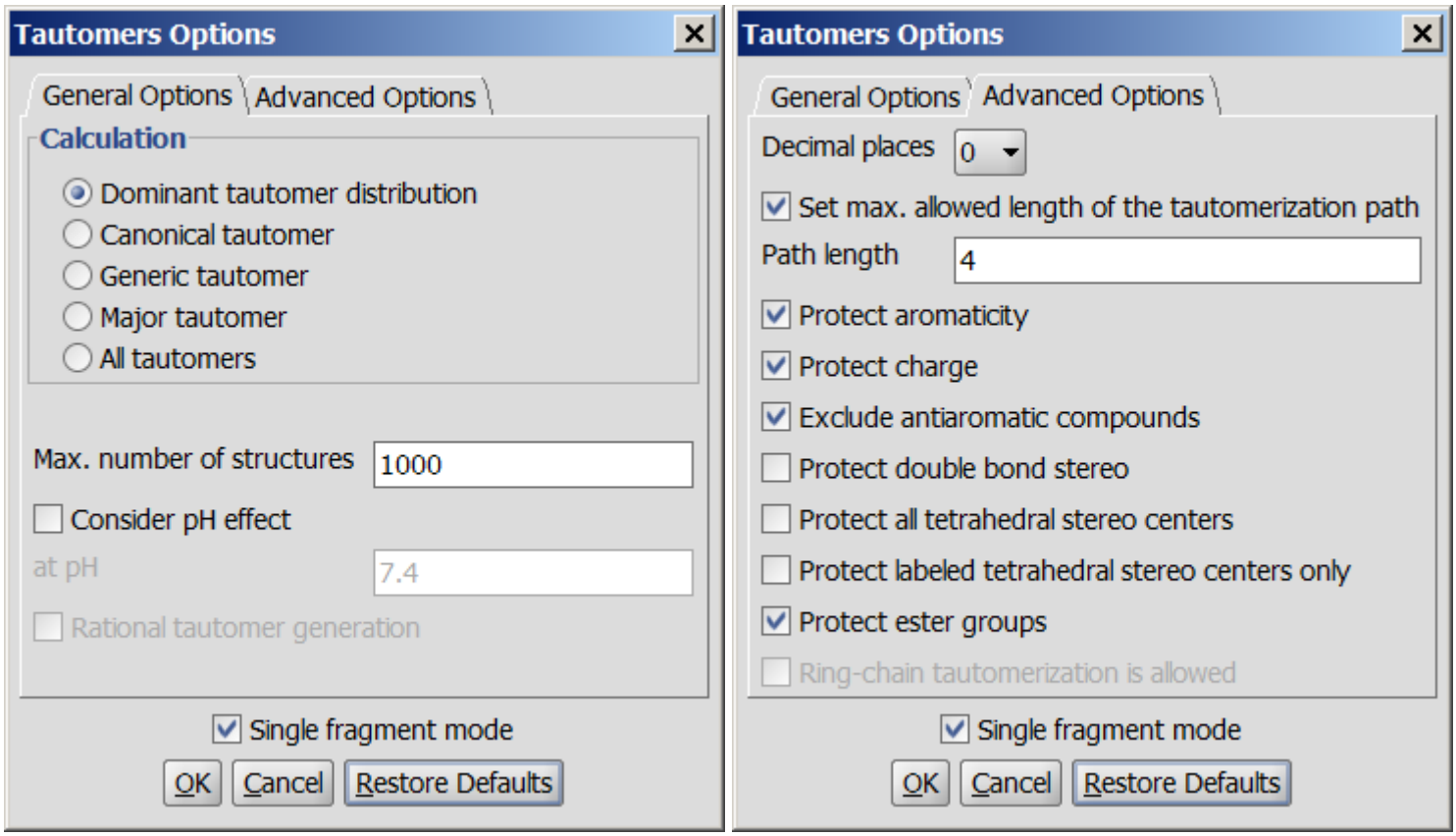
Isomers

Tautomer Generator Plugin

Tautomers are organic compounds that are interconvertible by tautomerization. Tautomerization reaction results in the formal migration of a hydrogen atom or proton, accompanied by a switch of a single bond and adjacent double bond. Commonly, the catalysts of these reactions are acids or bases. In solution a chemical equilibrium of the tautomers will be reached. Some types of tautomers: ketone-enol, amid-imidic acid, lactam-lactim, enamine-imine. Learn more about tautomerization and tautomers.

Tautomers of a compound can be determined with the help of Tautomer Generator Plugin.
Note: Tautomer Generator Plugin does not consider the three dimensional structure of molecules during tautomer generation, and symmetric structures are filtered out from the generated tautomer set.

Following options can be adjusted in the Tools > Isomers > Tautomers, **Tautomers Options** panel:



General options

- **Calculation:**
  - **Dominant tautomer distribution:** displays the percentage of different tautomers present at the given pH.
  - **Canonical tautomer:** calculates only the canonical tautomer of the structure. Rational tautomer generation mode can be activated.
  - **Generic tautomer:** used for the identification of tautomers in JChem databases. It is calculated according to these rules:
    - Tautomeric regions are identified.
    - All bond types in the tautomeric regions will be changed to ANY.
    - Each region will be assigned a data S-group with Sum(bonding electrons).
    - Explicit hydrogens are removed.
    - Isotope hydrogen:
      - outside of tautomer regions is kept as is
      - inside tautomer regions:
        - Non-mobilizable isotope hydrogen (attached to an atom which is neither donor nor

acceptor, so does not lose or gain H during tautomerization): the isotope is kept as is.
- Mobilizable isotope hydrogen (attached to a donor or acceptor atom in the tautomer region):
  the mobilizable isotopic hydrogens are removed, and the number of each type is included in the data sgroup description. For example: "36 e 2 D 3 T" (meaning 36 bonding electrons, 2 tautomerizable Deuterium and 3 Tritium atoms in the region).

- Only the protection or deprotection of tetrahedral stereo centers is taken into consideration.
- **Major tautomer:** gives the first species from the dominant tautomer distribution.
- **All tautomers:** calculates all possible tautomers. If any deuterium or tritium is involved in the tautomerization, it moves during enumeration. Rational tautomer generation mode can be activated.

- **Max. number of structures:** maximize the number of structures to display. This number is the sum of unique tautomeric count and degenerated tautomeric count; however, only unique tautormers are displayed their degenerated tautomeric pairs are not.
- **Consider pH effect:** takes into account the protonation states at given pH. Applicable for Major tautomer and Dominant tautomer distribution calculations.
- **Rational tautomer generation:** the tautomerization products are generated according to empirical rules. Rational tautomer generation narrows down the possible tautomerization paths and leads to chemically more feasible products.
- **Single fragment mode:** if checked (default), the results are displayed in separate windows; if unchecked, the calculation handles unlinked molecules together and results are in the same window.

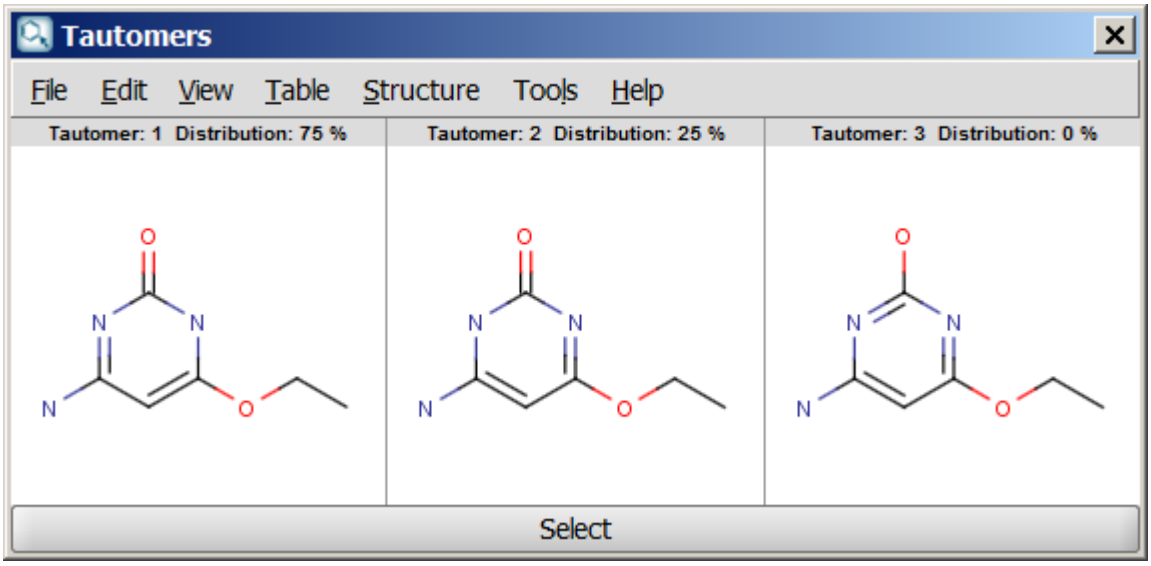
Advanced options

Note: the number of generated tautomers strongly depends on the options chosen.

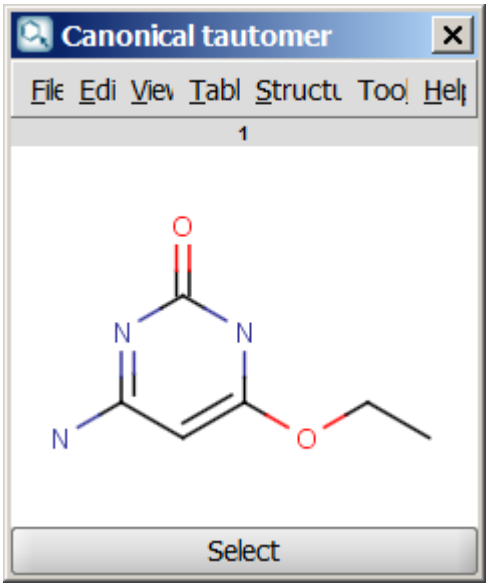
- **Decimal places:** setting the number of decimal places with which the tautomer distribution values are given.
- **Set max. allowed length of the tautomerization path; Path length:** sets the number of bonds which are considered by displacing a double bond.
- **Protect aromaticity:** if checked (default), the aromaticity will be maintained.
- **Protect charge:** if checked (default), defined charged atoms maintain their charge during calculation.
- **Exclude antiaromatic compounds:** if checked (default), any tautomer structure having an antiaromatic ring system will be discarded.
- **Protect double bond stereo:** if checked, all double bonds with stereo information remain intact. If unchecked (default), tautomer regions will lose the double bond stereo information, any other stereo information in the molecule is kept intact.
- **Protect all tetrahedral stereo centers:** if checked, stereocenters are not included in the tautomerization. If unchecked (default), tautomer regions will lose the tetrahedral stereo information, any other stereo information in the molecule is kept intact.
- **Protect labeled tetrahedral stereo centers only:** if checked, stereocenters labeled with chiral flag or MDL Enhanced Stereo Representation flags will not be included in tautomerization, other stereocenters will.
- **Single fragment mode:** if checked (default), the results are displayed in separate windows, if unchecked, the calculation handles unlinked molecules together and results are in the same window.
- **Protect ester groups:** if checked, ester is not taking part in tautomerization.
- **Ring-chain tautomerization is allowed:** this option can be activated when "All tautomers" function is selected. If it is checked, tautomer generation will take into account the possibility of ring closure.

For example, the following structures are the calculated tautomers of 4-amino-6-ethoxypyrimidin-2-ol:

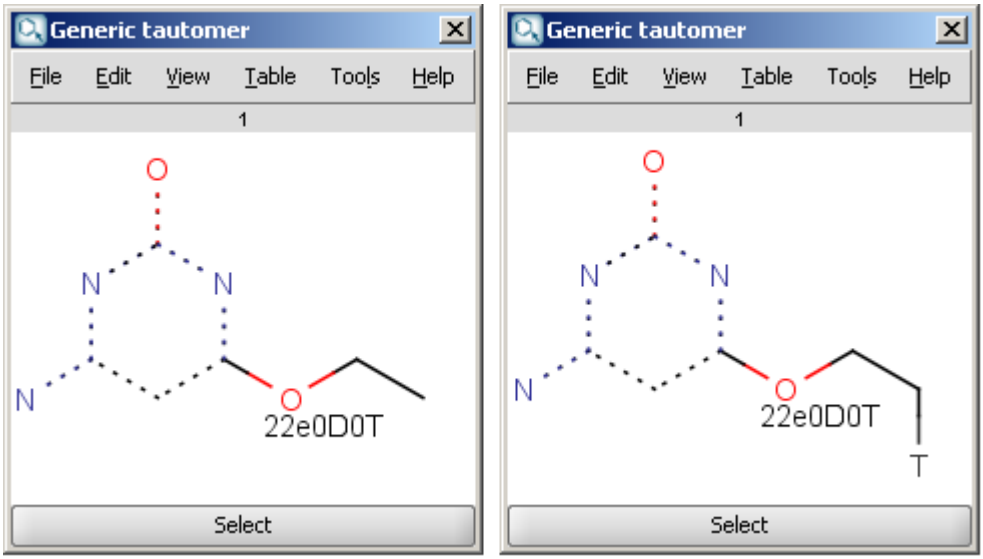
Dominant tautomer distribution



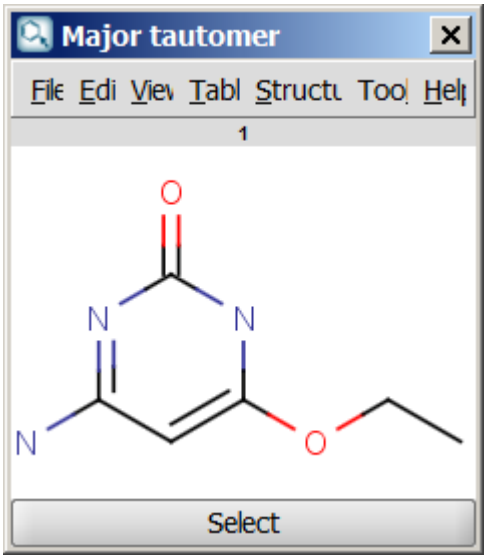
Canonical tautomer



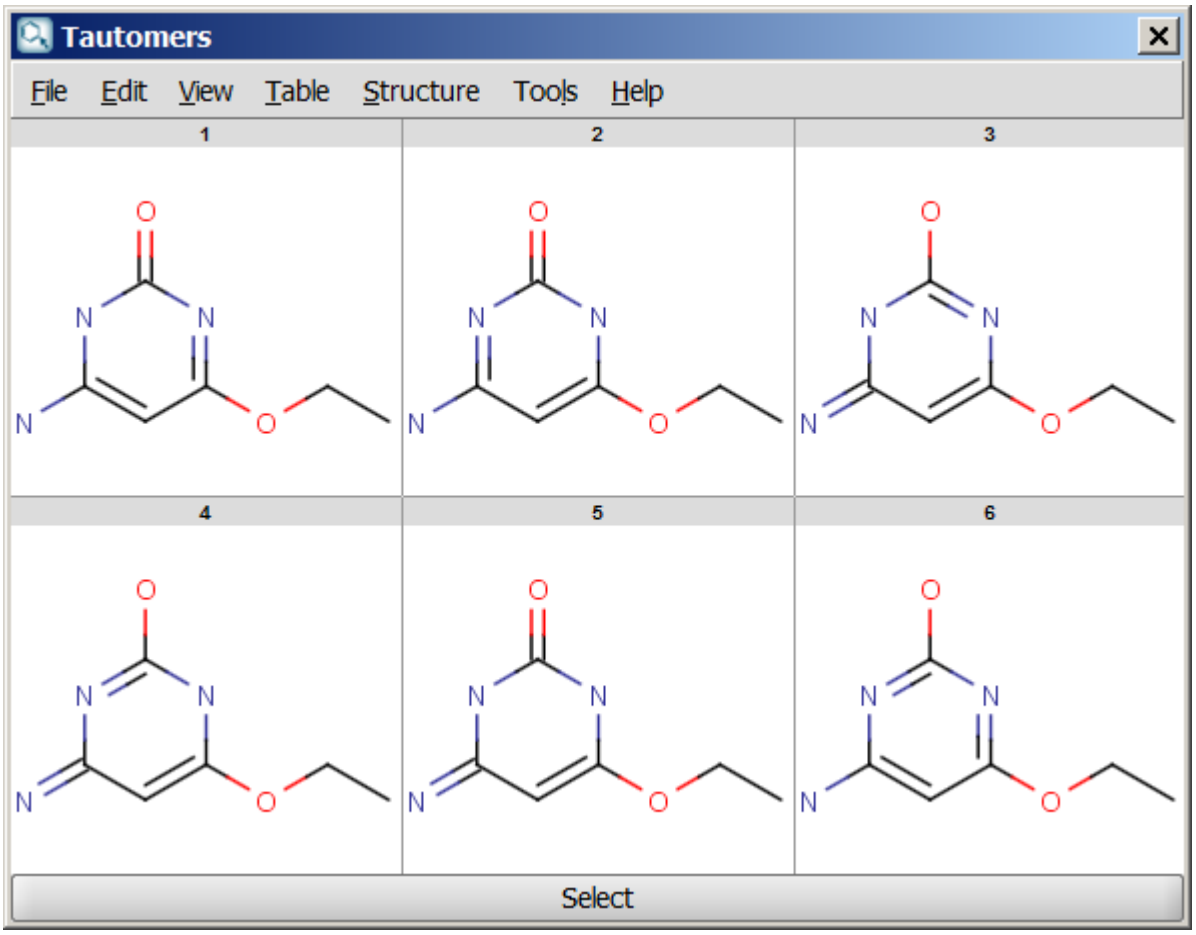
Generic tautomer and an isotope labeled example



Major tautomer

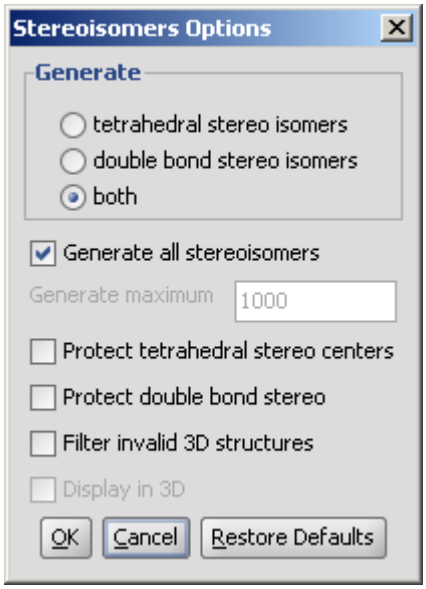


All tautomers



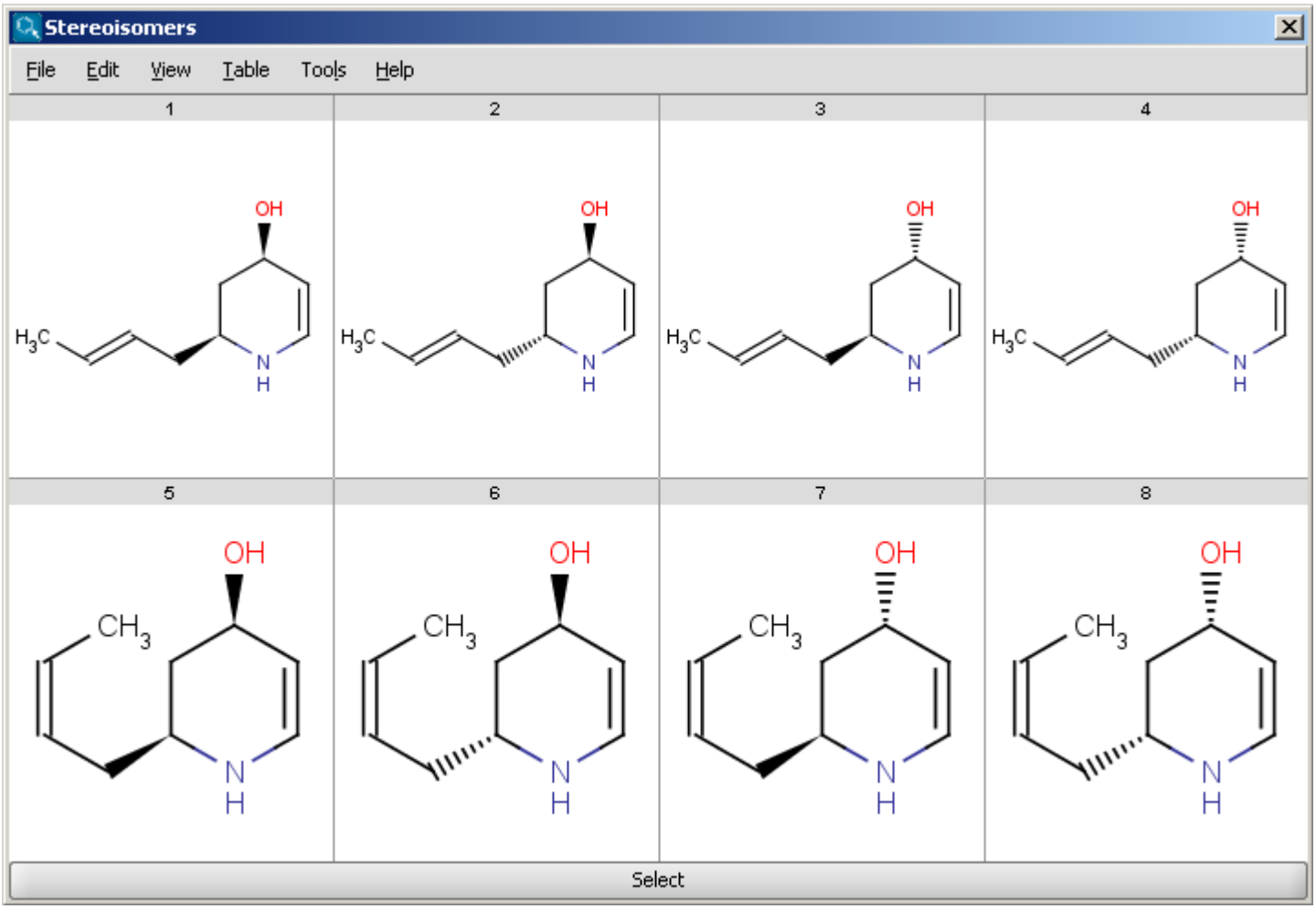
Stereoisomers Generator Plugin

The Stereoisomers Generator Plugin produces all possible stereoisomers of a given compound. The plugin handles both tetrahedral and double bond stereo centers.



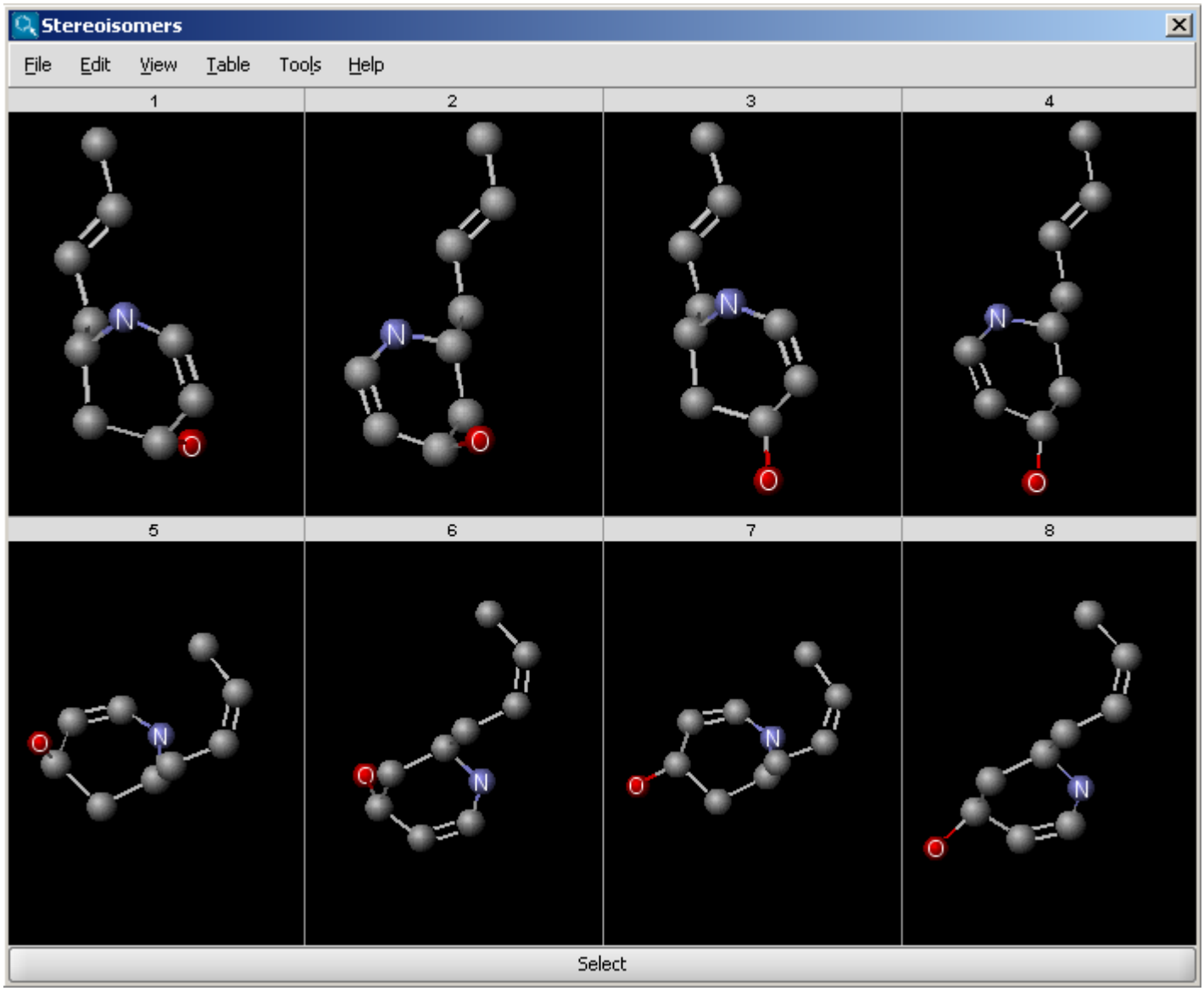
- **Generate**
  - **Tetrahedral stereo isomers:** only the R/S isomers are generated.
  - **double bond stereo isomers:** only E/Z isomers are generated.
  - **both:** both R/S and E/Z isomers are generated.
- **Generate all stereoisomers:** all isomers are generated
- **Generate maximum:** only the given number of structures are generated.
- **Protect tetrahedral stereo centers:** if checked, preset stereocenters are not included in the stereoisomer generation.
- **Protect double bond stereo:** if checked, all double bonds with preset stereo information remain intact.
- **Filter invalid 3D structures:** sterically restricted isomers are discarded.
- **Display in 3D:** results are displayed in a 3D viewer.

Results are displayed in a 2D viewer by default:



To replace your drawn molecule in the sketcher with any of the isomers shown, click on the structure then press "Select" at the bottom of the cells (the result window will be closed).

If "Filter invalid 3D structures" option is switched on in the **Stereoisomers Options** panel, the stereoisomers can also be displayed in 3D.



References

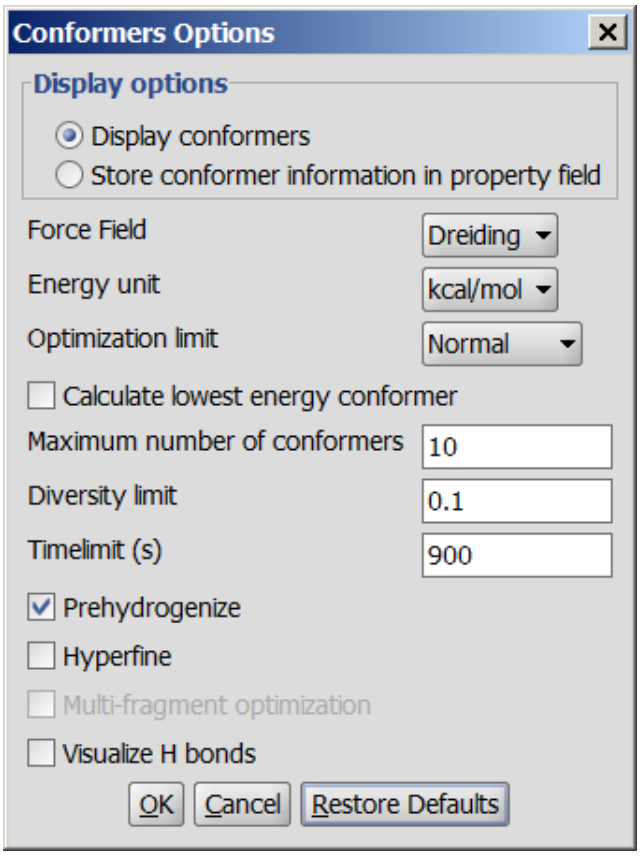
- Smith, M. B.; March, J. Advanced Organic Chemistry, 5th ed., Wiley Interscience, New York, 2001; pp 1218-1223. ISBN 0471585890

Conformation

Conformer Plugin

Conformational isomerism is a form of isomerism that describes the phenomenon of molecules with the same structural formula having different shapes due to rotations about one or more bonds. Different conformations might have different energies, can usually interconvert, and are very rarely isolatable.
Conformer plugin generates selected number of conformers or the lowest energy conformer of a molecule. For conformer calculation Dreiding force field is used.

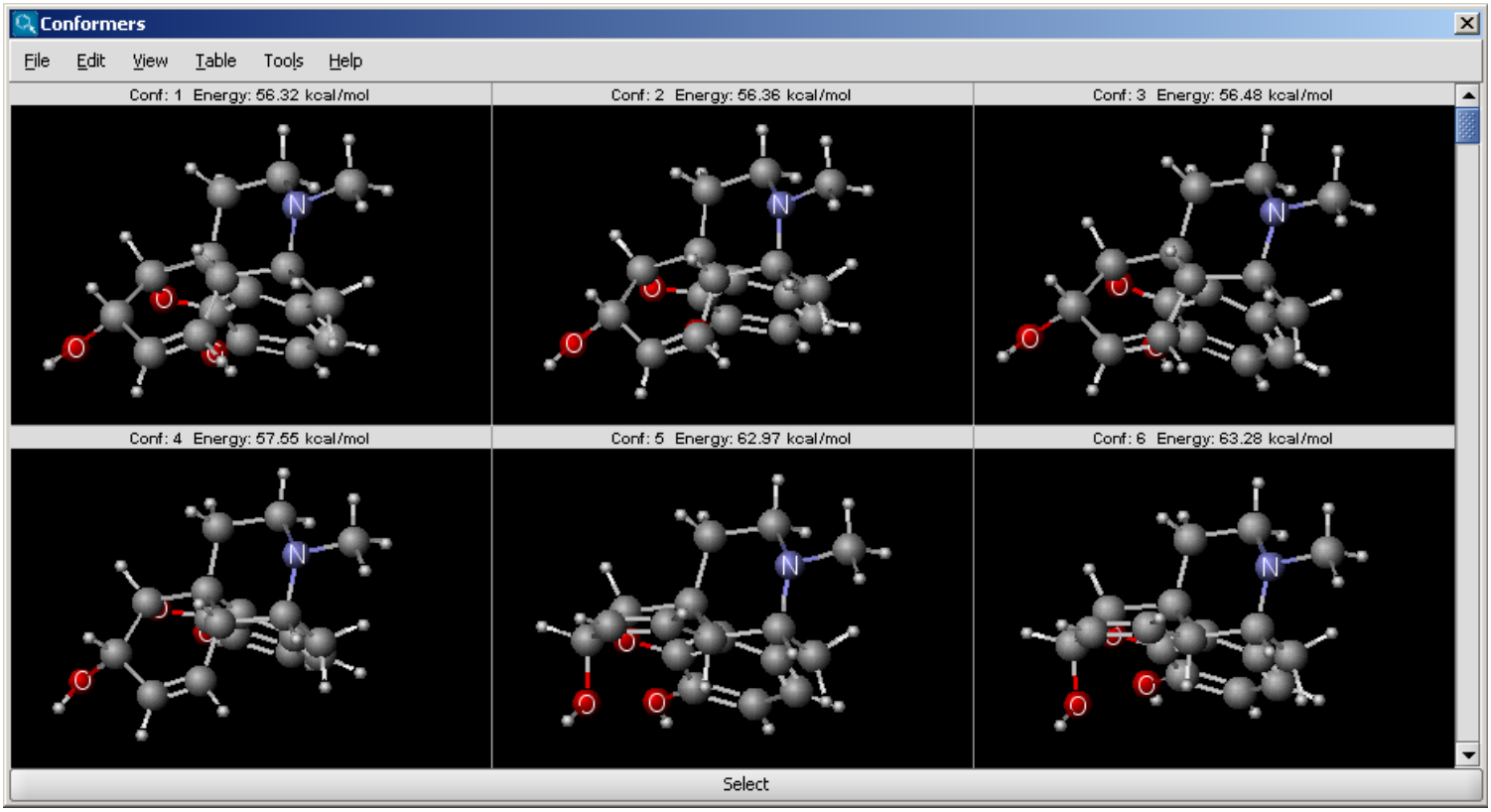
Different calculation parameters can be set in the **Conformers Options** panel:



- **Display options**
  - **Display conformers:** conformers are displayed in a MarivnView window.
  - **Store conformer information in property field:** the conformer data are calculated and stored with the structures. This option provides the calculations needed to select a specific conformer when using 3D cleaning (menu item Structure > Clean 3D > Display Stored Conformers). The conformers will only be stored if you select one result and click on "Select".
- **Force field:** force field used for calculation.
- **Energy unit:** giving results in kcal/mol or kJ/mol.
- **Optimization limit:** set the optimization to loose, normal, strict very strict (in this order increasing calculation times and precisity).
- **Calculate lowest energy conformer:** calculates and displays only the lowest energy conformer structure. When checking this option, max. number if conformers and diversity limit are disabled.
- **Maximum numbers of conformers:** limiting the number of calculated structures.
- **Diversity limit:** conformers within diversity limit will be considered the same and doubles removed.
- **Timelimit (s):** no conformers will be displayed if the calculation is stopped at the time limit set (e.g. there are too many conformers to calculate, the operation is cancelled after the given time had elapsed).
- **Prehydrogenize:** if checked, converts all implicit hydrogens to explicit hydrogens without removing them after the calculation. If unchecked, no explicit hydrogens will be added.
- **Hyperfine:** inserts more itineration steps in the calculations, gives more precision in results but the needed time becomes longer.
- **Multi-fragment optimization:** multi-fragment optimization with MMFF94.

- **Visualize H bonds**: marks intramolecular hydrogen bonds in the conformer where it is likely to occur.

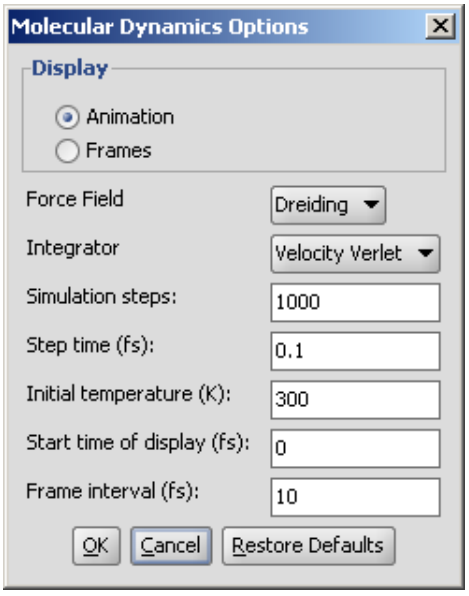
The results appear in a new window, containing all calculated conformers with their energy indicated:



Molecular Dynamics Plugin

The molecular dynamics plugin calculates the configurations of the system by integrating Newton's laws of motion.

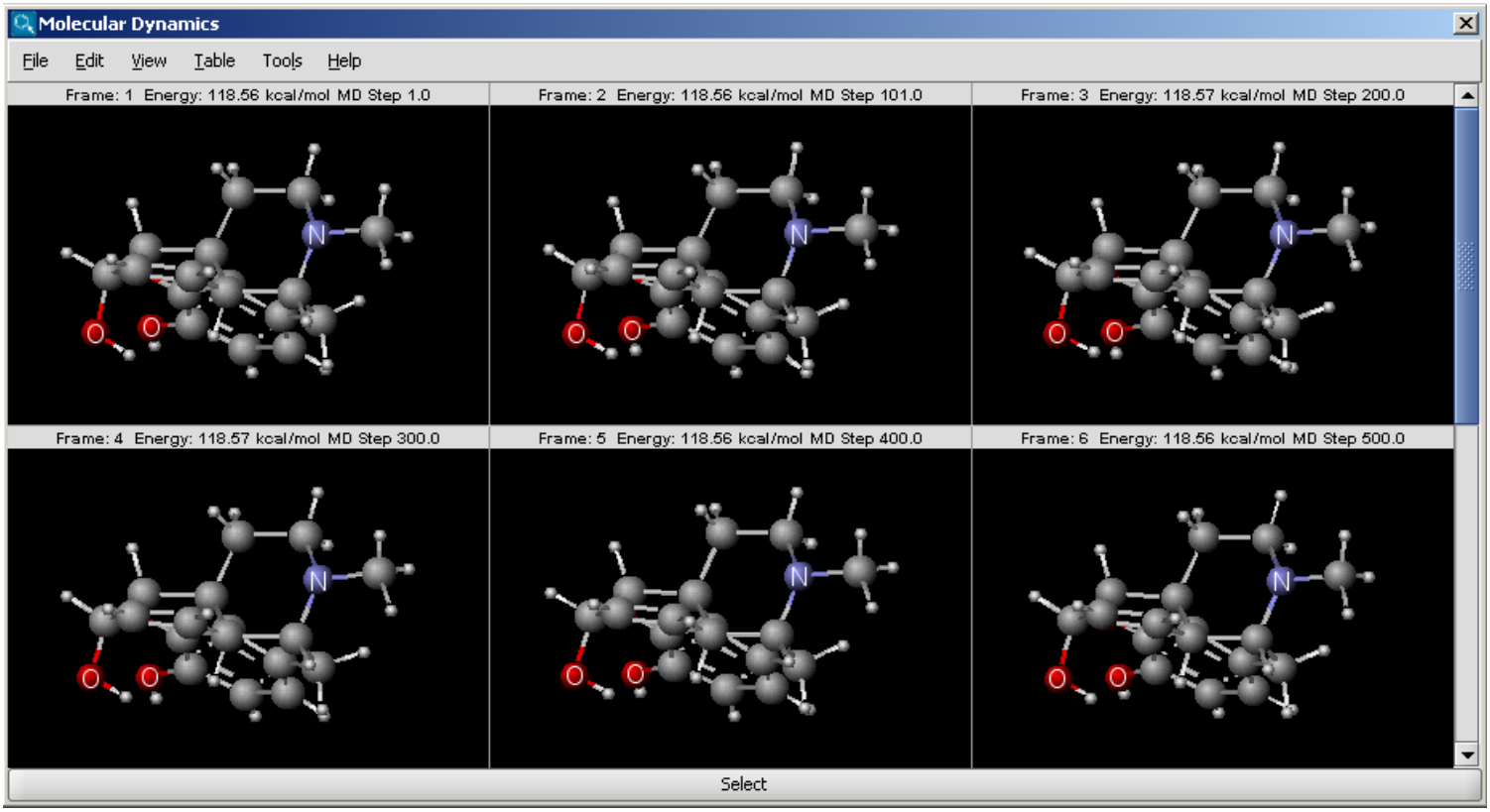
The calculation and the display options can be set in the **Molecular Dynamics Options** panel:



- **Display**: display mode
  - **Animation**: trajectory is displayed as an animation.
  - **Frames**: trajectory frames are displayed individually (see above).
- **Force field:** force field used for calculation.
- **Integrator:** integrator type used for solving Newton's laws of motion.
- **Simulation steps:** number of simulation steps.
- **Step time (fs):** time between simulation steps in femtoseconds.
- **Initial temperature (K):** initial temperature of the system in kelvin.

- **Start time of display (fs):** the time of the first simulation frame to be displayed in femtoseconds.
- **Frame interval (fs):** time between displayed simulation frames in femtoseconds.

The result is shown in a new window:



The window is a MarvinView window, with all its funcionalities to reach.

3D Alignment Plugin

3D Alignment overlays drug sized molecules onto each other in the 3D space.

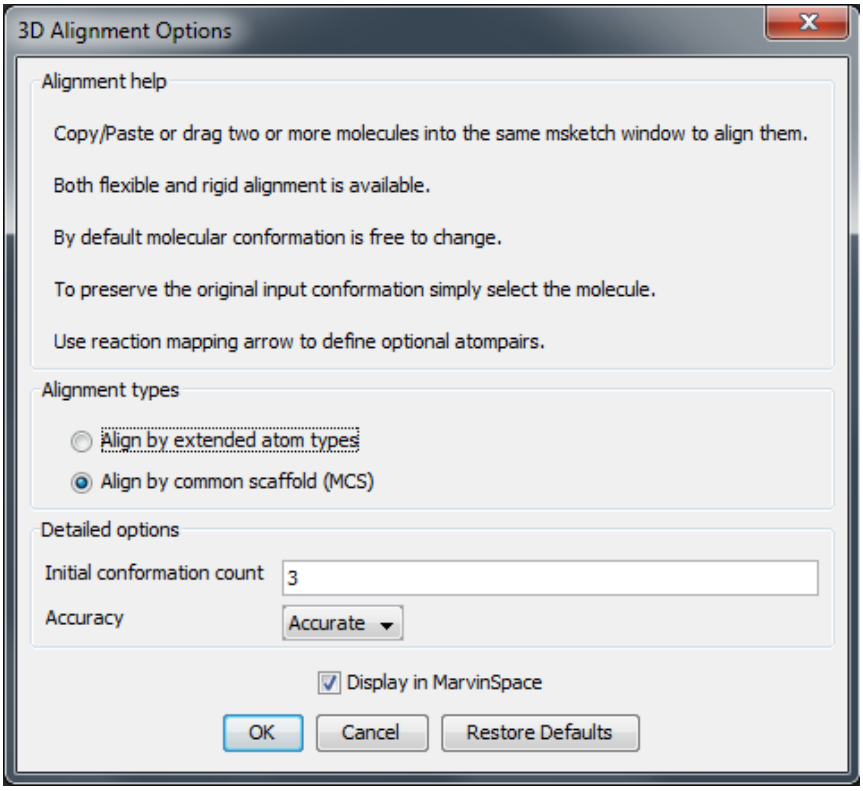
Input can be two or more molecules in 2D or in 3D. If 2D molecules are used their 3D structure is automatically generated by generate3D.

The conformation of the molecules can be treated flexible or the input conformation can be preserved. To preserve the input conformation simply select the molecule.

Usage: Molecules to align shoud be placed into the same MarvinSketch canvas by reading multiple molecules from a file. Alternatively, copy & paste or drag molecules from another sketch window.

Output is the aligned molecules in 3D. To save the aligned orientation use the popup menu: Click on the molecules with the second mouse button.

Following options can be set in the **3D Alignment Options** panel:



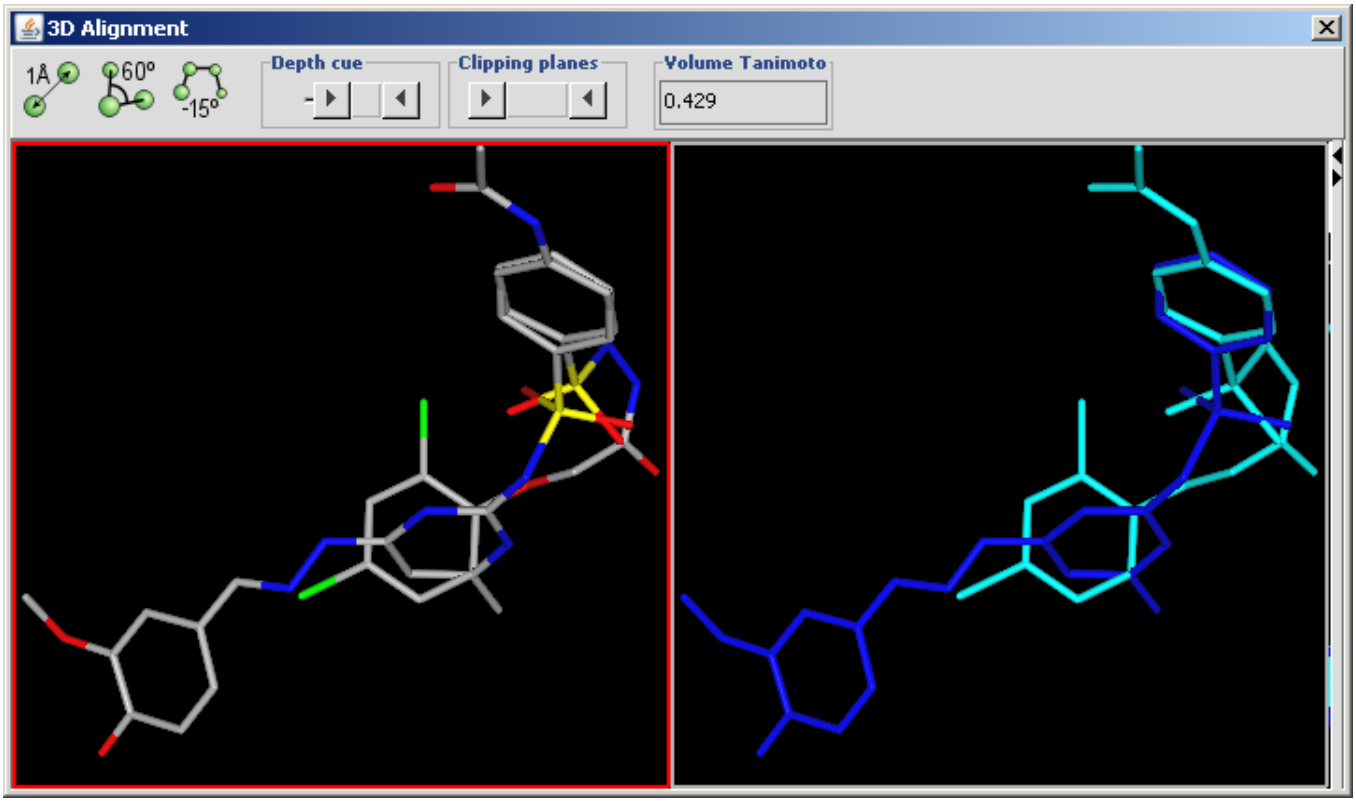
Alignment options

- **Align by extended atom types:** Extended atom types are assigned to each atom to enable chemically relevant atomic overlay. During the alignment process the overlap of the atoms of the same type is maximized. Types differentiate atomic number, hybridization state and aromaticity, e.g. aromatic nitrogen atom is not matched against a tertiary amine. These extended atom types correspond to the ones used in Dreiding force field.
- **Align by MCS:** The atom-atom pairing is obtained from the 2D maximum common substructure of the molecules. Alignment by extended atom types is applied on the non MCS atoms.

Detailed options

- **Initial conformation size:** Number of diverse conformations to generate as an input for the alignment.
- **Accuracy**: low, normal, high, very high: If lower selected the calcualtion is faster. The default is normal.

Display in MarvinSpace: the result window is a MarvinSpace 3D viewer. Molecules are visualized in different colors for better distinction of structures.



The aligned molecules are shown in a MarvinSpace window. Click and drag to rotate.

An example of usage

Suppose you have an SDfile contaning some molecules (called *wish.sdf*) that you wish to align. This must be converted for the alignment to a single molecule multi-fragment file where each fragment is a molecule from *wish.sdf*:

- Create an empty file in MarvinSketch called *empty.mol*
- Type at command prompt: `molconvert mol empty.mol -R wish.sdf -o wish_fused.mol`
- Open wish_fused.mol in MarvinSketch

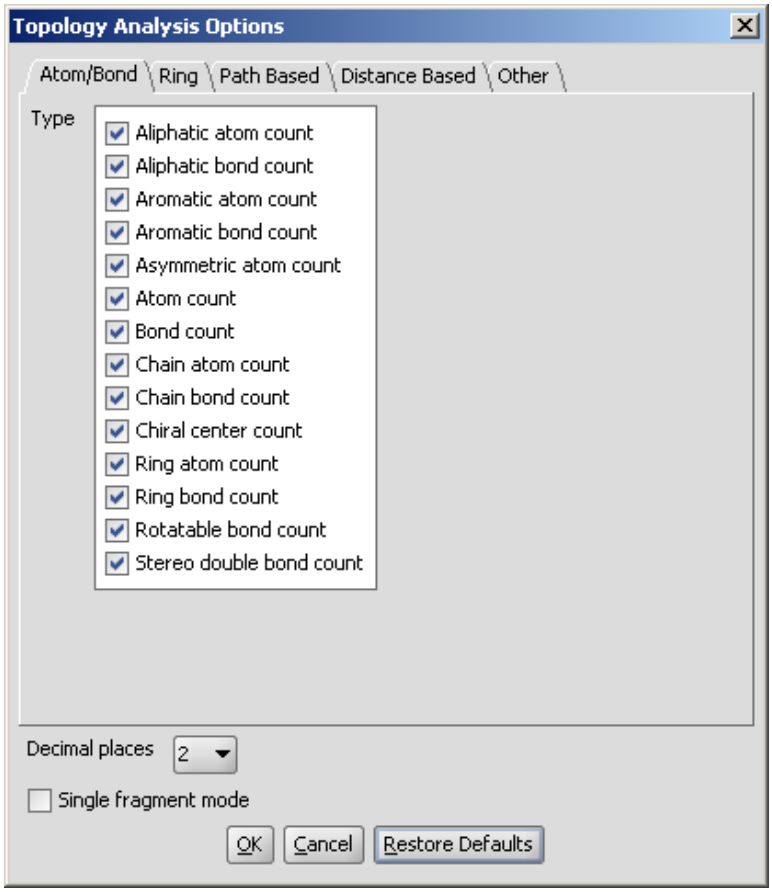
If you know which atoms to overlap use the Reaction arrow tool to connect them. This can improve the alignment. If you have only 3D molecules as input and you select one of them, its original conformation will be preserved during the alignment, while others remain flexible.

- Select Tools > Conformation > 3D Alignment
- Untick the Display in MarvinSpace option
- Alignment process can take a while, around a minute for 4 drugsize molecules
- Click on the result window with the right mouse button and select "Save As" from the pop menu.

Geometry

Topology Analysis Plugin

The Topology Analysis plugin provides characteristic values related to the topological structure of a molecule. These options can be set in the **Topology Analysis Options** panel, here shown with the Atom/bond tab opened:



Atom / bond

- **Aliphatic atom count:** number of atoms in the molecule having no aromatic bond (excluding hydrogens).
- **Aliphatic bond count:** number of non-aromatic bonds in the molecule (excluding bonds of hydrogen atoms).
- **Aromatic atom count:** number of atoms in the molecule having aromatic bonds.
- **Aromatic bond count:** number of aromatic bonds in the molecule.
- **Asymmetric atom count:** the number of asymmetric atoms (having four different ligands).
- **Atom count:** number of atoms in the molecule including hydrogens.
- **Bond count:** number of bonds in the molecule includingbonds of hydrogen atoms.
- **Chain atom count:** number of chain atoms (non-ring atoms excluding hydrogens).
- **Chain bond count:** number of chain bonds (non-ring bonds excluding bonds of hydrogen atoms).
- **Chiral center count:** the number of tetrahedral stereogenic centers. This function identifies two chiral centers in 1,4-dimethylcyclohexane, which does not contain asymmetric atoms.
- **Ring atom count:** number of ring atoms.
- **Ring bond count:** number of ring bonds.
- **Rotatable bond count:** number of rotatable bonds in the molecule. Unsaturated bonds, and single bonds connected to hydrogens or terminal atoms, single bonds of amides, sulphonamides and those connecting two hindered aromatic rings (having at least three ortho substituents) are considered non-rotatable.
- **Stereo double bond count:** number of double bonds with defined stereochemistry.

Ring

- **Aliphatic ring count:** number of those rings in the molecule that have non-aromatic bonds (SSSR based).
- **Aromatic ring count:** number of aromatic rings in the molecule. This number is calculated from the smallest set of smallest aromatic rings (SSSAR), which might contain rings which are not part of the standard SSSR ring set. As a

consequence, the sum of the aliphatic ring count and the aromatic ring count can sometimes be greater than the ring count value. The difference is the signal of a macroaromatic ring system.

- **Carbo ring count:** number of rings containing only carbon atoms.
- **Carboaliphatic ring count:** number of aliphatic rings containing only carbon atoms.
- **Carbooaromatic ring count:** number of aromatic rings containing only carbon atoms (SSSAR based).
- **Fused aliphatic ring count:** number of aliphatic rings having common bonds with other rings.
- **Fused aromatic ring count:** number of aromatic rings having common bonds with other rings.
- **Fused ring count:** number of fused rings in the molecule (having common bonds).
- **Hetero ring count:** number of rings containing hetero atom(s).
- **Heteroaromatic ring count:** number of aromatic heterocycles in the molecule.
- **Largest ring size:** size of the largest ring in the molecule.
- **Largest ring system size:** number of rings in the largest ring system.
- **Ring count:** number of rings in the molecule. This calculation is based on SSSR (Smallest Set of Smallest Rings).
- **Ring system count:** number of disjunct ring systems.
- **Smallest ring size:** size of the smallest ring in the molecule.
- **Smallest ring system size:** number of rings in the smallest ring system.

Path based

- **Platt index:** sum of the edge degrees of a molecular graph.
- **Randic index:** harmonic sum of the geometric means of the node degrees for each edge.

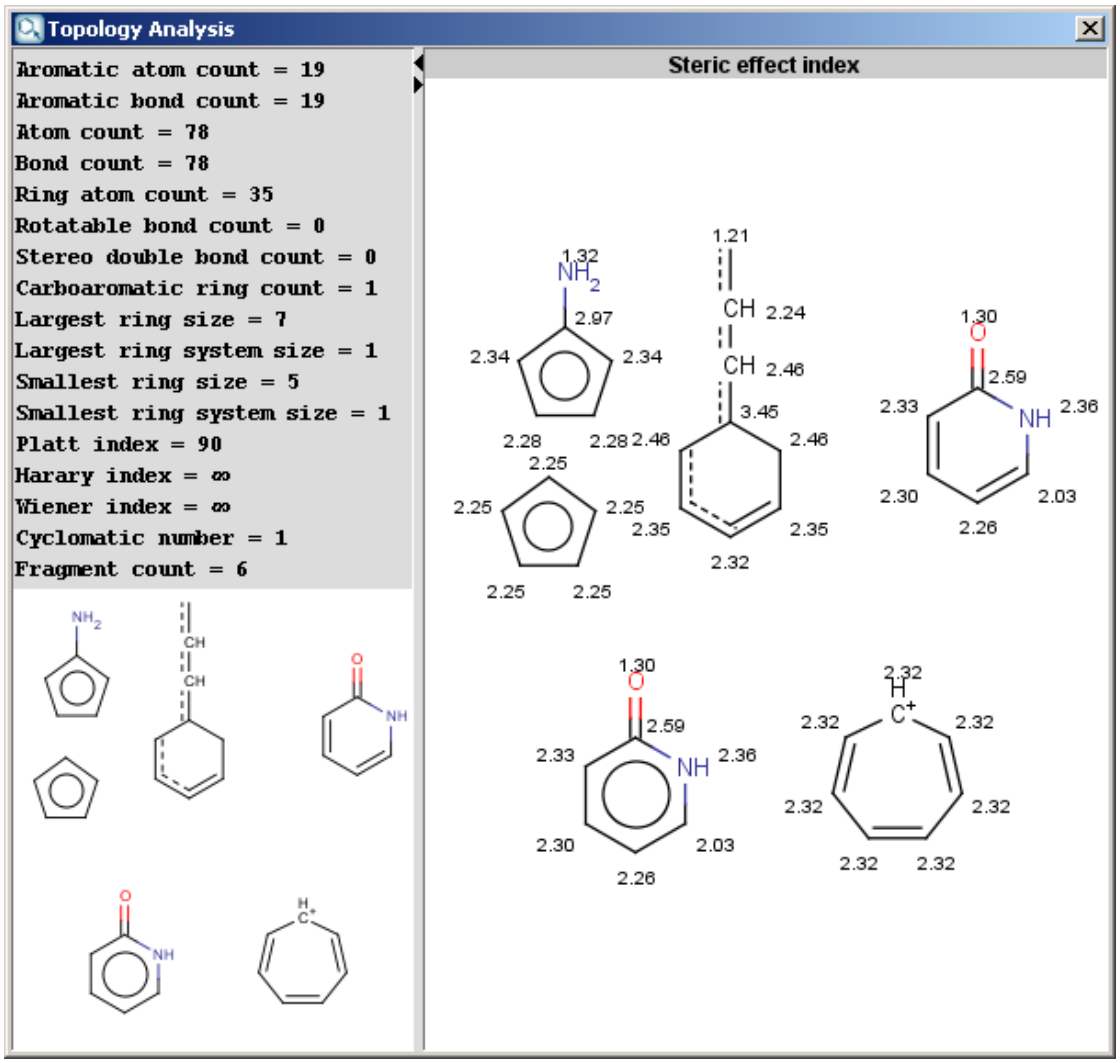
Distance based

- **Balaban index:** the Balaban distance connectivity of the molecule, which is the average distance sum connectivity.
- **Distance degree:** the sum of the corresponding row values in the distance matrix for each atom.
- **Eccentricity:** the greatest value in the corresponding row of the distance matrix for each atom.
- **Harary index:** half-sum of the off-diagonal elements of the reciprocal molecular distance matrix of the molecule.
- **Hyper Wiener index:** a variant of the Wiener index.
- **Szeged index:** The Szeged index extends the Wiener index for cyclic graphs by counting the number of atoms on both sides of each bond (those atoms only which are nearer to the given side of the bond than to the other), and sum these counts.
- **Wiener index:** the average topological atom distance (half of the sum of all atom distances) in the molecule.
- **Wiener polarity:** the number of 3 bond length distances in the molecule.

Other

- **Cyclomatic number:** the smallest number of bonds which must be removed so that no circuit remains. Also known as circuit rank.
- **Fragment count**: number of fragments in the sketch.
- **Steric effect index:** topological steric effect index (TSEI) of an atom calculated from the covalent radii values and topological distances. The stericEffectIndex is related to the steric hindrance of the given atom.
- **Fsp3**: number of sp^3 hybridized carbons diveded by the total carbon count

The result is shown in a separate window:

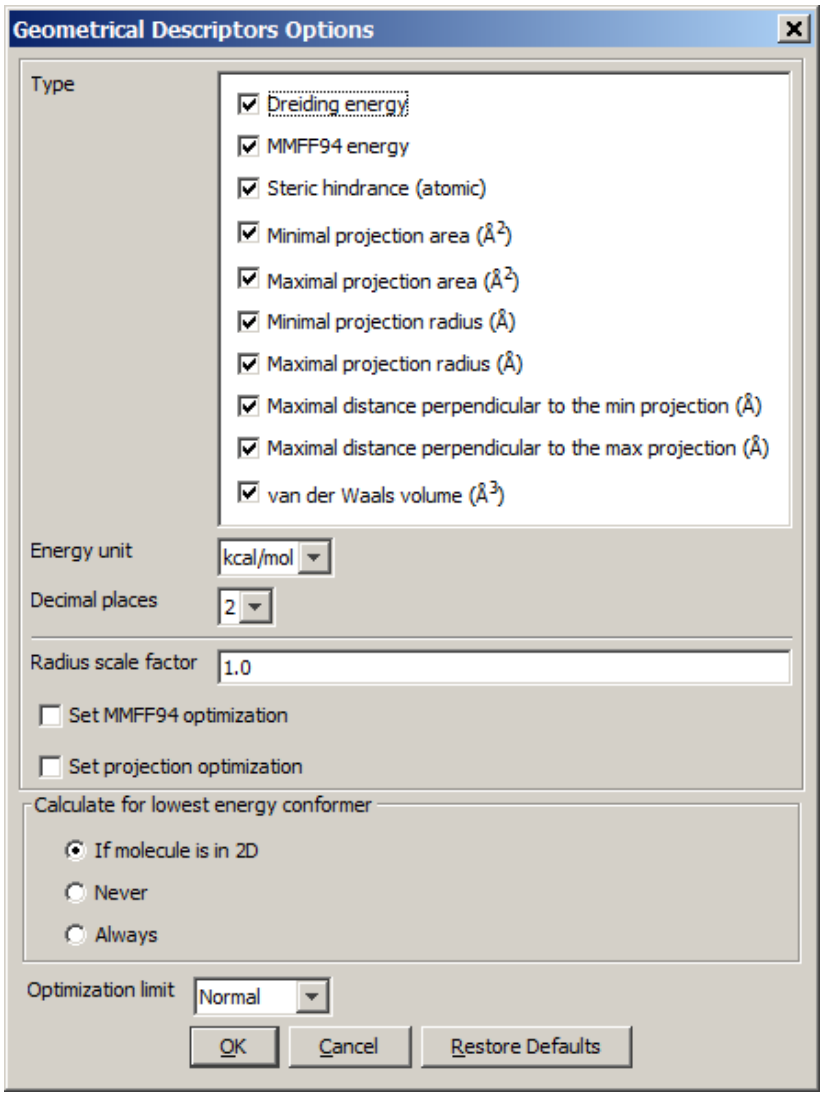


The contents of text field can be copied to the clipboard as text, the structure fields offers a MarvinView context menu.

Geometrical Descriptors Plugin

The Geometrical Descriptors plugin provides characteristic values related to the geometrical structure of a molecule. It can calculate steric hindrance and Dreiding energy. The calculation can predict and use the lowest energy conformer of the input structure.

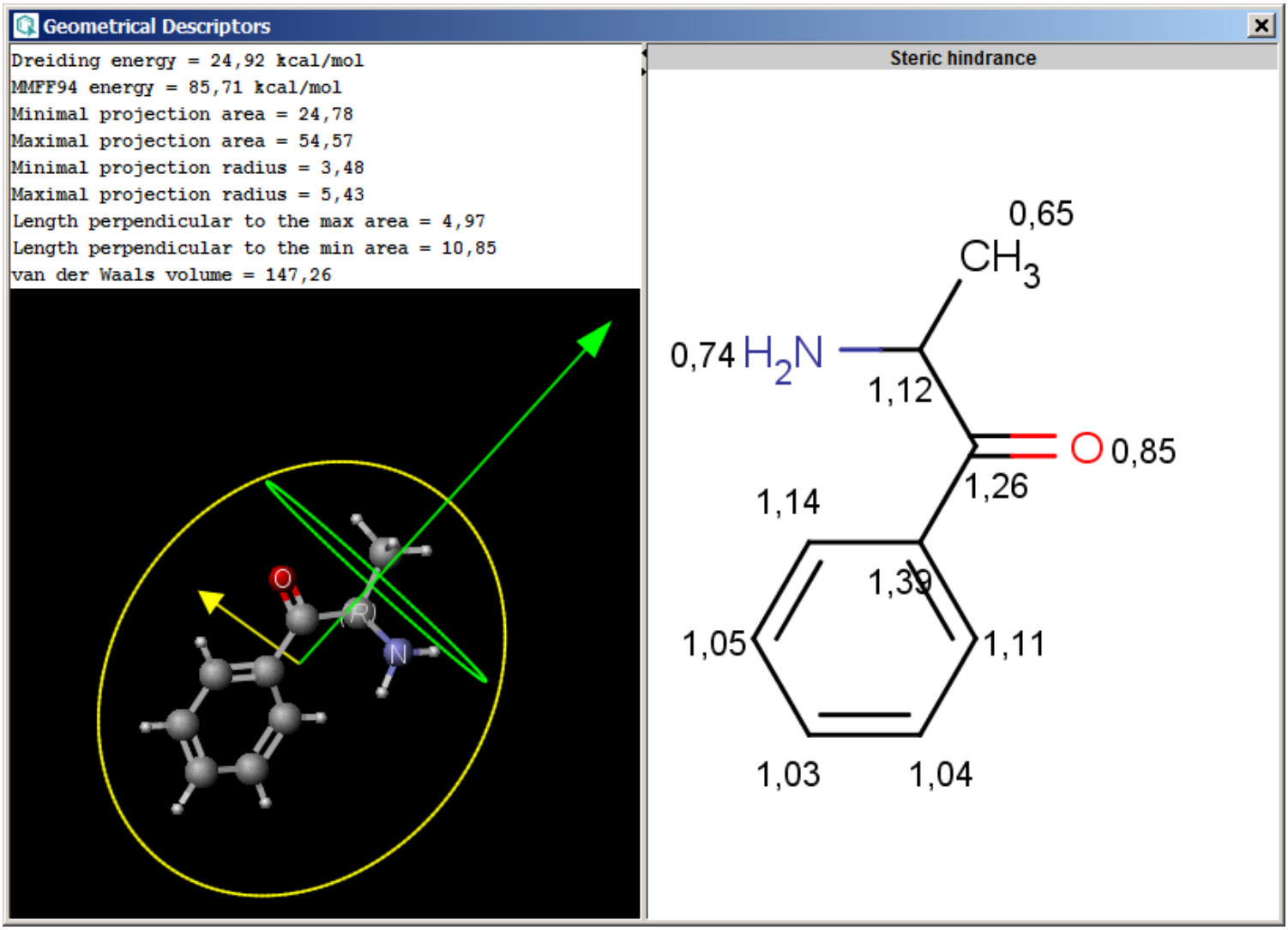
The calculation and the display options can be set in the **Geometrical Descriptors Options** panel:



- **Type**
  - **Dreiding energy:** calculates the energy related to the 3D structure (conformation) of the molecule using dreiding force field.
  - **MMFF94 energy:** calculates the energy related to the 3D structure (conformation) of the molecule using MMFF94 force field.
  - **Steric hindrance:** steric hindrance of an atom calculated from the covalent radii values and geometrical distances.
  - **Minimal projection area:** calculates the minimum of projection areas of the conformer, based on the van der Waals radius (in $Å^2$).
  - **Maximal projection area:** calculates the maximum of projection areas of the conformer, based on the van der Waals radius (in $Å^2$).
  - **Minimal projection radius:** calculates the radius for the minimal projection area of the conformer (in Å).
  - **Maximal projection radius:** calculates the radius for the maximal projection area of the conformer (in Å).
  - **Maximal distance perpendicular to the min projection:** calculates the maximal extension of the conformer perpendicular to the minimal projection area (in Å).
  - **Maximal distance perpendicular to the max projection:** calculates the maximal extension of the conformer perpendicular to the maximal projection area (in Å).
  - **van der Waals volume:** calculates the van der Waals volume of the conformer (in $Å^3$).
- **Energy unit:** gives dreiding energy in kcal/mol or kJ/mol.
- **Decimal places:**setting the number of decimal places with which the result value is given.
- **Radius scale factor:** atom radii from the periodic system are multiplied by this number.
- **Set MMFF94 optimalization**: The structure is optimized before MMFF94 energy calculation.
- **Set projection optimalization** The structure is optimized before projection area and projection radius calculation(s).
- **Calculate for lowest energy conformer:**
  - If molecule is in 2D: the lowest energy conformer of the 2D molecule is generated, and its parameters calculated. 3D input molecules are considered in the given conformation.
  - Never: the input molecule is used for calculation.

Always: the lowest energy conformer is generated (3D and 2D molecules as well), and its geometry parameters calculated.

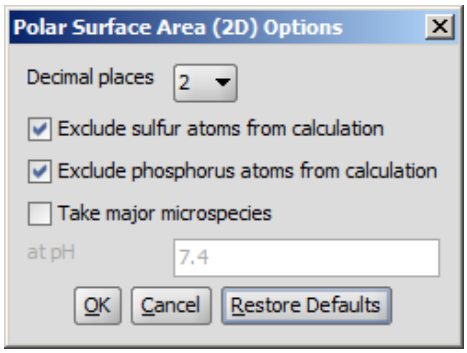
- **Optimization limit:**
  - Very loose
  - Normal
  - Strict
  - Very strict



Polar Surface Area Plugin (2D)

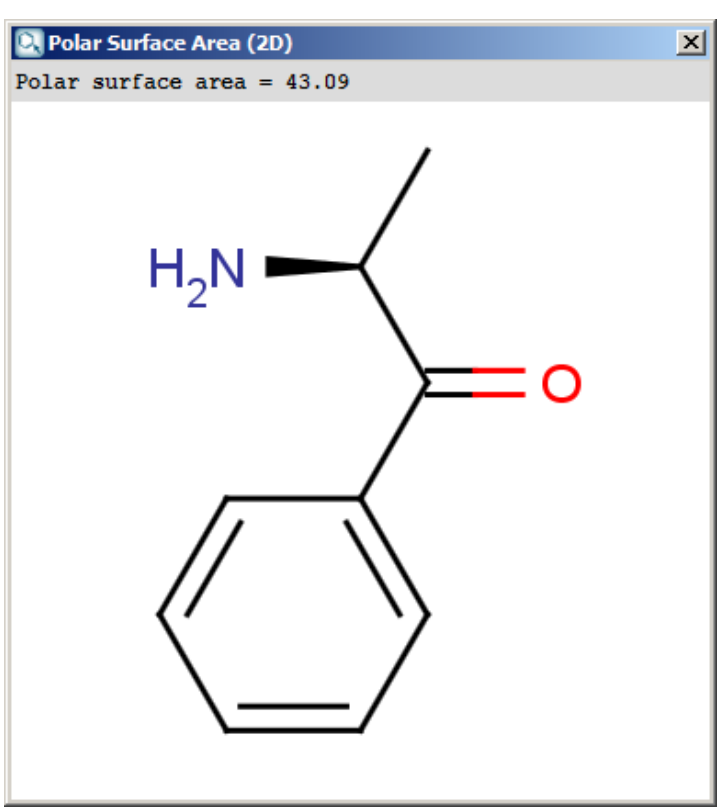
Polar surface area (PSA) is formed by polar atoms of a molecule. It is a descriptor that shows good correlation with passive molecular transport through membranes, and so allows estimation of transport properties of drugs. Estimation of topoligical polar surface area (TPSA) is based on the method given in this paper. The method provides results which are practically identical with the 3D PSA, while calculation time of TPSA is approximately 100-times faster. This method is more suitable for fast bioavailability screening of large virtual libraries. The TPSA value can be calculated both for the neutral form and the major microspecies.

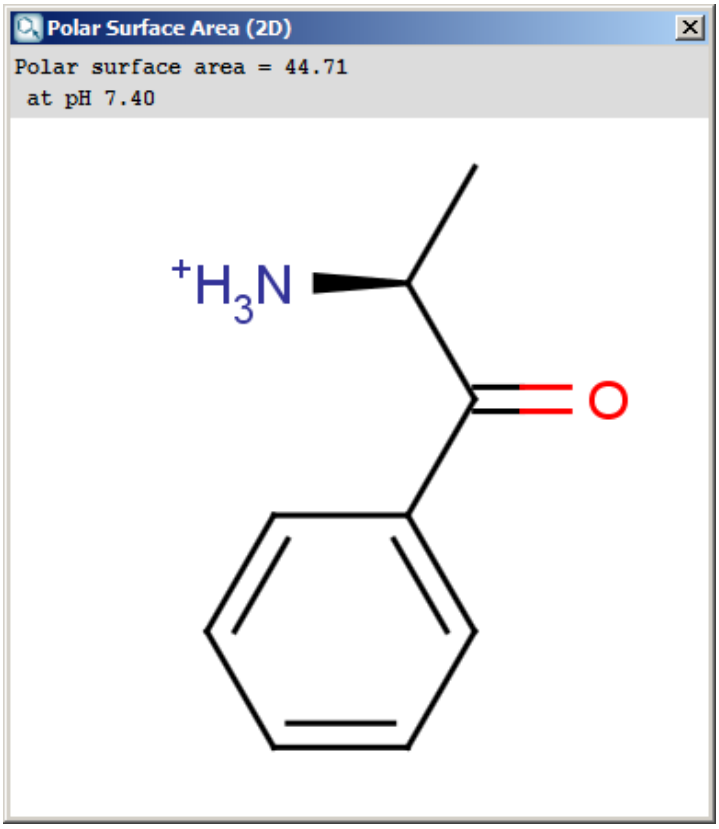
The calculation and the display options can be set in the **Polar Surface Area (2D) Options** panel:



- **Decimal places:**setting the number of decimal places with which the result values are given.
- **Exclude sulfur atoms from calculation**
- **Exclude phosphorus atoms from calculation**
- **Take major microspecies at pH:** calculates the polar surface area for the major microspecies present at the given pH.

The result appears in a separate window, if several structures were drawn navigation is possible with a scroll bar:



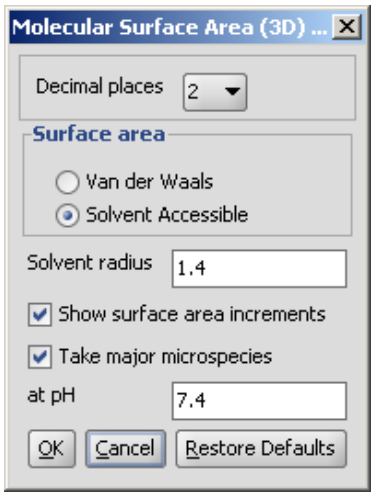


The contents of the text field can be copied to the clipboard by Ctrl+C, the structure field offers a context menu from MarvinView.

Molecular Surface Area Plugin (3D)

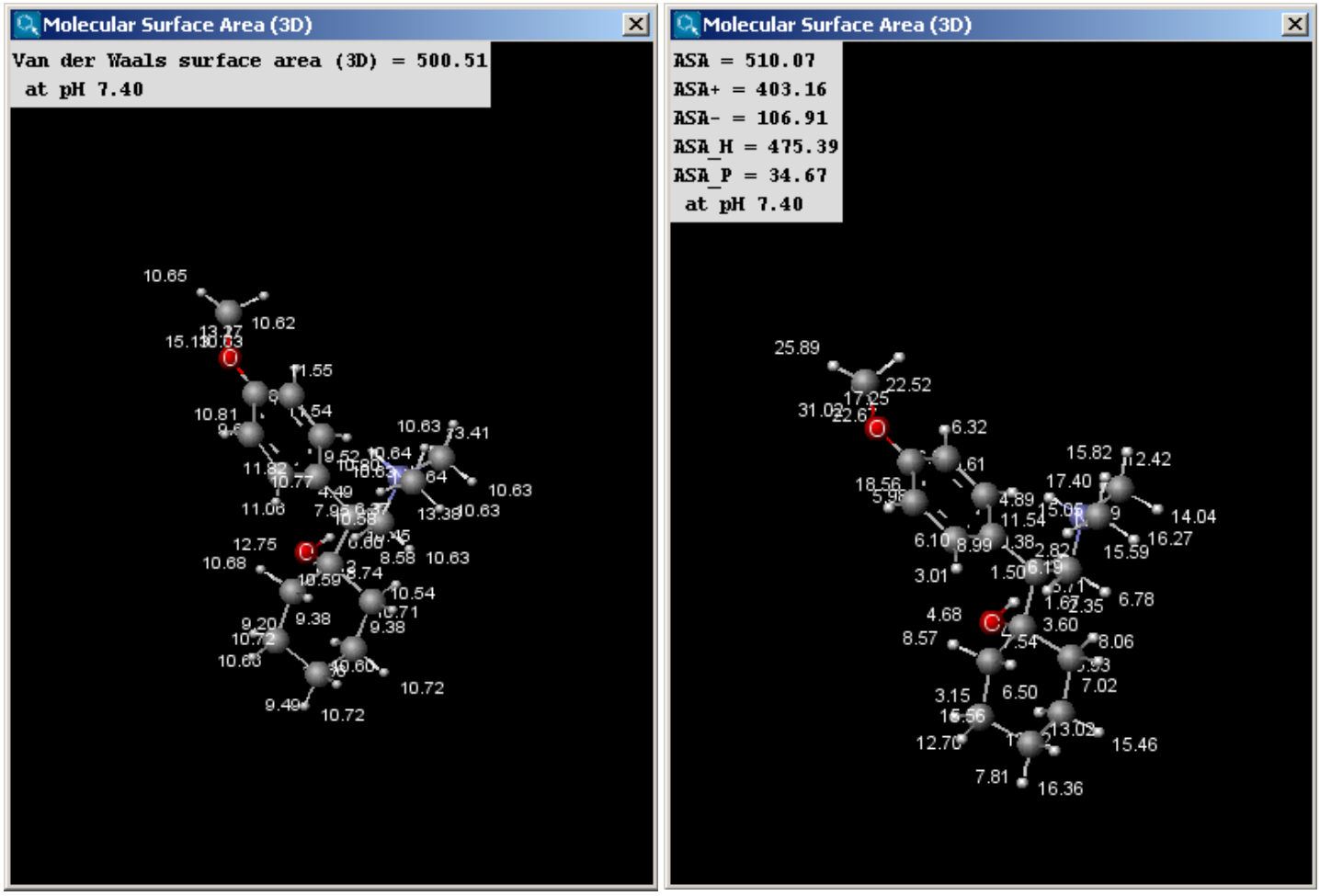
There are two types of available molecular surface area calculations, van der Waals and solvent accessible. Calculation method is based on the publication of Ferrara et al.

The calculation and the display options can be set in the **Molecular Surface Area (3D) Options** panel:



- **Decimal places:**setting the number of decimal places with which the result values are given.
- **Surface Area**
  - **Van der Waals:** calculates the van der Waals surface of the molecule (in $Å^2$).
  - **Solvent Accessible:** calculates the solvent accessible surface of the molecule (in $Å^2$).
- **Solvent radius:** setting here the radius of the solvent molecule (by default water, 1.4 Å).
- **Show surface area increments:** the increment by each atom is displayed.
- **Take major microspecies at pH:** the surface area of the major microspecies present at the given pH is calculated.

The result window contains the area values and the molecule in 3D view. The left picture shows the van der Waals surface and the right window the solvent accessible surface area:



The values indicated in the text field of the result window of the solvent accessible surface area calculations are the following (all in $Å^2$):

- **ASA:** solvent accessible surface area calculated using the radius of the solvent (1.4 Å for the water molecule).

- **ASA+:** solvent accessible surface area of all atoms with positive partial charge (strictly greater than 0).
- **ASA-:** solvent accessible surface area of all atoms with negative partial charge (strictly less than 0).
- **ASA_H:** solvent accessible surface area of all hydrophobic ($|q_i|<0.125$) atoms ($|q_i|$ is the absolute value of the partial charge of the atom).
- **ASA_P:** solvent accessible surface area of all polar ($|q_i|>0.125$) atoms ($|q_i|$ is the absolute value of the partial charge of the atom).

References

- Randic,M., *Chem. Phys. Lett.,* **1993**, *211,* pp 478-483; doi
- Lucic, B., Lukovits, I., Nikolic, S., Trinajstic, N., *J. Chem. Inf. Comput. Sci.,* **2001**, *41(3),* pp 527-535; doi
- Wiener, H., *J. Am. Chem. Soc.,* **1947,** *69(1)* pp 17 - 20; doi
- Ertl, P., Rohde, B., Selzer, P., *J. Med. Chem.*, **2000,** *43,* pp. 3714-3717; doi
- Ferrara, P,. Apostolakis J., Caflisch A., *Proteins* **2002,** *46,* 24-33; doi

Markush Enumerator Plugin

A Markush structure is a description of a compound class by generic notations, primarily used in patent claims and the description of combinatorial libraries. The library of a Markush structure is the total set of specific molecules that are described by the Markush structure.

The Markush enumeration plugin can be used to generate a whole or a subset of the library of a generic Markush structure. It is also capable of calculating the total number of specific structures present in a Markush library. The plugin is accessible from the followings:

- Marvin GUI (Structure > Markush Enumeration)
- Instant JChem
- Markush viewer
- cxcalc command-line program (see this link for the detailed usage of the plugin in command line)
- via API
- Markush search example JSP web application
- Chemical Terms functions in JChem

Markush features

- R-groups
- Atom lists
- Bond lists
- Link nodes
- Repeating units
- Position variation bond
- Homology groups

Functionality of the plugin

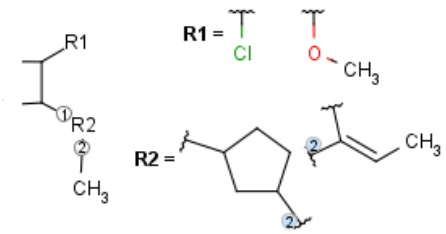
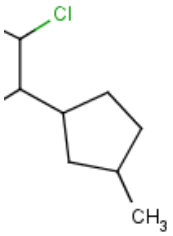
- Sequential enumeration
- Random enumeration
- Calculate library size
- Selected part enumeration
- Valence filter
- Homology group enumeration
- Scaffold alignment and coloring
- Markush code generation

Markush features

Currently, the Markush enumeration plugin supports the following features that describe Markush structures in combinatorial libraries:

- **R-groups**

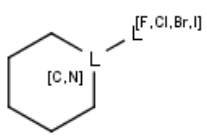
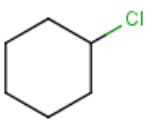
  R-groups (also referred to as "substituent variation") are the most widely known Markush generic features. The variable part of the structure is denoted by an R-atom (eg. R1), and the definitions are given separately. In each definition the connection points must be defined to show where the bonds of the R-atom are linked. R-atoms can appear in both rings and chains, and can have one or more than one attachments point. The same R-atom can appear multiple times, and the different occurrences are handled as different cases. (So they can be substituted with different definitions.) R-group nesting in R-group definitions is allowed to any depth, but without recursion. (An R-group definition cannot use the R-atom it is defining, not even through the use of other embedding R-atom(s).) R-groups up to number R32767 can be used.

Example	Example Markush library member
	

  R-group drawing in Marvin Sketch is described in the Marvin Sketch User's Guide.

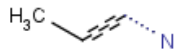
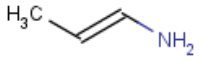
- **Atom lists**

  Atom lists are another example of substituent variation. They define lists of atom types at a given position. There is no restriction for the length of the list and for bond count of atom lists. Atom list drawing in Marvin Sketch is described here.

Example	Example Markush library member
	

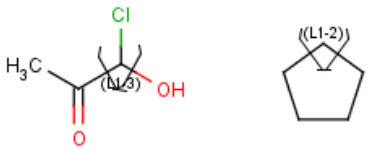
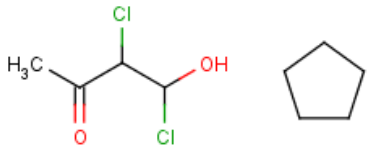
- **Bond lists**

The following bond lists (generic bond types) are supported by the plugin: single or double, any(single, double or triple), single or aromatic, double or aromatic. In Marvin Sketch, bond lists are accessible amongst query bond types in the bonds pop-up menu.

Example	Example Markush library member
	

- **Link nodes**

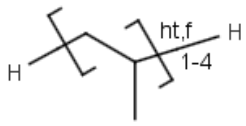
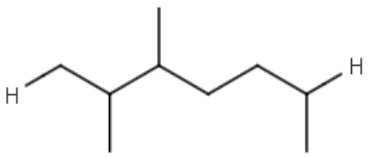
Link nodes are atoms that may repeat between two of their designated bonds (called outer bonds, denoted by brackets). All other substituents (if exist) repeat together with the atom. In the results, the new bonds between the repeating atoms will have the bond type of the lower order outer bond. Link nodes can be drawn in Marvin Sketch using the popup menu.

Example	Example Markush library member
	

- **Repeating units**

Repeating units represent structural parts that can be repeated several times. The repeating unit is enclosed in brackets with one or two head and the same number of tail crossing bonds. (Head crossing bonds go through the left bracket.) Two bond pairs represent ladder type repeating units. The repetition range is a comma-separated list of possible repetitions or repetition intervals, e.g. "1,3,5-9". The repetition pattern specifies the way how the subsequent repeated units are linked together: it can be head-to-head(hh), head-to-tail(ht) or either/unknown(eu) (the either/unknown case is not handled by the search software). In case of ladder type polymers there is also a flip(f) option that defines that the top and bottom crossing bonds are flipped during each connection. repeating groups with specified repetition ranges.

Repeating unit drawing is described in the Marvin Sketch Help here, and ladder-type bracket drawing is described at the polymer drawing section.

Example	Example Markush library member
	

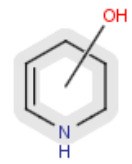
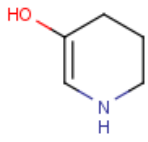
- **Position variation bonds**

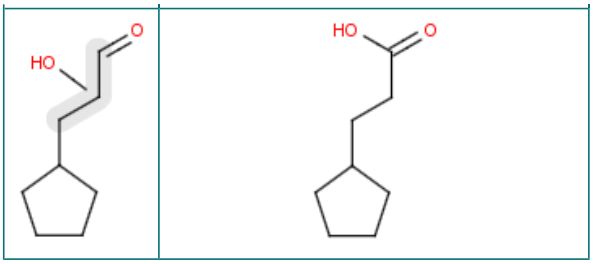
Position variation bonds are bonds attached to variable atoms at one or both end positions. The set of variable atoms is drawn as a multicenter group. A position variation bond connects one atom from one end position to one atom from the other end position. If the end position is a single atom then the bond is attached to this atom, if the end position is a multicenter group then the bond is attached to an arbitrary member of the group. Position variation drawing in Marvin Sketch is described in Help.

Limitations:

- Substructure search is not yet prepared to handle the case when both end positions are multicenter groups.
- A multicenter end position is not allowed to contain R-atoms.
- A multicenter end position is not allowed to contain another position variation bond (ie, position variation bonds cannot be nested).

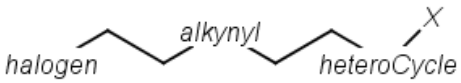
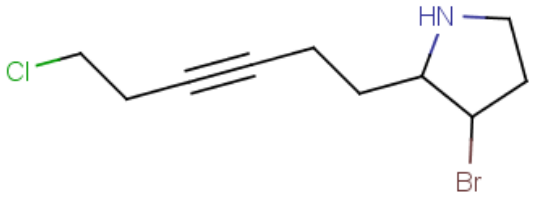
If a link node is a member of a multicenter group then the group will include the repeated atoms as well in case when the original multicenter group contains no more atoms from the link fragment, otherwise the position variation bond is part of the link fragment and repeated together with the link node. Although an R-atom is not allowed to take part in position variation, it can be the single-atom end position of a position variation bond, in which case its attachment point is connected to the bond.

Example	Example Markush library members
	



- **Homology Groups**

  Homology groups stand for sets of homologous molecular parts (e.g. functional groups). These are represented by pseudo atoms labelled with the common chemical annotation of the groups (alkyl, aryl, heterocycle etc.). See the detailed definition of these groups in a separate document. The pseudo atoms can be most easily drawn in Marvin Sketch using the Homology Groups template group.

Example	Example Markush library member
	

There are two major types of homology groups regarding their way of definition:

1. **Built-in groups** are defined by specific structural properties of the group. These groups are not enumerated during searching, but the query structure is recognized as fulfilling the requirements for such a structure. The possible number of covered structures is usually infinite, unless the number of atoms is limited. Examples of built-in groups are alkyl, aryl, heterocycle, etc.
2. **User-defined groups** are explicitly defined and only the listed structures can match on these homology groups. The definition is given in the form of an R-group definition, and any of the generic features discussed in this chapter can be used in the definition. These definitions can be customized by the user, and may be context-specific. (E.g. protecting group definition depends on which functional group it is protecting.)

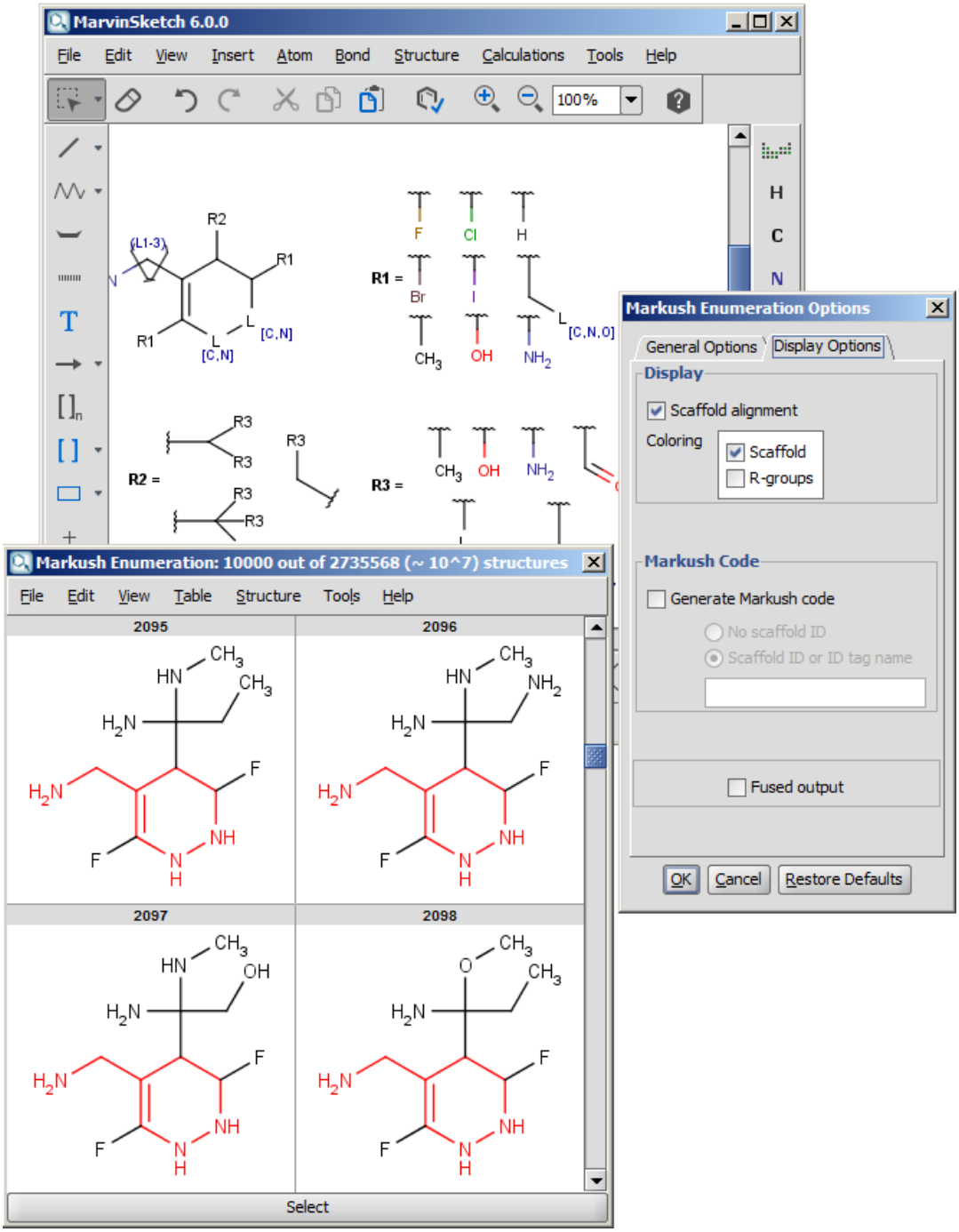
Read more about homology groups.

Functionality of the plugin

The plugin allows the following functionality. Examples are given using Marvin GUI.

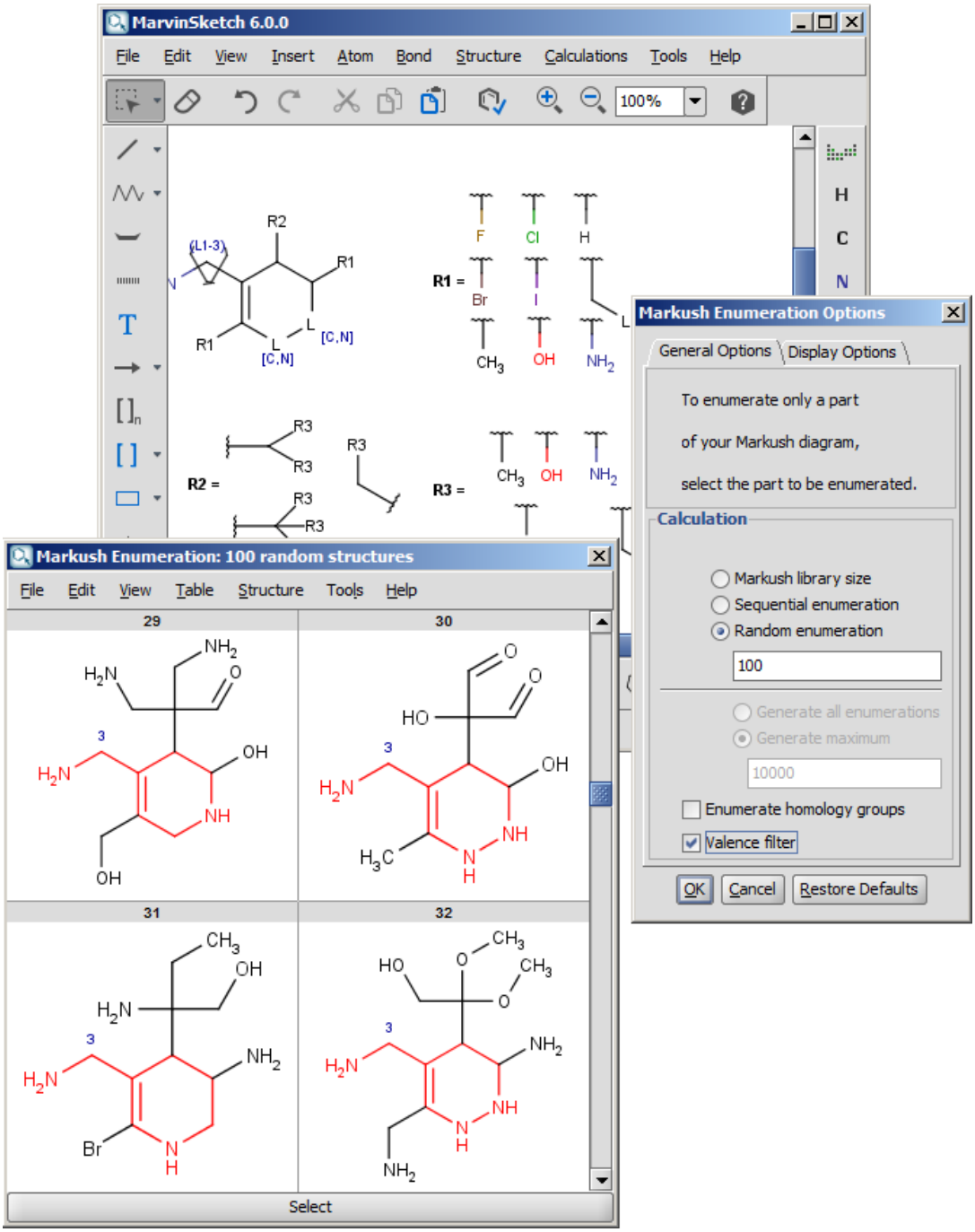
Sequential enumeration

Enumerates members of the Markush library in a sequential manner (by substituting the first definition of the first variable, etc). The results are specific structures. The plugin user interface allows the enumeration of all library members, or a specified number.



Random enumeration

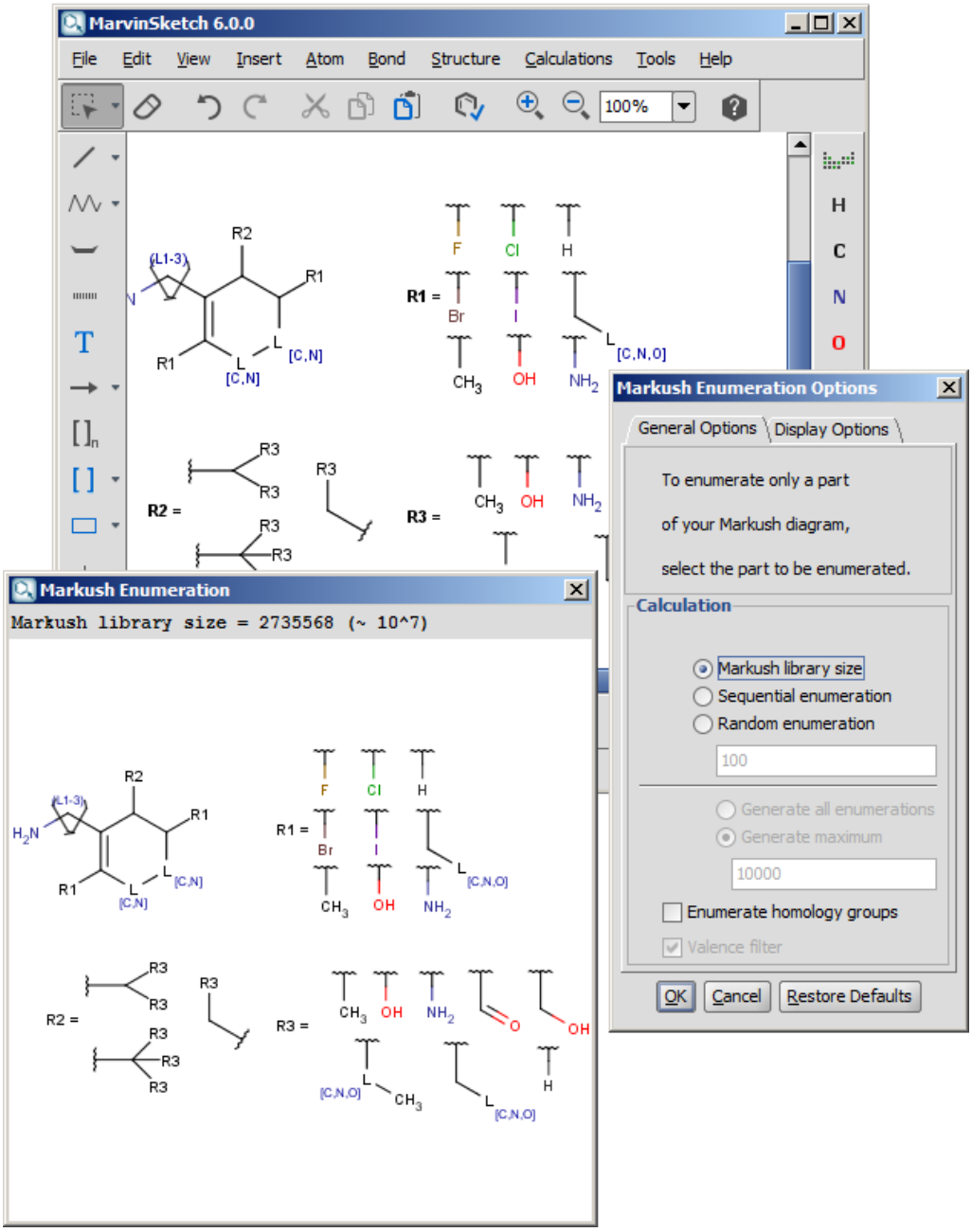
This mode generates a random subset of the Markush library to give a quick sampling. It is especially helpful for huge libraries, where full enumeration is impossible. In random mode variable parts are chosen randomly, and the substitution probability of each definition is proportionate with the fragment library size that the given definition generates. This ensures the generation of uniform distribution of representatives over the Markush library space.



Calculate library size

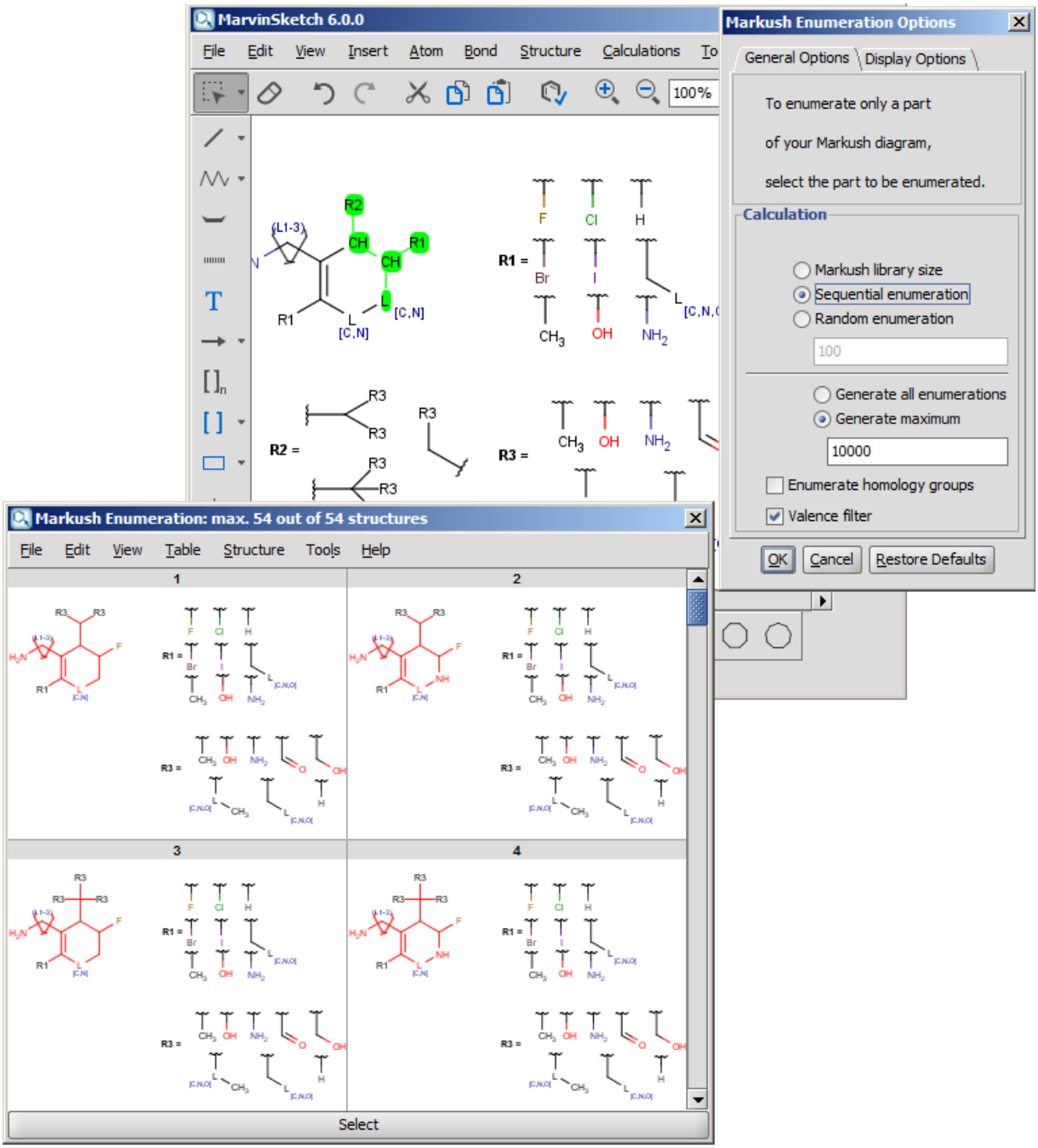
The size of the Markush library can be calculated by arbitrary precision. On the user interface, the exact value is displayed until 20 digits, above that only the magnitude is shown (for example, 10^28). The calculated number is the size of the whole library, and does not consider the valence check filter. (See below.)

If the 'Enumerate homology groups' option is enabled, the number of enumerated molecules increases accordingly, multiplied by the number of built-in species.



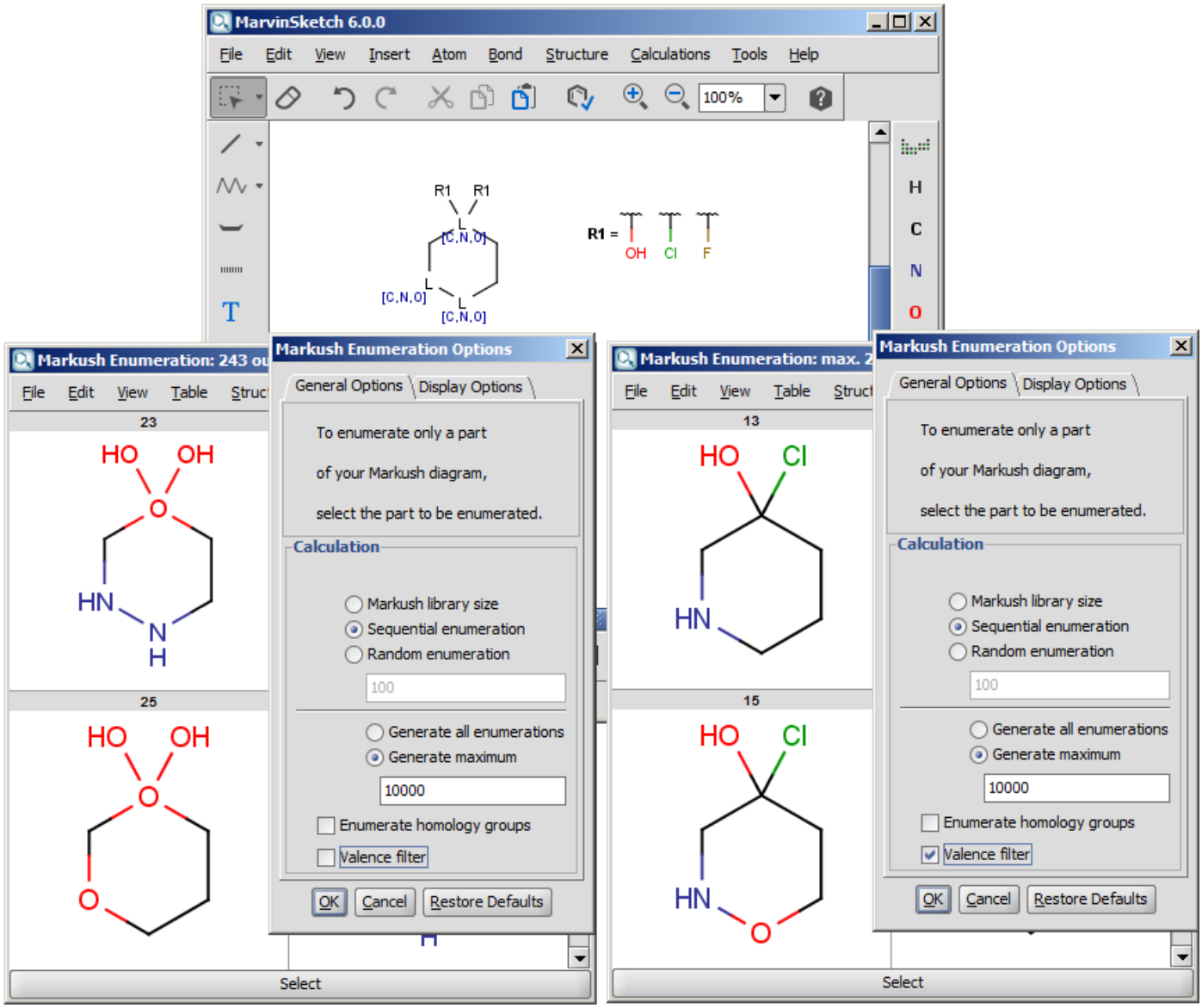
Selected part enumeration

If part of the Markush structure is selected, only the generic features in the selected part are considered for enumeration/calculation. This allows focusing on a particular area of the Markush structure. Enumeration of selected parts only may result in generating (more specific) Markush structures.



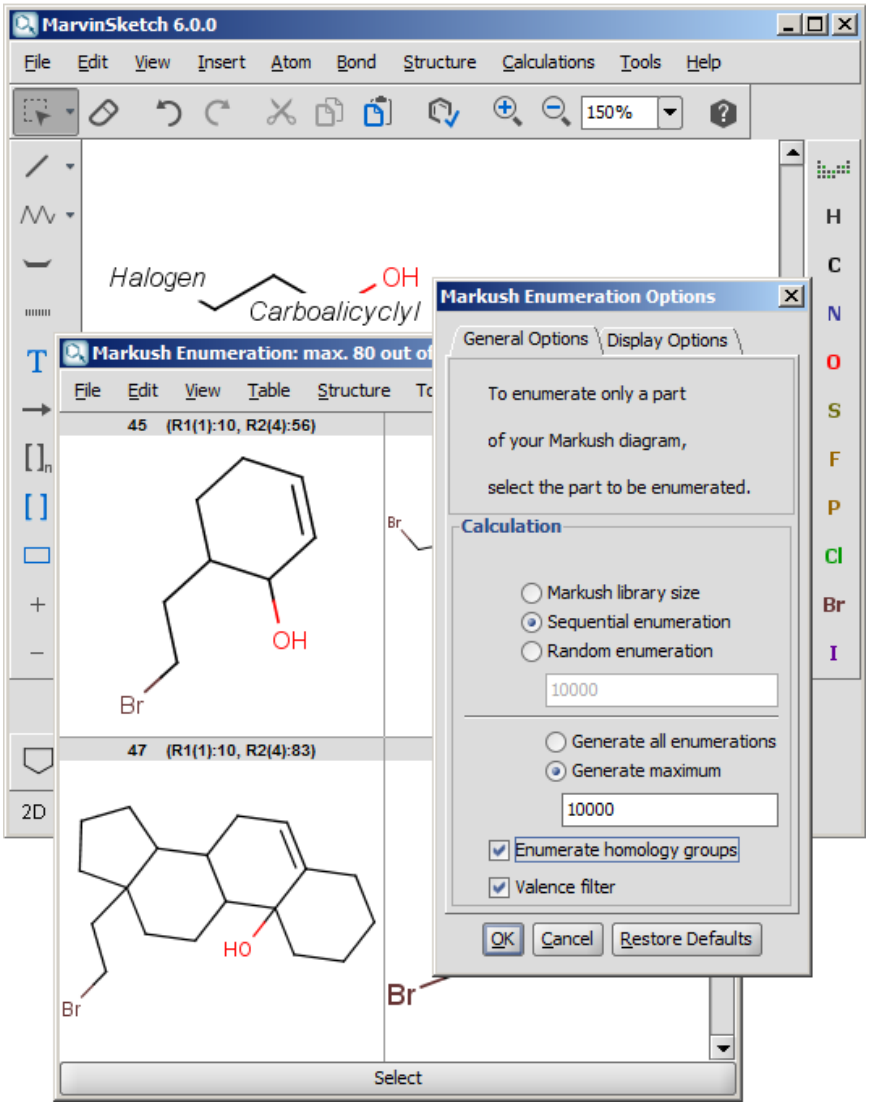
Valence filter

If the Markush structure is not properly (or too generally) formulated, it is possible that it describes structures with valence errors. In this case, the valence filter setting is useful to filter out the offending result structures. The default value is off (no filtering).



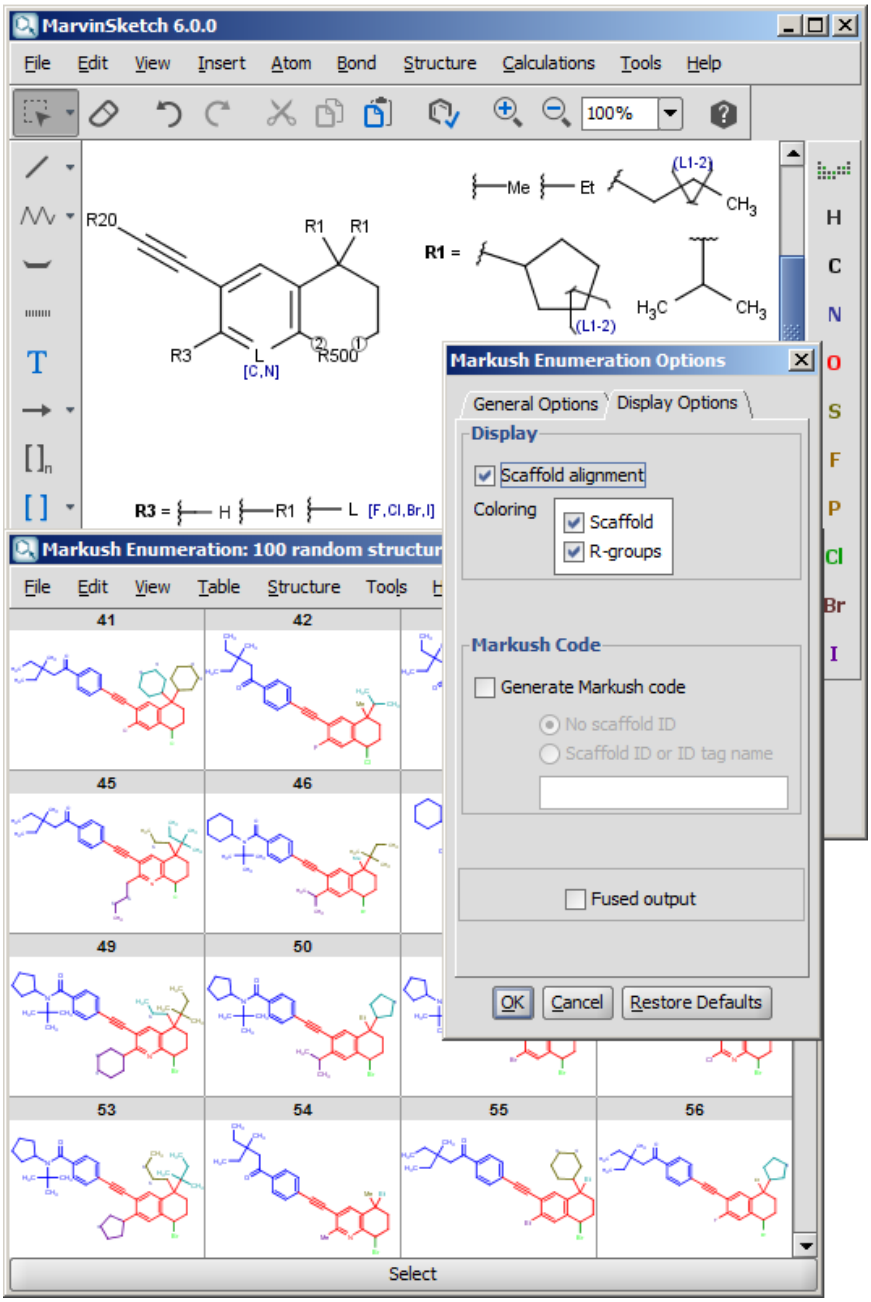
Homology group enumeration

Version 5.2 introduced the enumeration of homology groups. Homology groups are R-groups, represented as pseudo atoms - with the names covering a set of R-groups either built-in or user-defined. For detailed information on homology groups click here.



Scaffold alignment and coloring

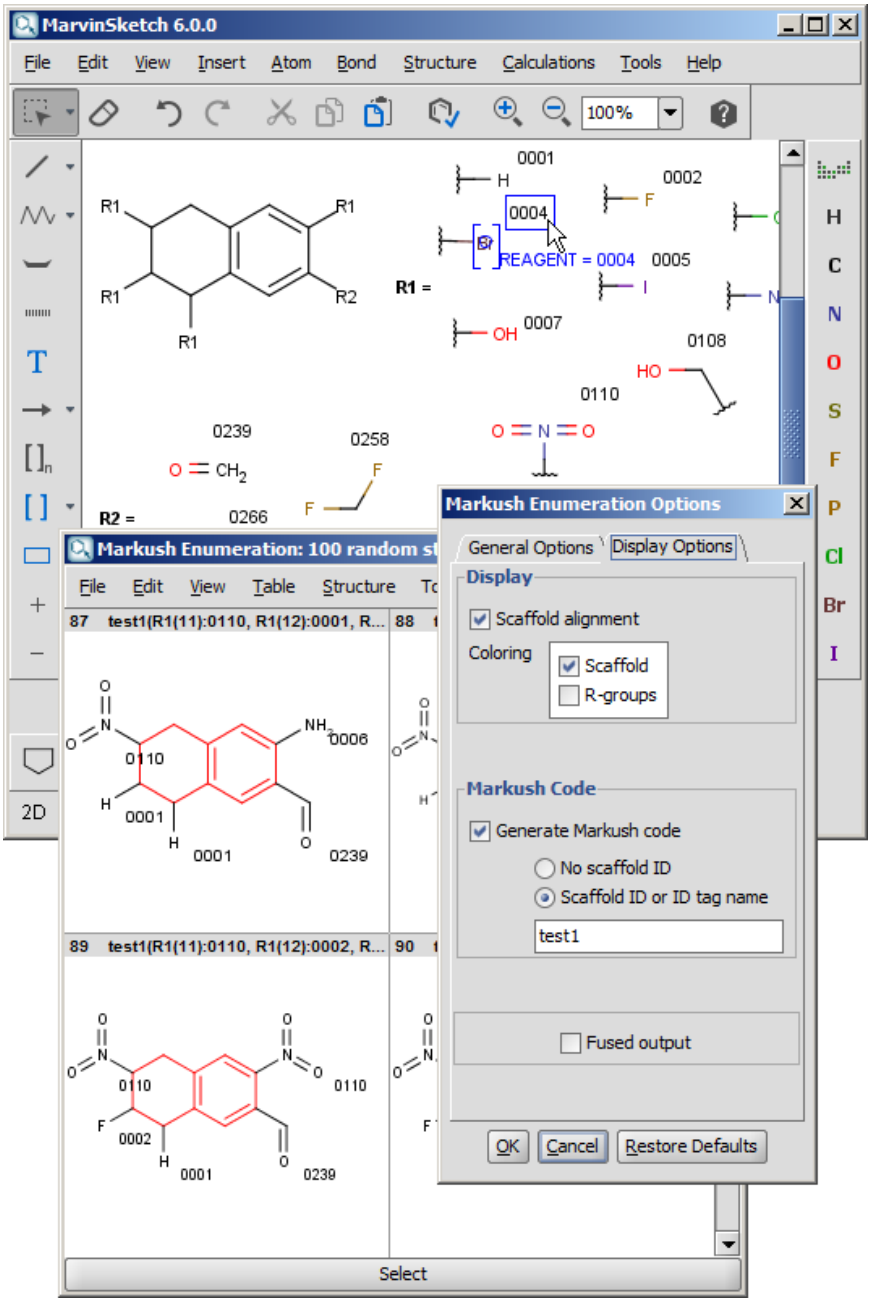
Coloring the scaffold (part of the structure containg no Markush features) and/or the R-groups in enumerated structures can help visual recognition of parts of the molecules. Differentiation of the structures is aided by alignment of all structures to the original scaffold. These options are available in sequential and random enumeration.



Markush code generation

A special ID number can be generated for the library members: every structure gets its own unique tag (molecule property), which can be saved in the structure file (in .mrv and .sdf formats) named as 'Markush Code'. This ID is visible in the plugin result window as well. It gives the following information:

- **Ri(n):x** R-group number *i* (at atom nr. *n*) is the ligand containing the atom numbered *x* (which is the smallest number in that fragment but not neccessarily the attachment point)
  Custom reagent codes: instead of atom index numbers, custom reagent codes (e.g. company identifiers) can also be used. Add attached data to R-group members with name 'reagent'. These reagent codes will appear in the enumerated structures both in the Markush code and in the generated molecule structures. (See example below)
- **ID tag name** the name you specified in the options panel (in this example Test1). If a tag with this name is attached to the Markush molecule, its value will be used.
- **Ln:x** link node on atom nr. *n* in the variation nr. *x* (in this example 1 or two methylene groups are inserted).
- **Bn-m:x** bond between atoms *n* and *m* is nr. *x* in the bond list (referring to the bond type)
- **PVn-m:x-y** position variation bond between *n* and *m* (multicenter numbered) occured between atoms *x* and *y*
- **An:x** atom nr. *n* is nr. *x* from the atom list

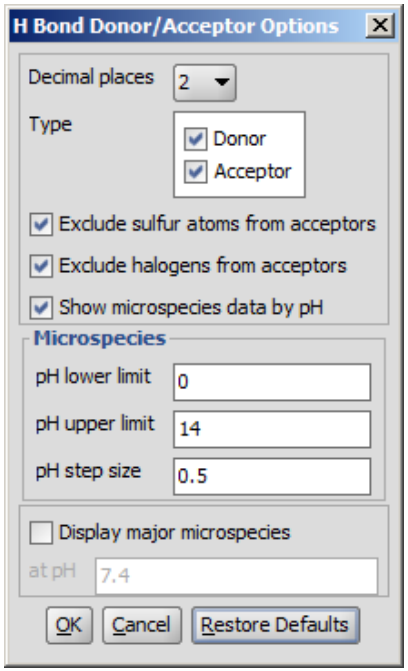

MarvinSketch 6.0.0
File Edit View Insert Atom Bond Structure Calculations Tools Help
100%
R1 =
REAGENT = 0004
R2 =
Markush Enumeration: 100 random st
File Edit View Table Structure
87 test1(R1(11):0110, R1(12):0001, R...
88
89 test1(R1(11):0110, R1(12):0002, R...
90
Select
Markush Enumeration Options
General Options
Display Options
Display
Scaffold alignment
Coloring
Scaffold
R-groups
Markush Code
Generate Markush code
No scaffold ID
Scaffold ID or ID tag name
test1
Fused output
OK
Cancel
Restore Defaults

Other Plugins

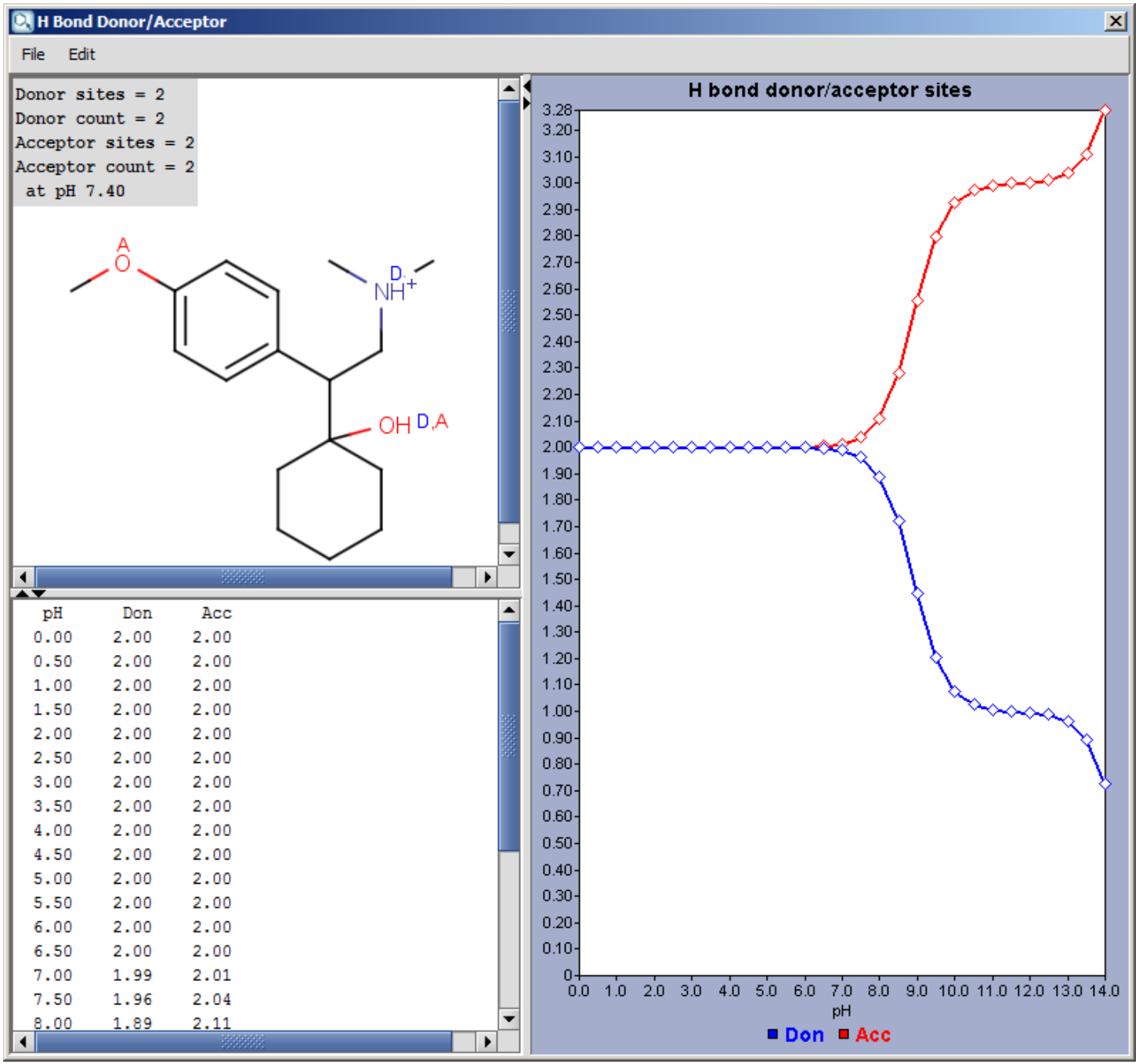
Hydrogen Bond Donor-Acceptor Plugin

Hydrogen Bond Donor-Acceptor calculates atomic hydrogen bond donor and acceptor inclination. Atomic data and overall hydrogen bond donor and acceptor multiplicity are displayed for the input molecule (or its microspecies at a given pH). The weighted average hydrogen bond donor and acceptor multiplicities taken over the microspecies and the proportions of their occurrences are computed for different pHs and displayed in a chart.

Different calculation parameters can be set in the **H Bond Donor/Acceptor Options** panel:



- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Type:**
  - **donor, acceptor:** specifying search for donor or acceptor characteristics.
- **Exclude sulfur atoms from acceptors**
- **Exclude halogens from acceptors**
- **Show microspecies data by pH:** the number of donor or acceptor sites vs. pH chart is displayed.
- **Microspecies:**
  - **pH lower limit; pH upper limit; pH step size:** the pH window of the chart is set here, with data points in the step size marks.
- **Display major mecrospecies:** the structure of the major form at the given pH is displayed.



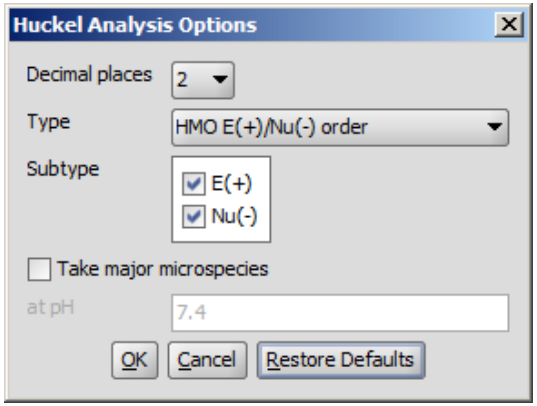
Hückel Analysis Plugin

Localization energies L(+) and L(-) for electrophilic and nucleophilic attack at an aromatic center are calculated by the Hückel method. The smaller L(+) or L(-) means more

reactive atomic location. Order of atoms in E(+) or in Nu(-) attack are adjusted according to their localization energies. The total pi energy, the pi electron density and the total electron density are also calculated by the Hückel method. Depending on the chemical environment the following atoms have optimal Coulomb and resonance integral parameters: B, C, N, O, S, F, Cl, Br, I. All other atoms have a default, not optimized parameter.

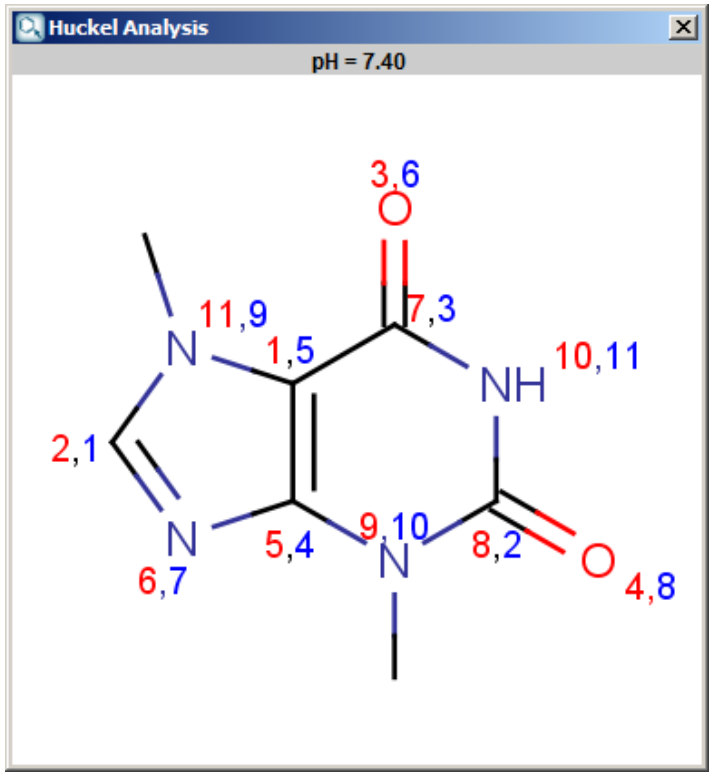
Theoretical background is taken from Isaacs' book. Additional literature for the Hückel's parameters is Streitwieser's book.

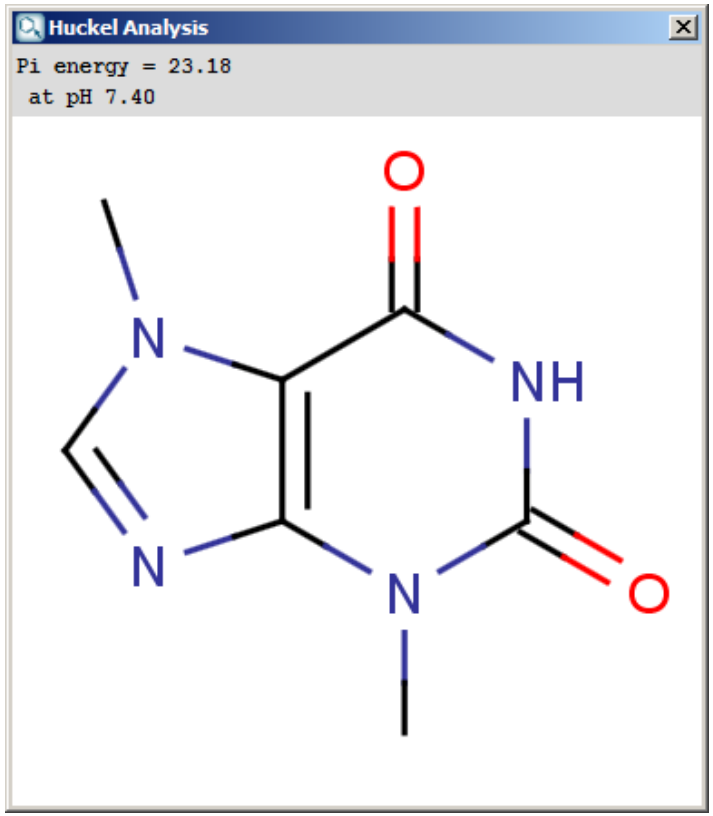
Following calculation parameters can be set in the **Huckel Analysis Options** panel:



- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Type**
  - **E(+)/Nu(-) order:** numbers the aromatic atoms according to their likeliness of being attacked by electrophiles or nucleophiles.
  - **Localization energy L(+)/L(-):** gives the localization energies of the aromatic center (dimension β).
  - **Pi energy:** calculates the pi energy of the aromatic ring(s) (dimension β).
  - **Electron density:** calculates the pi electron density.
  - **Charge density:** calculates total charge density on the ring atoms.
- **Subtype: E(+); Nu(-):** for E(+)/Nu(-)order and Localization energy L(+)/L(-), the electrophilicity and nucleophilicity approaches can be selected (at least one fo them). Results for E(+) are coloured red, and Nu(-) blue.
- **Take major microspecies at pH:** calculates the values for the major microspecies at the given pH.

The results appear in a new window, indicating all values at the corresponding atoms in the aromatic ring. The picture on the left is the result of Aromatic E(+)/Nu(-) order, the picture on the right the pi energy calculation:

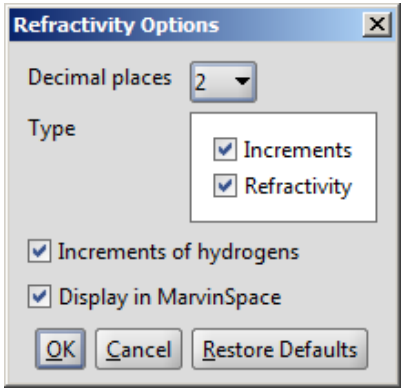




Refractivity Plugin

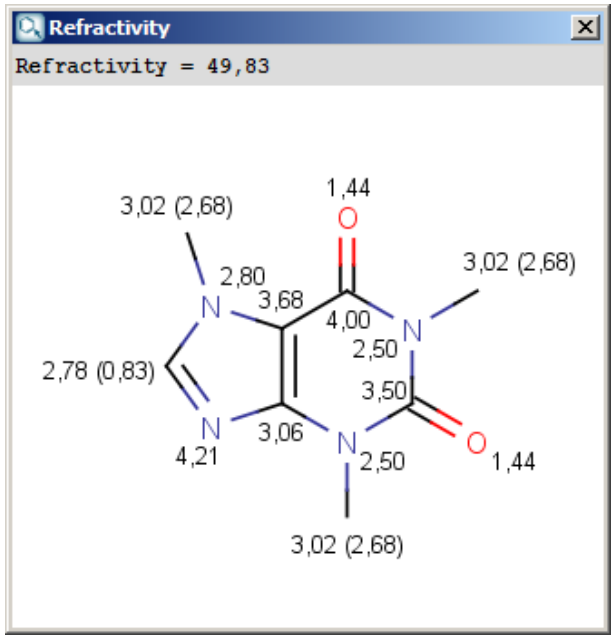
Our calculation is based on the atomic method proposed by Viswanadhan et al. Molar refractivity is strongly related to the volume of the molecules and to London dispersive forces that has important effect in drug-receptor interaction.

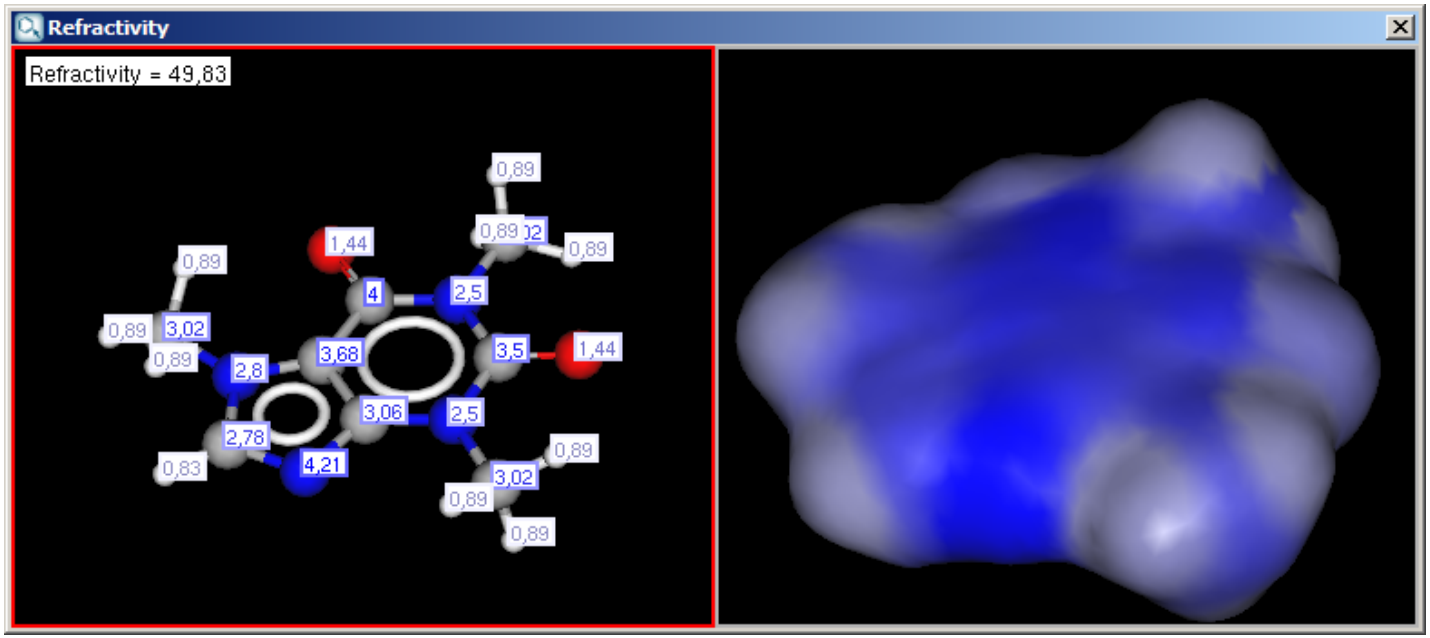
Different calculation parameters can be set in the **Refractivity Options** panel:



- **Decimal places:** setting the number of decimal places with which the result value is given.
- **Type**
  - **Increments:** displays the increments given by atoms.
  - **Refractivity:** calculates the value of the molar refractivity
- **Increments of hydrogens:** displays the increments given by hydrogens.
- **Display in MarvinSpace:** the result window opens as 3D MarvinSpace viewer. If unchecked, the results will be shown on a 2D picture.

The result appears in a new window, containing a text field with the value of refractivity (dimension: 10^6 [m^3 mol^{-1}] and the molecule in 2D or 3D view:

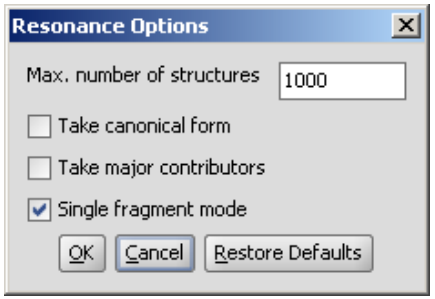




The numbers in brackets refer to the refractivity sums of the implicit hydrogen atoms.

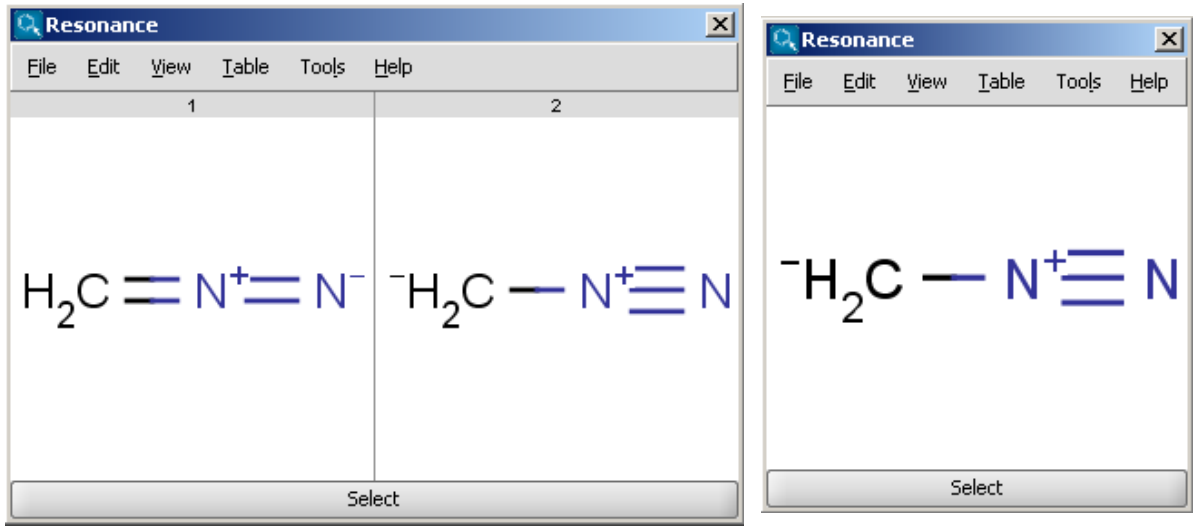
Resonance Plugin

The Resonance plugin generates all resonance structures of a molecule. The major contributors of the resonance structures can be calculated separately. Following options can be adjusted in the **Resonance Options** panel:



- **Max. number of structure:** maximize the number of structures to display (decrease calculation time).
- **Take canonical form:** displays the canonical structure of the molecule.
- **Take major contributors:** select the most relevant structures.
- **Single fragment mode :** if checked (default), the results are displayed in separate windows; if unchecked, the calculation handles unlinked molecules together and results are in the same window.

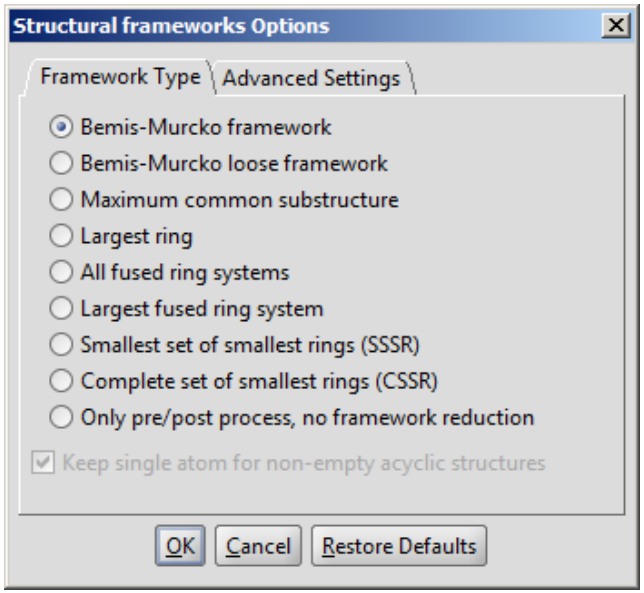
For example the two structures below, on the left are the major resonance contributors of diazomethane, while the structure on the right is the canonical form:



Structural Frameworks Plugin

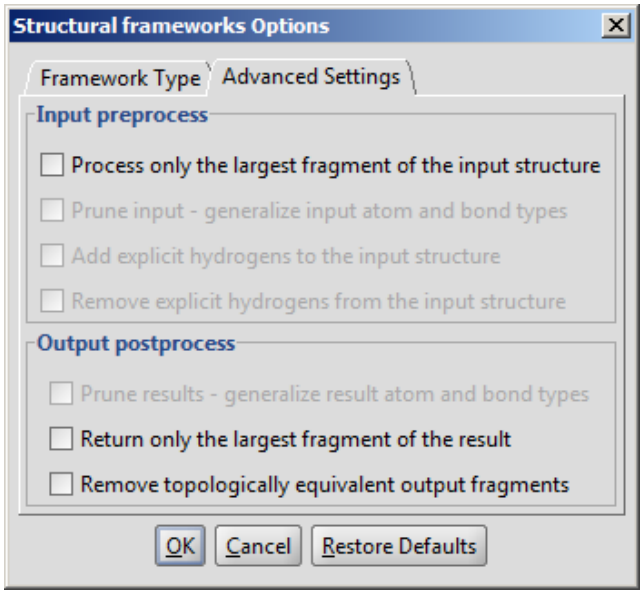
The plugin calculates Bemis and Murcko frameworks and other structure based reduced representations of the input structures.

The required calculation can be selected on the **Framework type** tab of the **Structural frameworks Options** panel:



- **Bemis-Murcko framework** is calculated by removing side chains from the input and generalizing atom/bond types. If **Keep single atom for non- empty acyclic structures** selected then acyclic inputs will not be erased completely; they will be represented by a single node.
- **Maximum common substructure** calculates MCS for every pairs of input fragments. The input must contain at least two disconnected fragments.
- **Largest ring** returns the largest SSSR ring of the input.
- **All fused ring systems** returns the fused ring systems of the input
- **Largest fused ring system** returns the largest the fused ring systems of the input
- **Smallest set of the smallest rings (SSSR)** returns the SSSR rings of the input.
- **Complete set of the smallest rings (CSSR)** returns the CSSR rings of the input.
- **Only pre / post process, no framework reduction** can be used to examine the optional preprocess and postprocess functionality. Selecting this option will skip any framework reduction/fragmentation.

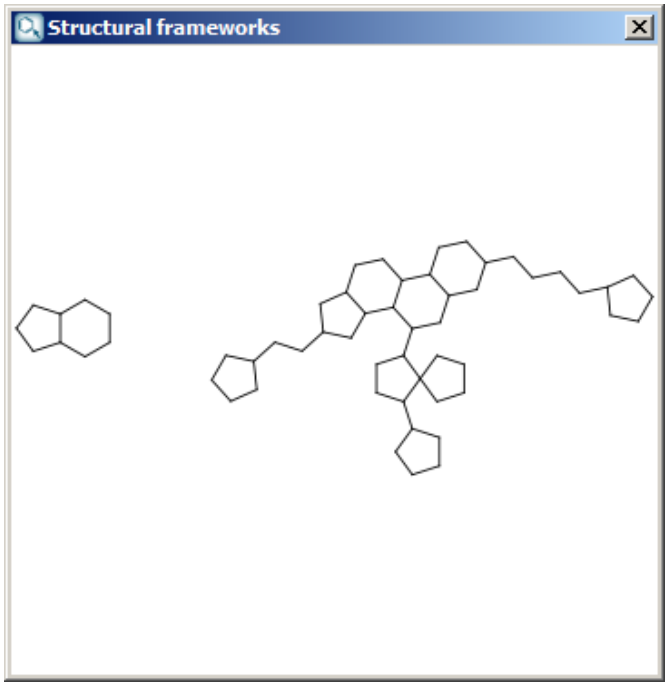
The **Advanced settings** tab allows options to fine tune the execution:



Note that redundant or not applicable options will be dinamically disabled based on the selected framework type or other calculations. (For example Bemis-Murcko framework calculation will generalize the input, so prune input/output will be disabled when it is selected.)

- **Input preprocess** steps are executed before the framework calculation.
  - **Process only the largest fragment of the input structure**: if selected then the largest fragment will be processed in the following steps
  - **Prune input** the input structure will be generalized by changing all atom types to carbon, all bond types to single and removing all stereo/wedge bond flags
  - **Add explicit hydrogens** will invoke hydrogenize on the input
  - **Remove explicit hydrogens** will invoke dehydrogenize on the input
- **Output postprocess** steps are executed after the framework calculation.
  - **Prune results** will generalize the resulting framework after the calculations
  - **Return only the largest fragment of the result** will keep only the largest resulting fragment
  - **Remove topologically equivalent output fragments** will remove duplicated result fragments

The result window contains the framework:



References

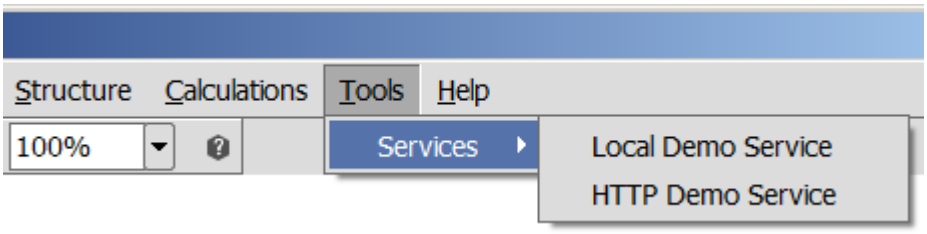
- Viswanadhan, V. N.; Ghose, A. K.; Revankar, G. R.; Robins, R. K., *J. Chem. Inf. Comput. Sci.*, **1989**, *29*, 163-172; doi
- Isaacs, N.S., *Physical Organic Chemistry*, John Wiley & Sons, Inc., New York, **1987**, ISBN 0582218632.
- Streitwieser, A., *Molecular Orbital Theory for Organic Chemists,* John Wiley, **1961**, ISBN 0471833584.

Marvin Services

Calculation integration as service

Services is a handy module of Marvin that helps to integrate third-party calculations* via the MarvinSketch GUI. The linked services will appear under the **Tools** > **Services** menu. The menu contains the names of the services in a formerly set order.

Figure 1. The location of the set services

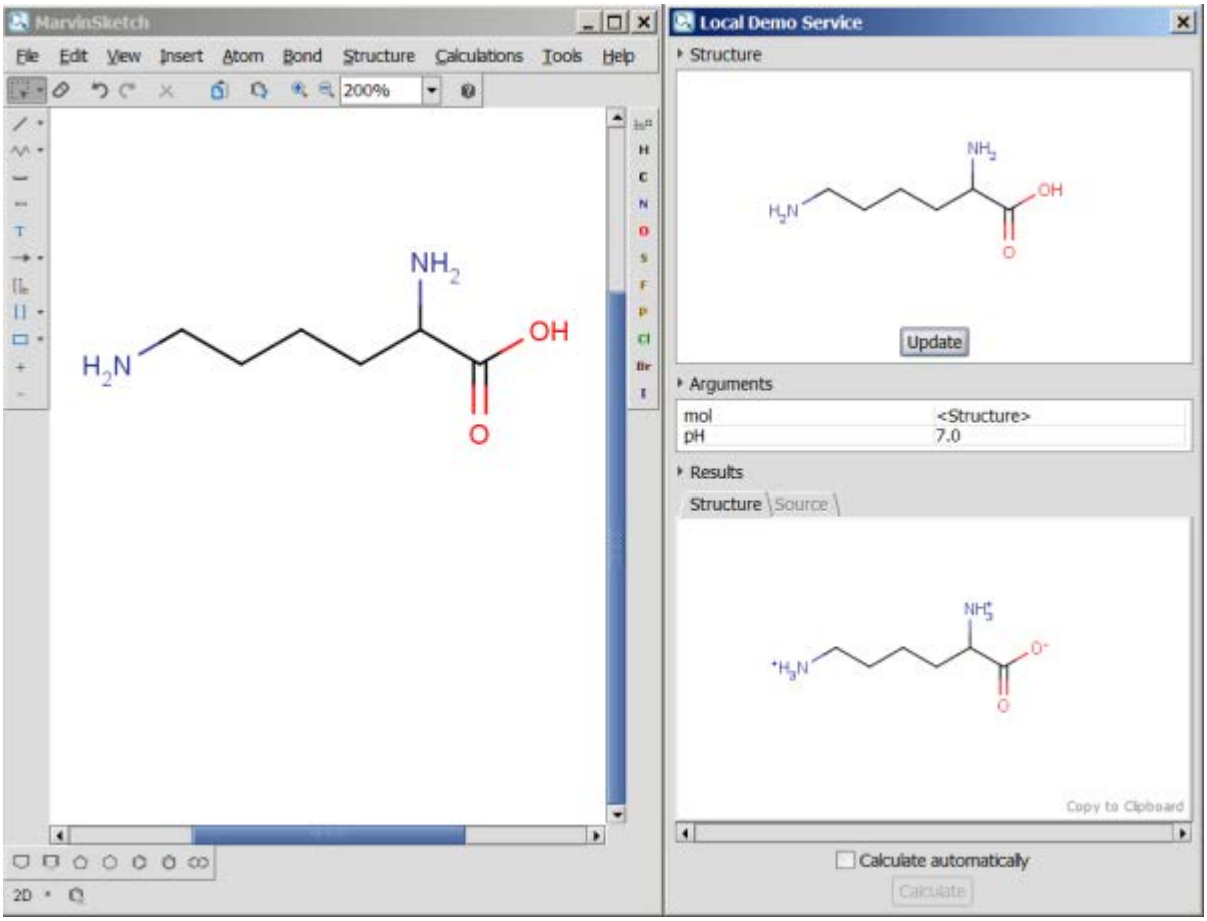


Note: When no Services are set in MarvinSketch, the **Tools** > **Services** menu will be disabled.

How to use

Select the desired third-party calculation under **Tools** > **Services**. The opening new window — right of MarvinSketch — has the same title as the service name.

Figure 2. MarvinSketch window (left) with the new service window (right)



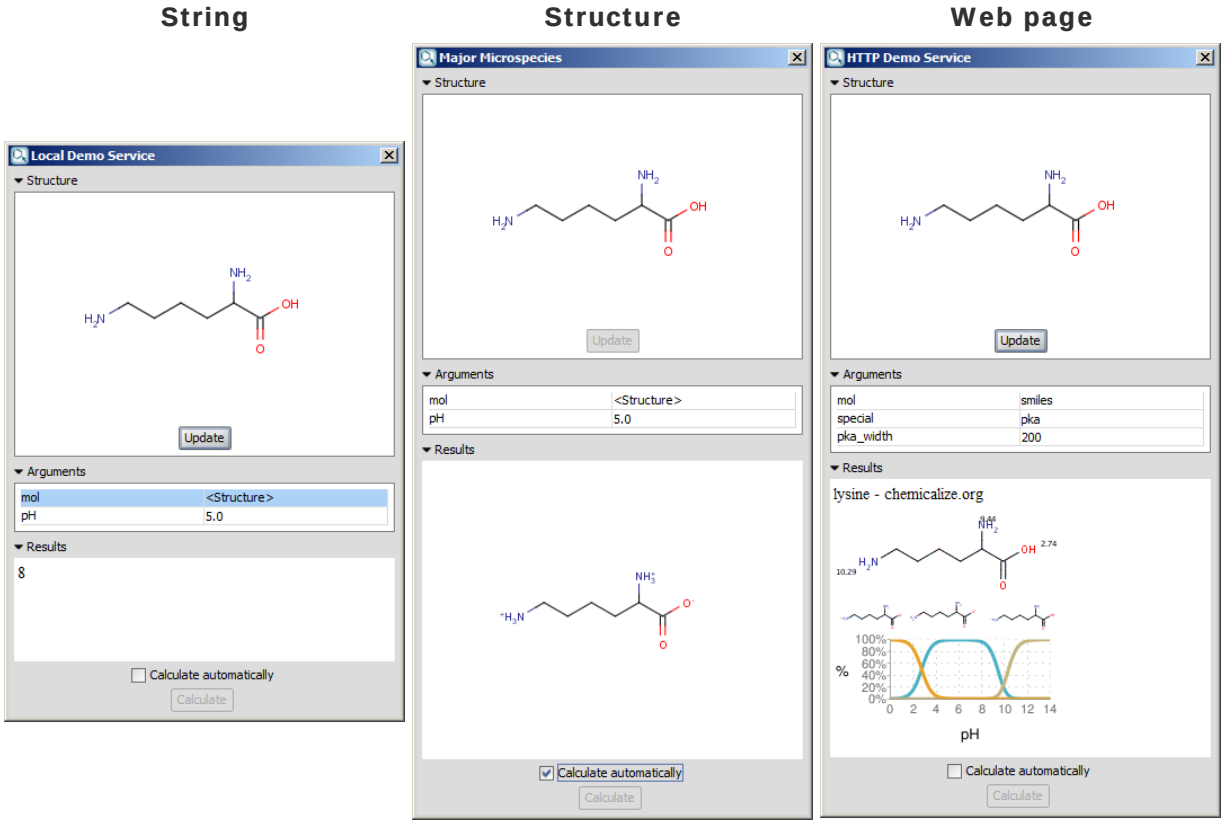
The collapsible panels of the window are the following:

- **Structure**: The upper panel will show the structure in question. The structure can only be edited in the MarvinSketch window.
  - **Update** button: If the structure is changed in MarvinSketch, press this button to refresh the

structure for the calculation. **Note**: The button will be disabled if **Calculate automatically** is checked;

- **Arguments**: The middle panel shows the calculation parameters. Unless the parameter is bold, it can be modified;
- **Result**: The lower panel will show the result of the calculation. The panel can present different output formats, e.g., string, structure, web page;
    - **Calculate automatically** check box: If the structure is changed in MarvinSketch, the update of the structure and the calculation will run automatically. **Note**: In case it is checked, the **Calculate** and **Update** buttons will be inactive;
    - **Calculate** button: Calculates and retrieves the result.

Figure 3. Different output type examples

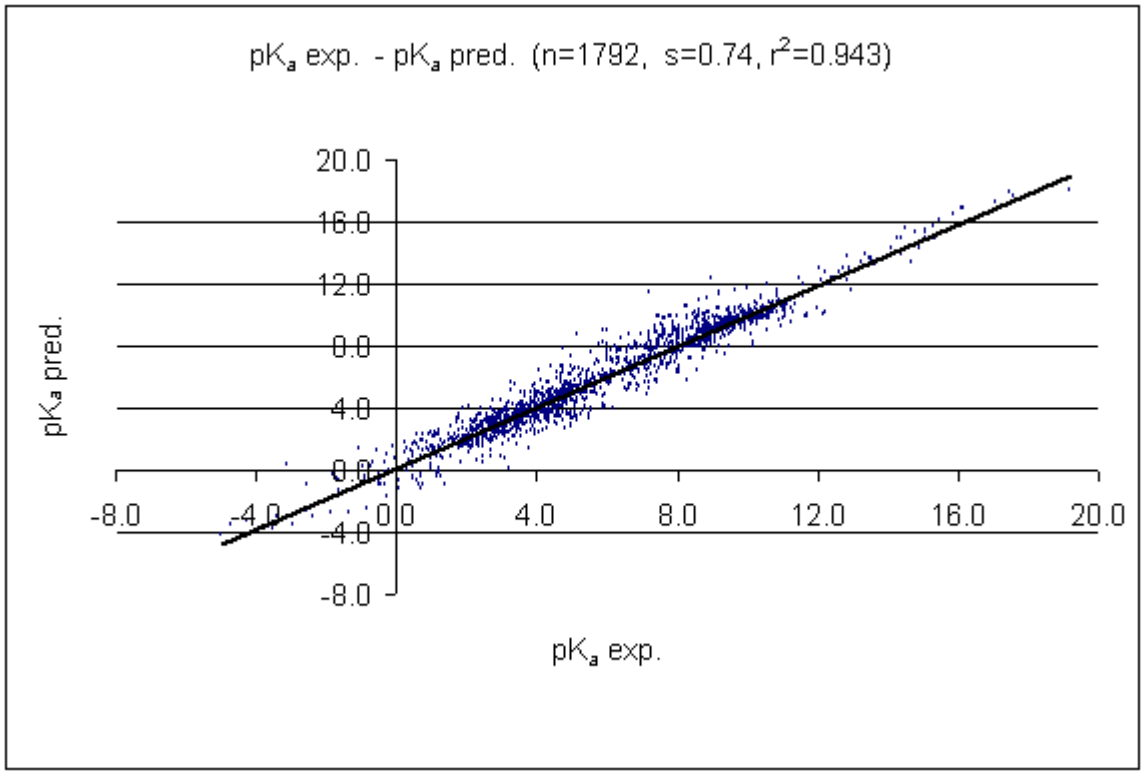


*All calculations not provided in ChemAxon's Marvin Beans or in its JChem package are referred to third-party calculations.

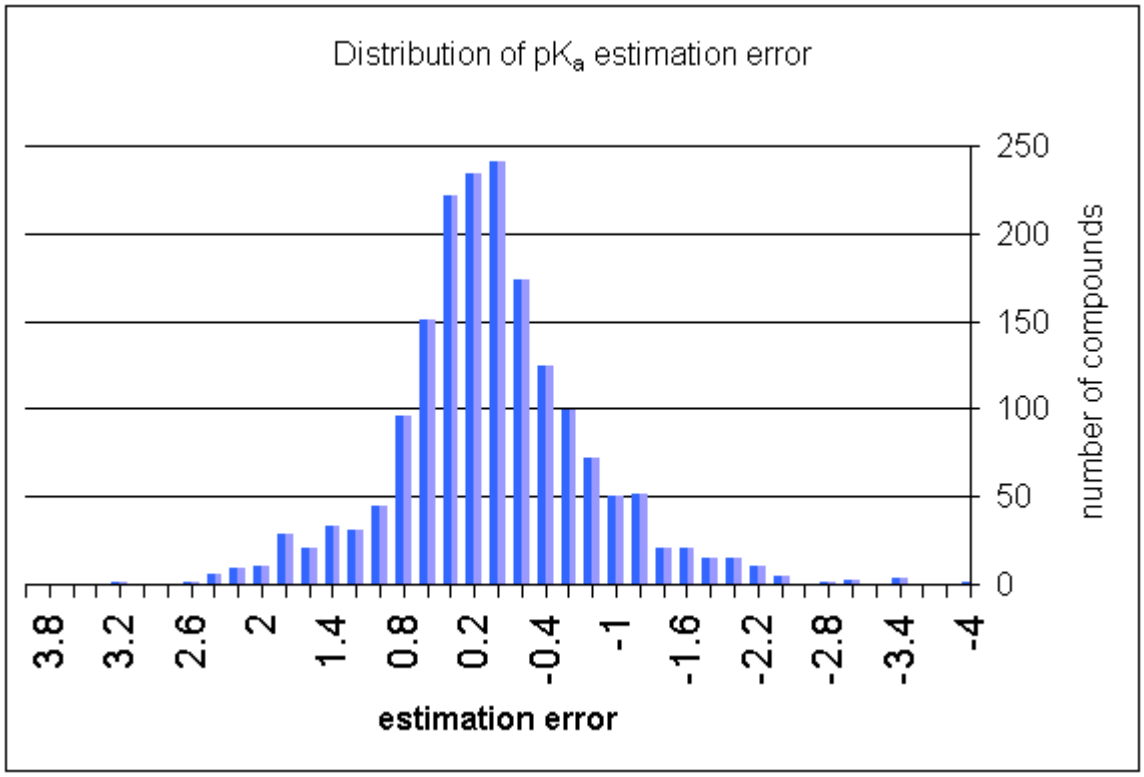
Test results of prediction tools

1. Test of pK_a prediction

pK_a predicted vs. pK_a experimental[1]

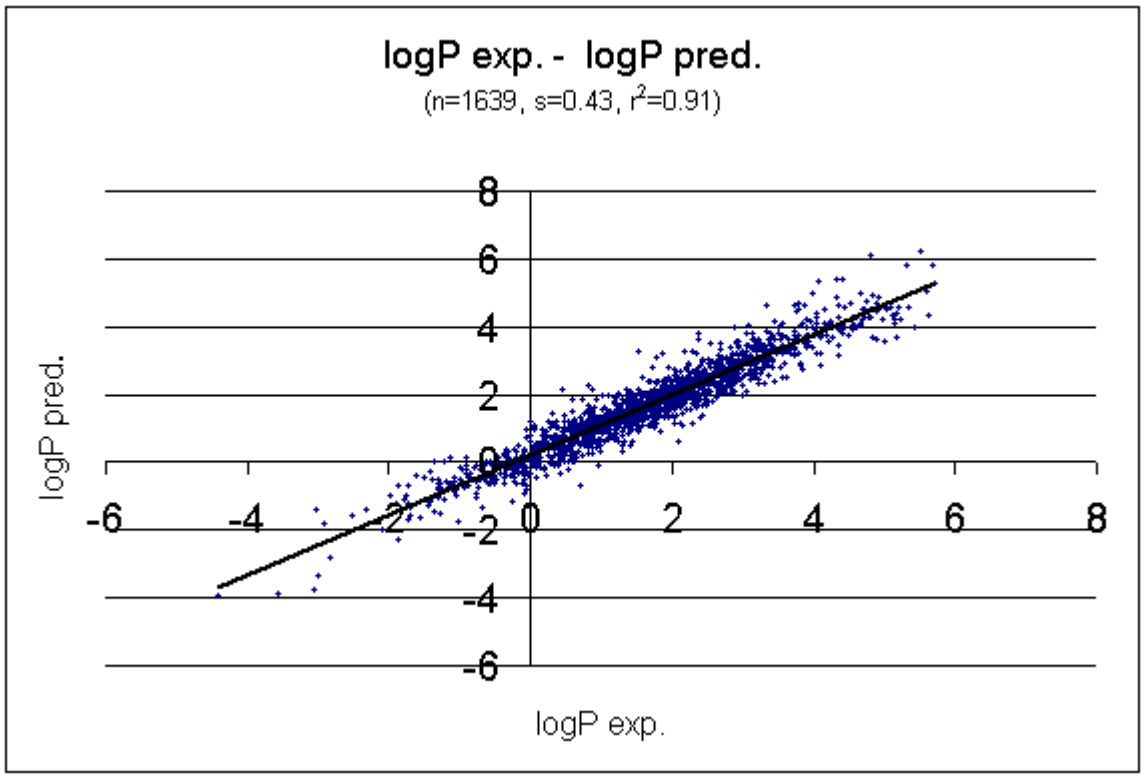


Distribution of pK_a estimation error

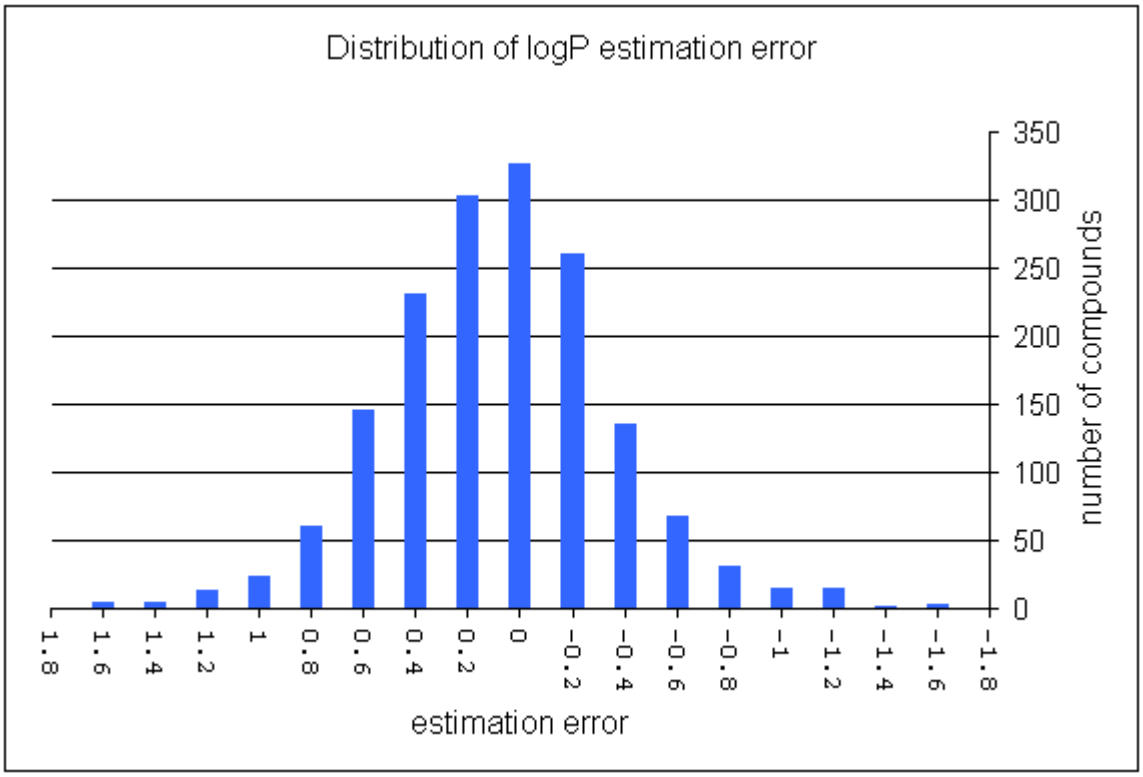


2. Test of log*P* prediction

log*P* predicted vs. log*P* experimental2

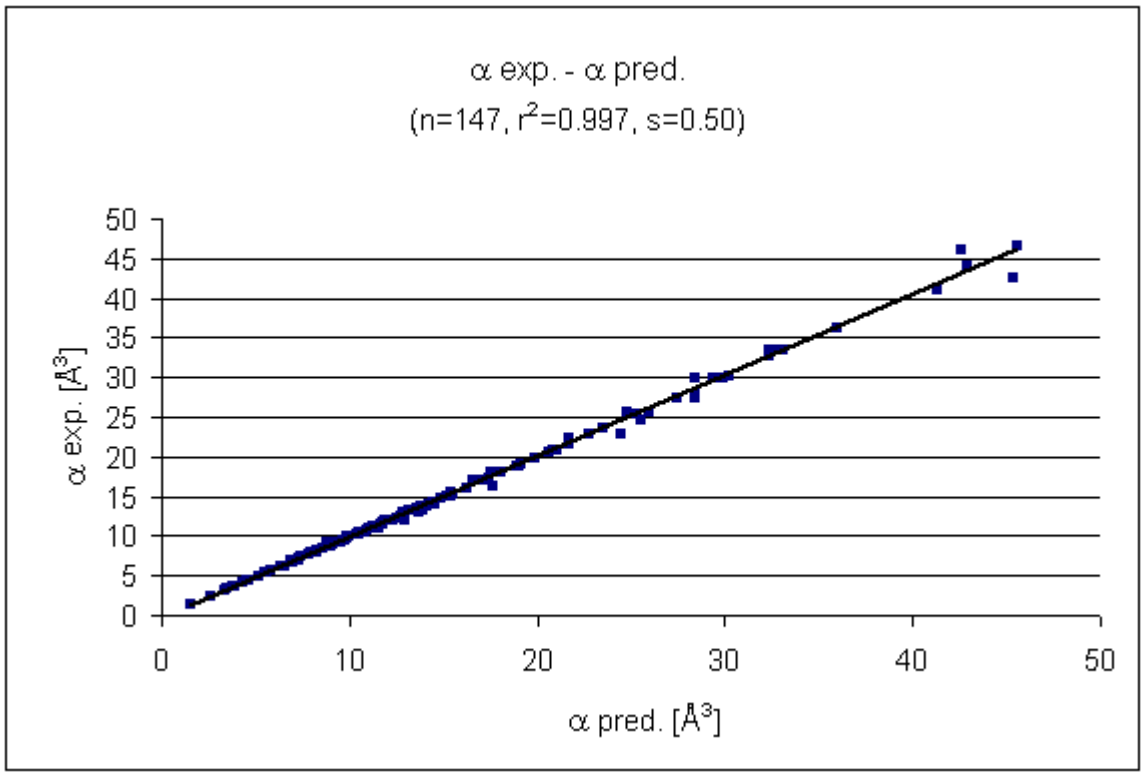


Distribution of log*P* estimation error



3. Test of average molecular polarizability prediction

Experimental3 vs. predicted molecular polarizability



Experimental3 and predicted data

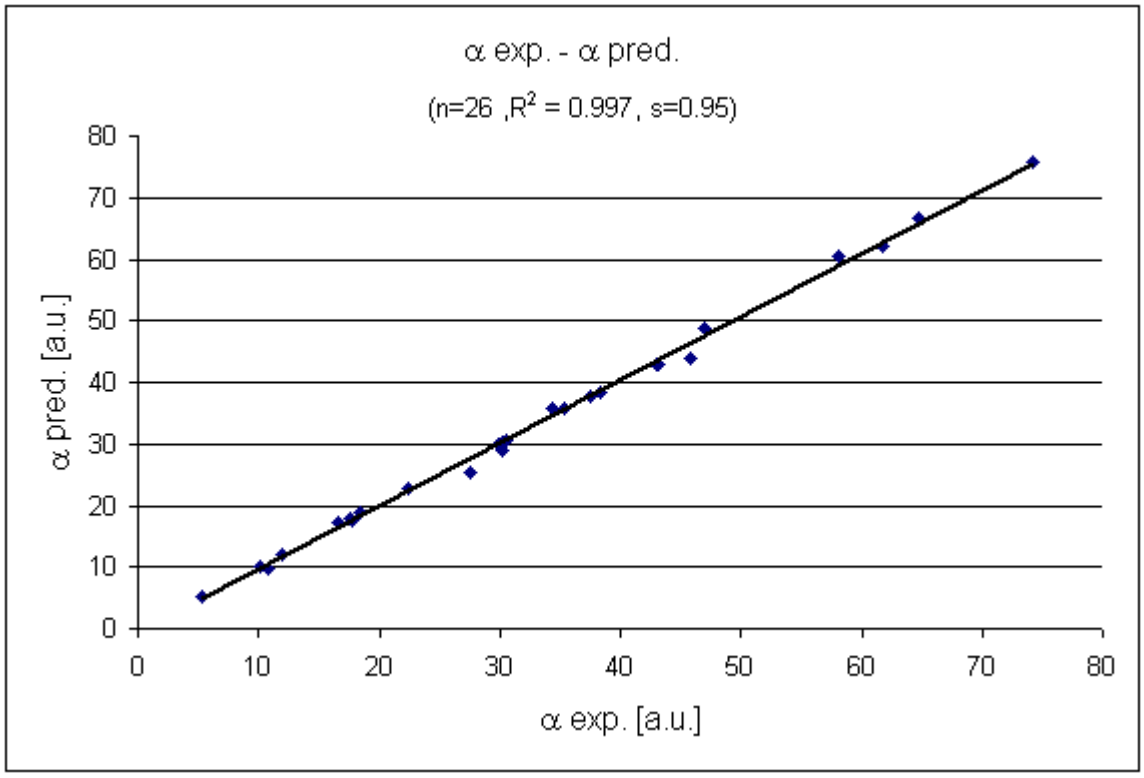
molecule	exp. α	pred. α	molecule	exp. α	pred. α
CH_3Br	5.53	5.55	1-propanol	6.77	6.87
C_2H_5Br	7.28	7.29	glycol	5.71	5.72
C_3H_7Br	9.07	9.06	dimethyl ether	5.16	5.11
C_4H_9Br	10.86	10.85	diethyl ether	8.73	8.79

$C_5H_{11}Br$	12.65	12.65	n-propyl methyl ether	8.86	8.79
$C_6H_{13}Br$	14.44	14.46	n-propyl ethyl ether	10.68	10.63
$C_7H_{15}Br$	16.23	16.27	di-n-propyl ether	12.55	12.48
$C_8H_{17}Br$	18.02	18.09	acetone	6.4	6.33
$C_9H_{19}Br$	19.81	19.92	methylethylketone	8.19	8.17
$C_{10}H_{21}Br$	21.6	21.75	diethyl ketone	9.93	10.01
$C_{12}H_{25}Br$	25.18	25.41	methyl propyl ketone	9.93	10.01
$C_{16}H_{33}Br$	32.34	32.75	di-isopropyl ketone	13.53	13.70
$C_{18}H_{37}Br$	35.92	36.43	n-propionaldehyde	6.35	6.33
CH_4	2.6	2.60	n-butyraldehyde	8.18	8.17
C_2H_5	4.47	4.44	furan	7.23	7.19
C_3H_8	6.29	6.29	formic acid	3.32	3.26
C_4H_{10}	8.12	8.14	acetic acid	5.15	5.03
C_5H_{12}	9.95	9.98	propionic acid	6.96	6.83
C_6H_{14}	11.78	11.83	methylpropionate	8.79	8.89
C_7H_{16}	13.61	13.68	methylacetate	6.81	7.07
C_8H_{18}	15.44	15.52	butyric acid	8.58	8.65
C_9H_{20}	17.35	17.37	methylbutyrate	10.41	10.72
$C_{10}H_{22}$	19.11	19.22	formamide	3.88	3.85
$C_{11}H_{24}$	21.04	21.06	acetamide	5.39	5.66
$C_{12}H_{26}$	22.75	22.91	benzamide	12.75	13.16
ethylene	4.26	4.23	p-fluroaniline	11.51	11.13
2-pentene	9.84	9.76	p-chloroaniline	13.5	13.32
1,4-hexadiene	11.49	11.38	p-bromoaniline	14.55	14.26
1-hexene	11.65	11.60	p-nitroaniline	13.9	13.36
1-heptene	13.51	13.45	3,4-dichloroaniline	15.18	15.26
acetylene	3.33	3.33	toluene	11.83	12.17
1-heptyne	12.87	12.56	p-fluorotoluene	11.7	11.74
methylchloride	4.56	4.43	p-chlorotoluene	13.7	13.95
methylenechloride	6.48	6.39	p-bromotoluene	14.8	14.83
chloroform	8.23	8.37	p-iodotoluene	17.1	17.18
carbontetrachloride	10.47	10.37	p-cyanotoluene	13.9	13.94
ethylchloride	6.4	6.25	p-xylene	13.7	13.93
chlorobenzene	12.25	12.19	mesitylene	15.38	15.69
bromobenzene	13.62	13.09	durene	17.4	17.45
p-dichlorobenzene	14.2	14.07	hexamethylbenzene	20.81	20.98
fluorobenzene	9.86	9.98	H_2S	3.78	3.78
1,2-difluorbenzene	9.8	9.74	C_2H_5SH	7.38	7.47
1,3,5-trifluorobenzene	9.74	9.62	$(C_2H_5)_2S$	11	11.17
1,2,4,5-tetrafluorobenzene	9.69	9.58	thiophen	9	8.97
pentafluorobenzene	9.63	9.60	CS_2	8.74	9.23
hexafluorobenzene	9.58	9.66	benzene	10.39	10.40
isopropylamine	7.77	7.80	naphthalene	17.48	18.08
diethylamine	9.61	9.65	anthracene	25.93	25.77
di-n-propylamine	13.29	13.34	phenantrene	24.7	25.77
triethylamine	13.38	13.34	naphthacene	32.27	33.47
tri-N-propylamine	18.87	18.88	1,2-benzanthracene	32.86	33.48
hydrazine	3.46	3.58	chrysene	33.06	33.48
N,N-dimethylhydrazine	7.21	7.27	1,2,5,6-dibenzanthracene	41.31	41.18
aniline	11.58	11.50	acenaphtene	20.61	20.82

N-methylaniline	13.5	13.34	fluorene	21.69	22.53
N-ethylaniline	15.32	15.19	pyrene	29.34	30.03
N,N-dimethylaniline	15.4	15.19	dodecahydrotriphenylene	29.89	30.15
N,N-diethylaniline	19.01	18.88	2,3-benzofluorene	30.21	30.21
pyrrole	7.94	8.04	fluoranthene	28.35	30.03
p-toluidine	13.47	13.26	coronene	42.5	46.28
nitrobenzene	12.92	12.20	difluoroenyl	42.82	44.30
p-nitrotoluene	14.1	13.96	anthraquinone	24.46	23.31
pyridine	9.47	9.44	quinoline	16.57	17.08
p-cyanotoluene	13.9	13.94	acridine	25.49	24.77
HCN	2.59	2.59	truxene	45.55	46.80
3-aminobutyronitrile	9.17	9.46	dixanthylene	45.27	42.78
3-dimethylaminobutyronitrile	12.87	13.15	9-chloroanthracene	27.35	27.43
pyrazole	7.23	7.14	9-bromoanthracene	28.32	28.00
1-methylpyrazole	8.99	8.89	9-cyanoanthracene	28.32	27.48
1,5-dimethylpyrazole	10.72	10.66	phenazine	23.42	23.78
1-ethyl-5-methylpyrazole	12.5	12.50	octafluoronaphthalene	17.64	16.41
H_2O	1.45	1.47	cytosine	10.33	10.26
methanol	3.26	3.21	adenine	13.11	13.36
ethanol	5.07	5.04	thymine	11.23	11.48

4. Test of 3D1 molecular polarizability prediction

Predicted vs. experimental4molecular polarizability



Experimental4 and predicted data

molecule	exp.[a.u.] α	calc. [a.u.] α	α_{xx} [a.u.]	α_{yy} [a.u.]	α_{zz} [a.u.]
acetamide	38.26	38.48	45.68	41.16	28.61
acetone	43.12	42.99	49.73	43.79	35.42
acetonitrile	30.23	28.82	24.63	24.63	37.18
bromo methane	37.45	37.71	32.86	32.86	47.30
chloro methane	30.57	30.62	27.12	27.12	37.51
cyclohexane	74.23	75.64	81.44	81.44	64.03
cyclopentane	61.75	62.09	65.51	65.51	55.19
dichloro methane	45.89	44.03	54.58	41.29	36.16
difluoro methane	18.42	18.71	19.90	18.49	17.74
dimethyl ether	35.36	35.83	31.91	43.86	31.64
ethane	30.23	30.09	28.61	28.61	33.13
ethanol	34.28	35.77	33.13	42.91	31.24
ethylene oxide	29.89	29.81	34.07	26.31	29.01
fluoro methane	17.61	18.05	17.61	17.61	18.89
formaldehyde	16.53	17.15	20.44	17.81	13.09
formamide	27.53	25.44	31.58	27.33	17.41
hydrogen	5.33	5.20	6.00	4.79	4.79
methane	17.68	17.48	17.47	17.47	17.47
methanol	22.4	22.83	20.31	21.39	26.72
nitrogen	11.88	11.91	14.30	10.66	10.66
oxygen	10.8	9.86	11.74	8.97	8.97
p-dioxane	58.04	60.59	59.31	71.18	51.14
propane	43.05	42.79	48.71	40.68	38.93
propanol	47.04	48.77	60.66	44.13	41.49
t-butyl cyanide	64.72	66.63	71.18	64.37	64.37
water	10.06	10.17	12.89	9.51	8.16

5. Comparative evaluation of pK_a estimation methods

A study comparing various pK_a calculation results versus the measured pK_a values of compounds was published by John Manchester et al. Read the article here.

6. References

1. ***PHYSPROP© DATABASE***
2. Klopman, G.; Li, Ju-Yun.; Wang, S.; Dimayuga, M.: *J.Chem.Inf.Comput.Sci.*, **1994**, *34*, 752; doi
3. Miller, K. J.; Savchik, J. A.: *J.Am.Chem.Soc.*, **1979**, *101*, 7206-7213; doi
4. Piet Th. van Duijnen.; Swart, M.: *J.Phys.Chem. A*, **1998**, *102*, 2399-2407; doi

7. Notes

1. 3D geometries of molecules were generated with Marvin.

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Elemental Analysis

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Name to Structure Conversion

ChemAxon's naming toolkit capabilities allow you to generate chemical structures from IUPAC, trivial, drug, CAS names and from CAS numbers.

Supported names include

- IUPAC names, CAS names and generally systematic names
- Common names (e.g. Toluene)
- Drug names (e.g. Paracetamol, Doliprane)
- Acronyms (e.g. ATP for "Adenosine Triphosphate")
- CAS numbers (Note, this feature uses a Web service.)
- For systematic names:
  - Chains
  - Monocycles
  - Retained/traditional names for ring systems with and without heteroatoms
  - Spiro ring systems
  - All cases of von Baeyer nomenclature for bridged ring systems
  - Fused ring systems
  - Ethers, esters, oximes, ...
  - Common characteristic groups
  - Ionic compounds
  - Compounds with one radical
  - Unlimited number of atoms and rings
  - All atom types
  - Substitutive and multiplicative nomenclatures
  - Isotopes
  - Stereochemistry

Current limitations

- Molecules containing multiple radicals (e.g. `ethane-1,2-diyl`) are not supported yet.

Supporting corporate IDs and custom dictionaries

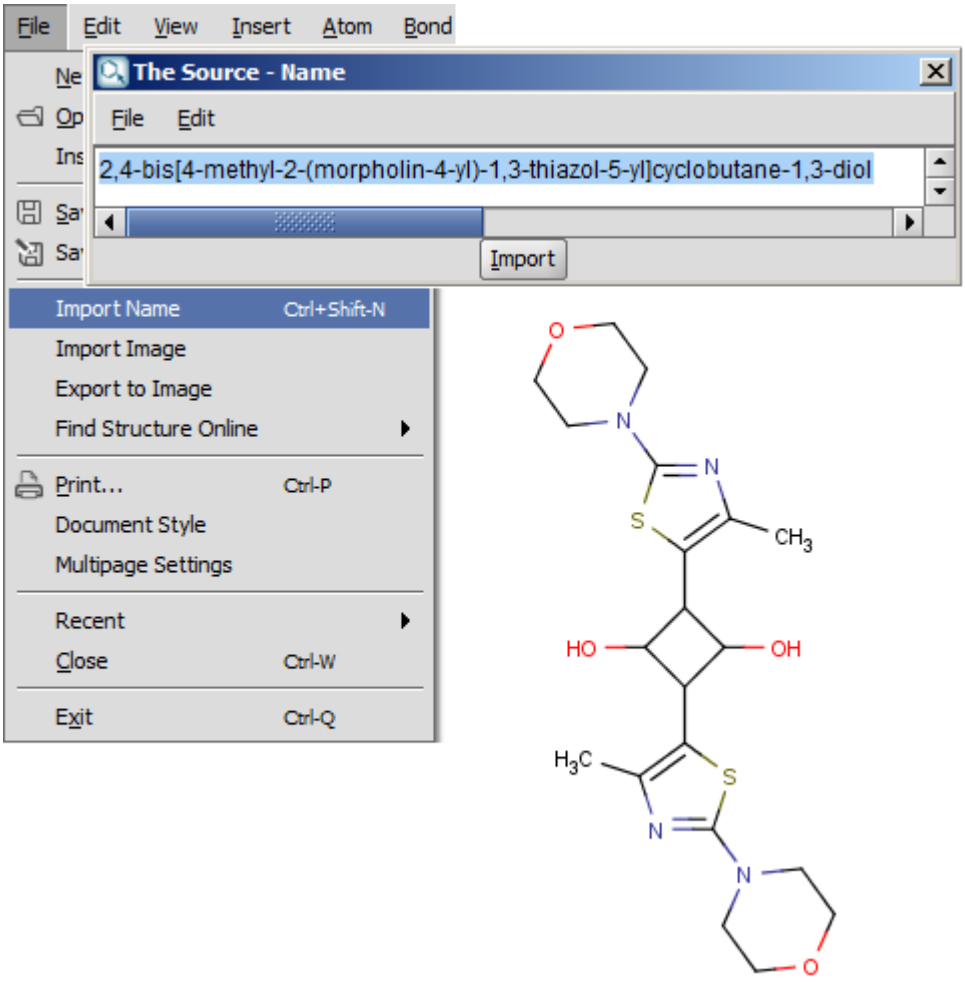
- It is possible to extend the name to structure conversion, for instance to support corporate IDs such as ABC0001234, or to make use of common name dictionaries in addition to the default one. This can be done by connecting to a webservice or by creating a custom dictionary file.

Name to Structure Conversion in MarvinSketch

There are different ways how you can import a name directly into MarvinSketch and convert it to a chemical structure.

- A simple method is to select the name in the text of any page and drag&drop or copy&paste it to MarvinSketch.

  OR
- Select the "Import Name" (Ctrl+Shift+N) option from the File menu, and write the name into the text field and click the "Import" button (Ctrl+I).



Name to Structure Conversion in MarvinView

Open a text file (.name) containing IUPAC names (one per row). MarvinView will open all the structures. Opening the same file in MarvinSketch, the program will ask you to select one structure (by its index number).

Name to structure conversion from command line

As a commandline tool, you can use MolConverter for name to structure conversion. Examples:

1. Converting "test.name" name file to MOL file:

   ```
   molconvert mol test.name -o test.mol
   ```

2. Converting "test.name" name file to "test.smi" SMILES file which also contains the name of the structures:

   ```
   molconvert smiles:n test.name>test.smi
   ```

The behavior of name to structure can be controlled using format options.

Marvin can also convert structures to names.

See also

- name format options
- Developer documentation for naming
- Document to Structure is used to find names in documents and free text

License information

- Name import is only available for a single molecule with the free MarvinSketch desktop application. For batch

conversion (with MarvinView, MolConverter, API, ...) you need the "Name to Structure" licence.

Document to Structure (d2s) Conversion

Document to Structure processes PDF, HTML, XML, text files and office file formats: DOC, DOCX, PPT, PPTX, XLS, XLSX, ODT. It recognizes and converts the chemical names (IUPAC, CAS, common and drug names), SMILES and InChI found in the document into chemical structures.

d2s conversion uses the name-to-structure converter. For the supported names and current limitation, see "Name to Structure Conversion" webpage. You can extend the document to structure conversion by creating a custom dictionary file.

d2s can be used via API, command line application (MolConverter), or MarvinView. Text mining can also be automatized by using d2s integrated into Knime or into Pipeline Pilot.

OCR and syntax correction

Chemaxon's d2s toolkit is able to correct several simple OCR and syntax error. For instance, given the incorrect name "3-rnethyl-l-me-thoxynaphthalene", it automatically corrects the name to "3-methyl-1-methoxynaphthalene" and generates the corresponding structure.

Document to Structure Conversion in MarvinView

Open a PDF file containing chemical names. MarvinView will display all the structures corresponding to the recognized names. The structures can then be saved, copy-pasted, opened in the MarvinSketch editor, ...

Document to structure conversion from command line

As a commandline tool, you can use MolConverter for d2s conversion. Example:

1. Converting "test.pdf" name file to MOL file:

```
molconvert mol test.pdf -o test.mol
```

Structure conversion from OLE objects

D2s converts the chemical structures from OLE objects – created by various chemical sketchers such as Marvin, ChemDraw, ISIS/DRAW, SYMYX DRAW, and Accelrys Draw – embedded in office documents.

Chemical image recognition

For structures represented as images in PDF or Office documents, d2s can make use of several **Image to Structure** tools (also called **Optical Structrure Recognition** or **Chemical OCR**). When such a tool is installed and successfully recognizes the image, the chemical structure become part of the output of d2s; it can be visualized, edited, indexed and search just like any other structure.

Currently the supported Image to Structure tools are:

- Keymodule CLiDE;
- NIH OSRA; and
- GGA Imago.

See configuration instructions to know how to make those tools recognized by d2s.

Note that structures present as vector graphics rather than bitmap are not converted, unless the `osraRendered` format option is used.

See also

- Developer documentation for d2s
- d2s code examples

License informations

- You need the "Document to Structure" licence.

Acknowledgements

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- *Aloe* Swing Extension Package: `cb.aloe.swing.tools` having LGPL license
- JGoodies Forms is a free library.
- JGoodies Looks is a free library.
- EasyCharts.
- Jep - Java Math Expression Parser, see license.
- Jacob Java - Com Bridge.
- IKVM, see license.
- InChI™ Material by IUPAC 2005©
- JNI-InChI is Copyright © 2006-2010, Sam Adams. JNI-InChI is free software: you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License e as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version. (See GPL, LGPL licence.)
- Image formats:
  - Apache SVG Toolkit, see license
  - JPEG Encoder by James R. Weeks and BioElectroMech©, Independent JPEG Group
  - PNG encoder by J. David Eisenberg is under LGPL license
  - PPM encoder by Jef Poskanzer©, see license
  - VectorGraphics package of FreeHEP Java Library is under LGPL license.
  - OSRA software by CADD Group Chemoinformatics Tools and User Services
  - Apache PDFBox -Java PDF Library
- MarvinSpace is based on JOGL, a Java interface to OpenGL under Berkeley Software Distribution (BSD) License
- MarvinSpace uses the DualThumbSlider component of Genomics Institute of the Novartis Research Foundation (GNF)
- Name to structure and Structure to name use names from the DrugBank database.