

MarvinSketch

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KEMIAN JA MATEMATIIKAN LEHTORI

HELSINGIN YLIOPISTON VIIKIN NORMAALIKOULU

Sisältö

1. Lataaminen
2. Asentaminen
3. Lisenssikuvio
4. ... Ohjeet
5. ... Ohjelman käyttö

KYSELY:

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



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.

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MAY 8, 2018

SciBite and ChemAxon to Deliver an Integrated Solution for Biology and Chemistry Research

[PARTNER](#) [PRESS RELEASE](#) [SCIBITE](#)

APR 23, 2018

ChemAxon European User Meeting, Budapest, March 20-22, 2018

[MEETING REPORT](#) [WENDY WARR](#) [WENDY WARR & ASSOCIATES](#)

MAR 19, 2018

Enamine collaborates with ChemAxon to create a convenient web-based search in immense chemical space

[CHEMAXON](#) [PRESS RELEASE](#) [PR](#) [ENAMINE](#)

DEC 12, 2017

ChemAxon and Simmaren Form Strategic Partnership to Accelerate the Development of New Software for the Prediction of Human Drug Metabolism

19th Annual Drug Discovery Summit

JUN 6 - 8, 2018 BERLIN, GERMANY - BOOTH #26

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JUN 14, 2018 7:00 PM CEST

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Marvin

A full featured chemical editor for making science accessible on all platforms

Marvin suite is a chemically intelligent desktop toolkit built to help you draw, edit, publish, render, import and export your chemical structures and as well as allowing you to convert between various chemical and graphical file formats. It is free for individual, academic and non-commercial use.

PLAY VIDEO



OVERVIEW

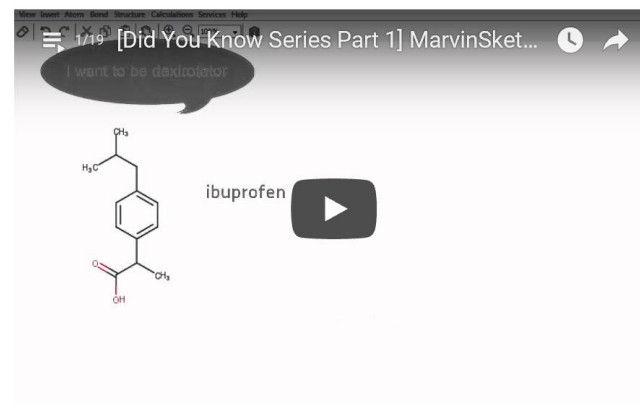
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MarvinSketch features an extensive set of functionalities to enable the fast and accurate drawing of chemical compounds, reactions, Markush structures and query molecules. Furthermore, MarvinSketch has built-in structure and valence checkers to provide guidance, and integrated property calculators to pull live results - upon your request. Not only does MarvinSketch translate chemistry into a digital environment, it also supports the widest selection of industrially acknowledged standard chemical file formats. For chemical drawing on the web, please also check our browser component [Marvin JS](#).



#	structure	code	MOLFORMULA	MOLWEIGHT	product_name	c_log_p	h_bond_donor	rotatable_bo
1		BTB 03727	C13 H7 Cl2 F2 N	286107000	N1-(2-chloro-5-(4-fluorobenzyl)phenyl)ethan-1-amine	5.13680000	0.00000000	3.00000000
					4-fluorobenzyl	0.00000e+000	0.00000e+000	0.00000e+000
					o-4-fluorobenzyl	0.00000e+000	0.00000e+000	0.00000e+000

MarvinView - View your molecules

Get started instantly

For drawing, calculations or bi-directional name to structure conversion you might not even need the Academic License.

Chemicalize

Calculate properties, draw, extract chemical data online

TRY ONLINE NOW

Marvin

THE chemical editor on desktop; free for non-commercial use

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Lataaminen

Lataaminen

- ❖ 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

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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 overlaid on the video player.

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

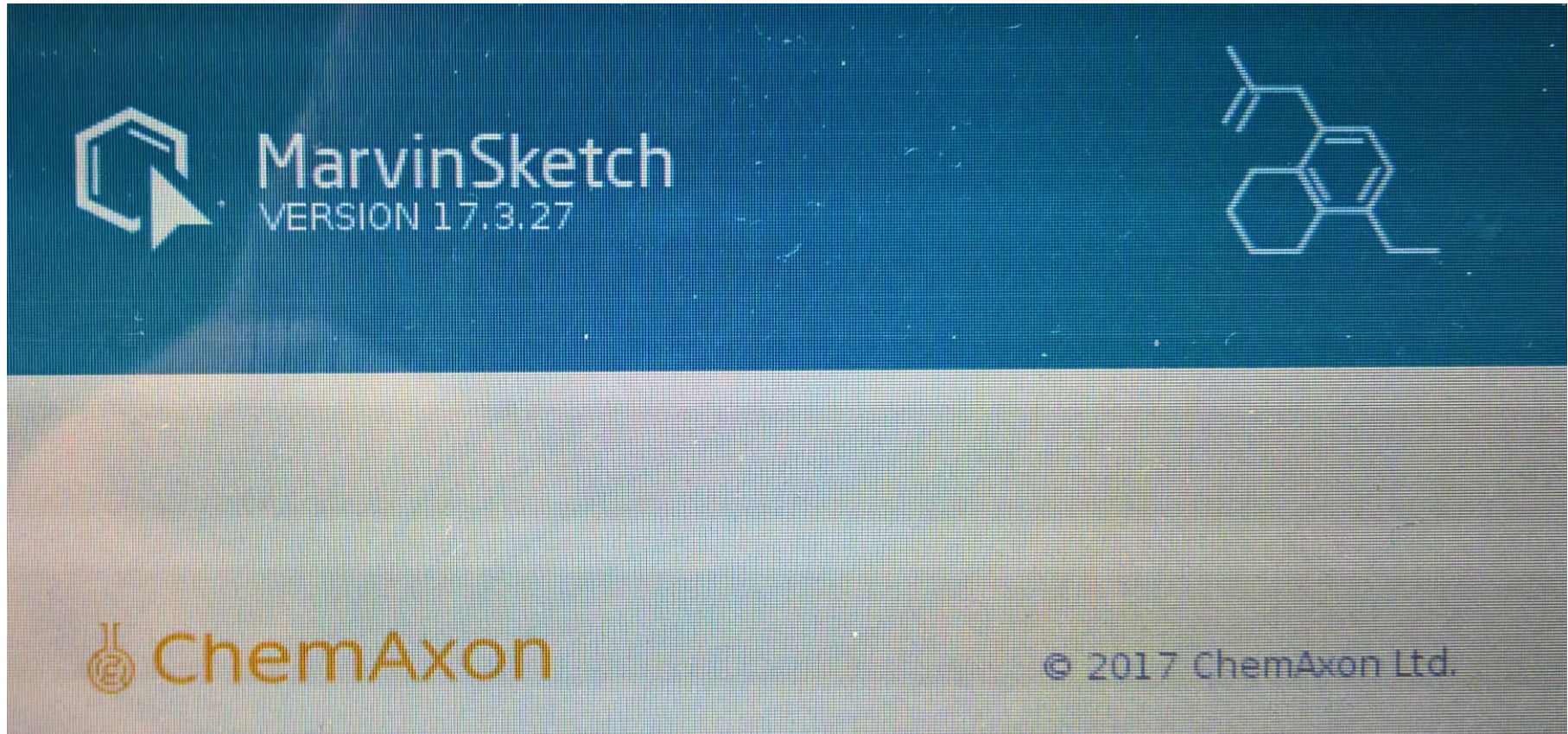
Includes Marvin desktop applications, API, examples, documentation.

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Mac OS X



Jakelussa oleva tuorein versio on 18.5.0

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Version 18.11

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Java versions & OLE Editor

Please note that from version 17.29.0 [our tools run on Java 8](#). Marvin is compatible with Java 10 too from version 18.11. Also please [install .NET Marvin component](#) with the Java OLE supported version to use OLE Editor functions in Marvin.

Windows

Includes Marvin desktop applications, API, examples, documentation.

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Mac OS X

Drag and Drop installer for Marvin desktop application.

[DOWNLOAD .DMG](#)

Linux

Kirjaudu järjestelmään ennen lataamista

JOS ET OLE VIELÄ
REKISTERÖITYNYT

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Marvin

THE chemical editor on desk

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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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 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

 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>

Tänään, 23:26

Anselmi Myllyviita ✎



Vastaa kaikille | ▾

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Thank you for registering to ChemAxon.

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

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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>

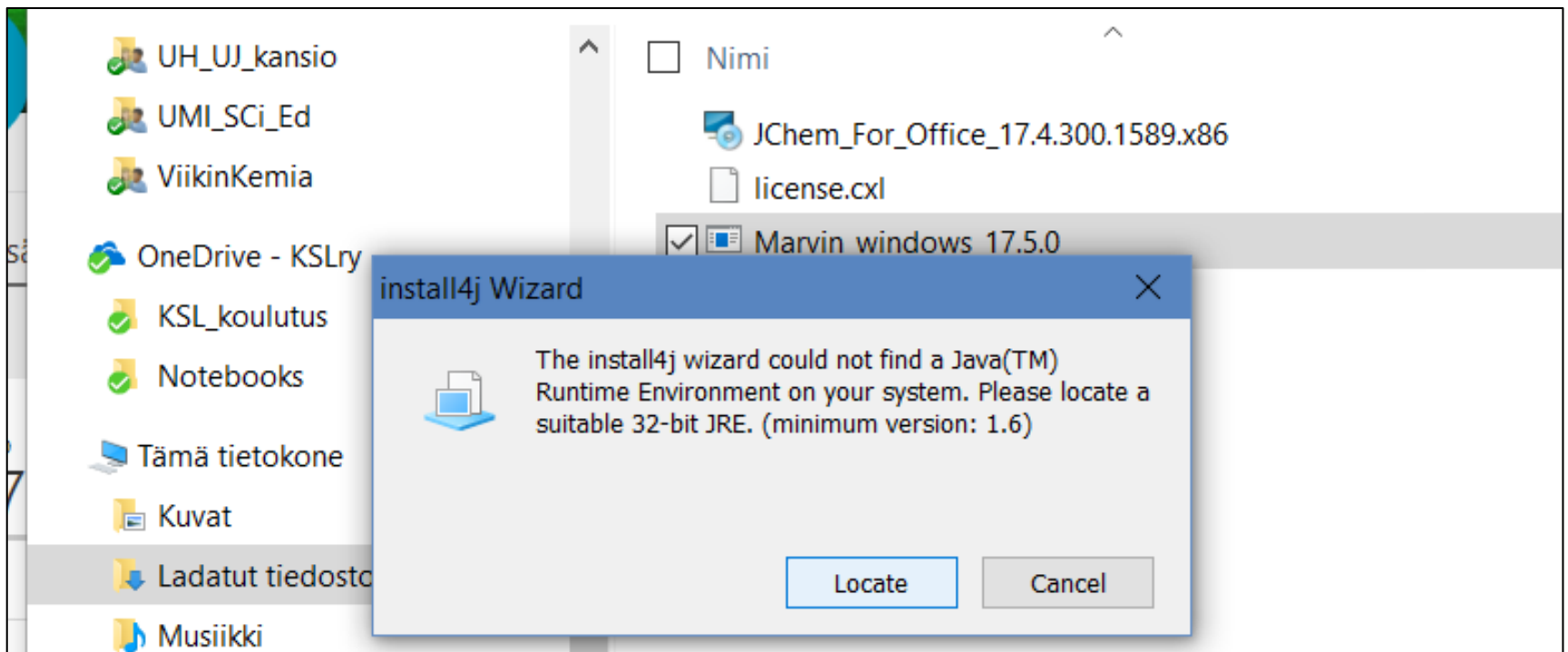
Should you have any technical difficulties, please do not hesitate to drop a line to the website-support@chemaxon.com.

Best regards,

The ChemAxon team

Asentaminen

Asennuksen yhteydessä tarkistetaan Javan olemassaolo



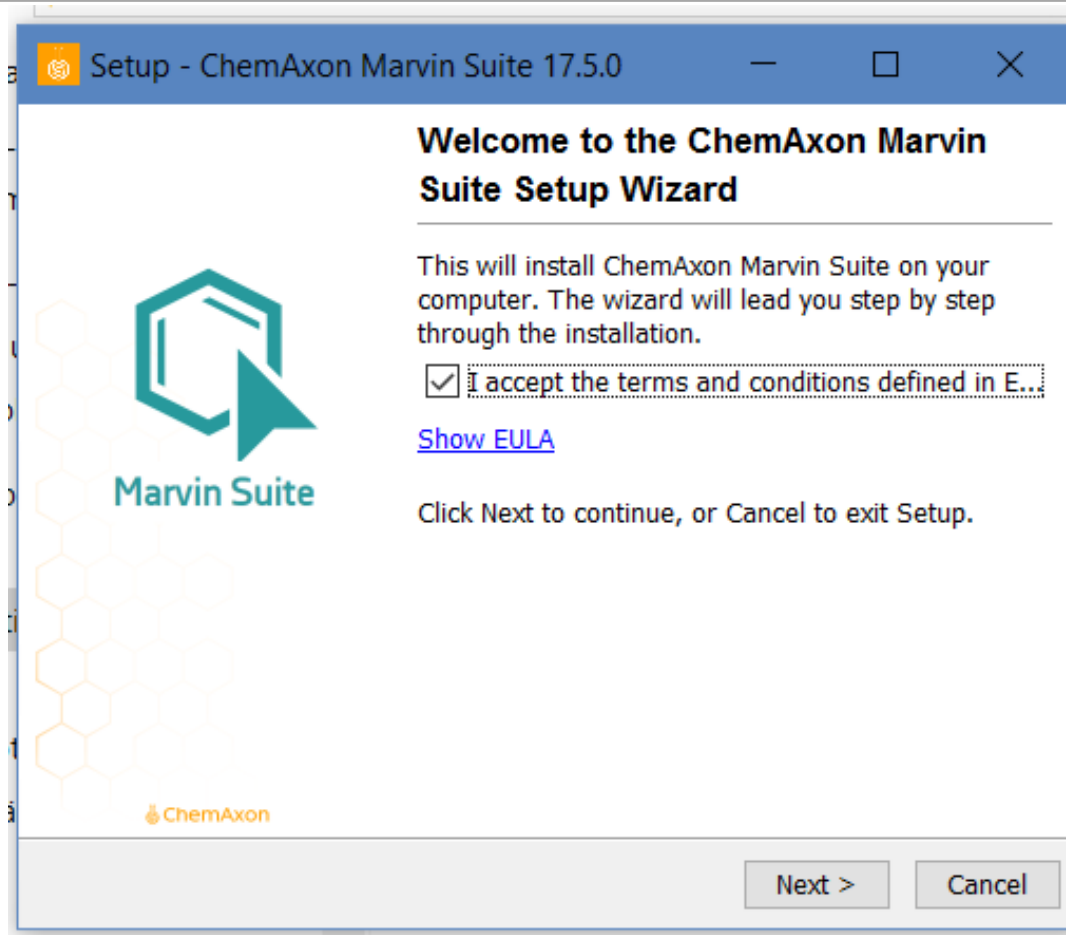
Javan asennus (asennus vaatii admin –oikeudet)

A screenshot of a search engine results page. The search bar contains the text "java runtime environment". Below the search bar, there are navigation tabs for "WWW", "Kuvat", and "Uutiset". The "WWW" tab is selected. Below the tabs, there is a link "2 270 000 TULOSTA" and a language filter "Kieli". The main search result is titled "JAVA-ohjelmistokehitystä | observis.fi" and includes a sub-link "Mainos · observis.fi". Below this, there is a snippet of text: "Vaativat asiakaskohtaiset java- palvelut meiltä toimitu".

A screenshot of the Java website's "Free Java Download" page. The page has a red header with the Java logo and navigation links for "Download" and "Help". A search bar is located in the top right corner. The main content area features a large red button labeled "Free Java Download". Below the button, there are links for "What is Java?", "Do I have Java?", and "Need Help?". The page also includes a section titled "Why download Java?" with a paragraph of text explaining the benefits of upgrading to the latest Java version for security.

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. The background window is titled "Setup - ChemAxon Marvin Suite 17.5.0" and shows the "Select Installation Type" screen. It asks "Which type of installation should be performed?" and provides two options: "Standard installation" (selected) and "Custom installation". The "Standard installation" option is described as installing all components for regular usage, while the "Custom installation" option allows for customizing components. The middle window, also titled "Setup - ChemAxon Marvin Suite 17.5.0", shows the "Installing" phase with the message "Please wait while Setup installs ChemAxon Marvin Suite on your computer." and a progress bar for "lib\calculations-elemanal-master-6729.jar". The foreground window, titled "Setup - ChemAxon Marvin Suite 17.5.0", shows the "Completing the ChemAxon Marvin Suite Setup Wizard" screen. It features the Marvin Suite logo and text stating "Setup has finished installing ChemAxon Marvin Suite on your computer. The application may be launched by selecting the installed icons." and "Click Finish to exit Setup." A blue arrow points from the Marvin Suite logo in this window to the desktop icons on the right. The desktop background is blue with a recycling bin icon labeled "Roskakori", a laptop icon labeled "Tämä tietokone", and two application icons: "MarvinSketch" and "MarvinView".

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.

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

Extracting files ...
lib\calculations-elemanal-master-6729.jar

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

Roskakori

Tämä tietokone

MarvinSketch

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, wavy lines, bonds, and various rings. On the right side, there is a vertical toolbar with a grid icon and a list of chemical elements: H, C, N, O, S, F, P, Cl, Br, and 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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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 (342.339 g/mol), Molecular formula (C₁₅H₁₀O₃), and Molecular weight (342.339 g/mol). A '3D' view of the molecule is also visible.

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Rekisteröi- tyminen

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About the applicant

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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Version 17.28.0

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Avaa Tallenna ^ Peruuta ×

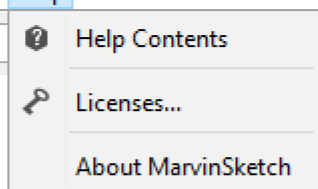
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Avaa Tallenna ^

Lisenssin asentaminen

MarvinSketch 17.4.3

File Edit View Insert Atom Bond Structure Calculations Services Help



Tiedosto asennetaan kohdasta
Help | Licenses ...

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 - Installing licenses
 - Frequently asked questions
 - Create report

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

Maximum Search/Minute:

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

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Marvin Beans	Vali d	Academic Teaching	The Universi	2 0

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After specifying the path, press the Install button.

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Install

If your e-mail client supports drag and drop of attachments, you can drag the license file you received by e-mail to this dialog.

The following licenses

Hae (Browse...) tiedosto omalta koneelta. Ja asenna (install) se.

Software

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 - Getting help
 - Installing licenses
 - Frequently asked questions
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After specifying the path, press the Install button.

License file: C:\Users\admin\Downloads\license.cd

If your e-mail client supports drag and drop of attachments, you can drag the license file you received by e-mail to this dialog.

The following licenses will be installed by pressing the Install button:

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

Asentamisen jälkeen:

The image shows a screenshot of 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 and editing. The main workspace is currently empty. An "About Marvinsketch" dialog box is open in the center, displaying the following information:

MarvinSketch

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

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The interface also features a vertical toolbar on the right with element symbols (H, C, N, O, S, F, P, Cl, Br, I) and a bottom toolbar with geometric shapes and a "2D" button.

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📁	17.28.0	-				2017-11-09 10:21:21
📁	17.29.0	-				2017-12-08 11:58:26
📁	17.3.13.0	-				2017-03-21 16:57:25
📁	17.3.27.0	-				2017-03-29 14:30:37
📁	17.4.3.0	-				2017-04-06 15:40:17
📁	17.5.0	-				2017-04-20 19:29:40
📁	17.6.0	-				2017-04-26 15:14:18
📁	17.7.0	-				2017-05-05 17:09:55
📁	17.8.0	-				2017-05-09 12:40:11
📁	17.9.0	-				2017-05-26 16:49:32
📁	18.1.0	-				2018-01-12 11:28:51
📁	18.2.0	-				2018-01-18 14:11:58
📁	18.3.0	-				2018-01-30 14:45:41
📁	18.4.0	-				2018-02-13 17:33:29
📁	18.5.0	-				2018-02-27 20:54:01

Ohjeet yms.

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Documentation

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

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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