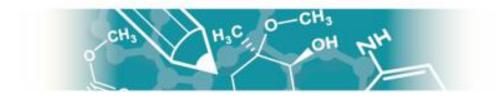
# Tutorial

by Dr. Markus Vogt

# ACD/ChemSketch

(for Windows)



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#### 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/

	Home	Platforms and Products	Solutions	Services and Support	Resources	About ACD/Labs							
	Pesouro	ces > Chemistry Software > ACD/Che	mSketch Ereeware										
ACD/ChemSketch for Academic and Personal Use													
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ACD/NMR Processor Academic Edition ACD/Column Selector			H <sub>3</sub>	H <sub>3</sub> C 0 C	H LAH								
ACD/Labs LC Method													
ACD/ChemSketch Freeware is a drawing package that allows you to draw chemical structures including organics polymers, and Markush structures. It also includes features such as calculation of molecular properties (e.g., mo density, molar refractivity etc.), 2D and 3D structure cleaning and viewing, functionality for naming structures (fe atoms and 3 rings), and prediction of log <i>P</i> . The freeware version of ChemSketch does not include all of the func- commercial version— <u>see a brief overview of the differences</u> . Visit <u>ACD/ChemSketch</u> to learn more about the cor													
	As a	n Educational Tool											
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		<ul> <li>versions of ACD/ChemSketch</li> <li>Free access to site licenses or</li> </ul>	n, ACD/ChemFo f ACD/ChemSke	lder, and ACD/l-Lab available etch Freeware are available.	e to their studer <u>Contact us</u> to le	2							
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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:

Resources > Chemistry Software > ACD/ChemSketch Freeware > ACD/ChemSketch Freeware Installation Instructions

#### Thank You for Downloading ACD/ChemSketch Freeware

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Chemistry Software ACD/ChemSketch Freeware ACD/NMR Processor	Your download should automatically begin. If it does not, please <u>click here</u> . Please ensure that your security settings permit downloading .exe files or contact your system administrator.
Academic Edition ACD/Column Selector ACD/Labs LC Method Translator	Installation Instructions <ol> <li>Locate the downloaded file.         <ul> <li>a. It is likely located in the C:\Users\"YOUR NAME"\Downloads folder on your hard drive.</li> <li>Double-click on the file: chemsk2015.exe. The ACD/Labs Software Web Setup Wizard appears.</li> <li>Click Next.</li> </ul> </li> </ol>
	<ol> <li>Choose the option to accept the license agreement and click Next.</li> <li>Clear any optional components that you do not wish to install (the installation of all components is recommended to provide access to the full capabilities of the software), then click Next.</li> <li>Click Install.</li> </ol>

7. Click Finish.



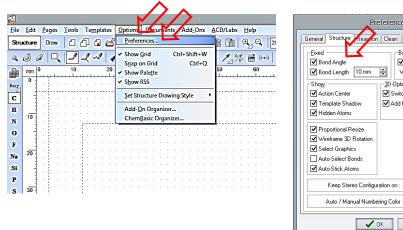
#### 2. First Steps

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

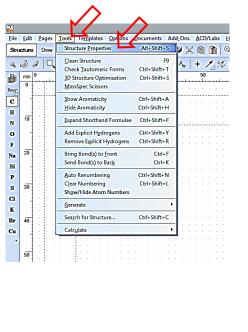
One minor drawback of the freeware version: With every start you have to first click the OK button in the small ACD/Labs Products presentation window.

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



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✓ Flips

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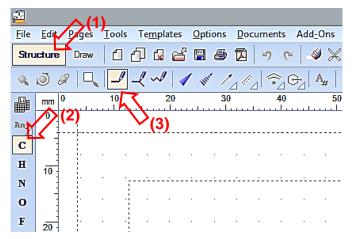
#### 3. Simple hydrocarbons: The alkane series

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**<sub>4</sub>.

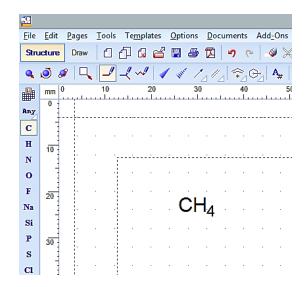
(Note: All free bonds of the selected C atom – and of any other atom – are automatically "saturated" with H(ydrogen) atoms.)

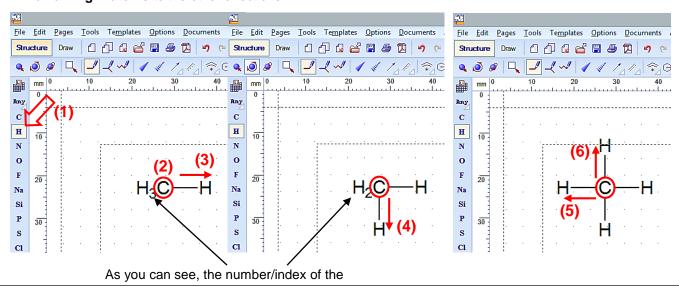
Now, we have the sum or shorthand formula. To expand to the complete **structural (LEWIS) formula** with explicit hydrogens, just

(1) select the H atom in the Atoms toolbar,

(2) click on the C in the  $CH_4,$ 

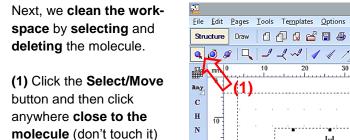
- (3) hold the button and move the mouse to any direction,
- (4) (6) repeat step (3) three times to "pull out" the remaining H atoms to the other directions.







remaining hydrogens is reduced correspondingly.



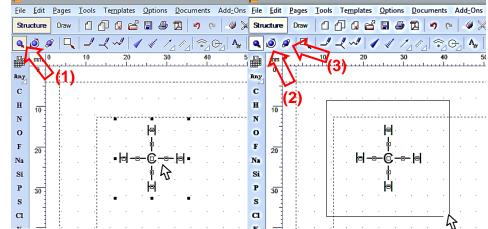
-> the whole structure is

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<sub>3</sub>) to get ethane.

(5) Starting with ethane, pull out another C(H<sub>3</sub>) to get propane, and so on.

In the same way, you can create branched molecules / isomers as well.

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ACD/ChemSketch (Freeware) - [noname01.s



#### 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

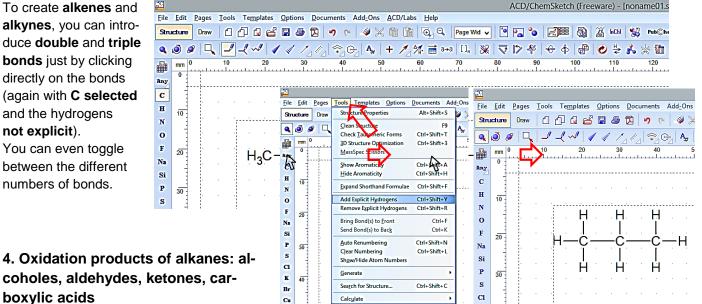
#### (or press Ctrl+Shift+Y).

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.

boxylic acids

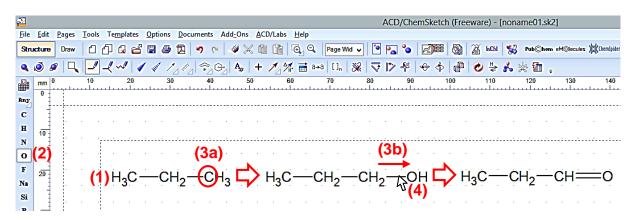
To create oxidation products of hydrocarbons you have to include oxygen.

(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.

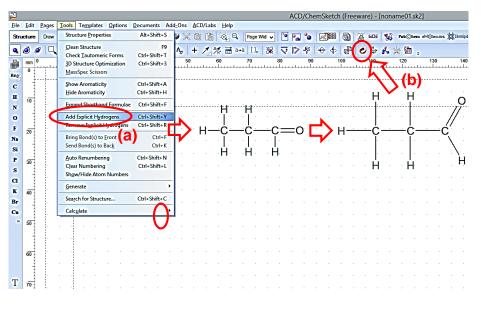


TIP: How to "Clean" a Structure



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.

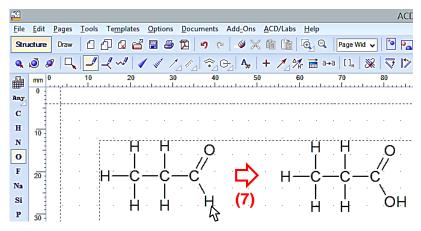


(5) To draw the ketone **propanone**, start with propane, select **O** in the Atoms toolbar and pull out from the **central C atom**.

(6) Click on the C–OH bond again to create the carbonyl (C=O) group.

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(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**.



### Tutorial ACD/ChemSketch (for Windows)

#### 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.

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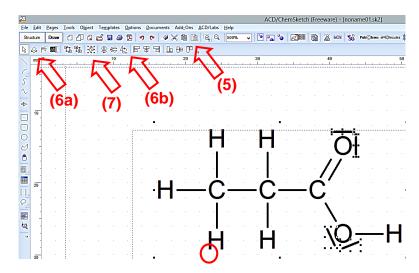
(2) Change from Structure to Draw mode. There you will find a bar with typical graphic tools.

(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 NH<sub>2</sub> 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

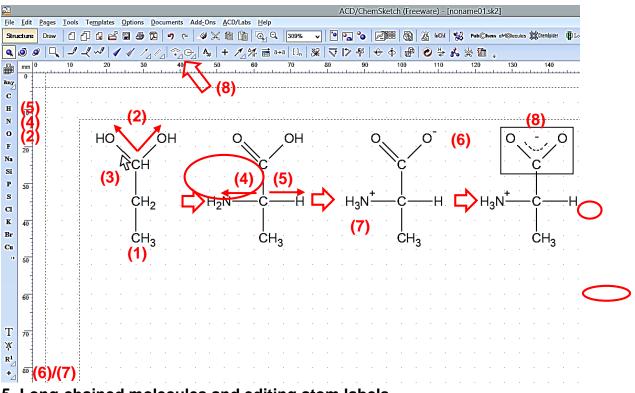
and select the **"Minus**" from the pull-out menu. Now click on the **OH** group to decrement the charge. (The hydrogen is removed accordingly.)

(7) Select the "Plus" from the pull-out menu of the Charge button and click on the  $NH_2$  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<sup>-</sup> group** and press the button for **Dotted/Solid Delocalization Curve**.



#### 5. Long-chained molecules and editing atom labels

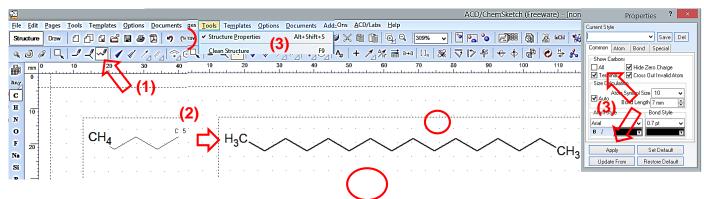
If you want to create hydrocarbons with longer C chains, e.g. **fatty acids**, it is advisable to use an alternative tool for drawing bonds.

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).

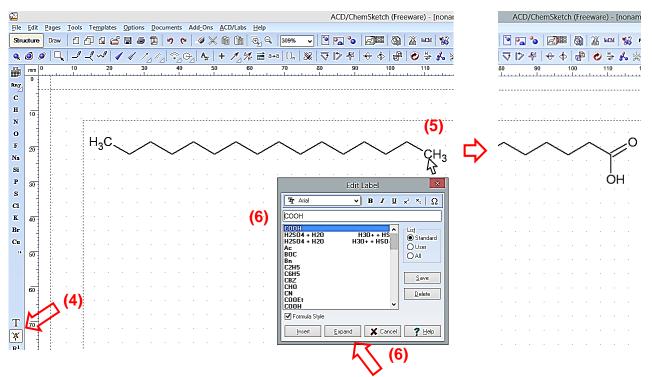
(3) Optional: For sake of clarity, you may want to select **Tools**->**Structure Properties** to change the **Show Carbon** option: Uncheck **"All**" and click **"Apply**" to only show the terminal Carbons or CH<sub>3</sub> groups.



(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<sub>3</sub> 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

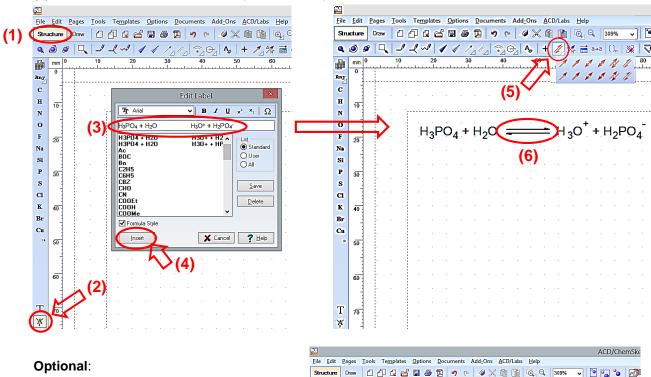
- (1) Select Structure mode.
- (2) Select Edit Atom Label.

(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.

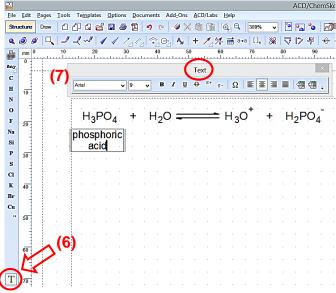
(5) Click on the **Reaction Arrow** button and use the default arrow, or click on the **white triangle** and choose any other arrow (here: equilibrium arrow) from the pull-out menu, respectively.

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



(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.

₽ Any C H N O F



(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.

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## 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.

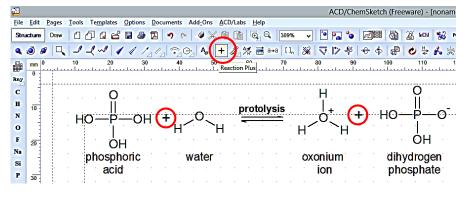
(2) Select the **Arrow** button at once to combine the arc with an arrowhead (a small window will open to change form and size of the arrow).

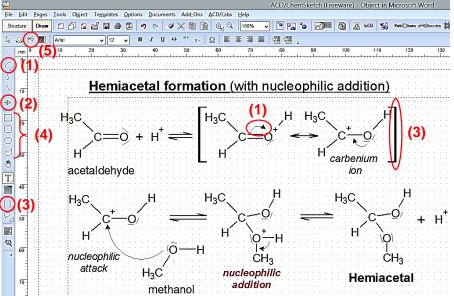
Arrows can also be combined with Lines, Curves and **Polylines**.

(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.

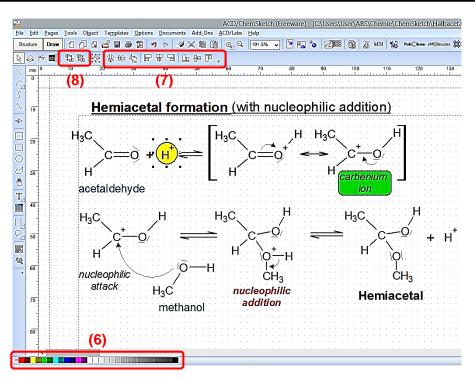




### Tutorial ACD/ChemSketch (for Windows)

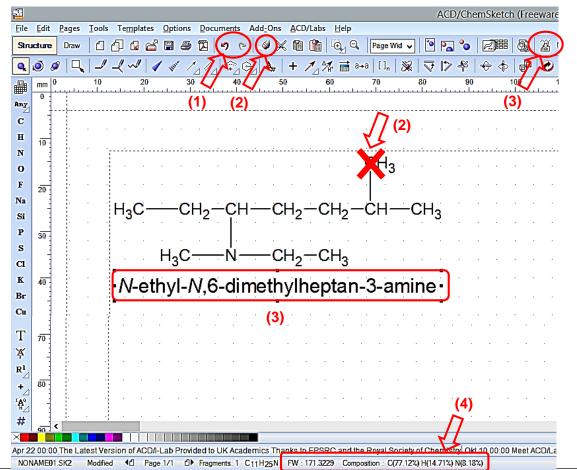
All objects (including text fields) can be selected & colored using the (6) Color buttons in the horizontal taskbar at the bottom of the workspace. In general, all objects can be (7) aligned, flipped and rotated or (8) brought to front/sent to

or (8) brought to front/sent to back with the corresponding buttons.

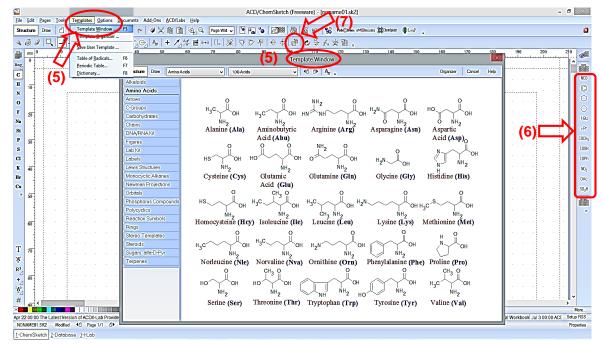


#### 7. Other useful functions, tools and gimmicks

- (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

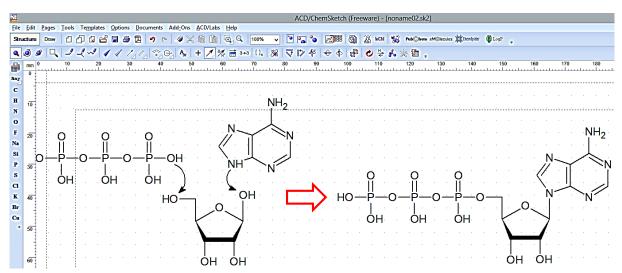


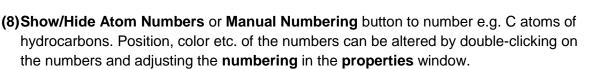
- (5) Templates->Template Window with dozens of ready-to-use formulas, e.g. amino acids, carbohydrates, DNA/RNA components, steroids etc., but also graphic templates, like arrows, lab material, figures, and labels.
- (6) **Template toolbar** with a collection of often used residues and functional groups 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**.

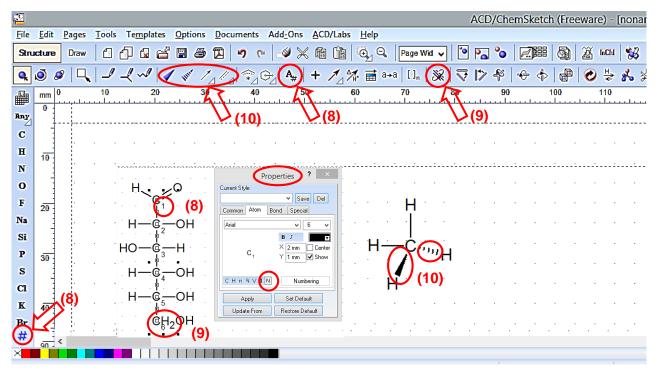
First, pick the components from the **Template Window** and paste them to the working space. To deactivate/release just click the **right mouse button** or press **esc**(ape). Then move the elements towards each other until they are automatically fused by a "virtual condensation reaction".



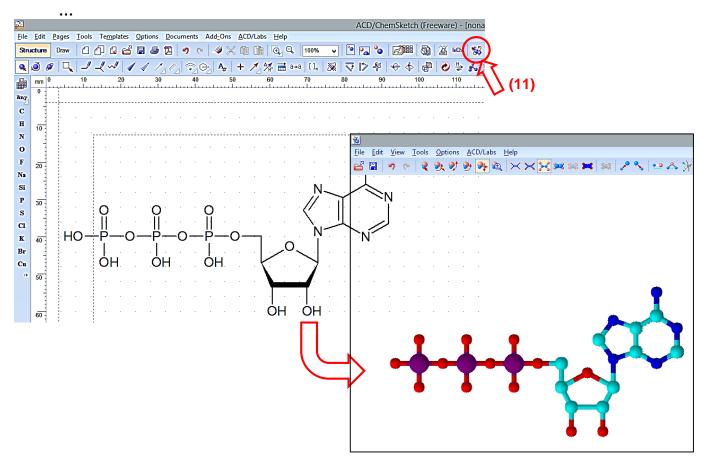


(9)Change Position button to alter the position of single atoms or groups in molecules

(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



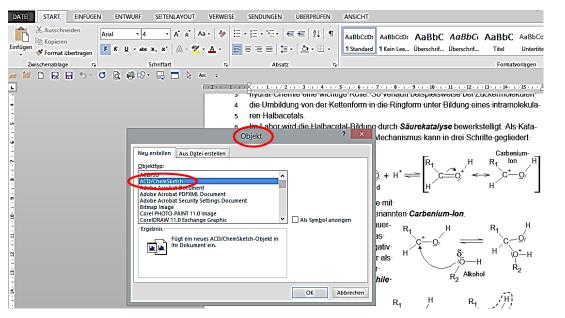


#### 8. Interaction with word processing programs

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.

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(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.

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