TopSpin

2D Structure Editor

User Manual

Version 003

Innovation with Integrity

NMR

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Contents

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1 About This Manual

This manual enables safe and efficient handling of the device.

This manual is an integral part of the device, and must be kept in close proximity to the device where it is permanently accessible to personnel. In addition, instructions concerning labor protection laws, operator regulations tools and supplies must be available and adhered to.

Before starting any work, personnel must read the manual thoroughly and understand its contents. Compliance with all specified safety and operating instructions, as well as local work safety regulations, are vital to ensure safe operation.

The figures shown in this manual are designed to be general and informative and may not represent the specific Bruker model, component or software/firmware version you are working with. Options and accessories may or may not be illustrated in each figure.

1.1 Policy Statement

It is Bruker's policy to improve products as new techniques and components become available. Bruker reserves the right to change specifications at any time.

Every effort has been made to avoid errors in text and figure presentation in this publication. In order to produce useful and appropriate documentation, we welcome your comments on this publication. Field Service Engineers are advised to check regularly with Bruker for updated information.

Bruker is committed to providing customers with inventive, high-quality, environmentally-sound products and services.

1.2 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All that you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All that you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REXPNO`

Table 1.1: Font and Format Conventions

2 Main User Interface Features

The new 2D molecule structure editor is integrated into the Structure tab of the TopSpin spectrum window.

The user interface of the editor consists of several main parts:

- The top horizontal quick access toolbar contains buttons to activate the main features of the editor like: drawing structures, selection and rotation capabilities, undo/redo support, file features, editing of the structure properties etc.
- Other toolbars allow selection of an element from the periodic table of elements to be used in a drawing. The user may also use a template to draw the structure more quickly.
- The drawing area: Used to draw and visualize the structure.
- The popup menu: Provides access to the same features as the toolbar in an alternative way.
- The status bar: Displays the full path and file name of the opened file.
- The user interface was designed to follow this criteria:
  - State of the art UI.
  - Simplified use, one click adds an atom (defined bond angle and length).
  - Smart utilization of Drag & Drop.

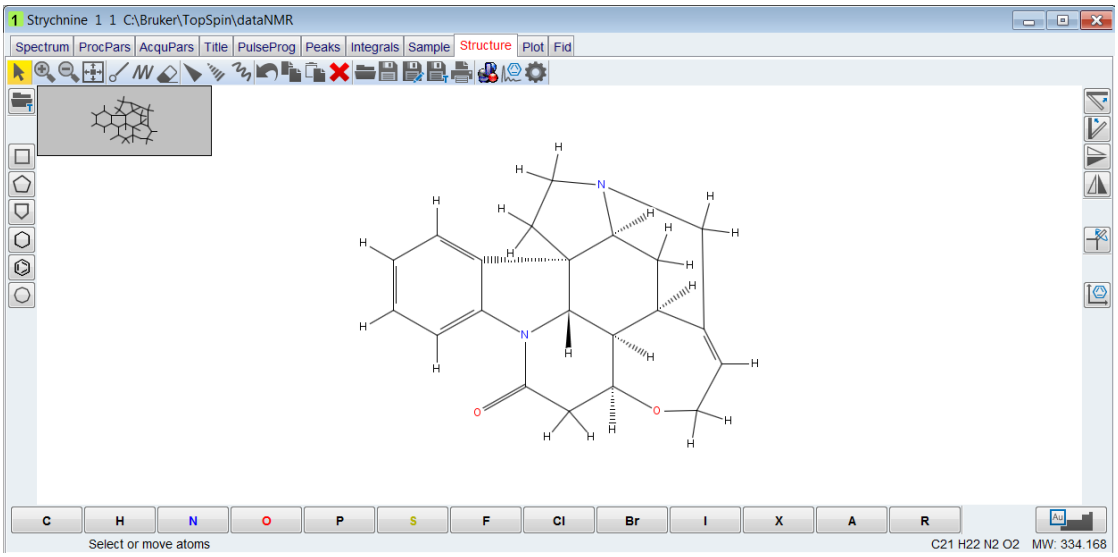
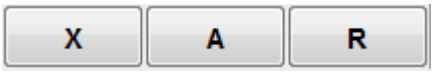


Figure 2.1: Molecule Structure Editor

The editor is similar to other chemical structure drawing programs, but a brief description of the key buttons is included here:

-  - Used to activate selection mode where object can be selected and moved.
-  - Used to control the zoom level.
-  - Used to scale the structure to its actual size.
-  - Activates the drawing mode for normal bonds or chains.

-  - Activates erase mode and deletes all touched bonds or atoms (highlighted in red before deleting).
-  - Deletes the selection.
-  - Used for stereo bond definition (note that at this time CMC-se ignores the stereo chemistry).
-  - Used to undo the last step.
-  - Simple ring templates.
-  - Used to save or open a user defined template.
-  - Used to open a structure or save changes.
-  - Used to copy and paste a selection.
-  - Used to rotate or flip structures.
-  - Used to clean a structure.
- 

- Use to add an atom.
- 

- Used to add a pseudo atom.
- 

- Used to open the periodic table to select additional elements. Refer to the CMC-se User Manual for a list of the atoms that are supported in CMC-se.

3 Working with Files

3.1 Automatic molfile Recognition

When the editor is started a molfile will open automatically if it is included in the NMR dataset. The search for the molfile begins in the *expno* directory and continues up to the project folder level if the file is not found.

3.2 Define Default molfile Folder

It is possible to set a default molfile source folder in the user preferences dialog. To set this directory, click **File**, then **Preferences**, enter the desired directory, then click **Apply**.

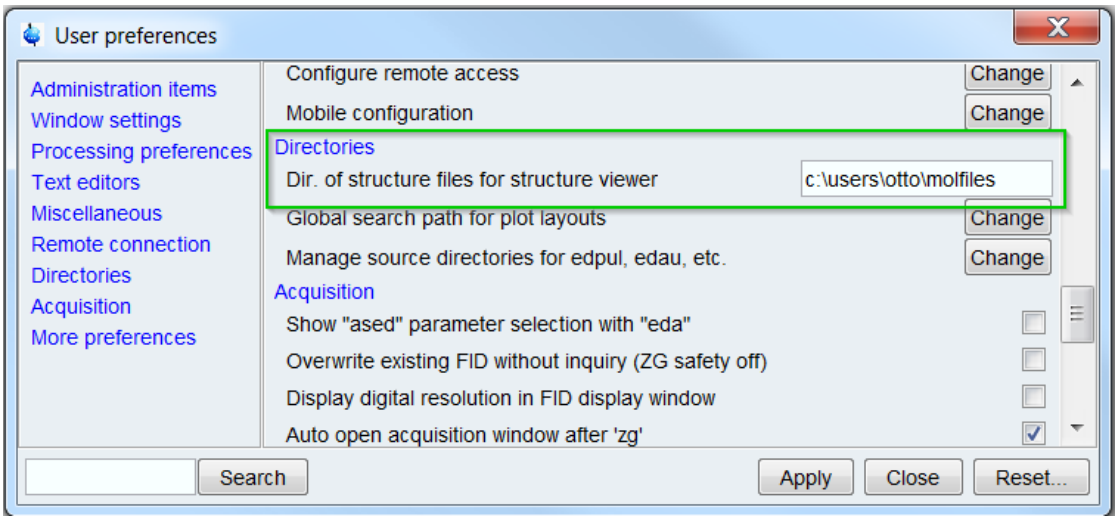


Figure 3.1: User Preferences used to Define the Default molfile Folder

3.3 Opening Files

The Structure Editor supports a variety of structure file types, including: `.mol, .sdf, .xyz, .pdb, .cml, .out.`

The editor uses the molfile format exclusively, therefore when a file with a 3D structure format is opened, the third (z) coordinate will be ignored.

Files can be opened by clicking the **Open** button and selecting the desired file, or by using *Drag and Drop* or *Copy and Paste* as described in the following sections.

3.3.1 Drag and Drop

To quickly open molfiles stored on the disk, it is possible to drag and drop the file to the editor screen:

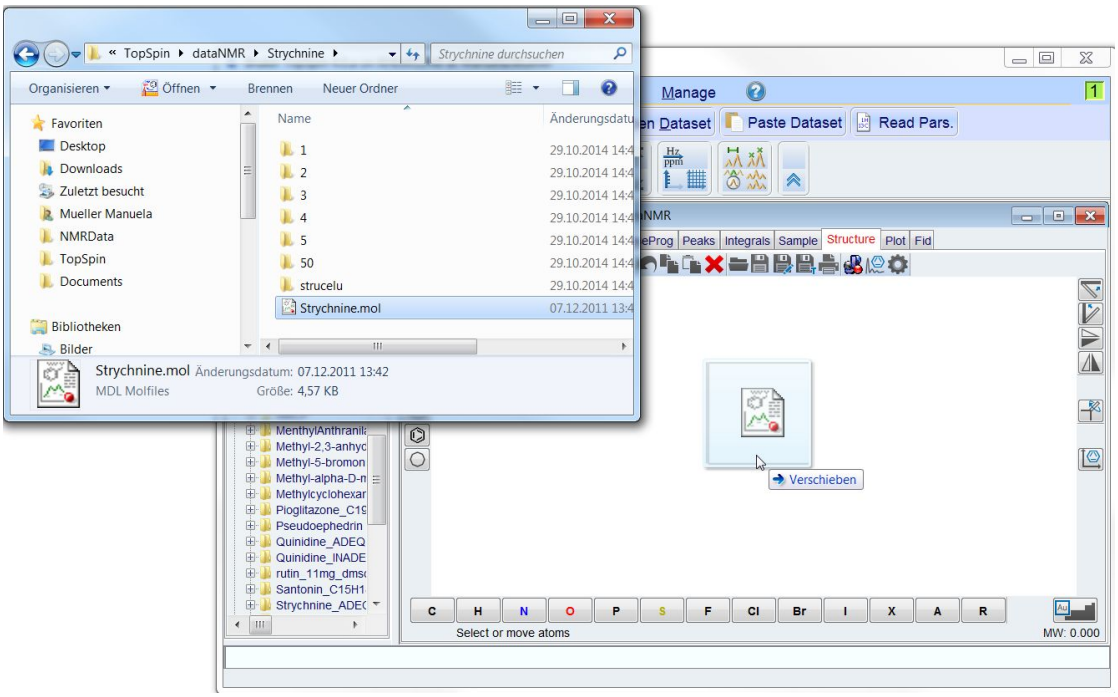


Figure 3.2: Drag and Drop Function

3.3.2 Copy and Paste

Another comfortable way to enter molecules from public libraries it to copy the SD file text from the browser and use the **Paste** button to import the structure.

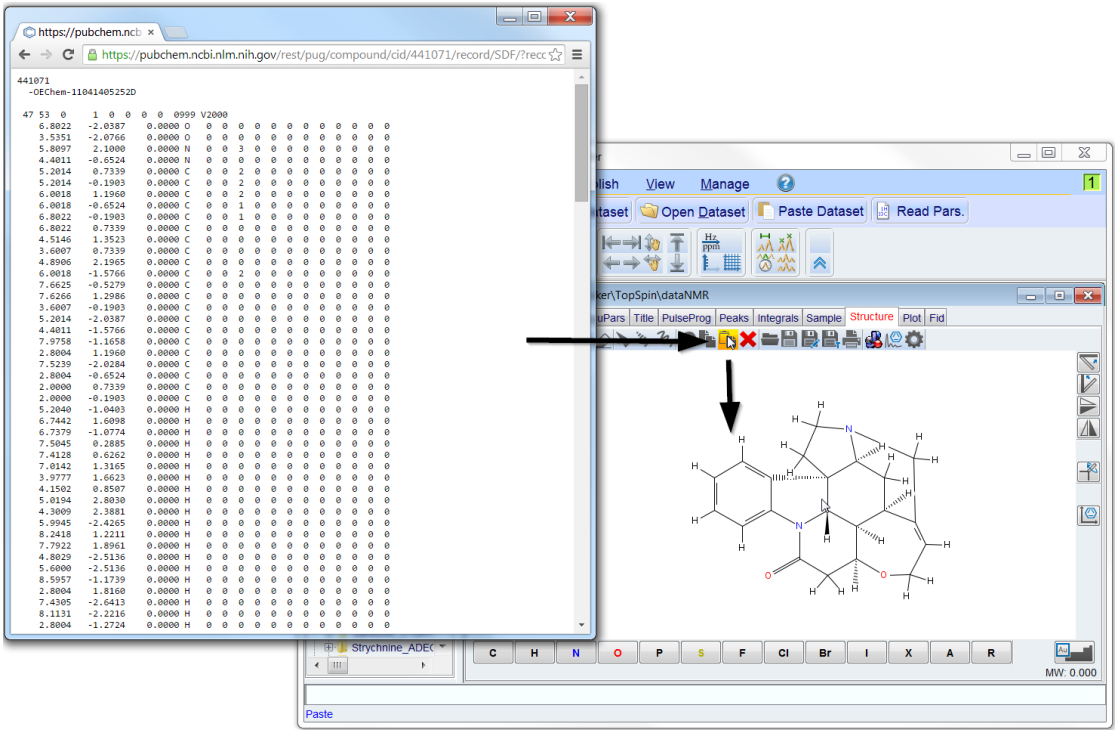


Figure 3.3: Copy and Paste Function to Import Structures from the Web

Copy and Paste can also be used to transfer data between different structure editors:

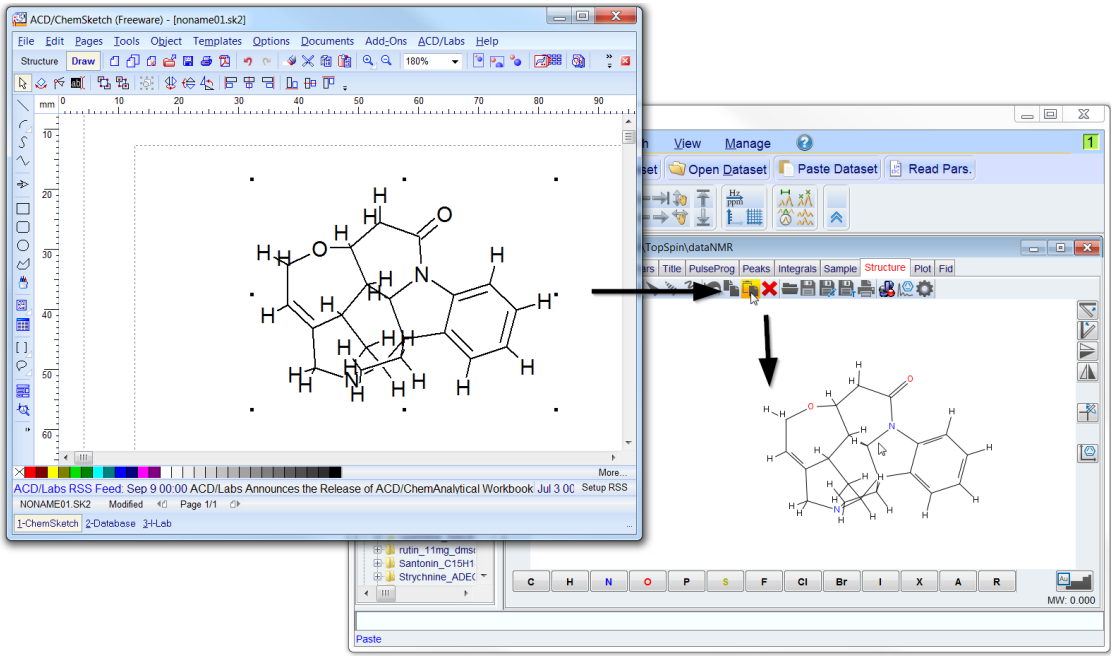


Figure 3.4: Copy and Paste Between Different Structure Editor

3.3.3 Open Templates

Another feature that provides a basis for structure drawing is access to a template library of commonly used fragments. The **Templates selection window** lists all of the available templates, to access this window click the button. It is possible to add additional templates to this window by saving them from the drawing area using the button.

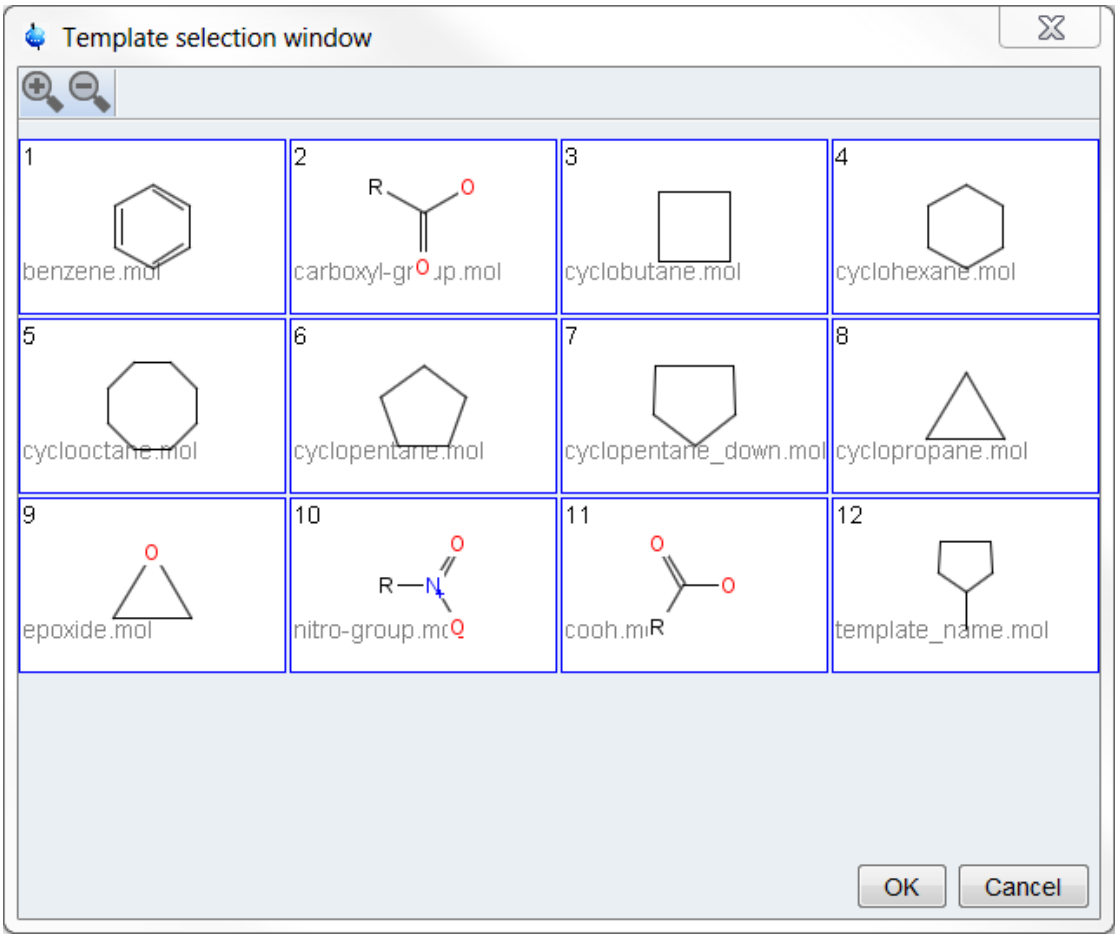


Figure 3.5: Template Selection Window

To open a template, select the fragment (left mouse click) and confirm the selection by clicking the **OK** button. Through this action the template is attached to the mouse and can be placed on the screen or docked to an existing structure.

3.4 Saving and Exporting Structures

Structures can be saved or exported from the structure editor in molfile format, or saved as a template for later use or for creating new structures.

3.4.1 Save and Save as

To save a structure, click the **Save** button. To save a structure under a new name click the **Save as…** button, and enter the name and path in the dialog that appears:

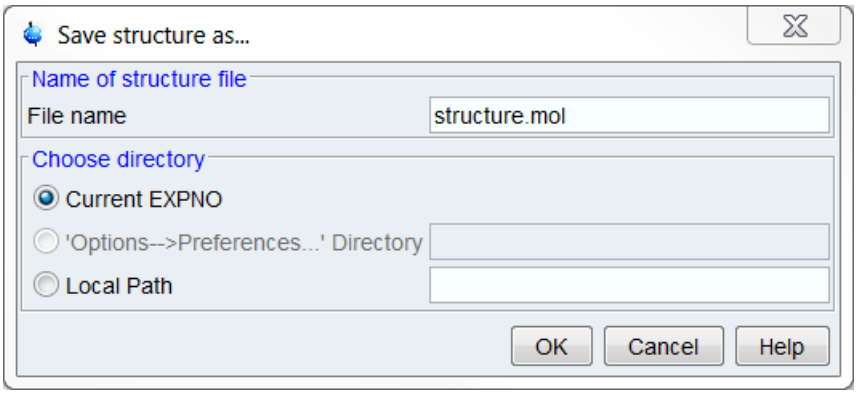


Figure 3.6: Save as… Dialog to Define the Name and Directory for the Structure

Three different directory options are available when saving a file:

- The current expno directory (default).
- A user defined standard molfile source folder (the path defined via **File | (User) Preferences | Directories | Directory of structure files for structure viewer**).
- A local path on the local file system.

3.4.2 Saving a Structure as a Template

A structure may also be saved as a template, where it can be used later for the quick drawing of structure fragments. To save a structure as a template, click the **Save Structure As Template** button. The following dialog appears:

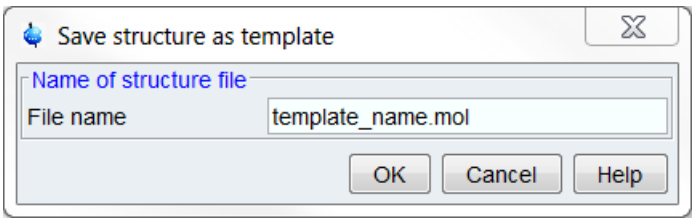


Figure 3.7: Save Structure As Template Dialog

Type the structure template name in the edit field and click **OK** to save the template. The saved templates can be accessed in the drawing process by clicking the **Open Templates** button on the vertical toolbar.

3.4.3 Export Structures

To use structures in a report, for example, it is possible to export the structure with the copy and paste function. Select the structure to be copied and click the button to copy the structure into the clipboard. In an external application it is possible to paste the structure as a picture or in molfile text format. Here are two examples:

Paste in a Word File

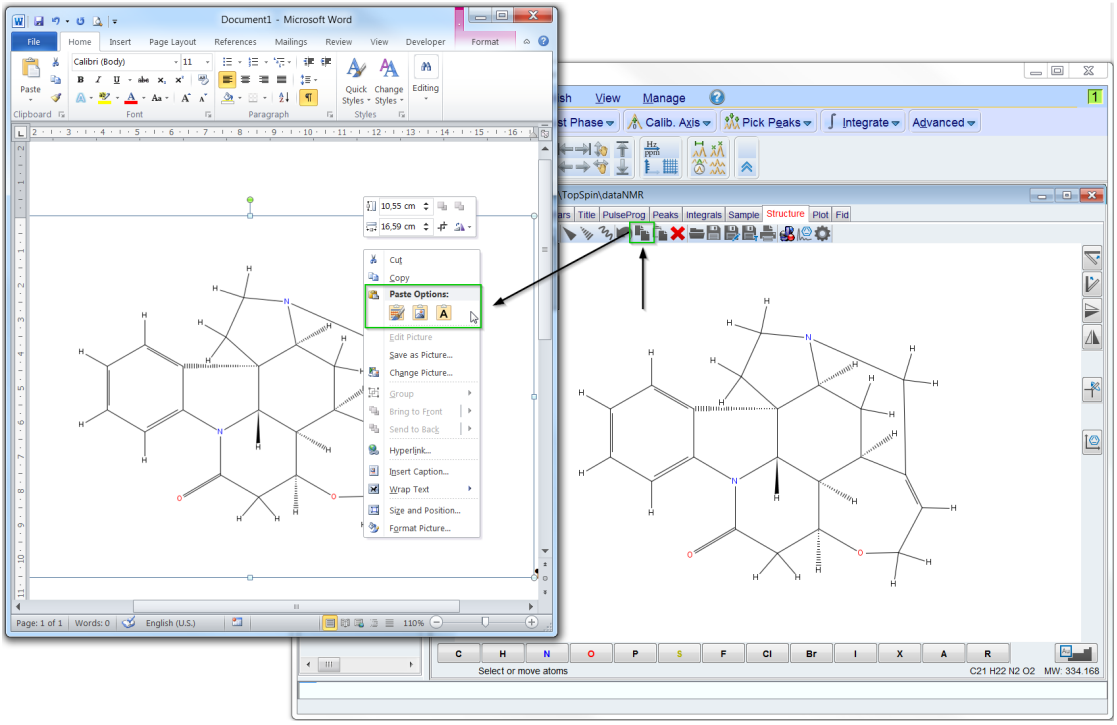


Figure 3.8: Copy Structure to Clipboard and Paste in Word as a Picture or molfile Text.

Paste in a OneNote File

It is possible to change the format, by selecting one of the options in **Paste Options**.

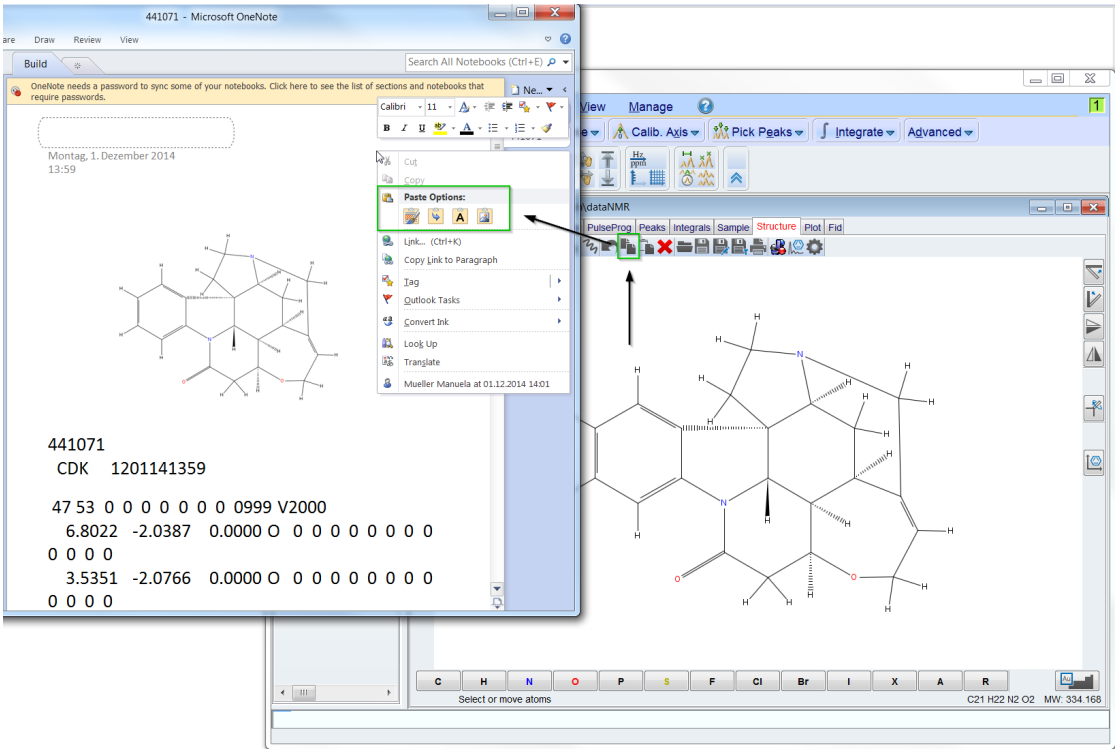


Figure 3.9: Copy Structure to Clipboard and Paste in OneNote as a Picture or molfile Text.

4 Selection Mode

To activate the selection mode press the button. The selection mode is necessary for the following tasks:

- To select bonds and atoms.
- To move, rotate and change their settings.

There are several ways to select atoms or bonds:

- Click on an individual atom or bond. Only one atom or bond will be selected.
- Use the Ctrl or Shift key while clicking on atoms or bonds to select more than one element.
- Click the left mouse button and drag the mouse while forming the shown rectangle to the optimal size and leave the mouse button again. All atoms and bounds inside the selection rectangle will be selected.
- Double click on an individual atom or bond to select the whole connected structure.

Selected atoms or bonds are always highlighted. When more than one element is in a selection, a rectangle is displayed around them with a red arrow symbol that can be used to rotate the selection:

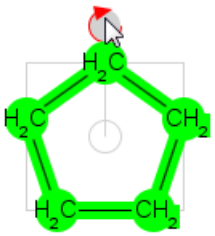


Figure 4.1: Fragment Editor in Selection Mode

To quickly change back to the selection modus, right-click with the mouse.

4.1 Moving a Structure

To move an individual atom, click on it and drag it to the required position. The same is true for bonds or any selection.

4.2 Rotating a Structure

To rotate a structure, click on the arrow , shown with the selection and drag the mouse in the preferred direction. Rotation is only possible with a selection consisting of at least two atoms connected with a bond.

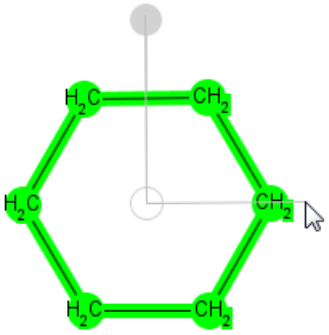


Figure 4.2: Structure Rotation

4.3 Setting a Bond Horizontally

A bond can be rotated to be exactly horizontal. This is especially useful because the selected part of the structure can be rotated together with this bond. Either a selection can be rotated, or (if no selection is available) it rotates the entire structure. Select the function **Set Bond Horizontal** in the context menu by right-clicking on the bond, or click the button and click on the required bond.

4.4 Setting a Bond Vertically

A bond can be rotated to be exactly vertical. This is especially useful because the selected part of the structure can be rotated together with this bond. Either a selection can be rotated, or (if no selection is available) it rotates the entire structure. Select the function **Set Bond Vertical** in the context menu by right-clicking on the bond, or click the button and click on the required bond.

4.5 Flipping On Bond

A selected part of the structure can be flipped on a bond, which may be important when switching between cis-trans isomerism:

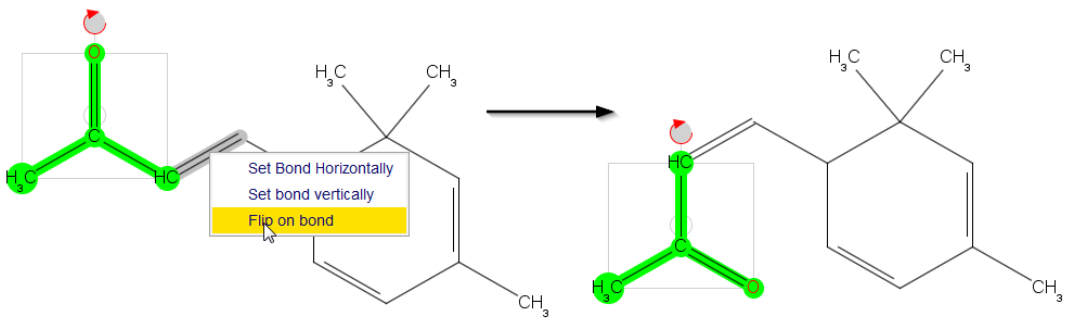


Figure 4.3: Change cis-trans Isomerism

To do this:

- Select the required part of the structure and click the  button.
- Click on the required bond.
- Click again if you want to select a different position of the selected structure.

The mode can also be activated for the desired bond by selecting **Flip on bond** in the context menu.

4.6 Flipping Horizontally

A structure can also be flipped horizontally by clicking the  button. Either the whole structure can be flipped, or an individual selection.

4.7 Flipping Vertically

A structure can also be flipped vertically by clicking the  button. Either the whole structure can be flipped, or an individual selection.

4.8 Refining a Structure

This feature allows the selected part of a structure to be refined automatically. To refine the structure, make a selection and click the  button.

Selection Mode

5 Drawing Mode

In the drawing mode it is possible to draw structures or to extend them. The following drawing modes are available:

- Normal draw mode , used to draw single bonds or add individual atoms.
- Draw chains mode , used for a quick and comfortable chains drawing.

5.1 Normal Drawing

Activate the **Draw normal** mode by clicking on the button. To add an individual atom (not connected with any other bond) to the structure, left click with the mouse on a location where the atom should be.

Another possibility is to add a set of connected atoms. To do this, either confirm the suggested bonds (considering the correct bond angle), or left-click and drag the mouse to an individual position, illustrated in the figures below.

When drawing a set of connected atoms, either draw an additional bond considering the correct bond angle, or draw individually positioned bonds. The suggested correct bond angle is shown highlighted when the mouse touches the atom. To confirm this angle click the left mouse button, as shown below:

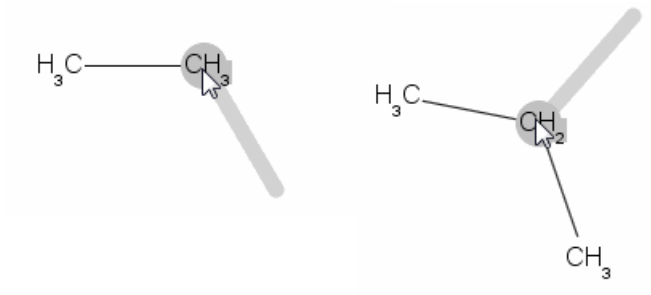


Figure 5.1: Draw Bonds with Considering Correct Bond Angles.

An individual drawing is possible by left-clicking and dragging the mouse to an individual position:

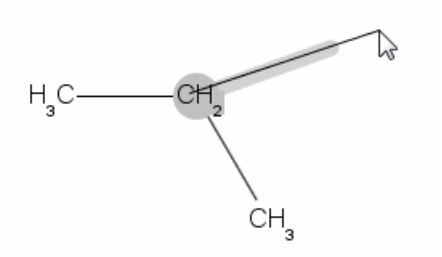


Figure 5.2: Drawing with Individual Bond Angle and Length

5.2 Drawing Chains

Activate the **Drawing Chains** mode by clicking on the  button. To build a chain, left-click and drag the mouse. During this process the current length of the chain is shown next to the mouse at the end of the chain. Release the mouse button when the desired length is reached:

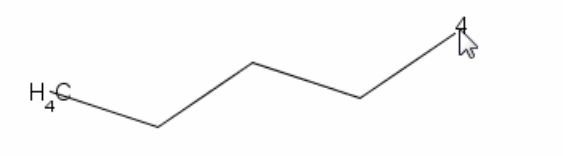
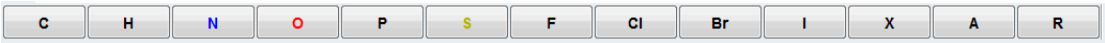


Figure 5.3: Drawing Chain Bonds

The default drawing element is carbon, to change this, select another element from the toolbar:



Or select one from the more comprehensive periodic table  .

It is also possible to replace an existing atom by selecting a different element and clicking the left mouse button on this atom. The old element will be changed to the current one. All atoms will be connected by bonds with order equal one.

5.3 Using Simple Templates

The editor also provides simple templates for a quick drawing. To use a template click on one of the available template  buttons. The selected ring template will appear next to the mouse on the screen and can be placed with a left mouse click. To extend a structure with a template, rotate the structure and try to dock the template to the desired binding site, until green circles indicate a successfully recognized binding:

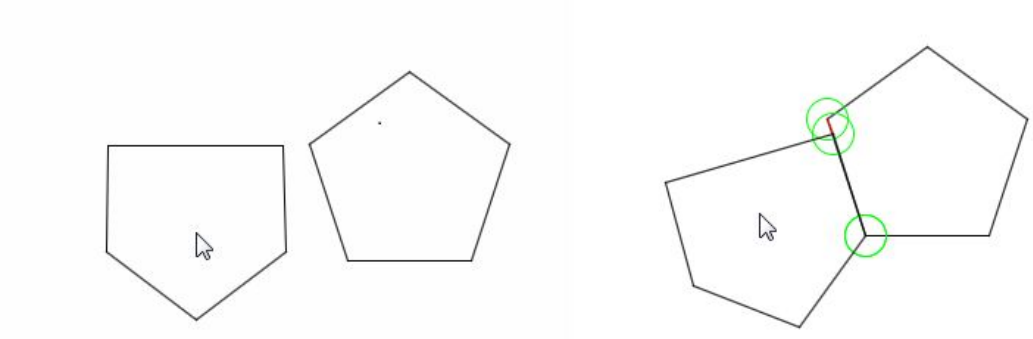


Figure 5.4: Illustration for the Simple use of Templates Through Docking.

6 Change Structure Settings

6.1 Stereo and Aromatic Bonds

The bond type can be changed using the following buttons:

-  : Up stereo bond
-  : Down stereo bond
-  . Undefined stereo bond

In this mode it is possible to toggle between the different possibilities (e.g. change the direction of the bond or change back to normal single bond) by repeatedly clicking on the already existing bond.

6.2 Bond Order

The bond order in the drawing modus can be changed by clicking on the required bond. Click the  button to enter the drawing modus, then click on the required bond repeatedly to change the bond order. This feature works in all of the drawing modes.

6.3 Atom Charge

The atom charge can be changed in the atom properties. To open the atom properties dialog in the context menu, right click on the atom and select **Atom Properties**:

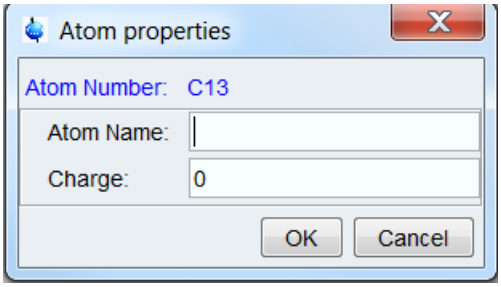


Figure 6.1: Atom Properties Dialog

Change the charge number and confirm it by clicking **OK**.

6.4 Removing Explicit Hydrogens

The structure editor always reads the molfile as IS. With the option **Remove explicit hydrogens** in the context menu (left mouse click) it is possible to remove explicit hydrogens. The hydrogens are not hidden, they are removed.

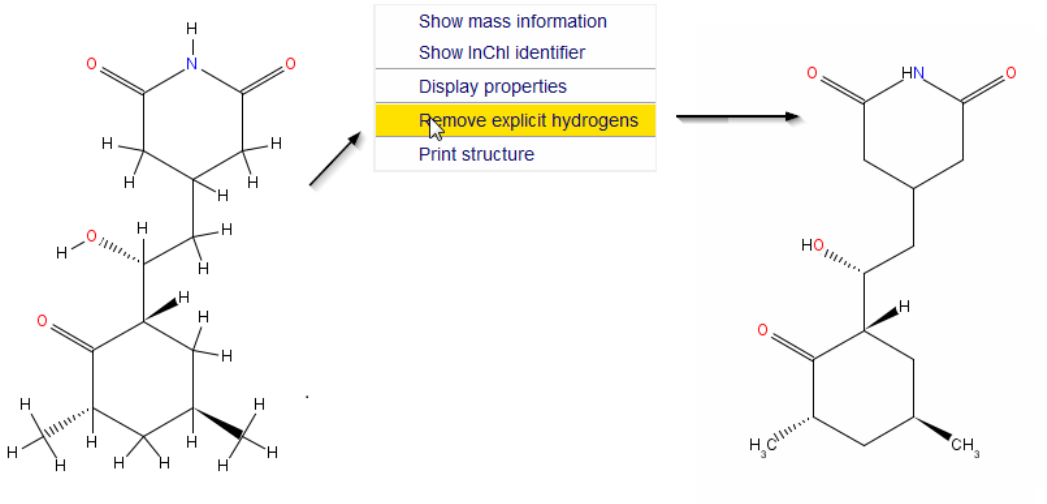


Figure 6.2: Remove Explicit Hydrogens

More changes to the illustration of the structure are available in the setting: **Display Properties**.

7 Periodic Table

In the periodic table it is possible to change the element selection to draw atoms. To open the periodic table dialog click the  button.

Figure 7.1: Periodic Table Dialog

The isotope value is *Auto* by default which means the isotope is not specified actually. If a change is necessary, specify a concrete isotope by selecting it from the **Nuclear Isotope** drop-down list box.

Periodic Table

8 Setting Display Properties

8.1 Display Properties

In the Display Properties dialog it is possible to change all or some part of the atoms in a structure. Click the button, or select the menu entry **Display properties** in the context menu (left mouse click), to open the dialog:

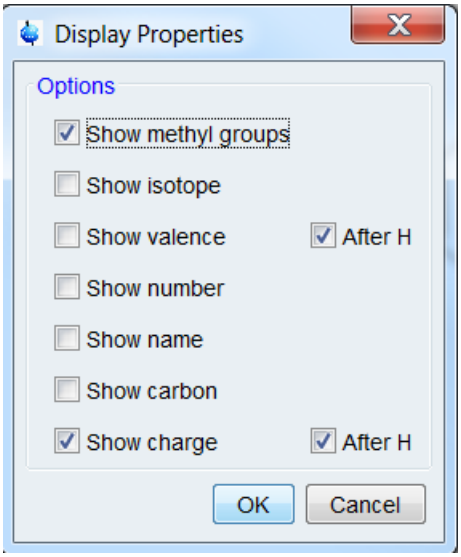


Figure 8.1: Display Properties with Default Settings

Check or uncheck the information that should be displayed. A checkbox is enabled when at least one atom selection is available, otherwise it will be disabled.

8.2 Zooming

There are the following zooming actions are possible:

- Zoom In
- Zoom Out
- : The structure will be scaled to its actual size.

8.3 Move Display Center

It is possible to move the focus of an object by using the miniature window in the left top window. Click with the mouse in this small window and drag the gray rectangle to the desired place. The focus will change at the same time:

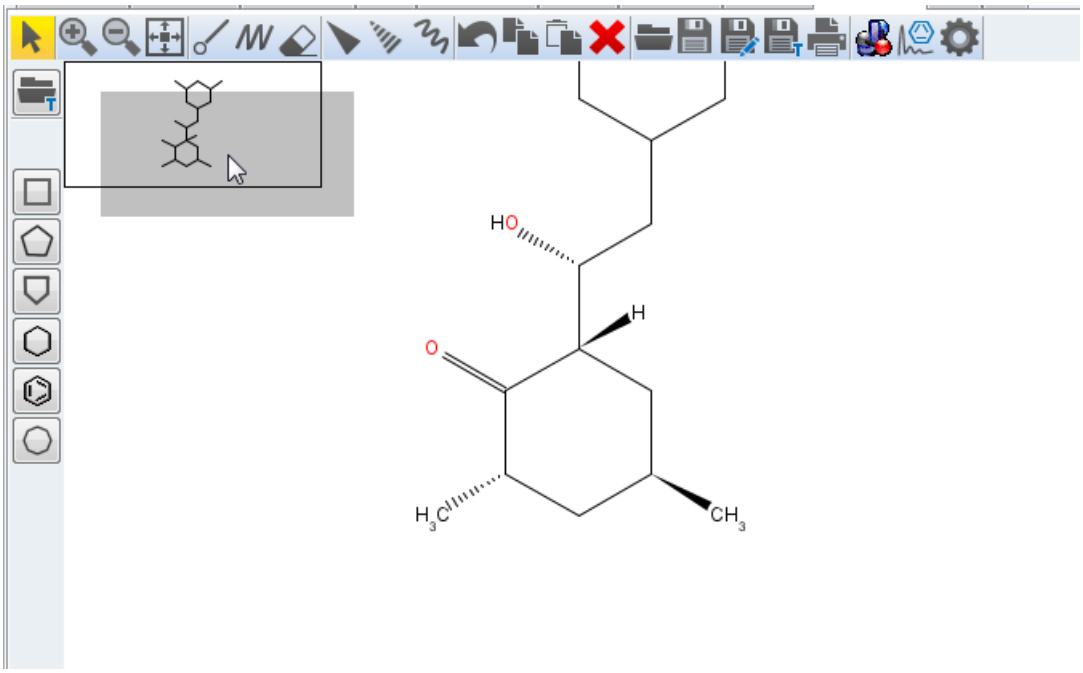


Figure 8.2: Move the Focus of the Display

8.4 Setting Colors

The structure and background colors, as well as other TopSpin options, can be selected using the **Options I Preferences** dialog. The editor uses the background color from the spectrum section of the dialog as the background color and the axes color as the color for the structure. To activate the new color settings the editor must be restarted.

9 Show Structure Information

This context menu option will display additional structure information, such as the mass information and international chemical identifier.

9.1 Mass Information

To display the mass information, click on **Show mass information** in the context menu: The following dialog appears, display two types of mass: molecular weight and mono isotopic mass:

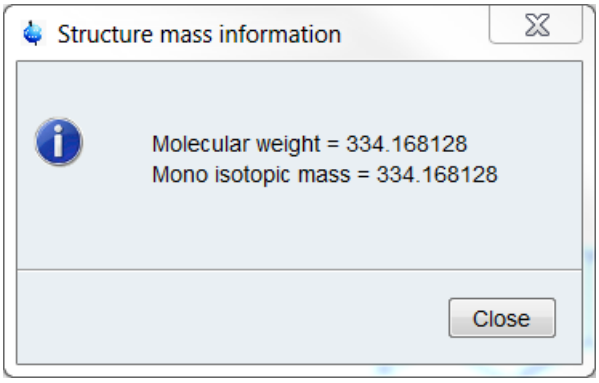


Figure 9.1: Structure Mass Information

9.2 International Chemical Identifier

Click the option **Show InChI identifier** in the context menu to display the International Chemical Identifier (InChI) identifier in a different file:

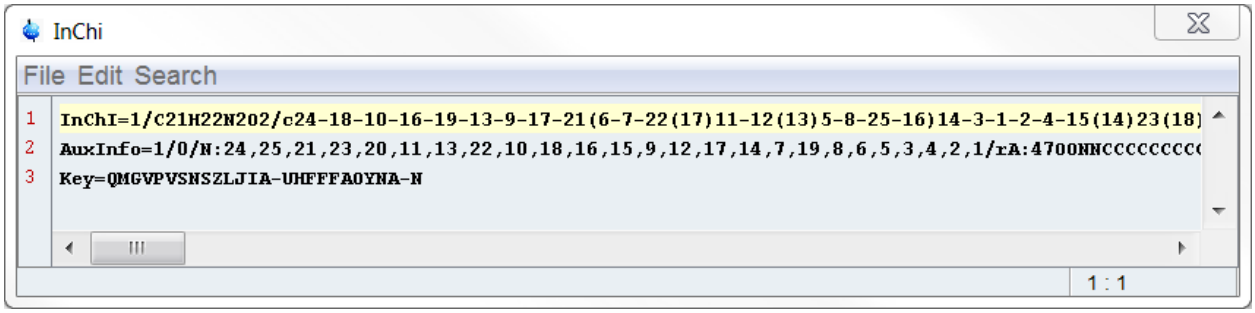


Figure 9.2: InChI Identifier

9.3 Starting Jmol

To work with the Jmol 3D Molecule Viewer click the  button. The current structure will be reopened in the Jmol Viewer. For this option it is necessary to save any changes.

9.4 Identify Structure with InChI Key

For a structure identification it is possible to search in different databases after the complete structure or the connectivity pattern only. To get access to the search interface choose **Identify structure** in the context menu of the structure editor (right clicking the mouse button) and the following dialog will appear:

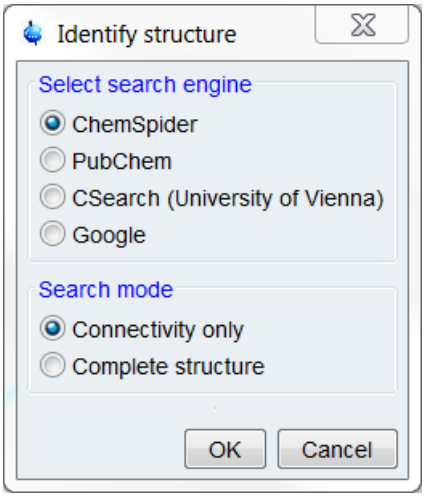


Figure 9.3: Identify Structure Dialog

The search is based on the InChI Key and shows the result in the default web browser. Internet access is necessary for all search engines.

10 View Spectrum Correlations

The View Spectrum Correlations is a special mode used to view the correlations between atoms in the structure and multiplets. The correlation assignment procedure is described in the Multiplet Analysis (**mana** command) documentation, refer this documentation more details.

To view the correlations defined in Multiplet Analysis, open the same dataset twice with one of both possibilities:

- Reopen the dataset with **File | Reopen**. The datasets will be arranged in stack automatically.
- Open the same dataset twice by using the context menu (right mouse click) from the dataset in the browser panel and selecting the **Display In New Window** item. The browser panel is located on the left side of TopSpin user interface. Select the **Window | Arrange in stack** item from the TopSpin main menu to view both windows at the same time.

To show the correlations:

- Click the Spectrum tab on the first window and the Structure tab on the second (optionally click the **Fit All** button to fit the structure into the sizes of the drawing area).
- Activate the correlation viewing mode by clicking the  button. The correlated atoms will be highlighted with different colors if correlations exist.
- Move the mouse cursor over the correlated atoms. The cursor in the first window will move to the corresponding multiplet as the mouse cursor passes over the correlated atoms.
- The correlation viewing works in the opposite direction as well, when you move the mouse cursor over the spectrum in the first window the corresponding atoms will be highlighted.

View Spectrum Correlations

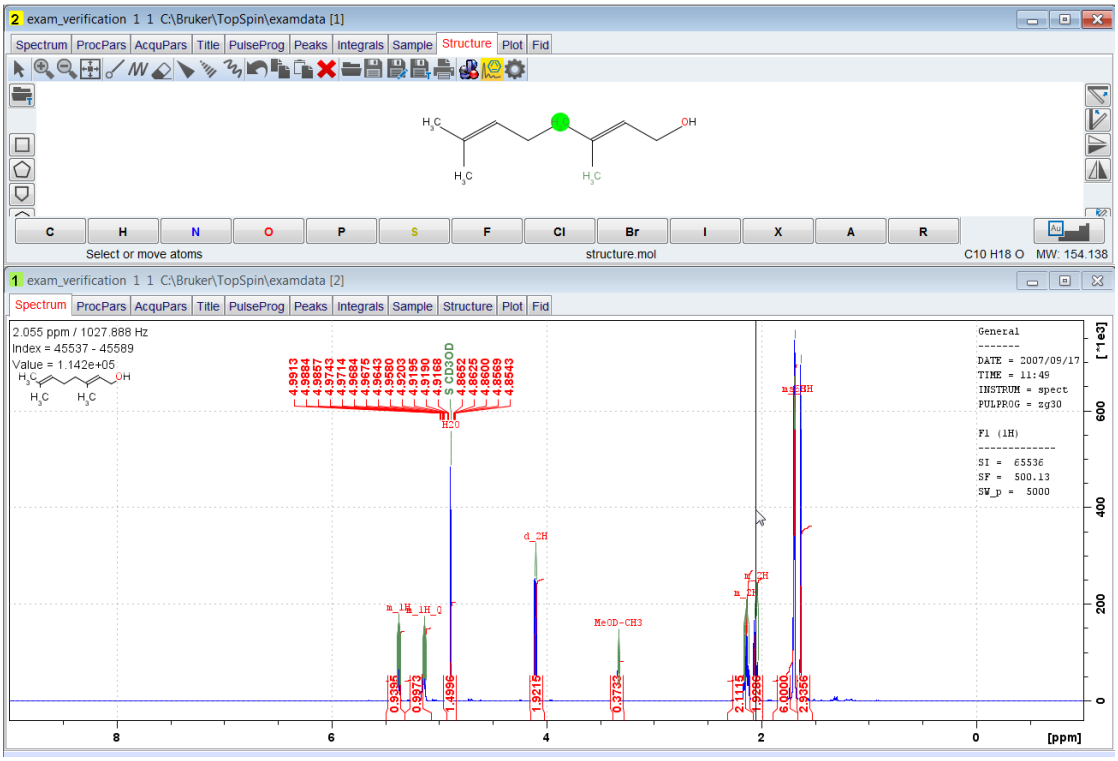


Figure 10.1: Show Spectrum Correlations

11 SD File Viewer

11.1 Main User Interface Feature

The Multi-Structure Viewer is a viewer with several features to visualize Structure Data (SD) files:

- The possibility of visualizing all structures in SD files.
- Scroll through a large amount of data and zoom into desired one.
- Working with compressed files save disk space (e.g. .zip or .gz files downloaded from PubChem without decompression).

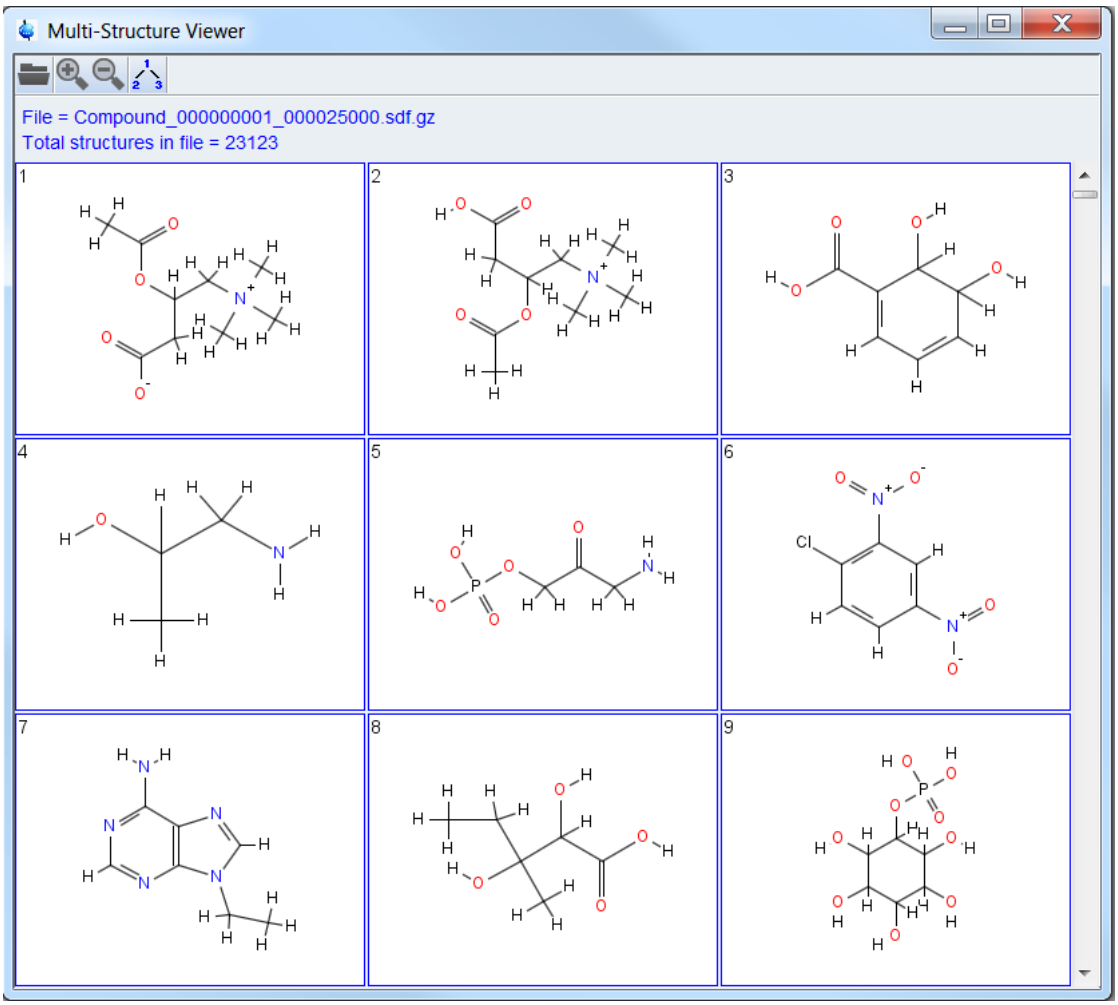


Figure 11.1: Multi-Structure Viewer

The editor provides a simple control with the following buttons:

- - Used to open a SD file.
- - Used to zoom in or zoom out to change the number of structures in the overview.

-  - Used to toggle between atom numbers and single atoms.

11.1.1 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All what you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All what you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST
Program Code **Pulse and AU Program Names** **Macros** **Functions** **Arguments** **Variables**	Courier	`go=2` `au_zgte` `edmac` `CalcExpTime()` `XAU(prog, arg)` `disk2, user2`
AU Macro	Courier in Capital Letters	`REX` `PNO`

Table 11.1: Font and Format Conventions

11.2 Open Files

The viewer supported the following strcture file types: `.mol`, `.sdf`, `.sdf.gz`, `.sdf.zip`.

Start the editor in the TopSpin menu bar by clicking **Analyse | Structures | 2D Multi-Structure Viewer** or by using the **vstrucs** command.

As the editor opens the desired file has to be selected. Once the editor is open, it is possible to change the file by clicking the **Open**  button.

12 3D Structure Viewer

12.1 About Jmol Molecule Viewer

Jmol is a 3D Structure Viewer for displaying chemical structures. It is TopSpin's implementation of the open source Jmol molecule viewer (cf. jmol.sourceforge.net). For general license information and Bruker changes to Jmol:

- Click **Help** => **License Info**

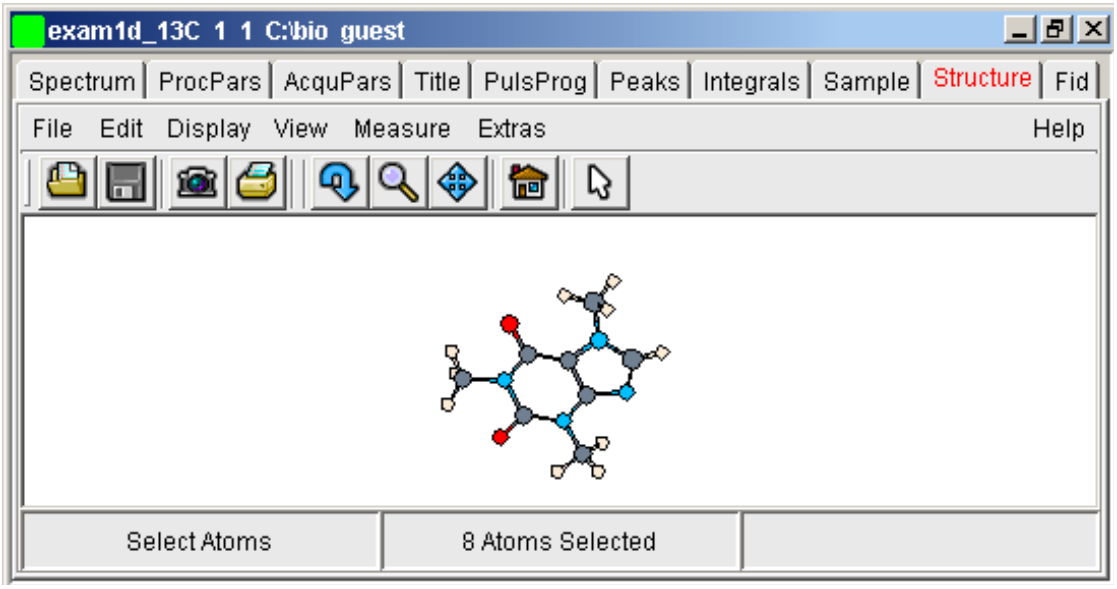
To start Jmol:

- Enter **jmol** on he command line

To start Jmol from the 2D Structure Editor, click the Jm button on the toolbar.

12.2 Jmol Functionality

The command **jmol** will switch the data window to the Molecule Viewer as shown:



TopSpin 1.3 and newer contains Jmol version 10. This has the following features:

- The viewer displays the structure file that resides in the expno of the current dataset. If this does not exist, the structure file defined by the acquisition parameter CHEMSTR is displayed. CHEMSTR can define a full pathname or a filename. In the latter case, the file is searched for in the directory defined in the User Preferences. To set this directory, click **Options** => **Preferences**, select **Directory pathnames**, enter a directory and click **OK**. If no structure file is found, you can open one by clicking **File** => **Open** in the Molecule Viewer
- The following structure file types are supported: `.xyz, .mol, .pdb, .cml, .out, .mmlgp, .res, .cif, .gpr, .hin, .nwo.`
- Secondary structure elements of proteins (backbone, cartoons, ribbons,...) can be displayed in selectable sizes and colors.
- Mouse button effects:

  - Rotate a molecule around the x- and y-axis by pressing the left mouse button, and moving the mouse left/right or up/down, respectively.
  - Rotate a molecule around the z-axis by pressing the middle mouse button and moving the mouse left/right.
  - Zoom in or out a molecule by pressing the middle mouse button, and moving the mouse up or down.
- RASmol command scripts are supported. To send a RASmol command to the currently displayed molecule enter:
  - **jmol <RASmol command>**
  - Here are some examples:

jmol zoom 400

jmol ribbon 200

jmol color ribbon yellow

You may create TopSpin macros containing RASmol commands. Just enter **edmac** on the TopSpin command line and insert the RASmol commands in the appearing editor. Here is an example:

jmol load /mystructures/alphahelix.pdb # load a structure

jmol backbone 0.7 # display its backbone with 0.7 Angstrom size

jmol color backbone yellow # change backbone color

jmol background green # change background color

jmol zoom 200 # zoom structure

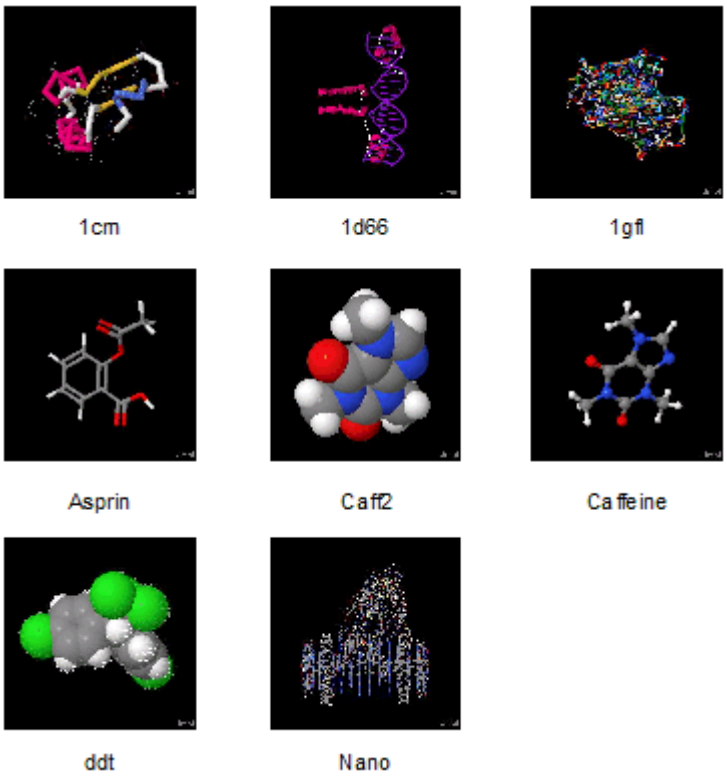
The available RASmol commands are described in the **Jmol Help** menu item **User Guide**.

- Multiple molecules (or multiple aspects of one molecule) can be displayed simultaneously. To do that just open multiple data sets or open the same dataset in multiple data windows and click on the **Structure** Tab in each window.

A set of molecule structure files is delivered on the TopSpin DVD and stored in the directory:

<tshome>/classes/prop/StructureSamples/*

The following figure gives an impression of the capabilities of Jmol. The images were extracted from the Jmol home page.



12.3 More Information on Jmol Molecule Viewer

More information on the Jmol molecule viewer is available under the Jmol **Help** menu in sub menu **User Guide**.

3D Structure Viewer

13 Contact

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