Tutorial

by Dr. Markus Vogt

ACD/ChemSketch
(for Windows)
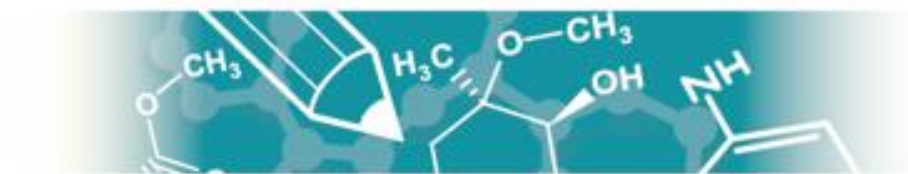
Content

1. Download & Installation

ACD/ChemSketch Freeware is a chemical drawing package for home and educational use, and can be **downloaded** from the following internet address:

http://www.acdlabs.com/resources/freeware/chemsketch/

However, before download you first have to **register**, but this takes only 1-2 minutes.

Next, locate the downloaded file **chemsk2015.exe** in your download folder, double-click on the file, and then just follow the installation instructions as shown below:

2. First Steps

To **start** the program select **Start** menu -> **Programs** folder
-> folder **ACDLabs Freeware 2015** -> **ChemSketch**

One minor drawback of the freeware version:
With every start you have to first click the **OK button** in the small ACD/Labs Products presentation window.

After first start you may want to set some **preferences**:

- Open menu point **Options** -> **Preferences** and then click on **Structure:**
  Activate **Fixed Bond Angle** and **Bond Length** (e.g. 10 mm)
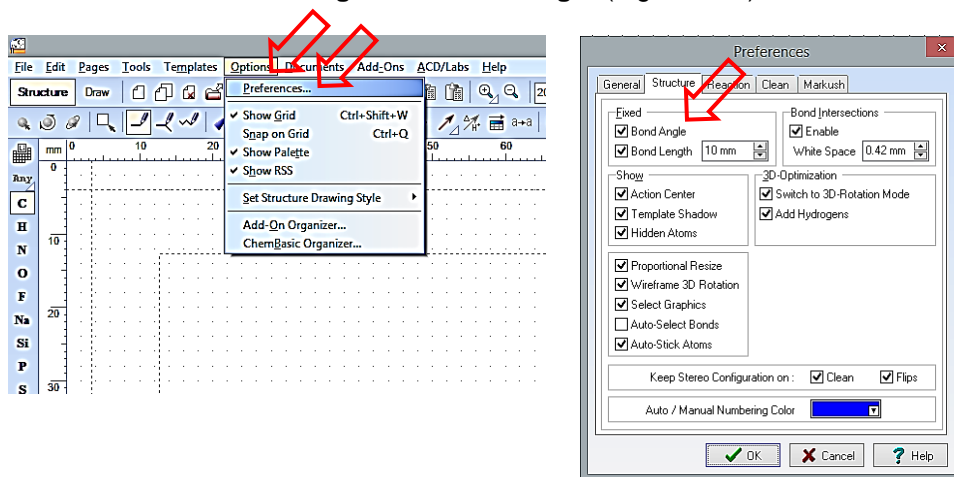
- Open menu point **Tools** -> **Structure Properties** -> **Common:**
  (1) Activate **Show Carbon: All** -> (2) **Set Default**
  -> *Optional:* (3) **Save** Current Style as e.g. Your Name/Your Initials
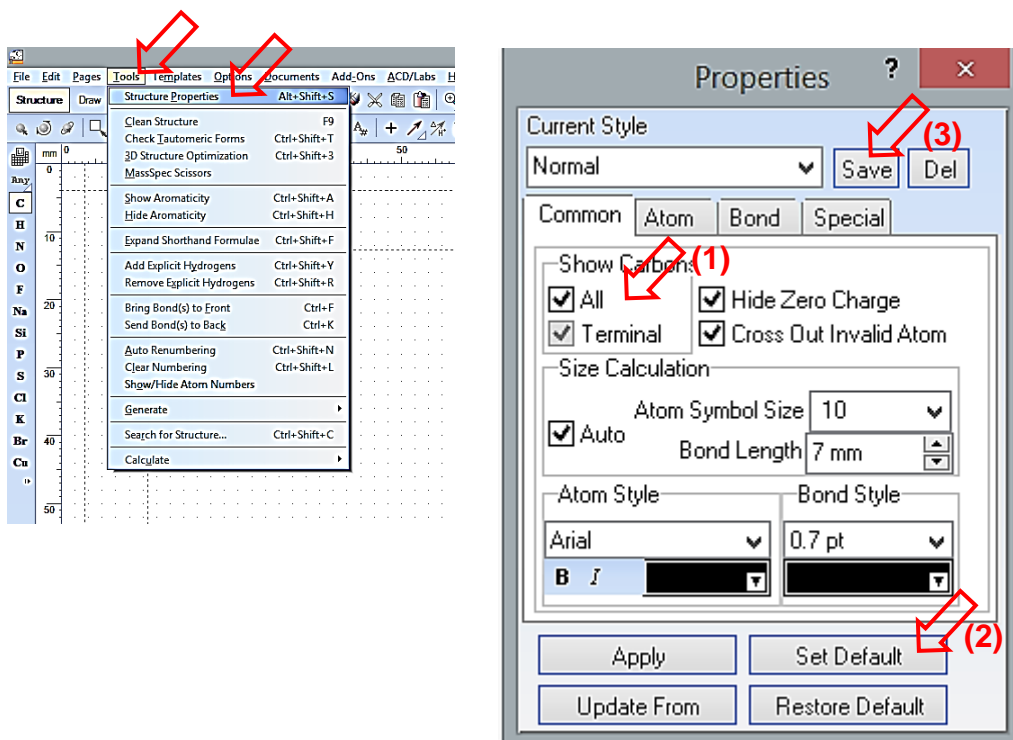
3. Simple hydrocarbons: The alkane series

At the beginning, you have an empty workspace
with a typical setup:
Since we typically draw **structural formulas** of
standard and modified **hydrocarbons,**
the following features are selected:

(1) Structure mode
(2) C(arbon) in the **Atoms** toolbar
(3) Draw Normal (bonds)
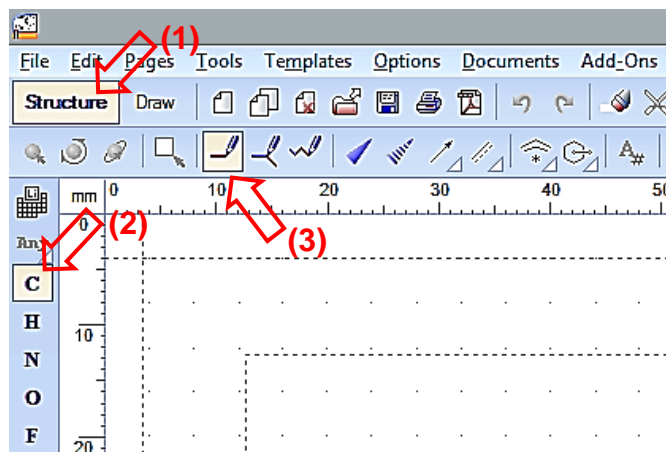
a) **Methane**, **ethane**, **propane** etc.

With this setup, click with the **left mouse-button**
anywhere in the workspace, and you immediately
get the formula of **methane** or **CH$_4$**.
(Note: All free bonds of the selected C atom – and
of any other atom – are automatically „saturated" with
H(ydrogen) atoms.)
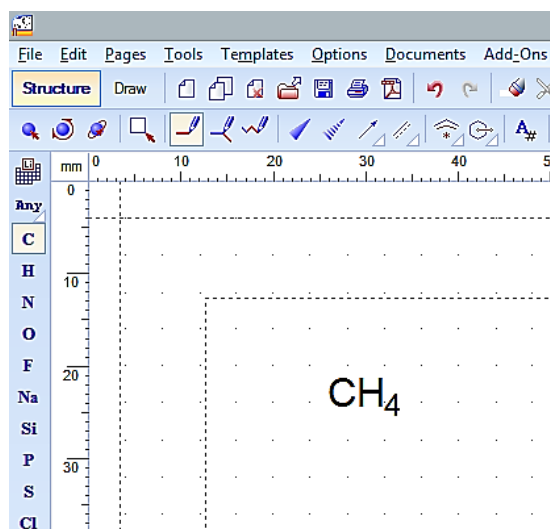
Now, we have the sum or shorthand formula.
To expand to the complete **structural (LEWIS) formula**
with explicit hydrogens, just
(1) select the **H atom** in the Atoms toolbar,
(2) click on the **C** in the **CH$_4$**,
(3) hold the button and **move** the mouse to any direction,
(4) – (6) repeat step (3) three times to „pull out" the
    remaining H atoms to the other directions.
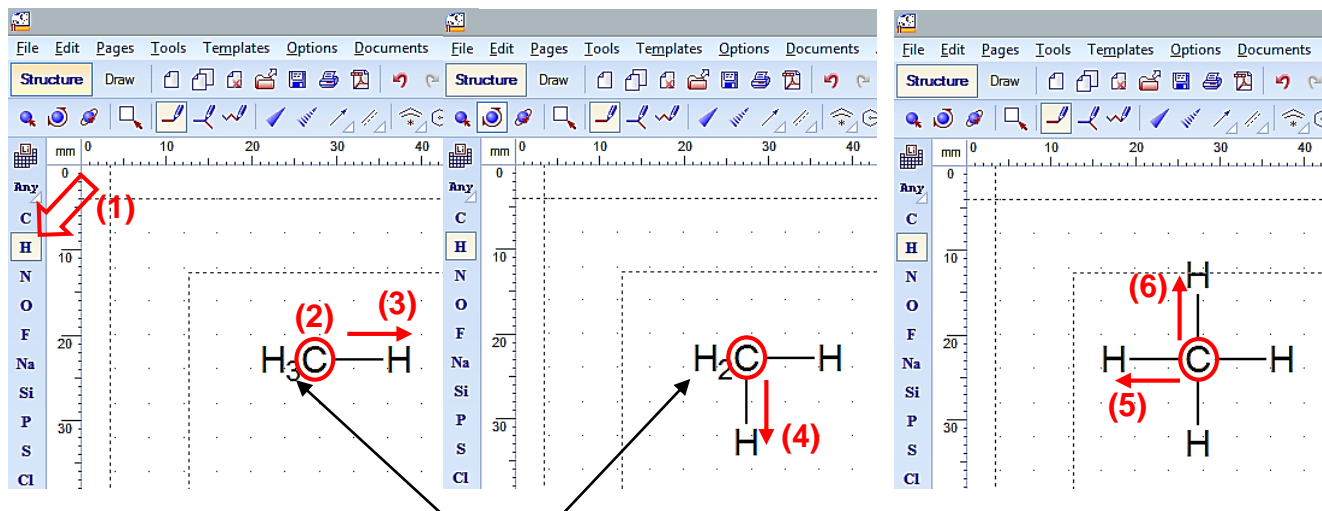
As you can see, the number/index of the

remaining hydrogens is reduced correspondingly.

Next, we **clean the work-space** by **selecting** and **deleting** the molecule.

(1) Click the **Select/Move** button and then click anywhere **close to the molecule** (don't touch it) -> the **whole structure** is selected with one click and can easily be **moved** away or also **removed** by pressing Del(ete).
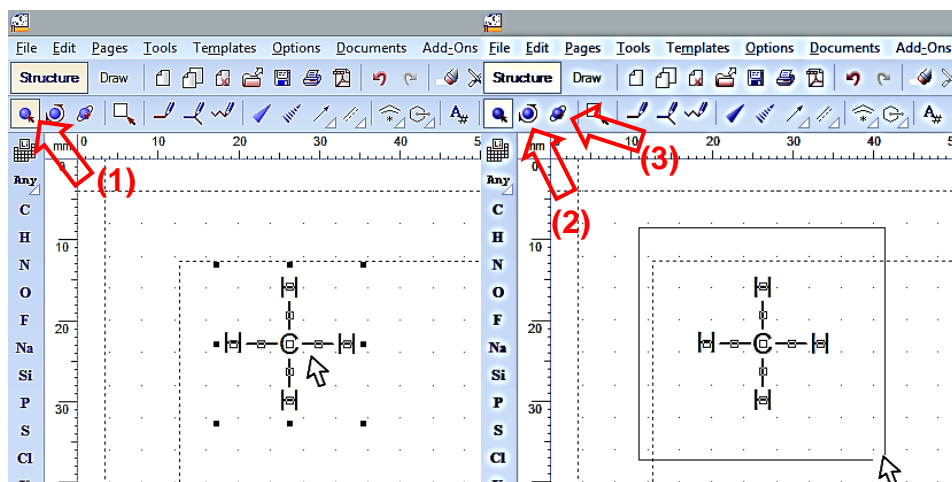
Another way to **select** single atoms, bonds, fragments or whole structures is to **directly click** on the atoms and bonds, or (just like in most programs) to **drag a rectangle around** the desired fragments / structures with the mouse-button pressed.

Two more **select buttons** can be used to additionally **(2) Rotate/Resize**, and **(3)** for **3D Rotation**.

To draw further members of the **alkane series**, proceed similarly:
(1) Start again with **methane** (with non-explicit hydrogens) by just clicking anywhere.
(2) Leave **C selected**, **(3)** click on the **C** in methane, **(4)** hold the mouse button and pull out another C(H$_3$) to get **ethane.**
(5) Starting with ethane, pull out another C(H$_3$) to get **propane,** and so on.
In the same way, you can create **branched molecules / isomers** as well.
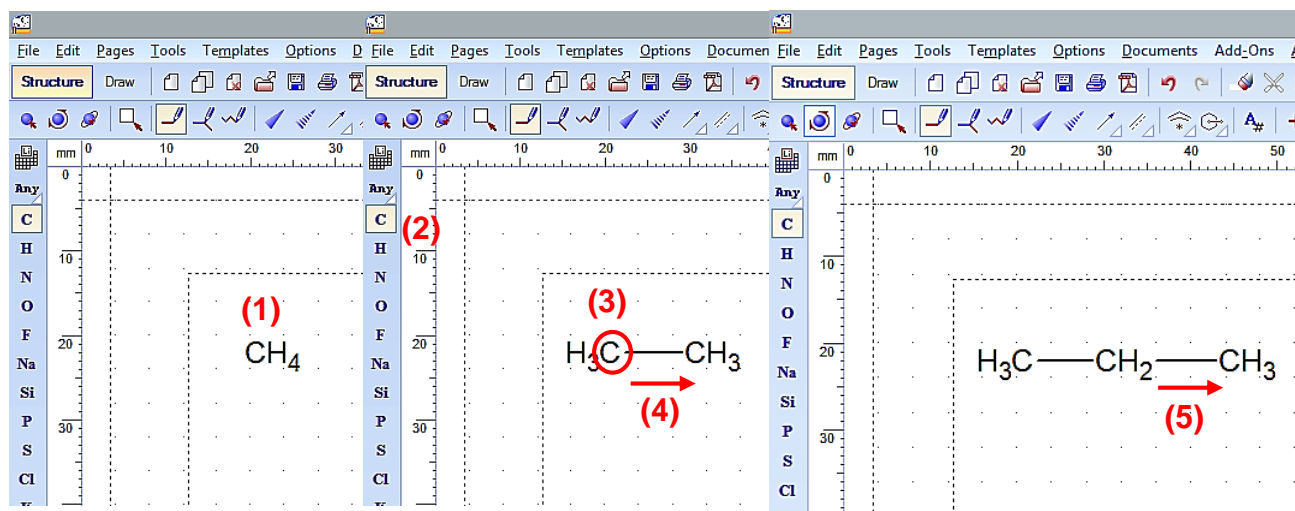
TIP: **How to expand all hydrogens at once**

If you want your hydrocarbons with all hydrogens fully expanded at once, just **select** the non-expanded molecule(s), and click on **Tools -> Add Explicit Hydrogens** (or press **Ctrl+Shift+Y).**

To return to the non-expanded condition, **select** and click **Tools -> Remove Explicit Hydrogens** (or press **Ctrl+Shift+R).**

You can also apply this tool on **fragments of molecules.** Select them by dragging a rectangle around the relevant atoms and bonds and then apply.

To create **alkenes** and **alkynes**, you can introduce **double** and **triple bonds** just by clicking directly on the bonds (again with **C selected** and the hydrogens **not explicit**).

You can even toggle between the different numbers of bonds.

4. Oxidation products of alkanes: alcoholes, aldehydes, ketones, carboxylic acids

To create oxidation products of hydrocarbons you have to include **oxygen**.

(1) Draw a **C chain** of any length, e.g. **propane** (hydrogens not explicit).
(2) Select **O**(xygen) in the Atoms toolbar.
(3) Click on the **(a) terminal C atom**, hold the button and **(b)** move the mouse to get **propanol**.
(4) Click on the C–OH bond to introduce a **double bond** (C=O) and get **propanal**.

TIP: How to „Clean" a Structure

If you now **(a)** add explicit hydrogens to your structure(s), e.g. to **propanal**, you may not be completely satisfied with the appearance, especially of the aldehyde group.

To render your structure more like „standard", you can use the **(b) Clean Structure** button.

This tool mainly adjusts binding lengths and angles. As you may experience, it is not useful in every case. Sometimes it may be better to apply on fragments of the molecule only.
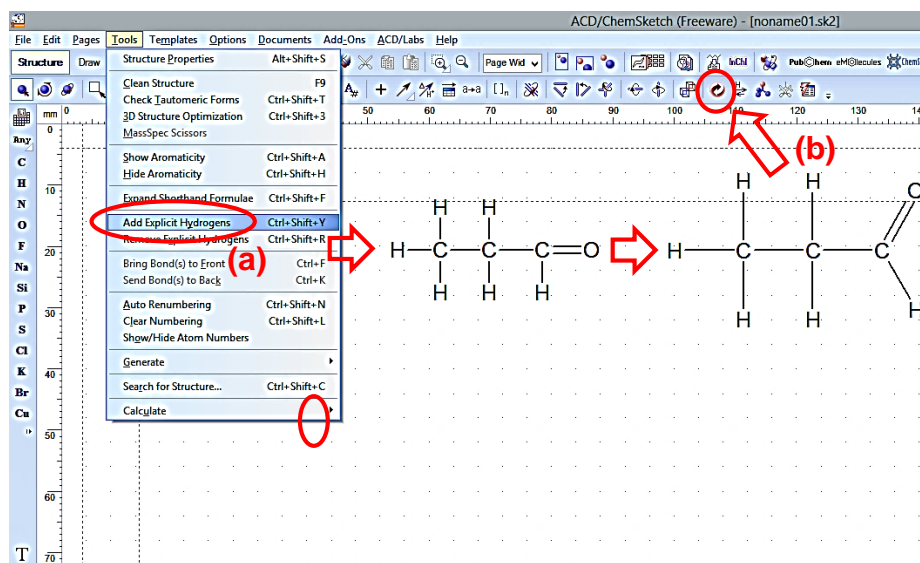
(5) To draw the ketone **propanone**, start with propane, select **O** in the Atoms toolbar and pull out from the **central C atom**.

(6) Click on the C–OH bond again to create the carbonyl (C=O) group.
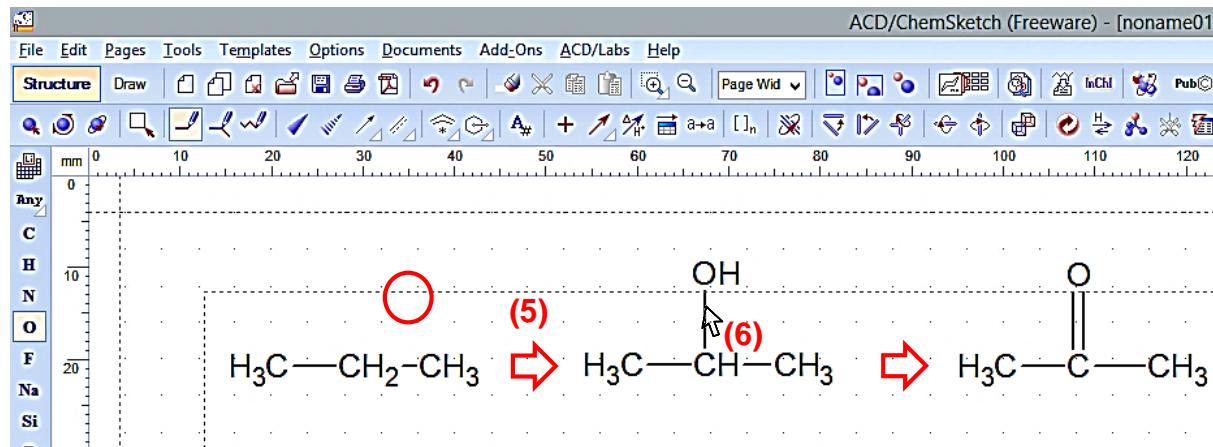
(7) To draw **propanoic acid** you may start with **propanal**, select **O** in the Atoms toolbar and just **click directly** on the H in the aldehyde group -> H ist replaced by OH, and you have the **carboxylic group.**
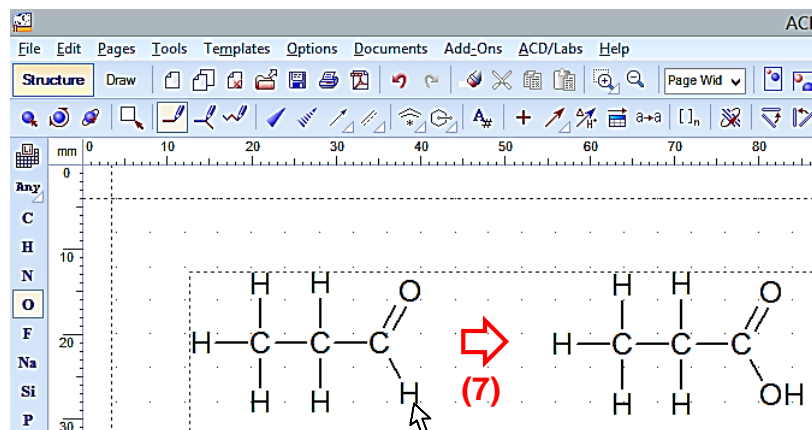
TIP: How to add free / non-binding electron pairs

When working with oxidation products, it may be desirable to add **free/non-binding electron pairs** to the oxygen(s). ChemSketch appears not to provide any particular tool for this procedure, therefore you need to add the electron pairs **manually**.

(1) Draw any oxygen containing molecule, e.g. **propanoic acid.**

(2) Change from Structure to **Draw mode**. There you will find a bar with typical graphic tools.

(3) For ease of adjusting the electron pairs, **zoom** into the molecule with the button **Fit All.**

(4) Select **Line** from the toolbar and draw one electron pair. Hold **Shift** while drawing to get a straight line more easily.

(5) In case you like your electron pair, select it and use **Copy** and **Paste** to reproduce exactly the same line.
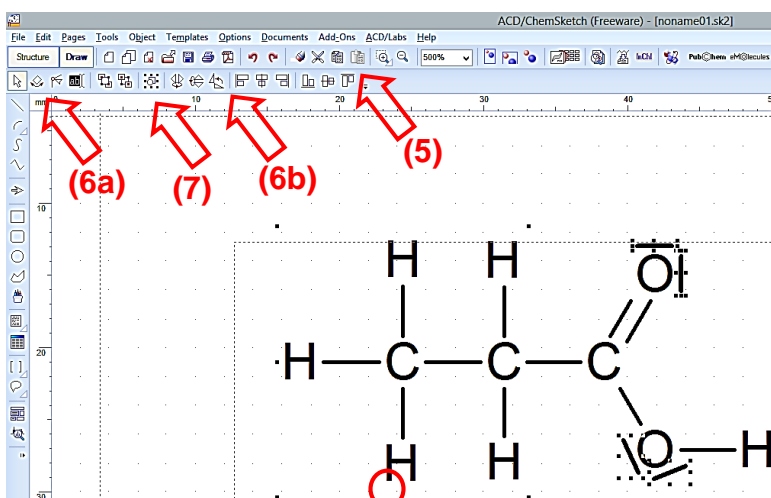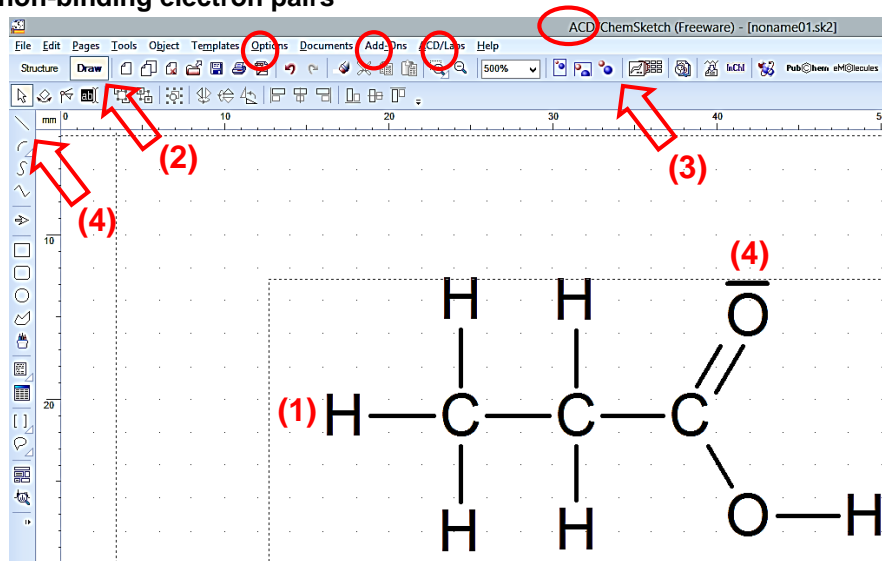
(6) To get electron pairs in different angles, use the **(a) Select/Move/Rotate** or the **(b) Rotate 90°** button.

Optional:

(7) When you have finished and do not plan any further changes to the molecule, it may be reasonable to **group all elements** by selecting **Select/Move/Resize**, dragging a rectangle around everything and click on **Group**.

TIP: How to add charges (+/-) to atoms

In some cases, you may want to display the charges of certain atoms, e.g. the negative charge of the deprotonized/anionic form of carboxylic groups or the positive charge of the protonized/cationic form of amino groups.

Example: Amino acid **Alanine** (2-aminopropanoic acid) in FISCHER projection.

(1) Start with **propane** in vertical orientiation.

(2) Select O, click on the terminal C and pull out **two OH** groups.

(3) Select the C–O bond of one OH group and click to create a **C=O** group.

(4) Select N and pull out from the alpha C atom to create an **NH₂** group.

(5) Select H and pull out from the alpha C atom.

(6) Select the (Increment/Decrement) **Charge** button, click on the small **white triangle** down right and select the „**Minus**" from the pull-out menu. Now click on the **OH** group to decrement the charge. (The hydrogen is removed accordingly.)

(7) Select the „**Plus**" from the pull-out menu of the Charge button and click on the **NH₂** group to increment the charge. (One hydrogen is added accordingly.)

By clicking several times you can further increase or decrease the charges step-by-step.

Optional: **(8)** If you wish to display the **delocalized electrons** of the anionic carboxylic group, select the **COO⁻ group** and press the button for **Dotted/Solid Delocalization Curve**.
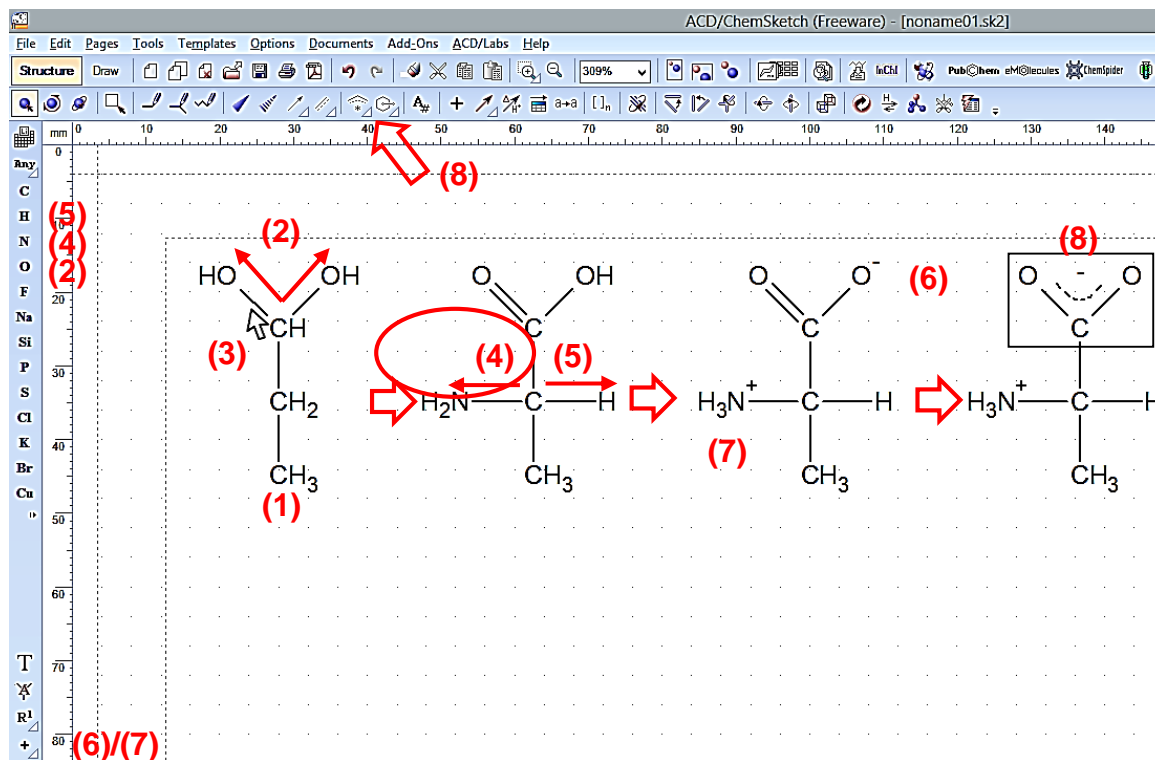
5. Long-chained molecules and editing atom labels

If you want to create hydrocarbons with longer C chains, e.g. **fatty acids**, it is advisable to use an alternative tool for drawing bonds.

Example: **Palmitic acid** or **hexadecanoic acid** (C16:0).
(1) Select the **Draw Chains** button.
(2) Click anywhere and **hold** the mouse button, then **move** the mouse until 16 C atoms are drawn (the number of C atoms is counted up while drawing).
(3) Optional: For sake of clarity, you may want to select **Tools**->**Structure Properties** to change the **Show Carbon** option: Uncheck „**All**" and click „**Apply**" to only show the terminal Carbons or CH_3 groups.
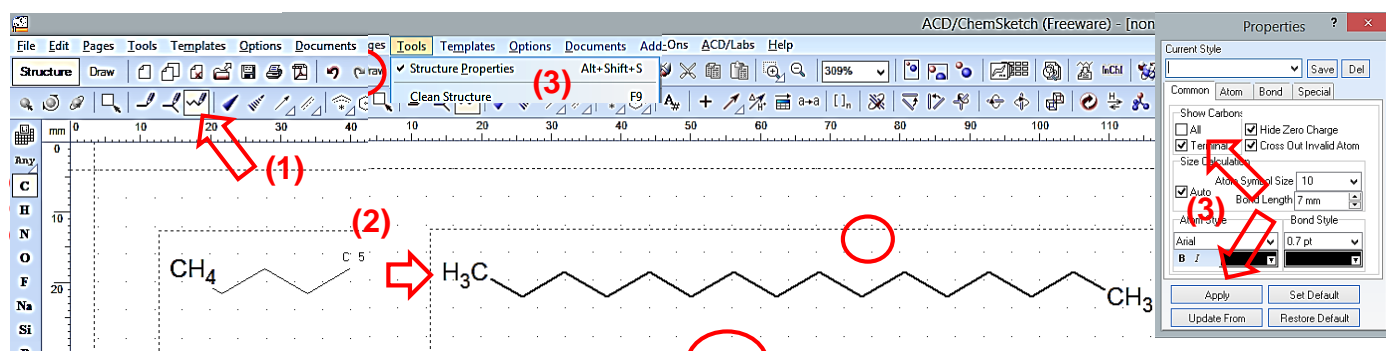
(4) To add the **carboxylic group** more quickly now, select the button **Edit Atom Label**.
(5) Next, click on one of the terminal C atoms of your chain, and the **Edit Label** window will open.

(6) Choose the **COOH** group from the list and click **Expand** (make sure, the feature **Formula Style** is checked) -> the terminal CH_3 group is now replaced with the (expanded) structure of the COOH group.

Optionally, you may also click **Insert** in the Edit Label window, if you just want to insert a different atom or the shorthand formula of a group. If you later still want to have the complete structural formula, click on the respective group, then select the **Tools** menu and click on **Expand Shorthand Formulae**.

6. Reaction equations, mechanisms, and graphic tools

a) Equations with sum/shorthand formulas

Simple reaction equations with non-structural formulas can be created in any word processing program. However, this can be time-consuming, since subscript and superscript numbers/symbols have to be included frequently.

In ChemSketch, such reaction equations can simply be created with the **Edit Atom Label** function.

Example: **Protolysis** (1st step) of phosphoric acid in water
(1) Select **Structure** mode.
(2) Select **Edit Atom Label**.
(3) Enter the desired **text**/**equation** (subscript/superscript numbers are in most cases inserted automatically). In the edit window, you can also make changes to **font** style, **subscript/superscript** yourselve or add **symbols** in Greek font. Make sure you leave some **space** between educts and products for the **reaction arrow**.
(4) Click on **Insert**.
(5) Click on the **Reaction Arrow** button and use the default arrow, or click on the **white triangle** and choose any other arrow (here: equilibrium arrow) from the pull-out menu, respectively.

(6) Draw the arrow with the mouse (click or move).

Optional:
(6) You can **label** your components:
Select the **Text** button, click where you wish to have your label and enter your text.
(7) A window (**Text**) opens simultaneously, which provides basic editing functions.
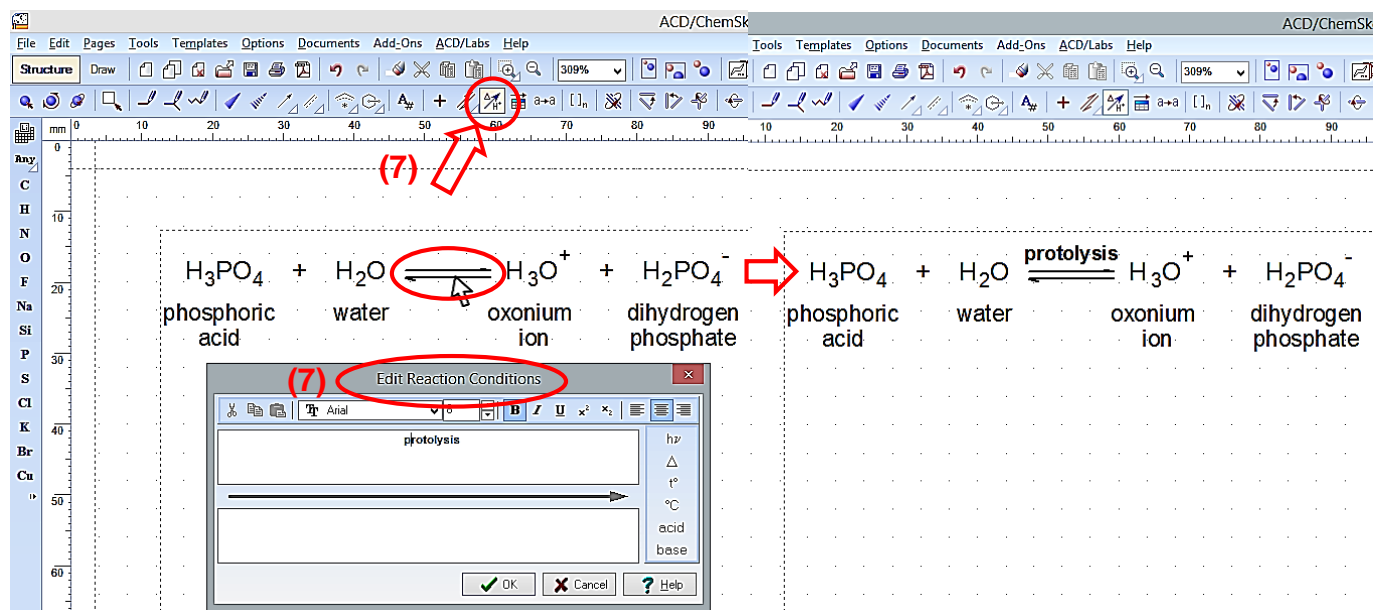

(7) You can add **reaction conditions** to the arrow: Select the **Reaction Arrow Labeling** button, click on the arrow and enter **free text** above or below the arrow, or choose from a set of **predefined**
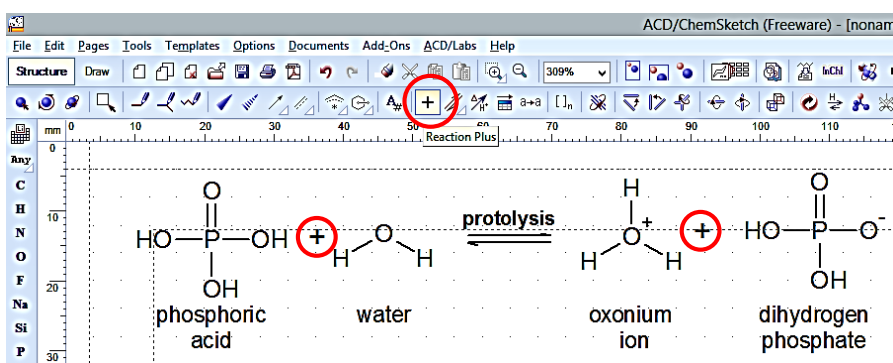
symbols/words.

b) Equations with structural formulas

To setup reaction equations with **structural** formulas, you only need one more function:
the **Reaction Plus** button to connect the different educts and products of the equation.
Another way to insert the „+" is to use the **Text** function.

c) Reaction mechanisms

In the **Draw mode**, there are several graphic tools, which facilitate the development of reaction mechanisms:

(1) Select the **Arc** function (with pull-out menu) to have arcs with five different angles at your disposal.

(2) Select the **Arrow** button at once to combine the arc with an arrowhead (a small window will open to change form and size of the arrow).
Arrows can also be combined with **Lines**, **Curves** and **Polylines**.

(3) Use the **Brackets** function (with pull-out menu) to show e.g. mesomeric formulas or intermediate products.

(4) Use the **Rectangle**, **Rounded Rectangle**, **Ellipse** or **Polygon** functions to **highlight** certain structures or functional groups.

(5) Optional: **Adjust** the angle/structure/length of any line continuously with the **Edit Nodes** function.
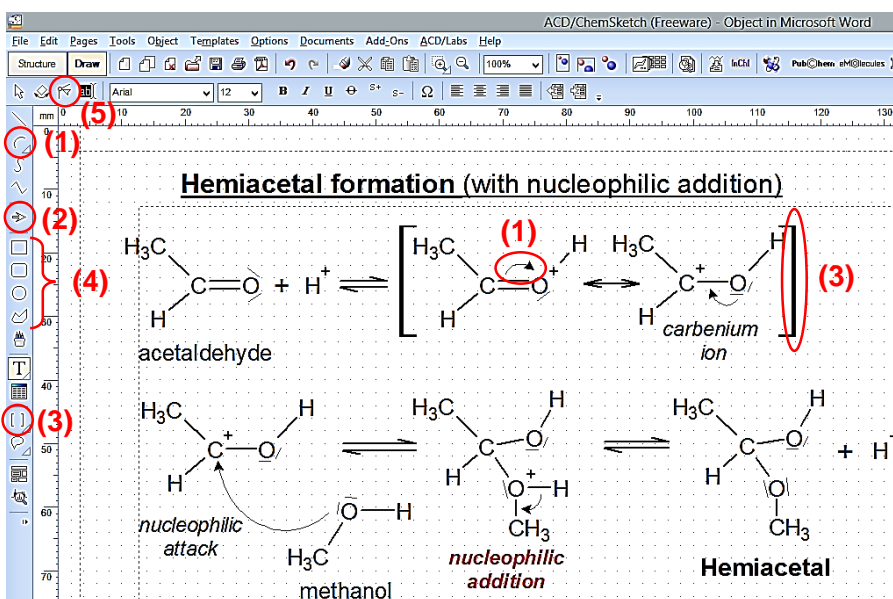
All objects (including **text** fields) can be **selected** & **colored** using the **(6) Color** buttons in the horizontal taskbar at the bottom of the workspace.

In general, all objects can be **(7) aligned, flipped and rotated** or **(8) brought to front/sent to back** with the corresponding buttons.
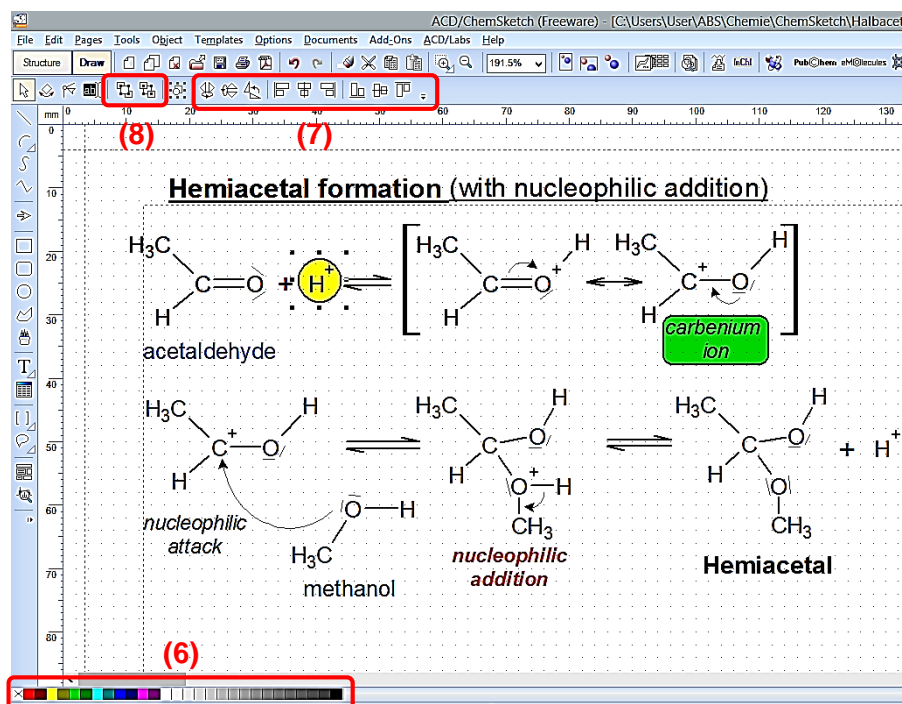

7. Other useful functions, tools and gimmicks

(1) **Undo/Redo** button to correct mistakes

(2) **Delete** button to remove single atoms or groups from formulas

(3) **Generate Name for Structure** to label selected structural formulas (consisting of up to 50 atoms) with their (IUPAC) names

(4) Display of **Molecular Weight** (**FW**) and **Composition** for depicted formulas
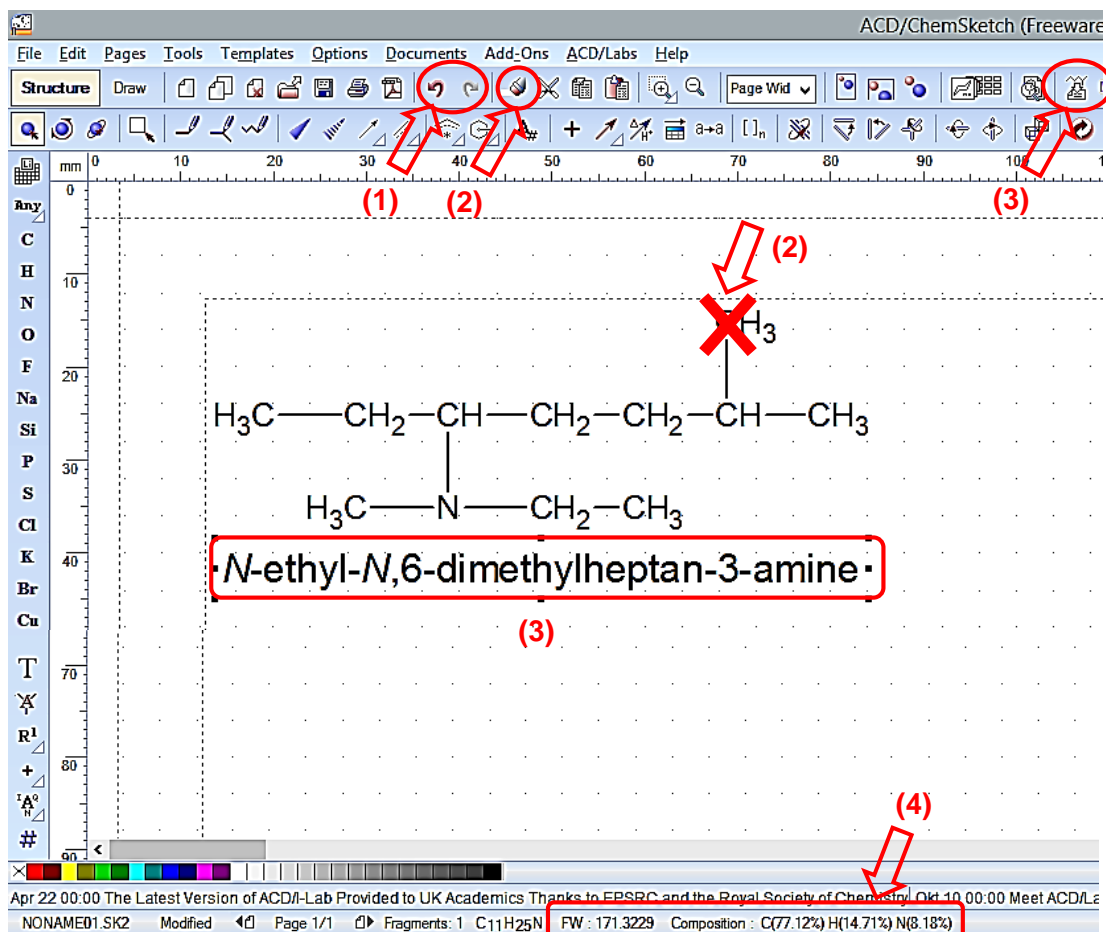
(5) **Templates->Template Window** with dozens of ready-to-use formulas, e.g. amino acids, carbohydrates, DNA/RNA components, steroids etc., but also graphic templates, like arrows, lab material, figures, and labels.

(6) **Template toolbar** with a collection of often used residues and functional groups to stand alone or add to existing structures

(7) **Instant Template** button to create templates from newly drawn structures and „clone" them
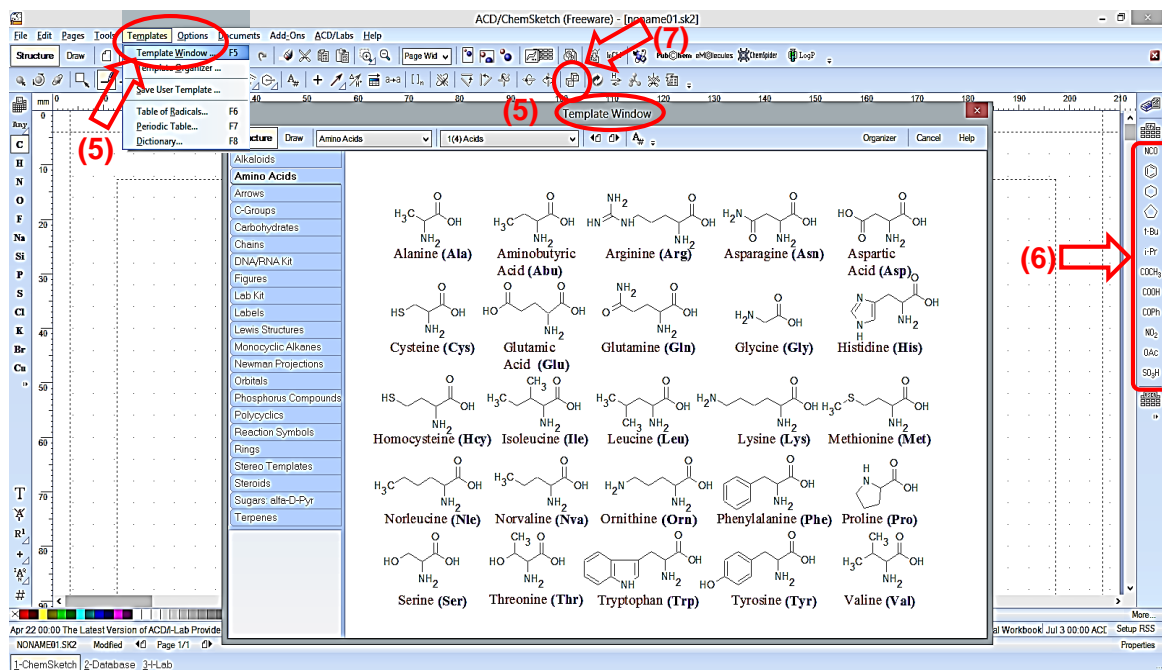
Templates can also be used to construct more complex molecules simply by combination of single components,e.g. **Adenosine triphosphate** (**ATP**) from components of the **DNA/RNA kit**.

First, pick the components from the **Template Window** and paste them to the working space.
To deactivate/release just click the **right mouse button** or press **esc**(ape). Then move the elements towards each other until they are automatically fused by a „virtual condensation reaction".
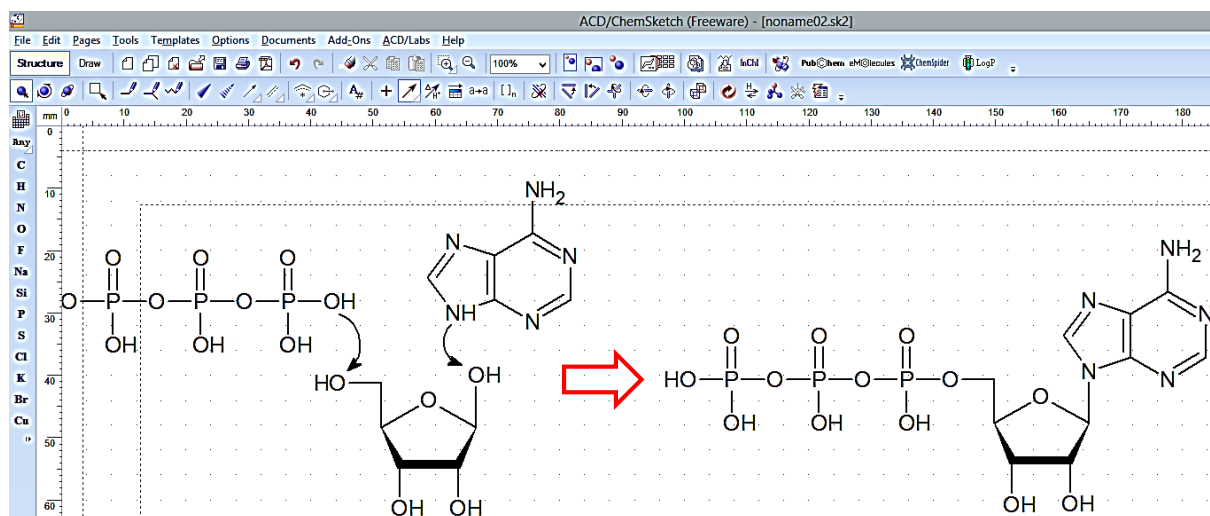
(8) **Show/Hide Atom Numbers** or **Manual Numbering** button to number e.g. C atoms of hydrocarbons. Position, color etc. of the numbers can be altered by double-clicking on the numbers and adjusting the **numbering** in the **properties** window.

(9) **Change Position** button to alter the position of single atoms or groups in molecules

(10) **Up Stereo/Down Stereo/Coordinating/Delocalized Bonds** buttons to adjust bond structures
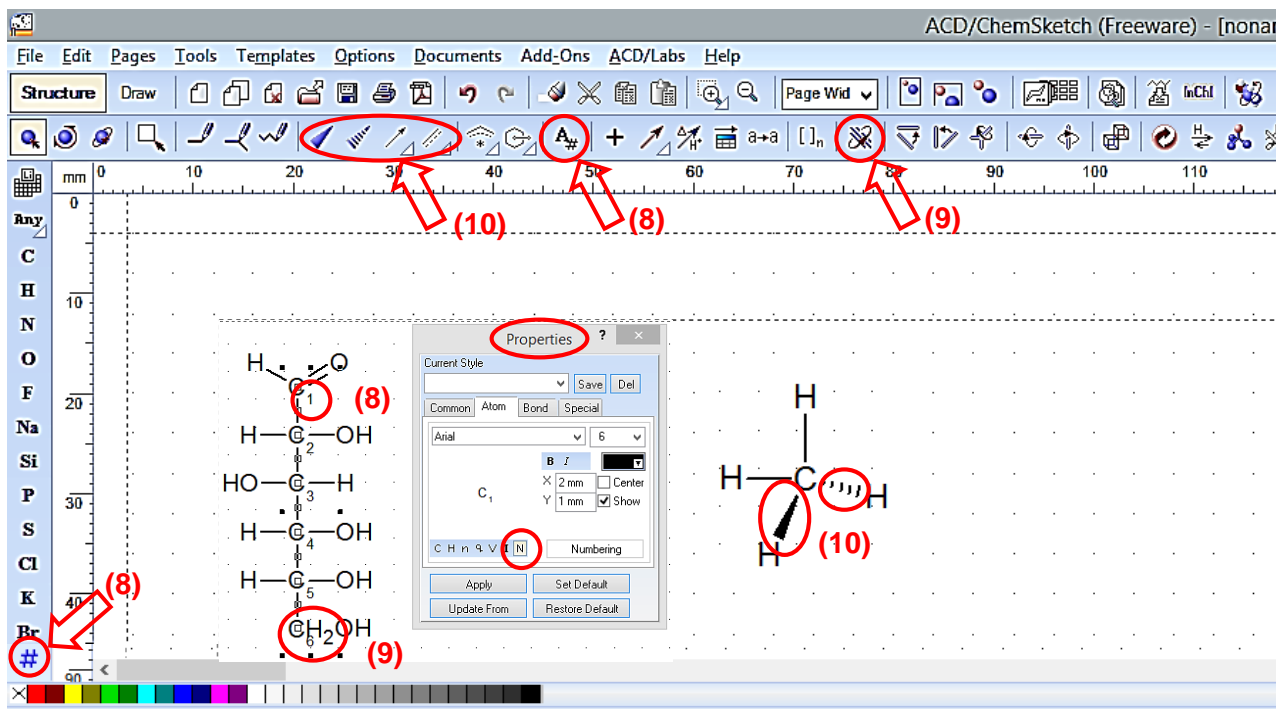
(11) **3D Viewer** function to generate various 3D models from drawn formulas

...
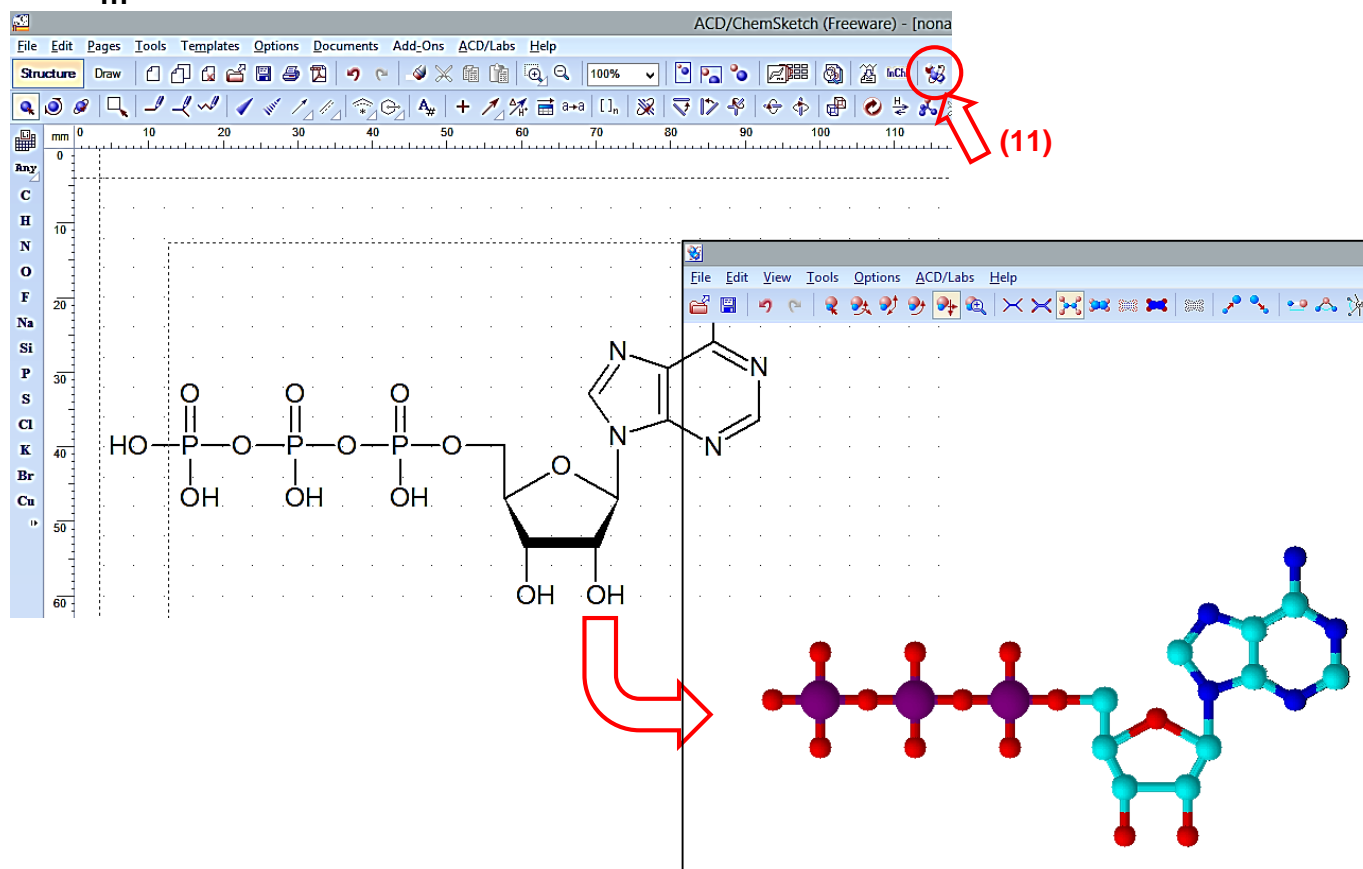
8. Interaction with word processing programs

Formulas, reaction equations and mechanisms are usually not created as an end in itself, but as a part of a worksheet, an exercise, a presentation etc.

To insert ChemSketch objects into the pages of a word processing program, there are two advisable ways:
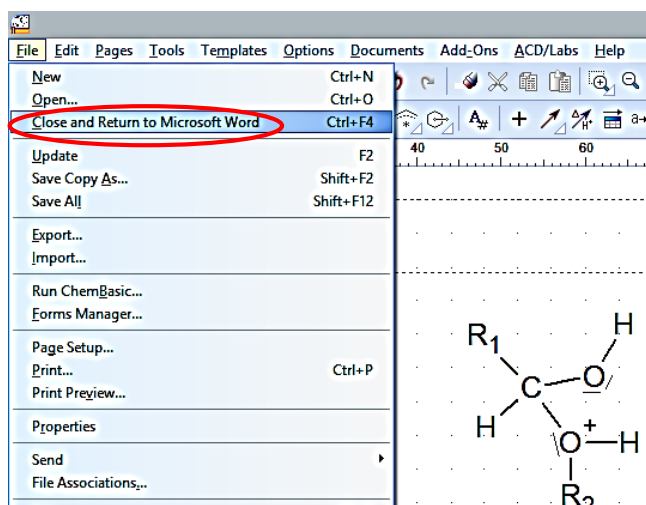
(A) Start working with your word processing program. To directly insert a ChemSketch object select **Insert -> Object** and then choose **ACD/ChemSketch** from the list of object types.
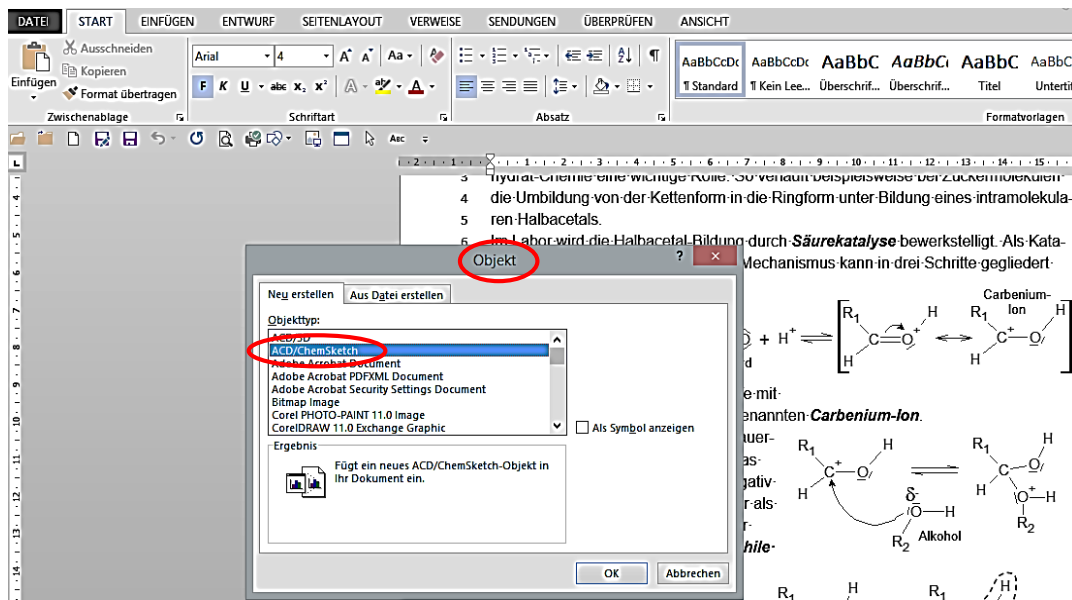
ChemSketch will open and you can draw your formula, reaction, scheme etc.

When you have finished and want to go back to your worksheet, press **File -> Close and Return to …**
You are then asked whether you (really) want to update the embedded object, and if you answer with **Yes**, you return to your word processing program with the properly inserted and **free scalable ChemSketch object**.

(B) Alternatively, you can do **Copy&Paste**: start working in ChemSketch, then **copy** your object(s), e.g. by selecting and clicking **Ctrl+C.** Next, you start or open or change to your word processing program, open your file and press **Ctrl+V** to **paste**.

Editing inserted ChemSketch objects is also quite comfortable:
Just **double-click** on the ChemSketch object or (if you e.g. have changed the formate) click with the **right mouse button** and choose **ChemSketch object -> Edit** from the pull-down menu.