

# MarvinSketch

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## Sisältö

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1. Lataaminen
2. Asentaminen
3. Lisenssikuvio
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KYSELY:

<https://peda.net/p/myllyviita/marvinsketch/tutkimus>

# SO

## TOOLS TOO COOL NOT TO USE

ChemAxon's entire product portfolio offers out-of-the-box solutions for scientists, back-end tools for IT professionals, components to add extra functionality, and integrations to make our technology available from 3rd party software like Microsoft Excel or KNIME.

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### Marvin

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Web-based molecule design, collaboration & report

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### Plexus Suite

Web-based chemical data management solutions

### Chemicalize

Calculate properties, draw, extract chemical data online

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### International Chemistry & CR Summit

28, 2017 · LONDON, UK

### ChemAxon Invent 2017

2017 · LAS VEGAS, NV, US

# Lataaminen

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## Lataaminen

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- ❖ Ohjelman voi **ladata osoitteesta:**  
<https://www.chemaxon.com/products/marvin/marvinsketch/>
- ❖ **Opettaja:** Akateeminen lisenssi, opettajien kannattaa rekisteöityä ja hakea oppilaitos-lisenssin (tsekkaus vie muutaman päivän)
- ❖ **Kaikki:** Varmista, toimiiko laitteessa 64-bittinen vai 32-bittinen versio (jos 64-versio ei toimi, kokeile 32-versiota)
- ❖ **Marvin Sketch** on koneelle asennettava ohjelma, **Marvin JS** on selaimessa toimiva ohjelma (kuten MolView), kyseisen työkalu on upotettu useaan palveluun, sen voi asentaa jopa omille www-sivuille



# Marvin

A full featured chemical editor for making science accessible

Marvin runs smoothly on desktops allowing you to import, draw, edit and publish your daily chemistry workflows. Marvin allows users to quickly draw molecules with the interface and advanced functionalities, such as: sprout drawing, customisable shortcuts, abbreviated groups, default and user-defined templates and context-sensitive popup menus.

PLAY VIDEO



OVERVIEW

FEATURES

RESOURCES

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## Create and Design

Marvin features an extensive set of functionalities to enable fast and accurate drawing of discrete chemical compounds, Markush structures, reactions and query molecules. Furthermore, these functionalities have built-in structure and valence checkers to provide guidance, and integrated property calculators to pull live instant results - upon your request. Not only is Marvin capable of drawing general organic

The screenshot shows the Marvin software interface. At the top, there's a title bar with "New Sketch Atom Bond Structure Calculation Services Help". Below that, a video player is embedded with the title "[Did You Know Series Part 1] MarvinSket...". A speech bubble above the video says "I want to be dextrorotator". The main area displays the chemical structure of ibuprofen, which is a chiral molecule with a carboxylic acid group and a chiral center. The name "ibuprofen" is written next to the structure, and a play button icon is visible to the right.

# DOWNLOAD MARVIN

Version 17.28.0

[DOWNLOAD LATEST FOR WINDOWS \(64 BIT\)](#)

By downloading, you automatically accept our [End User License Agreement](#). Read more about the [upcoming changes in EULA](#).



## Switch to Java8

Please note that from version 17.29.0 our tools run on Java8. Read more about these changes [here](#).

### Windows

Includes Marvin desktop applications, API, examples, documentation.

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### Mac OS X

# Kirjaudu järjestelmään ennen lataamista

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PHONE (OPTIONAL)

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## Marvin

THE chemical editor on desktop

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The screenshot shows the ChemAxon website's download page for Marvin. At the top left is the ChemAxon logo. The navigation menu includes PRODUCTS, SUPPORT, and COMPANY, along with search and user icons. The main heading is "DOWNLOAD MARVIN" with a sub-heading "Version 17.28.0". A prominent orange button says "DOWNLOAD LATEST FOR WINDOWS (64 BIT)". Below this is a notification banner with a bell icon, titled "Switch to Java8", which states that from version 17.29.0, tools run on Java8 and provides a link "here". The "Windows" section features the Windows logo and text: "Includes Marvin desktop applications, API, examples, documentation." Below this are three buttons: "DOWNLOAD 64 BIT", "DOWNLOAD 32 BIT", and "DOWNLOAD 32 BIT + OLE SUPPORT". At the bottom, the "Mac OS X" section is partially visible.

ChemAxon

PRODUCTS SUPPORT COMPANY

## DOWNLOAD MARVIN

Version 17.28.0

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**Switch to Java8**  
Please note that from version 17.29.0 our tools run on Java8. Read more about these changes [here](#).

**Windows**  
Includes Marvin desktop applications, API, examples, documentation.

[DOWNLOAD 64 BIT](#) [DOWNLOAD 32 BIT](#) [DOWNLOAD 32 BIT + OLE SUPPORT](#)

Mac OS X

HUOM!  
Valitse  
oikea  
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 ChemAxon PASSCHECK YOUR E-MAILS

You have successfully created your ChemAxon Pass, but we need you to verify your e-mail address.

To complete your registration, please check your e-mails and click on the activation link inside.

If you have not received it yet, first check your junk or spam folder, otherwise please drop an e-mail to [website-support@chemaxon.com](mailto:website-support@chemaxon.com)

 ChemAxon PASSYOUR PASS IS READY TO USE

You have successfully activated your ChemAxon Pass.

You may continue exploring ChemAxon at:

- [ChemAxon Website](#)
- [ChemAxon Support Tickets](#)
- [Chemicalize - Instant Cheminformatics Solutions](#)

## Welcome to ChemAxon

ChemAxon Pass <[pass@chemaxon.com](mailto:pass@chemaxon.com)>

Tänään, 23:26

Anselmi Myllyviita ✉



Vastaa kaikille | ▾

Dear Anselmi,

Thank you for registering to ChemAxon.

In order to activate your account, please click on the button below.

[ACTIVATE MY ACCOUNT](#)

If the button does not show, you can also visit the the following link to activate: <https://pass.chemaxon.com/activate/anselmi.myllyviita@viikinnormaalikoulu.fi/8902c1b58b92d51647ccf686b641bb0ae46090f45df8faca0d14e0a027e33498>

Should you have any technical difficulties, please do not hesitate to drop a line to the [website-support@chemaxon.com](mailto:website-support@chemaxon.com).

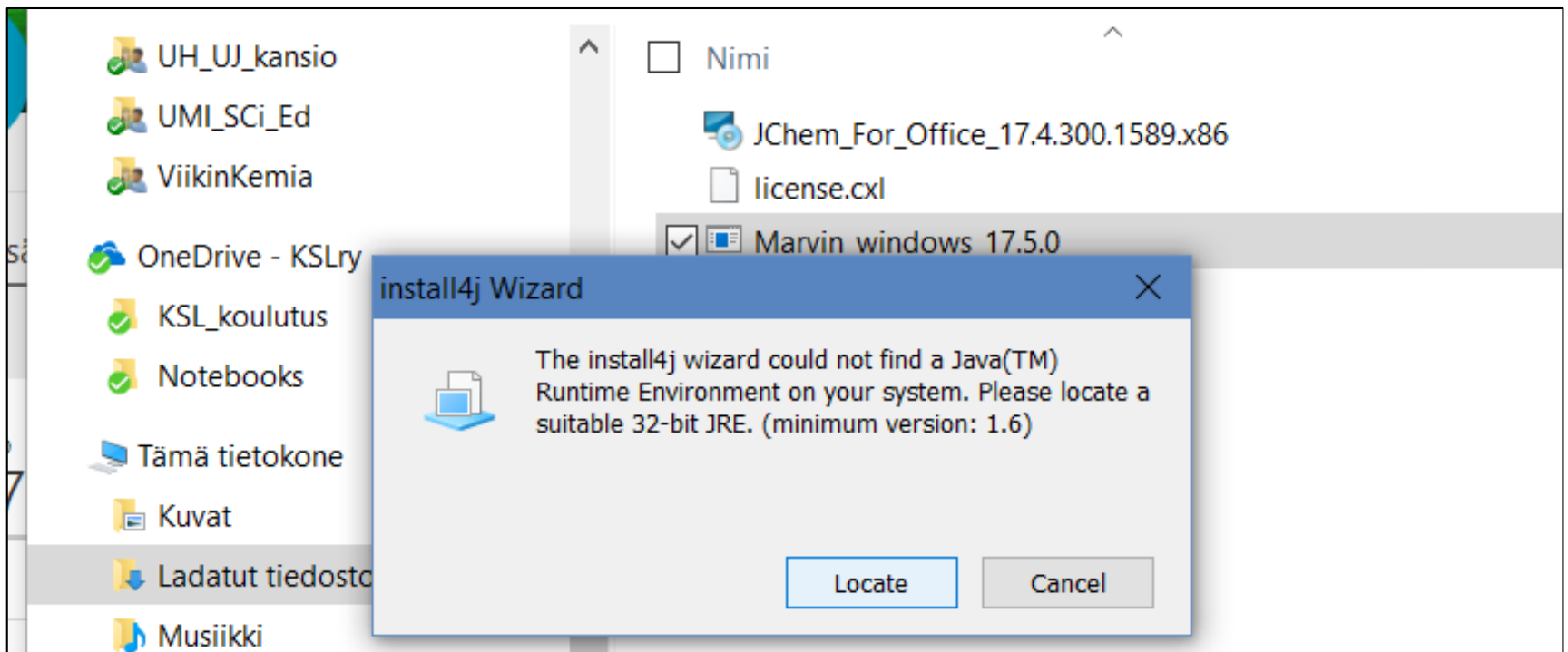
Best regards,

The ChemAxon team

# Asentaminen

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# Asennuksen yhteydessä tarkistetaan Javan olemassaolo



## Javan asennus (asennus vaatii admin –oikeudet)

Search: java runtime environment

WWW Kuvat Uutiset

2 270 000 TULOSTA Kieli ▾ Alue ▾

**JAVA-ohjelmistokehitystä | observis.fi**  
Mainos · [observis.fi](#)  
Vaativat asiakaskohtaiset java- palvelut meiltä toimitu

**Download Free Java Software**  
<https://java.com/en/download>  
This page is your source to download or update your  
Environment (JRE, Java Runtime), also known as t

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Release date April 18, 2017

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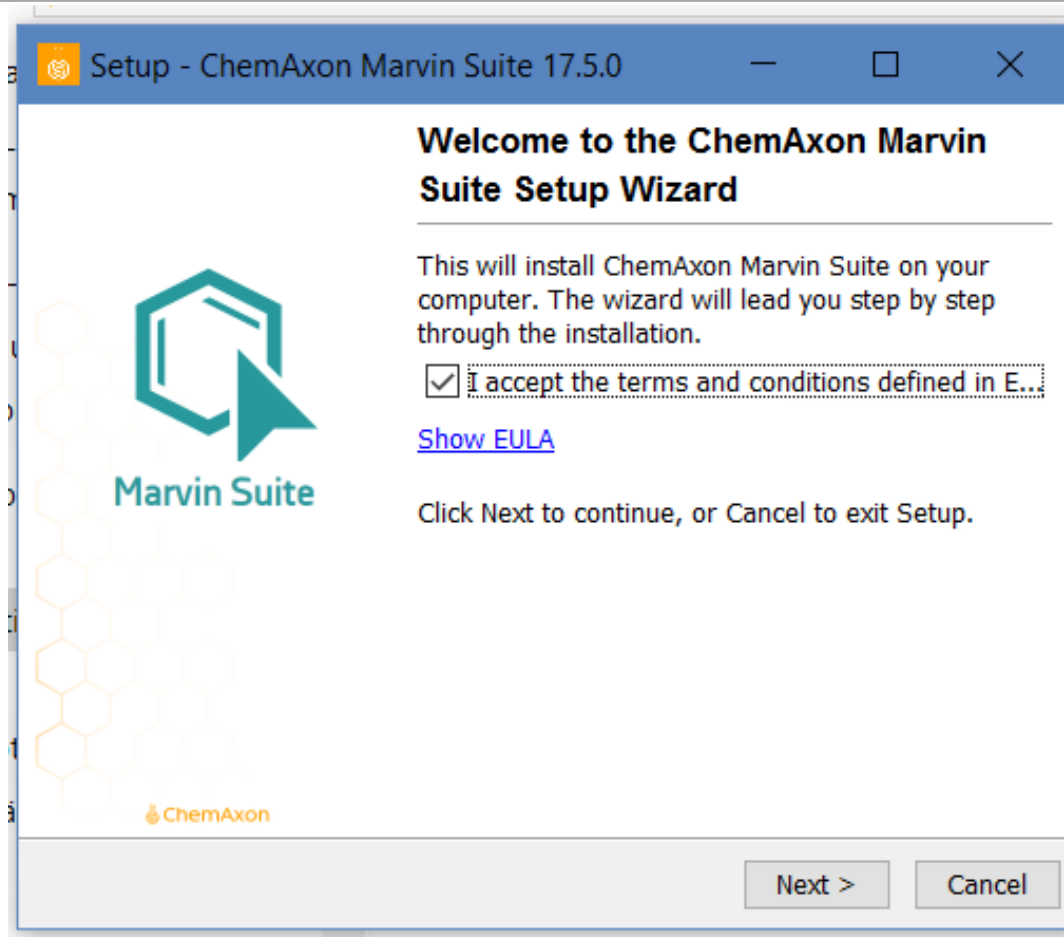
» [What is Java?](#) » [Do I have Java?](#) » [Need Help?](#)

**Why download Java?**

Java technology allows you to work and play in a secure computing environment. Upgrading to the latest Java version improves the security of your system, as older versions do not include the latest security updates.

# Marvin Suite -asennus

Kun Java-asennus on hoidettu, käynnistetään (Ladattut kansioista) Marvin –ohjelman asennus





The image displays three overlapping windows from the ChemAxon Marvin Suite 17.5.0 installation wizard:

- Top-left window: "Select Installation Type"**

Which type of installation should be performed?

Select the type of installation that you want to perform. Click Next when you are ready to continue.

  - Standard installation**

All components required for regular usage are installed. Some rarely used components are not installed in order to save space.
  - Custom installation**

In the next step you can customize the components installed. The initial selection is set to the standard installation.
- Top-right window: "Installing"**

Please wait while Setup installs ChemAxon Marvin Suite on your computer.

Extracting files ...  
lib\calculations-elemanal-master-6729.jar
- Bottom window: "Completing the ChemAxon Marvin Suite Setup Wizard"**

Setup has finished installing ChemAxon Marvin Suite on your computer. The application may be launched by selecting the installed icons.

Click Finish to exit Setup.

**Marvin Suite**

ChemAxon

Finish

The desktop background shows icons for Roskakori, Tama tietokone, MarvinSketch, and MarvinView.

File Edit View Insert Atom Bond Structure Calculations Services Help

The screenshot displays the MarvinSketch software interface. At the top, a menu bar includes 'File', 'Edit', 'View', 'Insert', 'Atom', 'Bond', 'Structure', 'Calculations', 'Services', and 'Help'. Below the menu bar is a toolbar with icons for selection, erasing, undo, redo, cutting, copying, pasting, and zooming. A zoom level of 100% is indicated. The main workspace is a large white area for drawing chemical structures. On the left side, there is a vertical toolbar with icons for drawing lines, zig-zag lines, curves, dashed lines, text, and various rings. On the right side, there is a vertical toolbar with icons for selecting atoms and a list of elements: H, C, N, O, S, F, P, Cl, Br, I. At the bottom, there is a horizontal toolbar with icons for drawing rings (cyclopentane, pyrrolidine, cyclopentane, cyclohexane, benzene, naphthalene) and a '2D' button.

# Lisenssikuvio

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## Academic License for Teaching or Research

**Please note that your request will be queued in our system, and we might get back with an answer to you after several working days.**

This option is yours if you've checked the drawing, calculation and naming functionalities of [Chemicalize](#) and [Marvin](#), yet you need a more sophisticated and complex software solution. To apply you must be affiliated with an educational institution that grants academic degrees, and you are allowed to run non-commercial research only. If you receive money from a 3rd party (company or government), please scroll down to read more about discounts for you. [Read more about license condition conditions](#) The Academic License is valid for 2 years, including the new product versions released until expiry. This period can be extended if you publish a scientific paper where ChemAxon is cited.

**Application for the Academic License not available before  
November 27th.**

# DISCOUNTED LICENSES

Academic and non-profit scientific communities have always been supported by ChemAxon via free or discounted software solutions, as well as we are offering custom tailored options for startups and research institutes.

## Free tools for chemical drawing and calculations

**Chemicalize** provides a variety of physico-chemical calculations and properties, chemical drawing and name - structure conversion as an online service. If you prefer a desktop tool, you can use **Marvin** - our advanced chemical editor - offers quality publication drawings, physico-chemical calculations and name - structure conversion too.

**The free version of Marvin is for non-commercial, individual users only.**

The screenshot displays the Marvin software interface. On the left, a chemical structure of a substituted benzene ring is shown. The main panel is divided into two sections: 'Basic properties' and 'Structural properties'. The 'Basic properties' section includes fields for Name, Molecular weight, Exact mass, Formula, Composition, and Lipinski's rule of five. The 'Structural properties' section lists various counts: Atom count (21), Heavy atom count (13), Aromatic atom count (8), Rotatable bond count (1), Ring count (1), Aromatic ring count (1), and Hetero ring count (0). On the right, a 'Properties' panel shows Molecular weight (326.339 g/mol), Molecular formula (C<sub>16</sub>H<sub>12</sub>O<sub>3</sub>), and Molecular weight (326.339 g/mol). A 'Basic properties' window is also visible, showing the chemical structure and its properties.

[TRY CHEMICALIZE ONLINE](#)   [DOWNLOAD MARVIN](#)

# Rekisteröi- tyminen

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First name (\*)  
Ari

Last name (\*)  
Myllyviita

Your academic email address (\*) (Please use your institutional e-mail)  
ari.myllyviita@helsinki.fi

Occupation / Position (\*)  
Lecturer, Chemistry and Mathematics

Telephone number (\*)  
+358 50 3199411

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Update application

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## DOWNLOAD MARVIN

Version 17.28.0

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## Lisenssin asentaminen

MarvinSketch 17.4.3

File Edit View Insert Atom Bond Structure Calculations Services Help

- Help Contents
- Licenses...
- About MarvinSketch

ChemAxon License Manager

Install license file

- License overview
- Product license details
- Help
  - ChemAxon licensing
  - ChemAxon products
  - Request license
  - Getting help
  - Installing licenses
  - Frequently asked questions
- Create report

### License overview

Default license file location: C:\Users\arimyl\chemaxon\license.cxl

Maximum Search/Minute:

Licenses are read from: C:\Users\arimyl\chemaxon\lic

| Software       | Sta...    | License Term         | Licensee        | E      |
|----------------|-----------|----------------------|-----------------|--------|
| Marvin Applets | Vali<br>d | Academic<br>Teaching | The<br>Universi | 2<br>0 |
| Marvin Beans   | Vali<br>d | Academic<br>Teaching | The<br>Universi | 2<br>0 |

# AEEF Licenssin hyväksyminen (asentaminen)

## Install license file

Please enter the location of the license file or press the Browse button to select path from the file system.

**After specifying the path, press the Install button.**

License file:

Browse...

Install

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The following licenses

Software

- Install license file
- License overview
- Product license details
- Help
  - ChemAxon licensing
  - ChemAxon products
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  - Getting help
  - Installing licenses
  - Frequently asked questions
  - Create report

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Please enter the location of the license file or press the Browse button to select path from the file system.

**After specifying the path, press the Install button.**

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| Software       | Status          | License ...       | Licensee     | Expiratio... | Support ... | Restriction                                   | Number of ... | Comment           |
|----------------|-----------------|-------------------|--------------|--------------|-------------|---|---------------|-------------------|
| Marvin Applets | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | Server Use: Not Allowed                       | Unlimited     | academic teaching |
| Marvin Beans   | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | Server Use: Not Allowed                       | Unlimited     | academic teaching |
| Instant JChem  | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | B/S/P/E: Standard Server Use: Not Allowed     | Unlimited     | academic teaching |
| JChem Base     | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | Search/Min: Unlimited Server Use: Not Allowed | Unlimited     | academic teaching |
| Standardizer   | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | B/S/P/E: Standard Server Use: Not Allowed     | Unlimited     | academic teaching |
| Screen         | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | Server Use: Not Allowed                       | Unlimited     | academic teaching |
| Reactor        | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | Server Use: Not Allowed                       | Unlimited     | academic teaching |
| JKluster       | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | B/S/P/E: Standard Server Use: Not Allowed     | Unlimited     | academic teaching |
| Metabolizer    | To be installed | Academic Teaching | The Universi | 2019-04-04   | 2019-04-04  | Server Use: Not Allowed                       | Unlimited     | academic teaching |

The screenshot shows the MarvinSketch 17.5 software interface. The main window title is "MarvinSketch 17.5". The menu bar includes "File", "Edit", "View", "Insert", "Atom", "Bond", "Structure", "Calculations", "Services", and "Help". The toolbar contains various icons for file operations, editing, and viewing. The main workspace is currently empty. A vertical toolbar on the right side shows element symbols: H, C, N, O, S, F, P, Cl, Br, I. At the bottom, there are icons for 2D and 3D views and a set of chemical rings (pentagon, hexagon, heptagon, octagon, nonagon, decagon).

An "About Marvinsketch" dialog box is open in the center, displaying the following information:

**MarvinSketch**

|                            |   |
|----------------------------|---|
| <b>Product Version:</b>    | MarvinSketch 17.5.0                     |
| <b>Build Date:</b>         | 2017-04-18                              |
| <b>Internal build id:</b>  | 17.5.0-6729                             |
| <b>Operating System:</b>   | x86 Windows 10 10.0                     |
| <b>Character encoding:</b> | windows-1252                            |
| <b>Java:</b>               | Oracle Corporation Java 1.8.0_131       |
| <b>Memory:</b>             | 247,5M maximum, 38,3M total, 11,1M free |
| <b>Environment:</b>        | Application                             |
| <b>Browser:</b>            | -                                       |

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Close

## Ohjeet yms.

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[HTTPS://DOCS.CHEMAXON.COM/DISPLAY/DOCS/MARVINSKETCH+USER%27S+GUIDE](https://docs.chemaxon.com/display/docs/marvinsketch+user%27s+guide)

# MarvinSketch –ohjeet 1

Pages

## Documentation

Created by Unknown User (jvasco), last modified by Nikolett Minala on Apr 06, 2017

Welcome to ChemAxon's documentation home page! We provide here documentation for our products. If you still have a question please create a ticket in our [Support Ticket System](#).

✔ **Are you looking for other versions?**  
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|  |   |  |
|--|---|--|
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Pages / Documentation

## MarvinSketch

Created by Dora Barna, last modified by Nikolett Mihala on Aug 11, 2016

## MarvinSketch User's Guide

Created by Dora Barna, last modified by Nikolett Mihala on Jul 11, 2016

### Getting started

- Start to draw in MarvinSketch
- Select
- Delete
- Move / Rotate / Zoom / Scale
- Tricks and Tips

### MarvinSketch Graphical User interface

- Canvas
- Menus of MarvinSketch
- Toolbars of MarvinSketch
- Pop-up Menus of MarvinSketch
- Status bar of MarvinSketch
- Dialogs of MarvinSketch
- Shortcuts of MarvinSketch
- Customizing MarvinSketch GUI

### Working in MarvinSketch

- Structure Display Options
  - Customizing structure drawing styles
    - Drawing settings
    - Drawing styles
  - Structure Display
  - Colors
  - Implicit/Explicit Hydrogens
  - Displaying the label of carbon atoms
  - Error Highlighting in MarvinSketch
  - Saving Display Options
- Basic Editing
  - Selecting a Structure
  - Copy-Paste and Drag&Drop
  - Geometric transformation of

### Marvin OLE User's Guide

- Install and Uninstall
- How to Use
- Customize Marvin OLE editing mode
- Redirecting other Vendors' OLE objects to Marvin OLE
- Logging
- Troubleshooting and Administration
- Known Issues

### Additional information

- Calculator Plugins
- File formats in Marvin
- Name to Structure
- Scientific Background
- Structure Checker
- Structure to Name

MarvinSketch User's Guide

# MarvinSketch – ohjelman käyttö

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ABITTI-TIKUSSA MARVINSKETCH 17.3.27

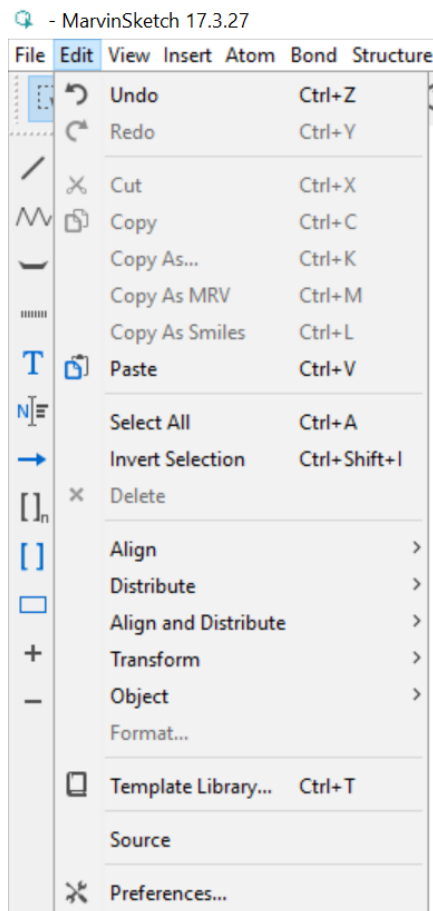
## Mihin MarvinSketch ”taipuu”

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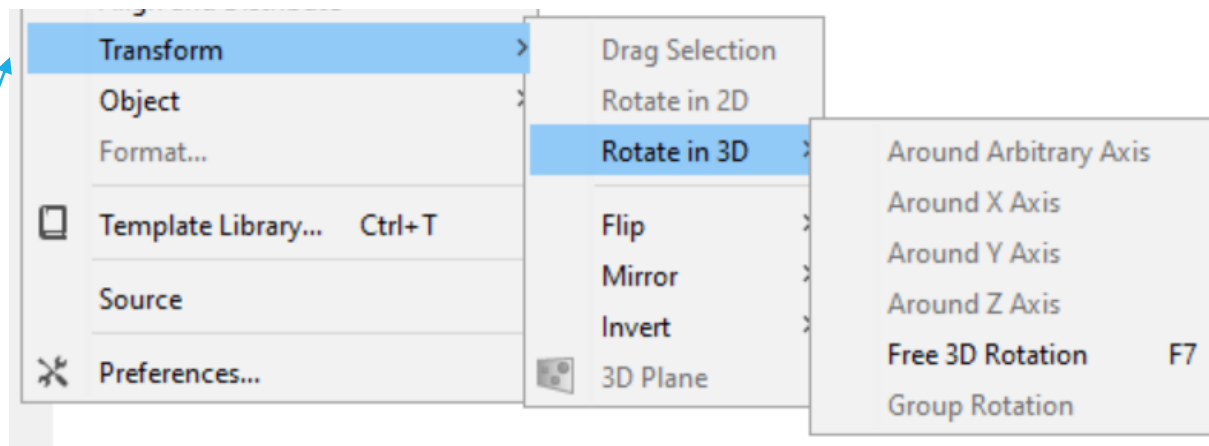
- Molekyylien piirtäminen 2D – 3D
- Reaktioyhtälöiden kirjoittaminen (orgaaninen kemia)



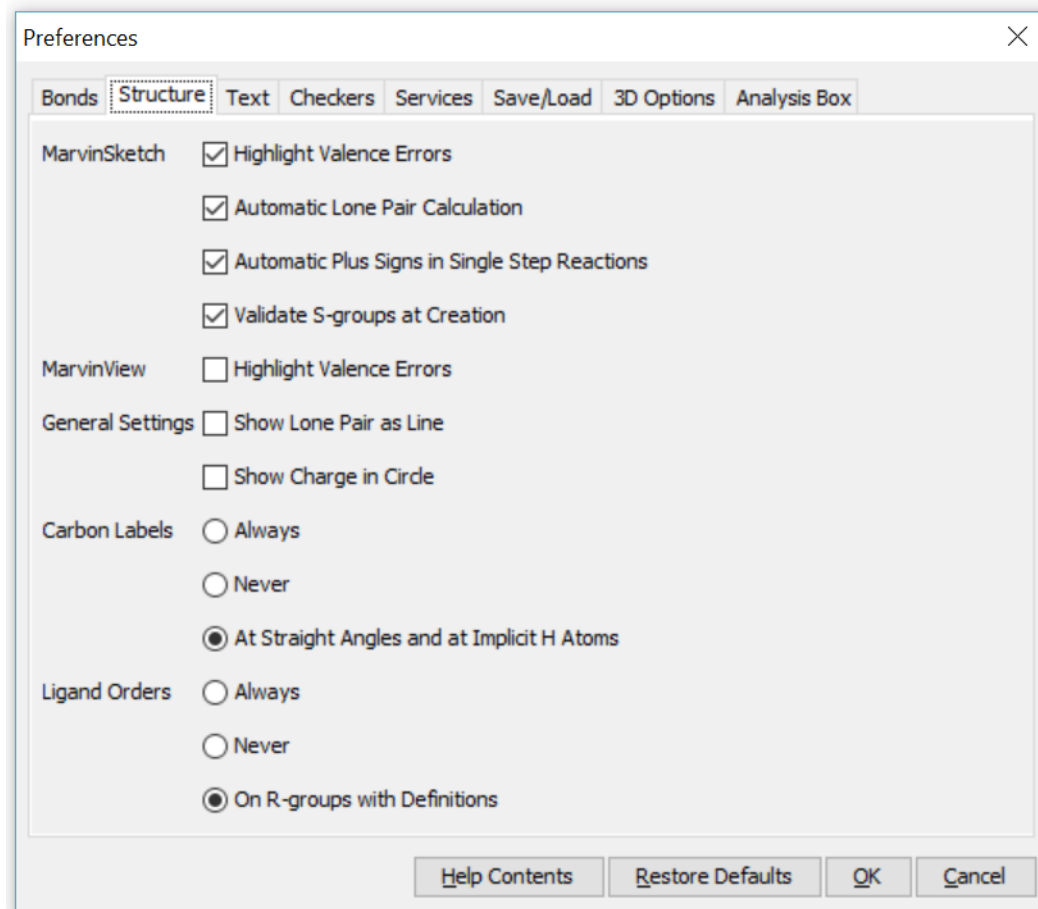
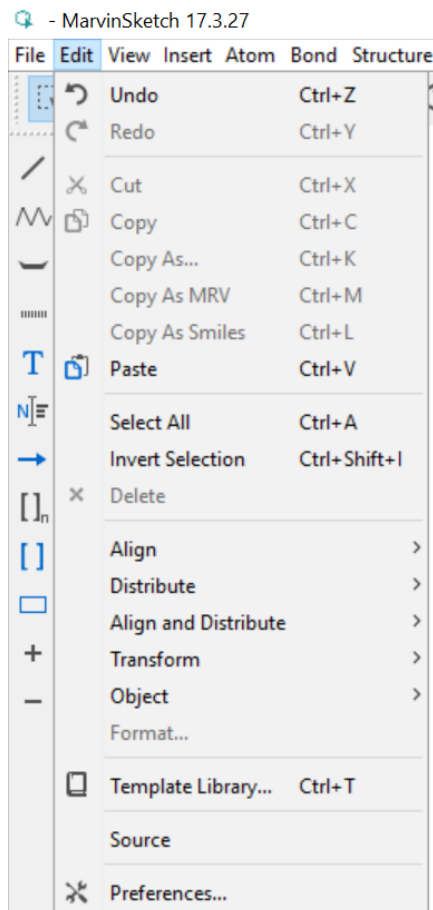
## Valikot - Edit



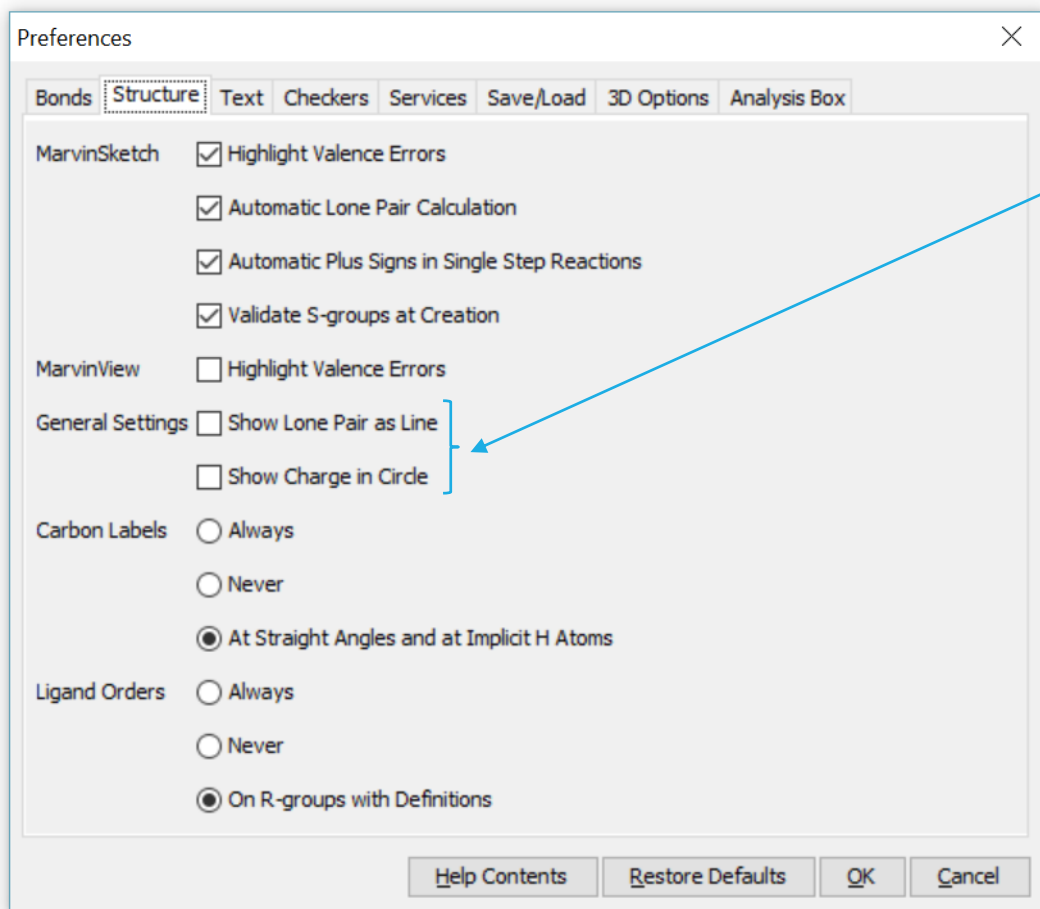
Molekyylin ”pyöritys”, paina F7 vrt. valinta -painike



## Valikot – Edit – Preferences...



# Vapaat elektroniparit näkyviin



EI TOIMI NORMIOHJELMALLA?

## Valikot - View

MarvinSketch 17.3.27

File Edit View Insert Atom Bond Structure Calculations Services Help

- Mouse mode
- Zoom Level
- Structure Display
  - Atom Symbols in 3D
  - Wireframe
  - Wireframe with Knobs
  - Stick
  - Ball and Stick
  - Spacefill
- Colors
- Stereo
- Implicit Hydrogens
- Peptide Display
- Advanced
- Pages
- Toolbars
- Menubar F11
- Status Bar
- Grid Shift+F9
- Guidelines Ctrl+Shift+F9
- Editor style

Atom Numbering: Off, Atom Numbers, IUPAC Numbering

3D Ball and Stick Model

## Valikot – View – Bond Length

MarvinSketch 17.4.3

File Edit **View** Insert Atom Bond Structure Calculations Services Help

The screenshot shows the MarvinSketch 17.4.3 interface. The 'View' menu is open, and 'Bond Lengths' is selected. The chemical structure of 3-aminobutan-2-ol is displayed with the following bond lengths:

- C-N bond: 1.47
- C-C bond (top): 1.55
- C-C bond (middle): 1.56
- C-O bond: 1.43
- C-C bond (bottom): 1.55

Name: 3-aminobutan-2-ol  
 Molecular weight: 89,14  
 Formula: C<sub>4</sub>H<sub>11</sub>NO

## Valikot - Insert

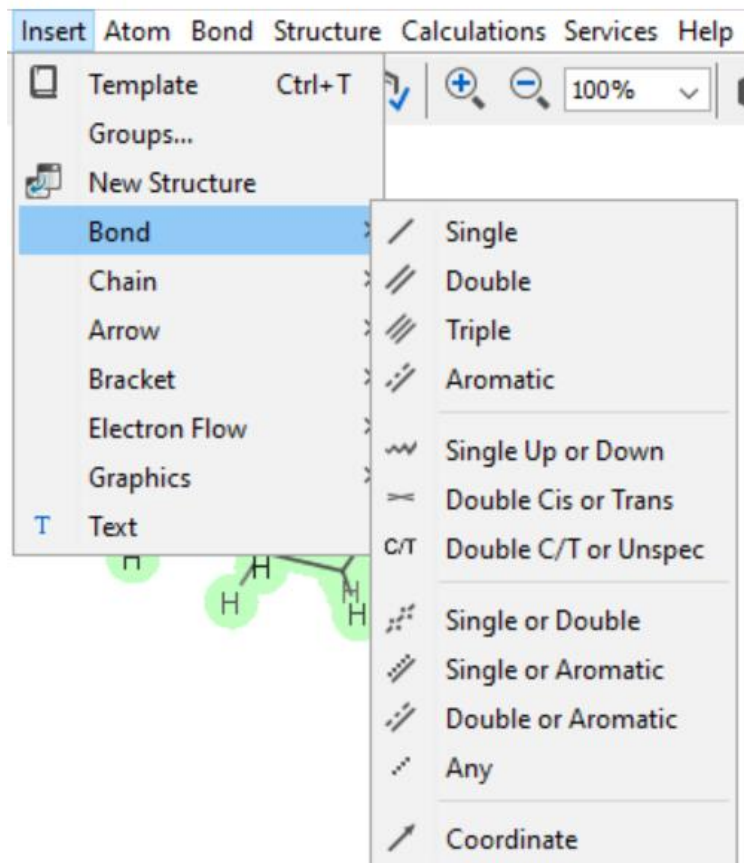
Vasen reuna

MarvinSketch 17.3.27

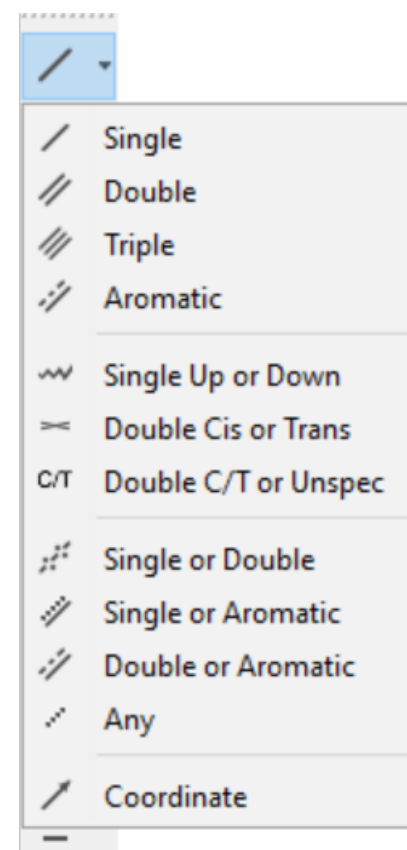
The image displays the MarvinSketch 17.3.27 software interface. The 'Insert' menu is open, showing various options. The 'Chain' option is highlighted, and its sub-menu is shown, containing 'Chain' and 'Curved Chain'. The 'Arrow' option is also highlighted, and its sub-menu is shown, containing 'Straight Arrow / Reaction', 'Retrosynthetic Arrow', 'Equilibrium Arrow', 'Resonance Arrow', 'Curved Arrow', 'Dashed Arrow', and 'Crossed Arrow'. A small chemical structure is visible in the background.

## Bond - Pikavalikosta

tch 17.3.27



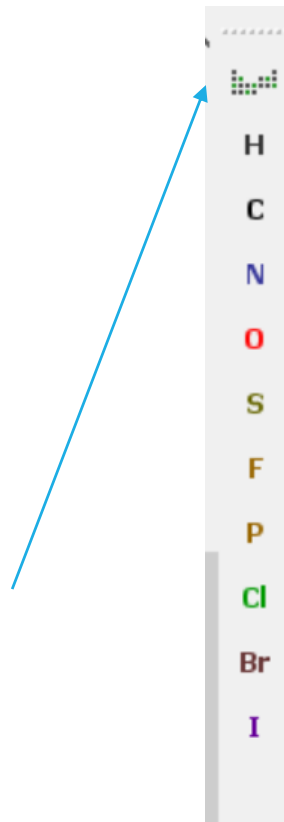
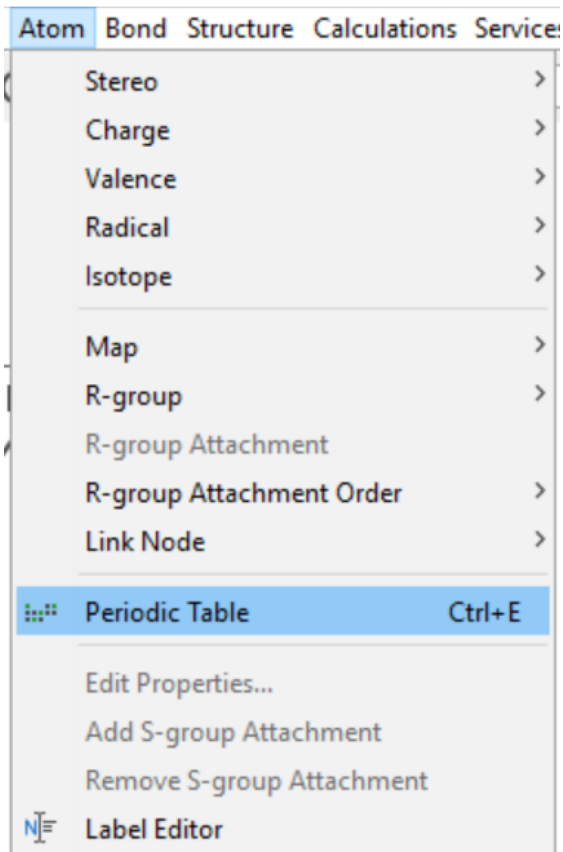
## Vasen reuna



## Valikot - Atom

Oikea reuna

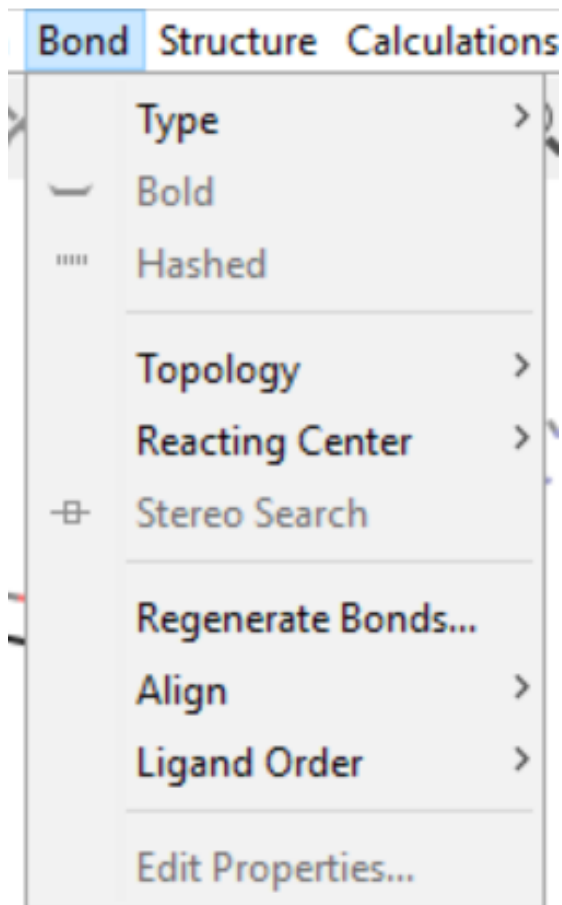
3.27



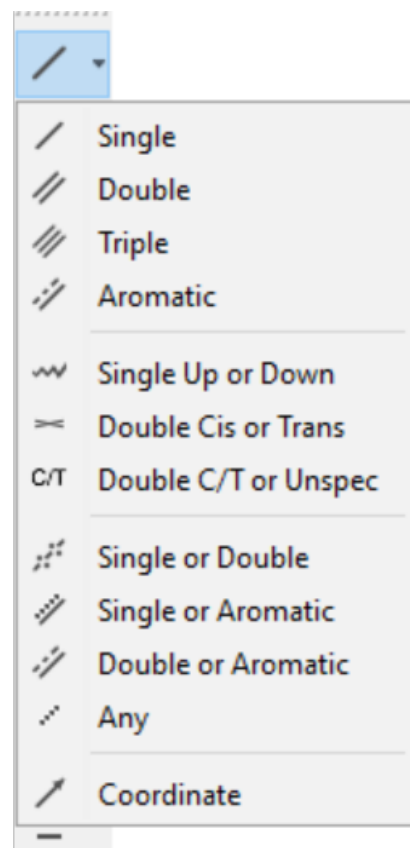
Valitse alkuaine



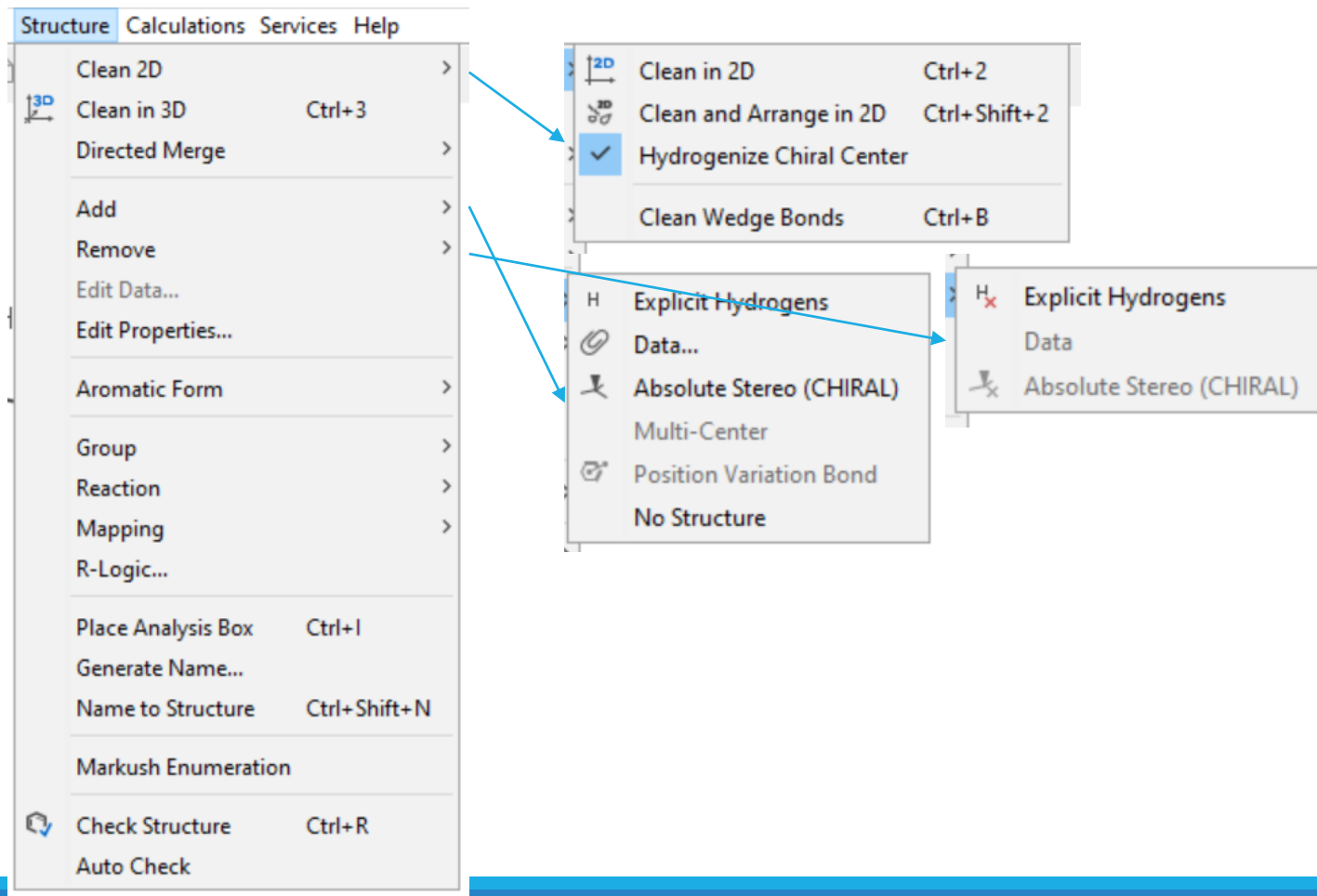
## Valikot - Bond



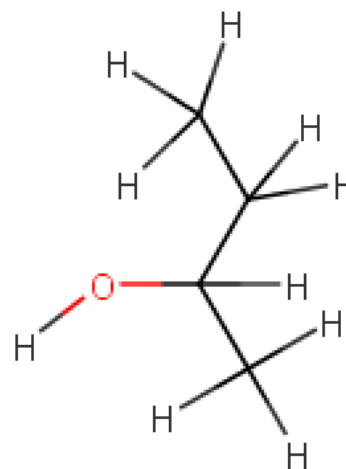
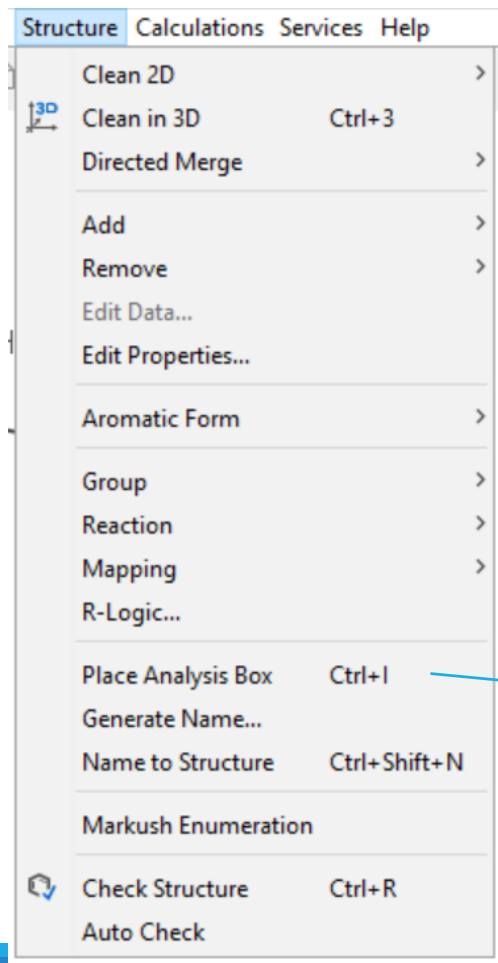
## Vasen reuna



## Valikot – Structure

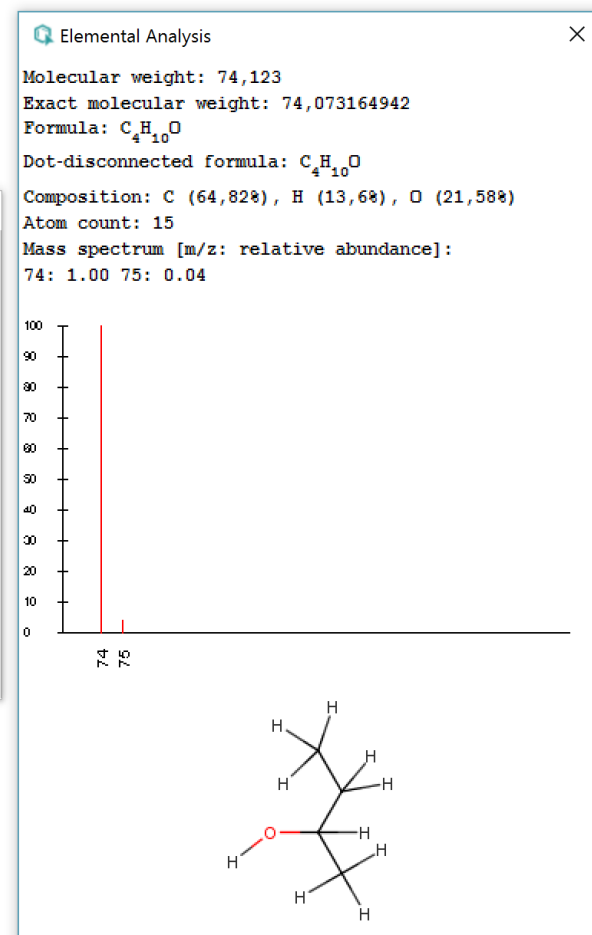
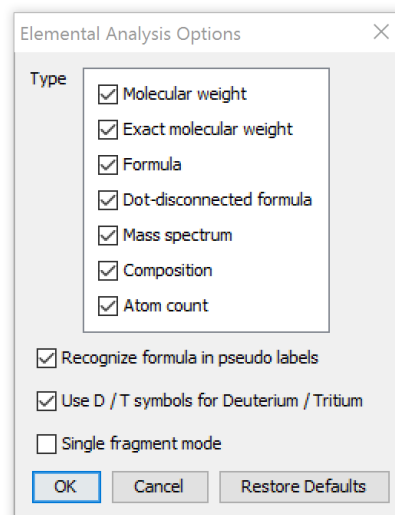
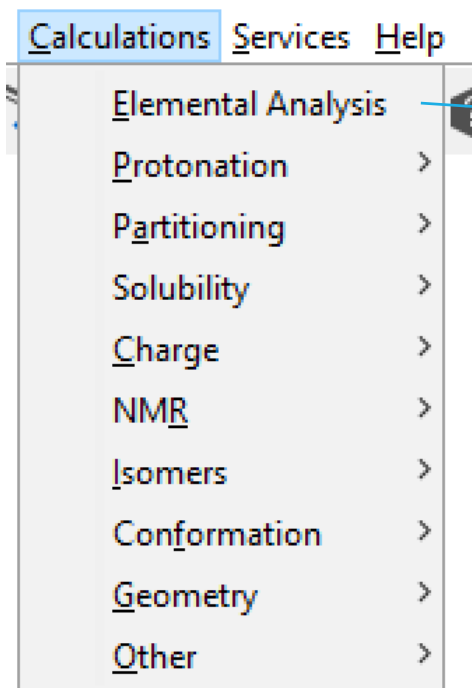


## Valikot – Structure



Name: butan-2-ol  
 Molecular weight: 74,12  
 Formula: C<sub>4</sub>H<sub>10</sub>O

## Valikot – Calculations



## Valikot – Calculations - Charge

The screenshot displays the AEEF software interface. The main menu bar includes 'Bond', 'Structure', 'Calculations', 'Services', and 'Help'. The 'Calculations' menu is open, showing options like 'Elemental Analysis', 'Protonation', 'Partitioning', 'Solubility', 'Charge', 'NMR', 'Isomers', 'Conformation', 'Geometry', and 'Other'. The 'Charge' option is selected, and a sub-menu is visible with 'Charge', 'Polariza', 'Orbital', and 'Dipole I'.

A 'Charge Options' dialog box is open, showing the following settings:

- Decimal places: 2
- Type: Total
- Charges of implicit hydrogens
- Take resonant structures
- Take major microspecies
- at pH: 7.4
- Display in MarvinSpace

Buttons for 'OK', 'Cancel', and 'Restore Defaults' are at the bottom of the dialog.

The 'Charge' window shows a 3D ball-and-stick model of a molecule with partial charges labeled on each atom. The charges are: 0,02, -0,06, 0,02, 0,03, -0,03, 0,05, 0,06, 0,03, -0,04, 0,03, 0,03, 0,21, and -0,39.

To the right of the ball-and-stick model is a 3D electrostatic potential (ESP) map of the molecule, showing regions of positive (red) and negative (blue) charge.

## Valikot – Calculations - Charge

The image shows the AEEF software interface. The 'Calculations' menu is open, with 'Charge' selected. The 'Orbital Electronegativity Options' dialog is open, showing 'Pi' selected in the 'Type' dropdown. The 'Orbital Electronegativity' window displays a chemical structure of a branched alkane with a highlighted oxygen atom (red) and a value of 3,16 next to it.

**Calculations Menu:**

- Elemental Analysis
- Protonation
- Partitioning
- Solubility
- Charge**
  - Charge
  - Polarizability
  - Orbital Electronegativity
  - Dipole Moment Calculation
- NMR
- Isomers
- Conformation
- Geometry
- Other

**Orbital Electronegativity Options:**

- Decimal places: 2
- Type: Pi (selected), Sigma, Pi
- Take resonance
- Take major microspecies
- at pH: 7.4
- Buttons: OK, Cancel, Restore Defaults

**Orbital Electronegativity Window:**

- Chemical structure: A branched alkane with a highlighted oxygen atom (red) and a value of 3,16 next to it.

## Valikot – Calculations - Charge

Bond Structure **Calculations** Services Help

