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MarvinSketch

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KEMIAN LEHTORI

HELSINGIN YLIOPISTON VIIKIN NORMAALIKOULU

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Asentaminen

- 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

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MarvinSketch

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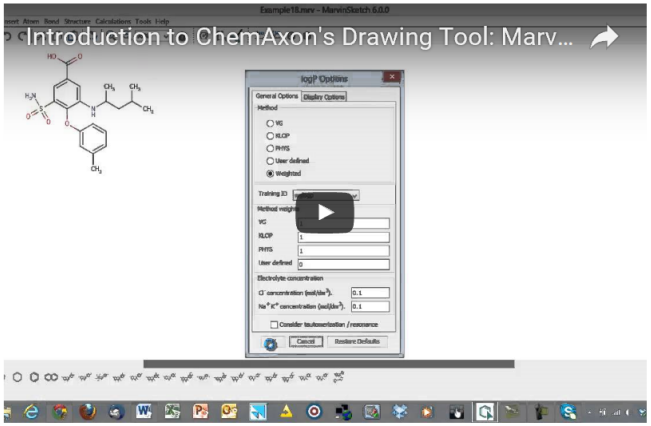
ADVANCED CHEMICAL EDITOR FOR DRAWING CHEMICAL STRUCTURES, QUERIES AND REACTIONS

MarvinSketch allows users to quickly draw molecules through basic functions on the GUI and advanced functionalities such as sprout drawing, customisable shortcuts, abbreviated groups, default and user-defined templates and context-sensitive popup menus.



PRODUCT TYPE: application
INTERFACES: GUI (Desktop) API (Java, .NET)
AVAILABLE IN: JChem Base, Instant JChem, JChem for Office, JChem for SharePoint, Plexus Suite, Biomolecule Toolkit, chemicalize.org, KNIME, Pipeline Pilot

Chemical structure drawing

Atom and Bond properties

MarvinSketch has a rich support for atom and bond properties. Users can assign stereochemistry, charge, valence, radicals and isotopes to each atom. Single, double, triple bonds and aromatic forms are supported.

Reaction drawing

You can draw single step reactions in MarvinSketch by placing a reaction arrow in any position, pointing in any direction in relation to reaction products. The structures 'in front' of the arrow will be recognized as reactants, structures

Query drawing

Atom lists, bond lists, not lists, generic atoms, R-groups, and lone pairs are among the query building features available in MarvinSketch. Link nodes, repeating units, pseudo atoms and homology groups, S-groups with attached data

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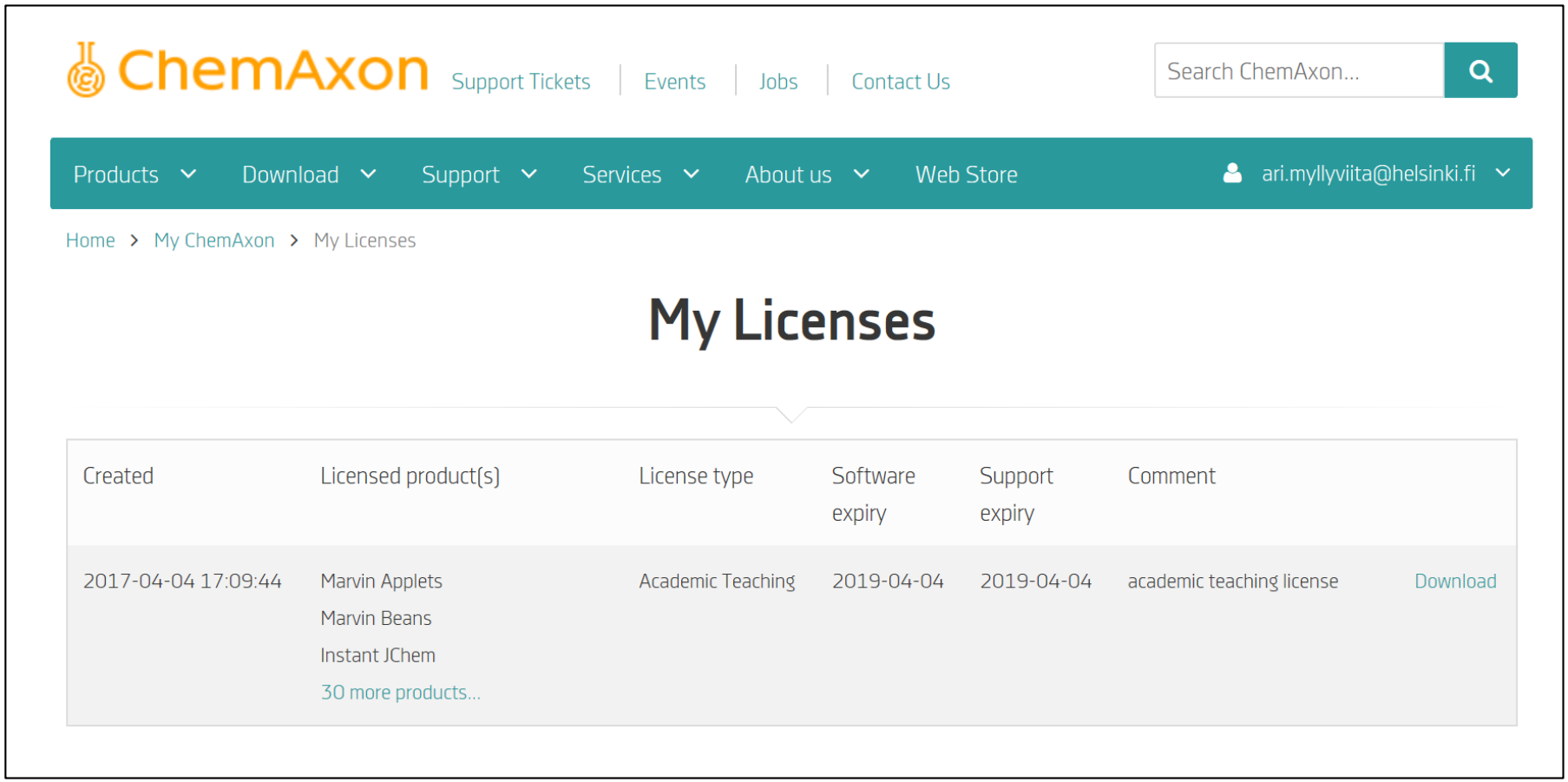
Oppilaitos-lisenssi



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Lataaminen ja lisenssit

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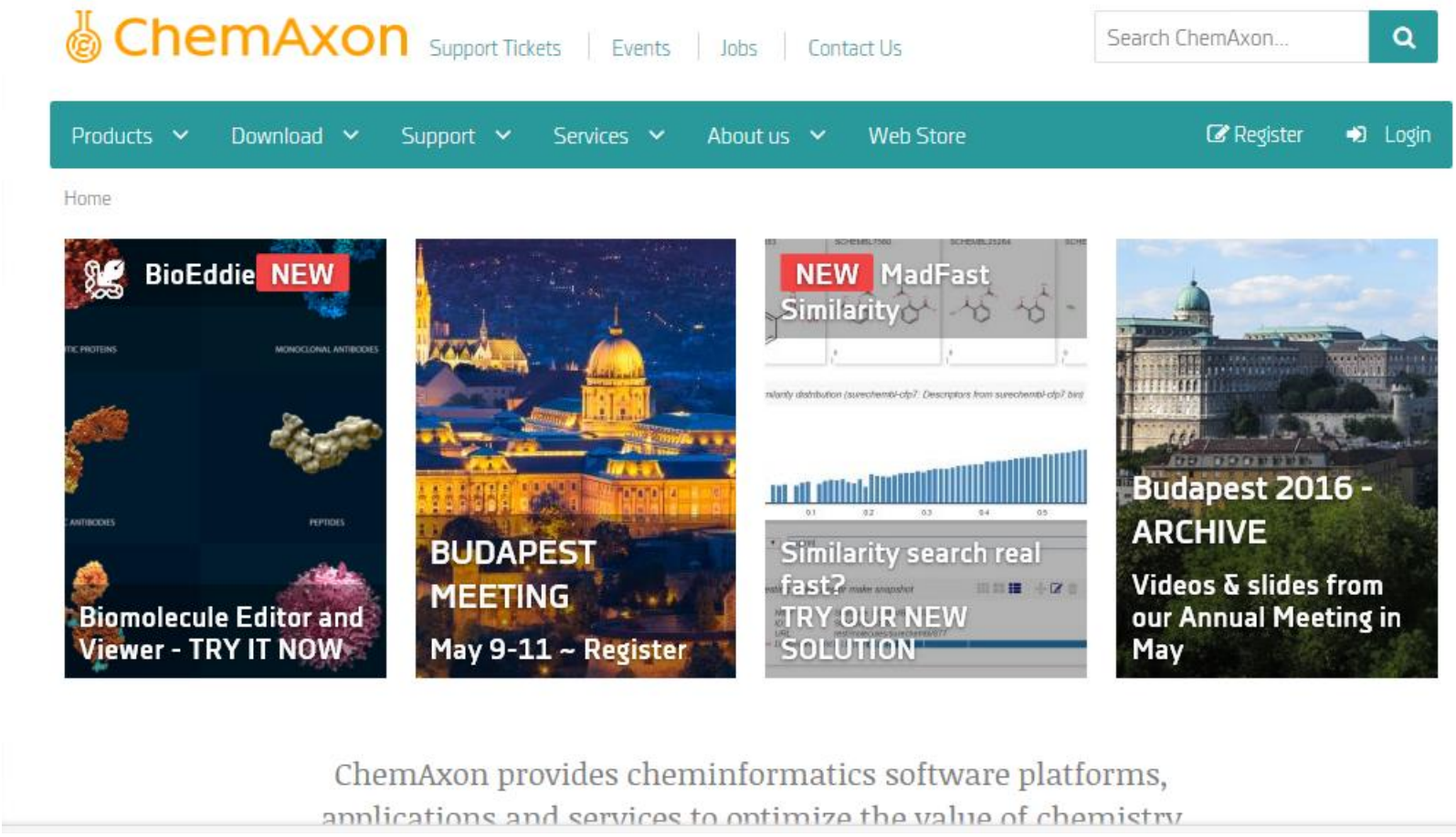

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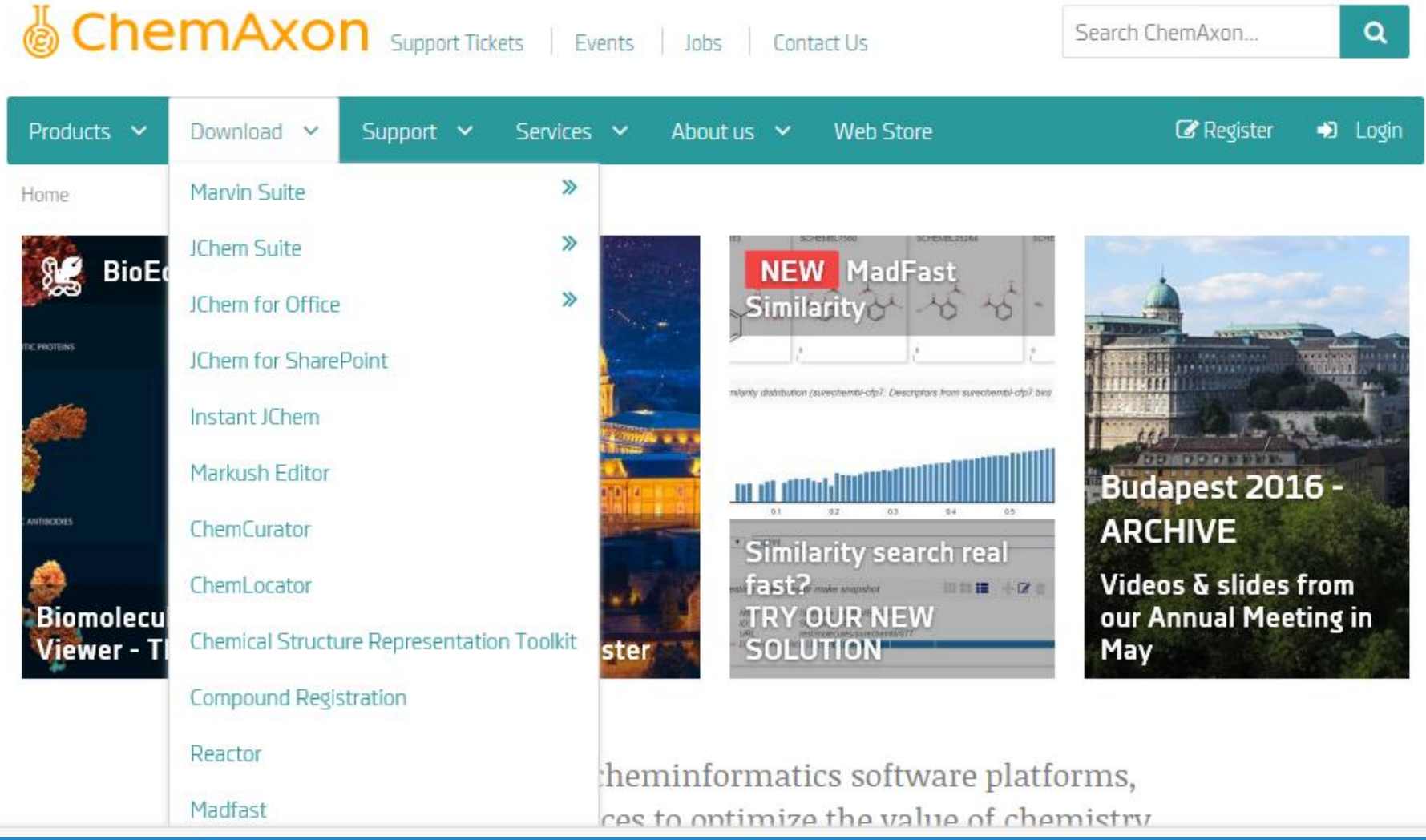
Kuten ChemSketch –ohjelman tapauksessa

Lataussivu – ennen sitä rekisteröidy



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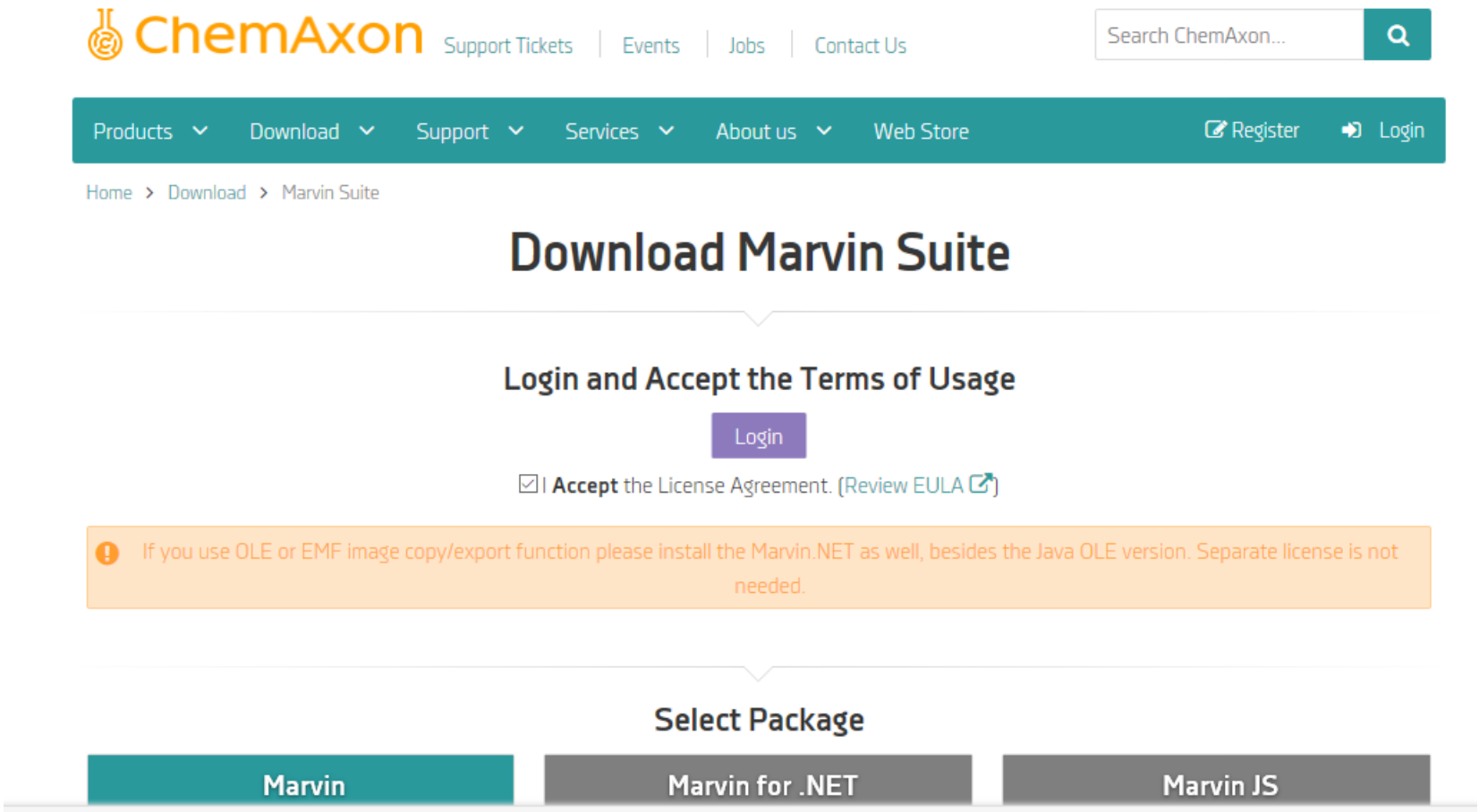
Lataussivu – hyväksy sopimusehdot



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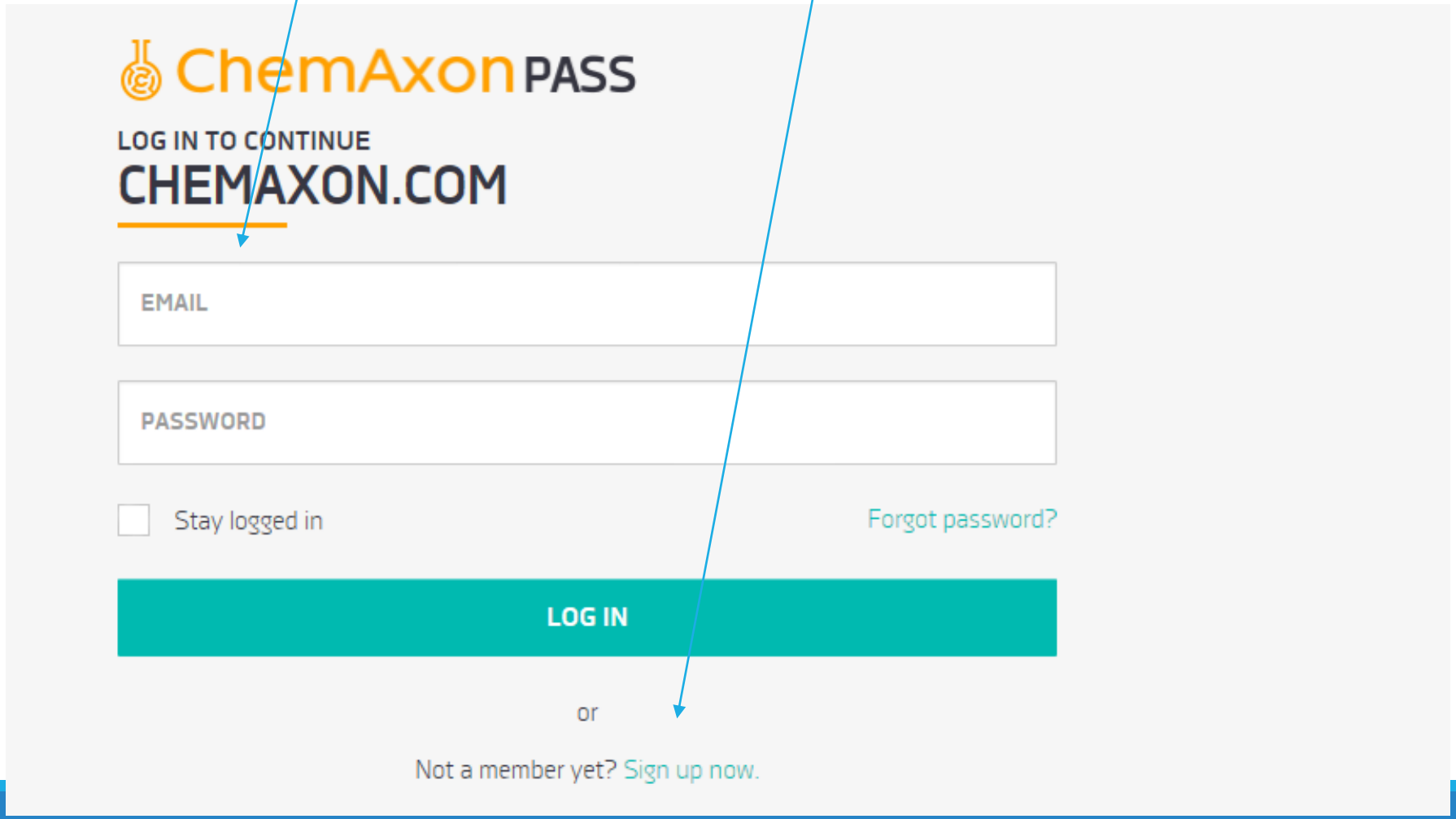
Kirjaudu tai rekisteröidy



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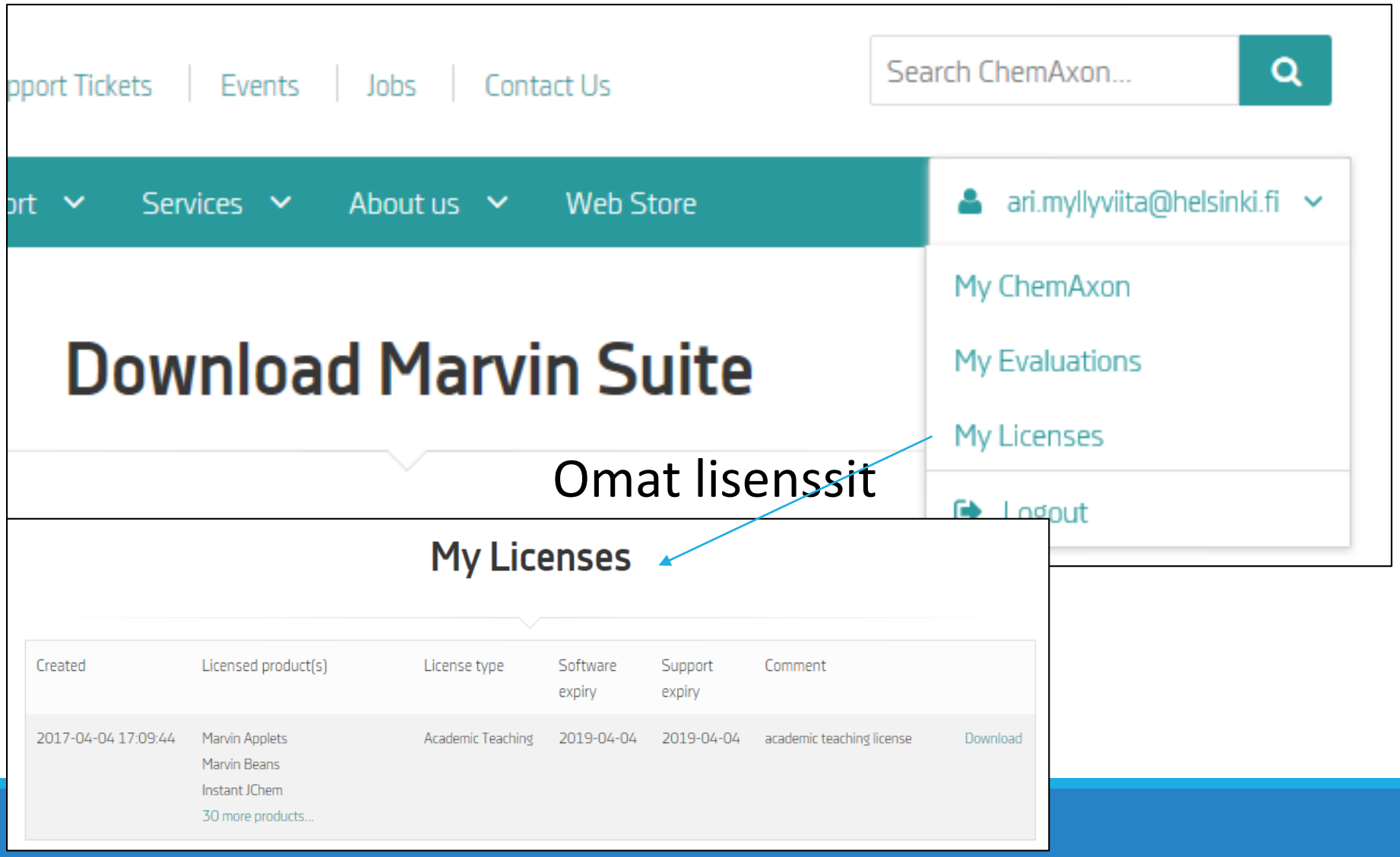
Kirjautumisen jälkeen



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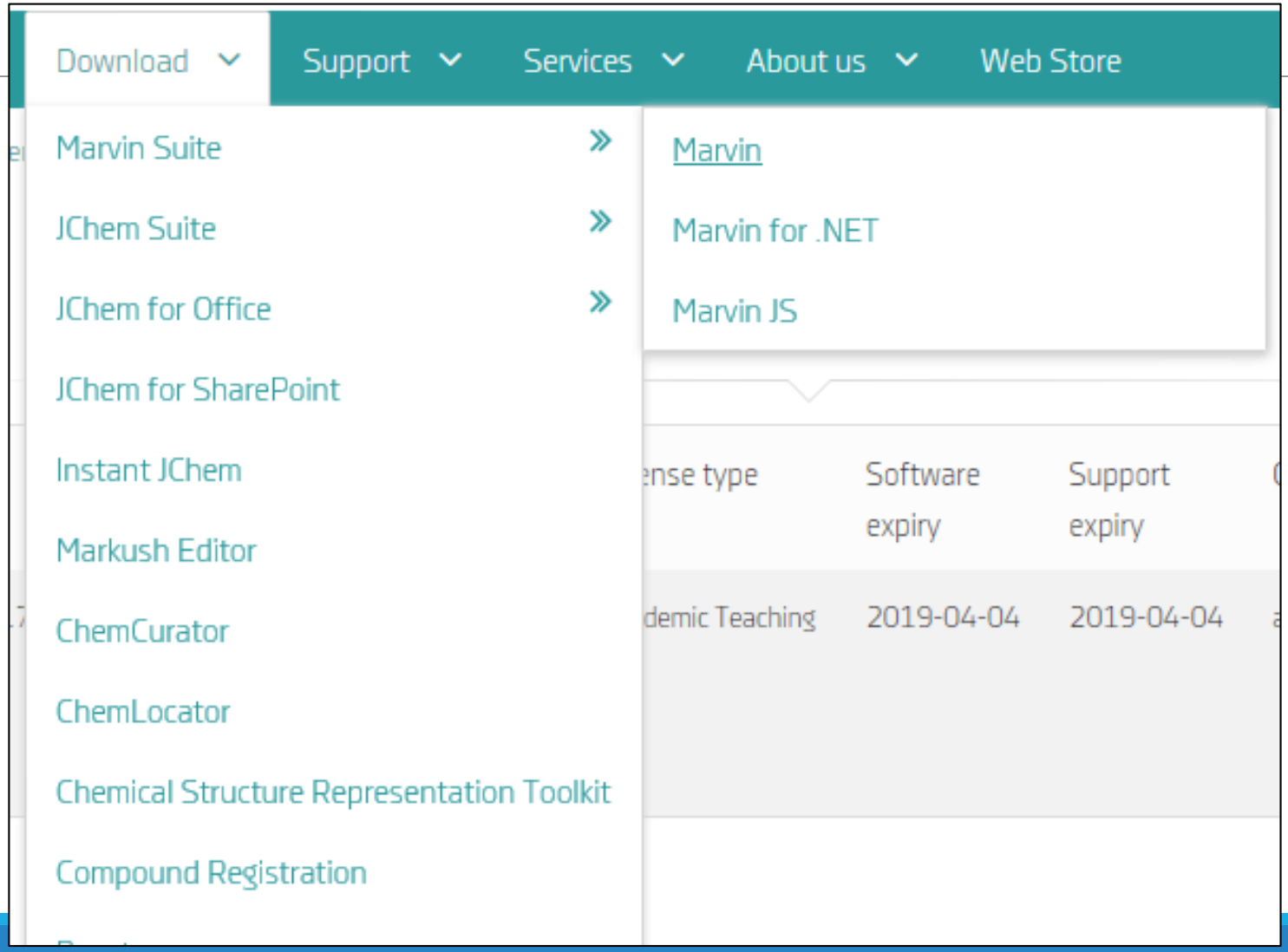
Ohjelmien lataaminen



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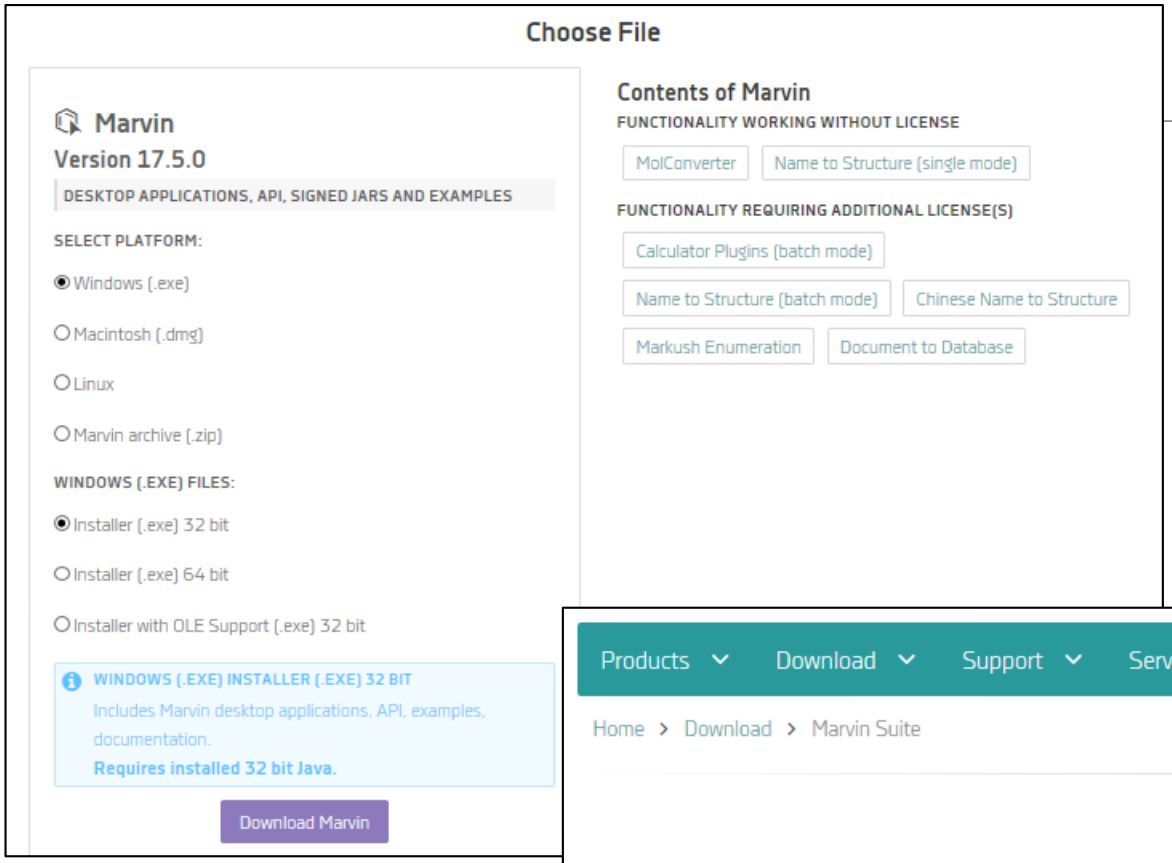
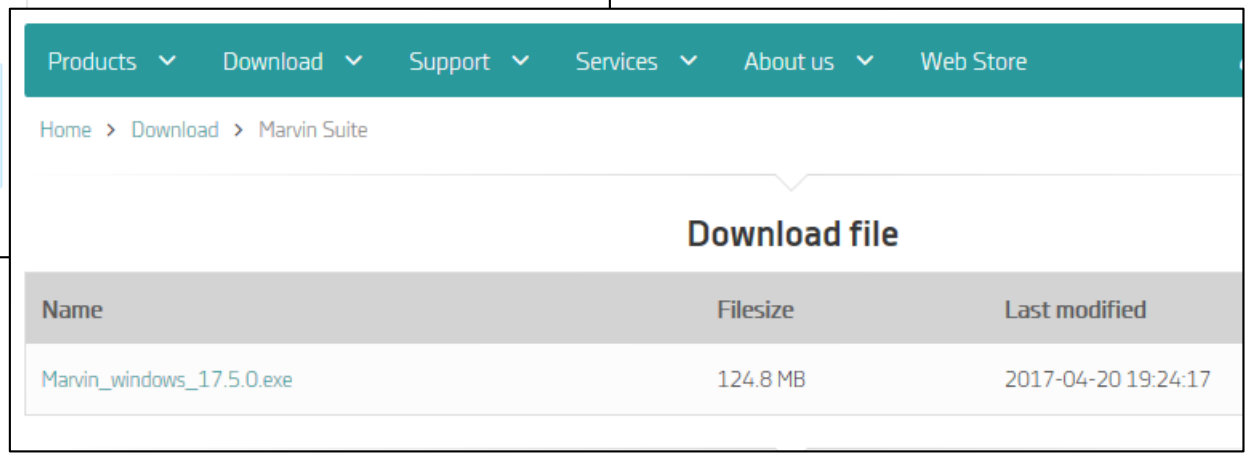
Lataaminen (jatkuu)





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Ohjeet yms.

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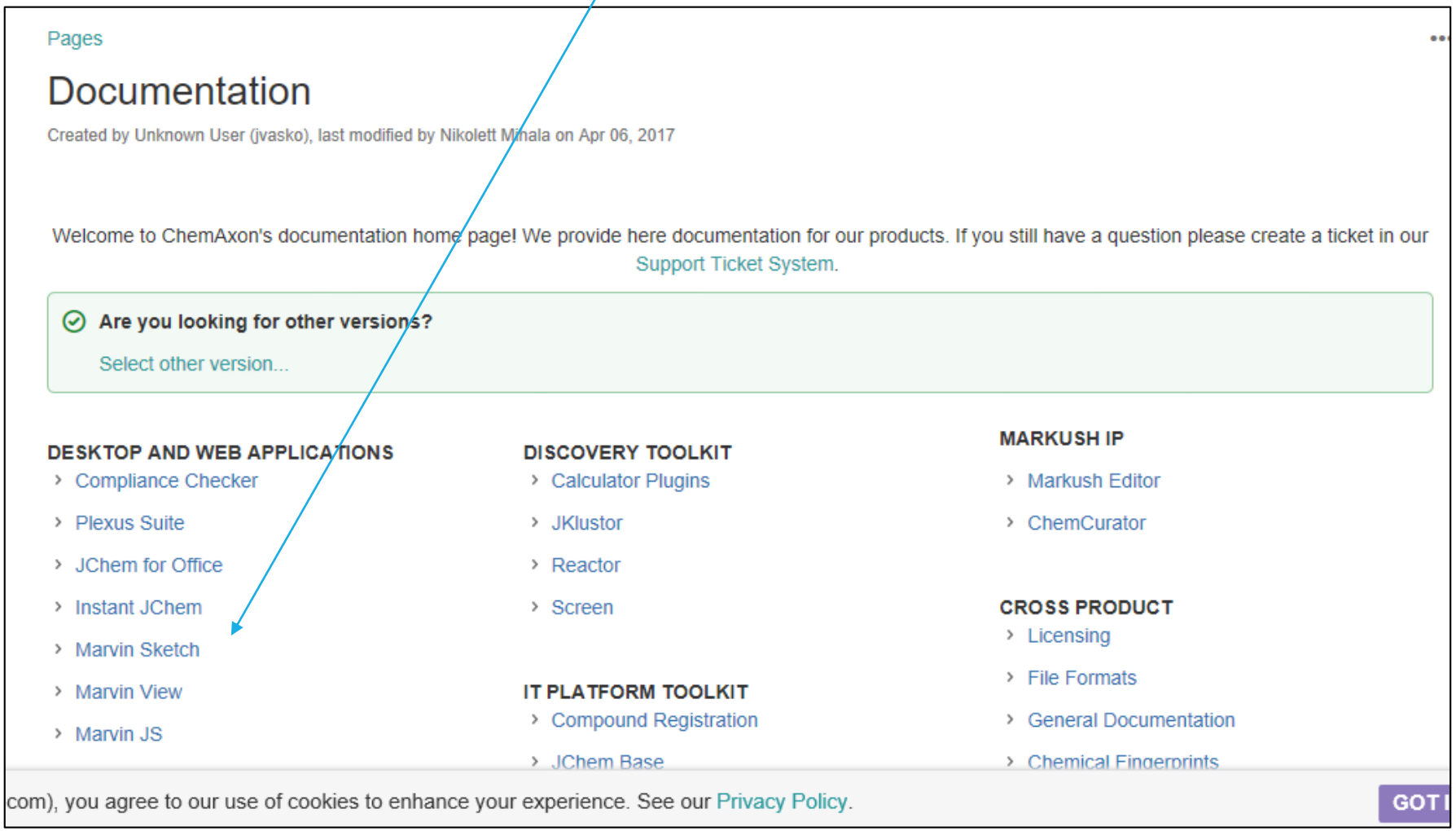
MarvinSketch –ohjeet 1



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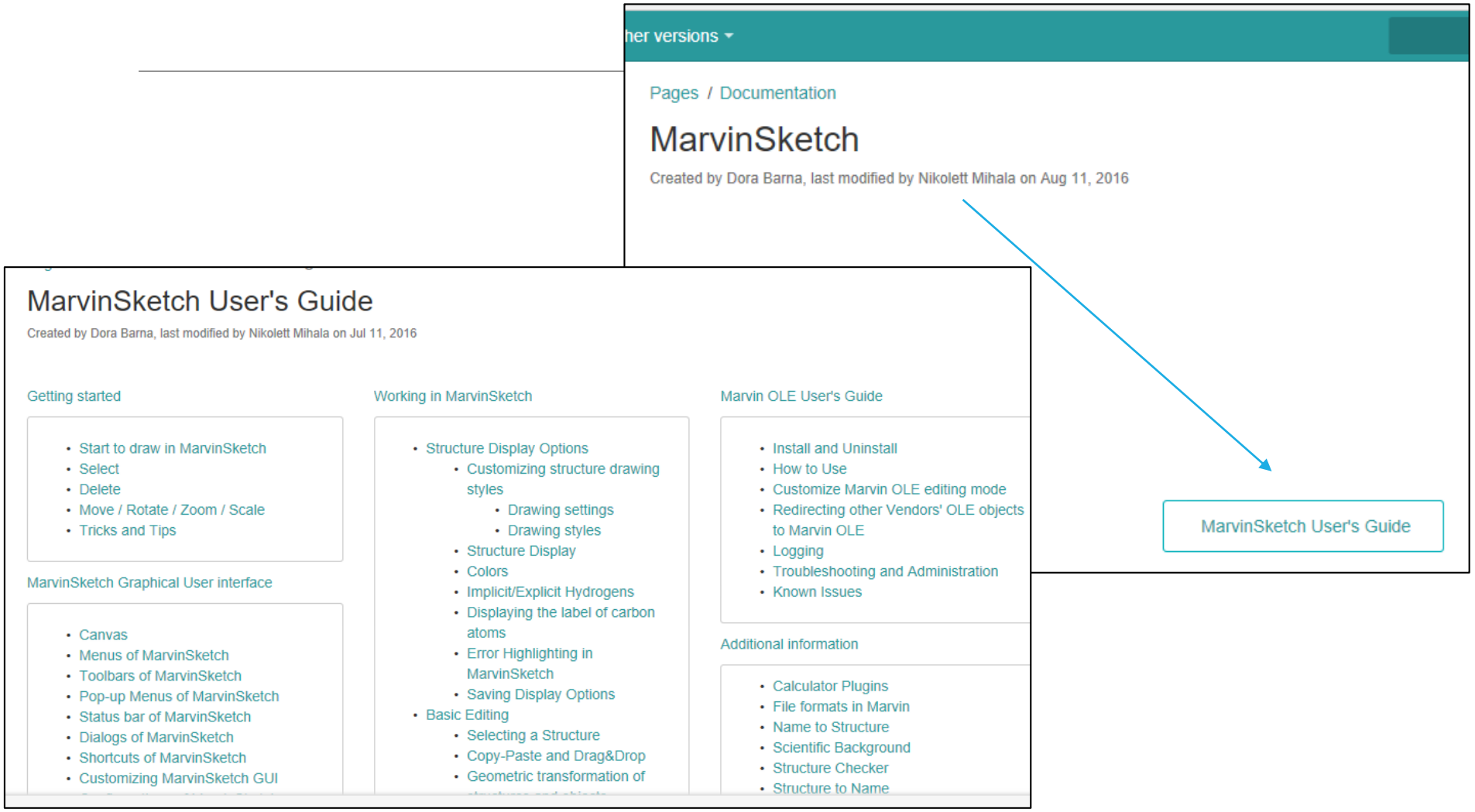
MarvinSketch –ohjeet 2



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Käyttöönotto

VAATII JAVAN …

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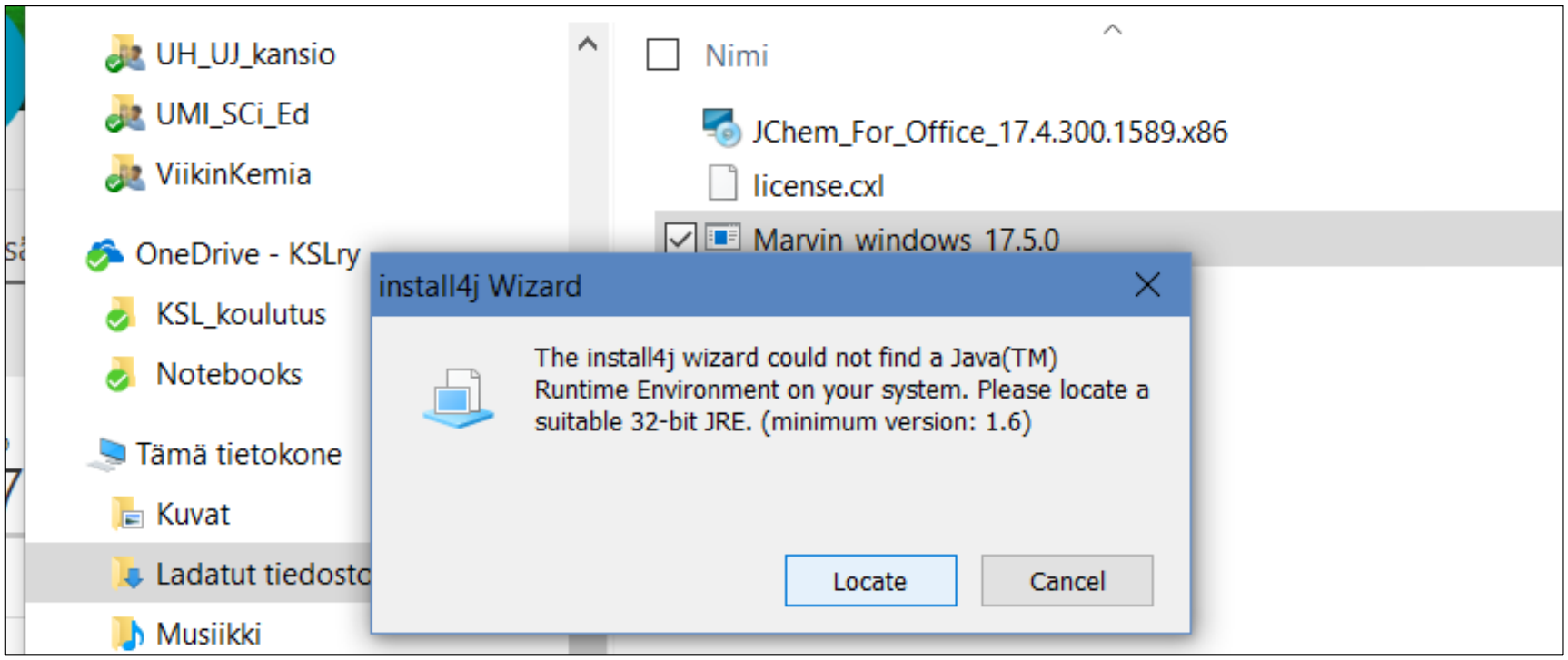
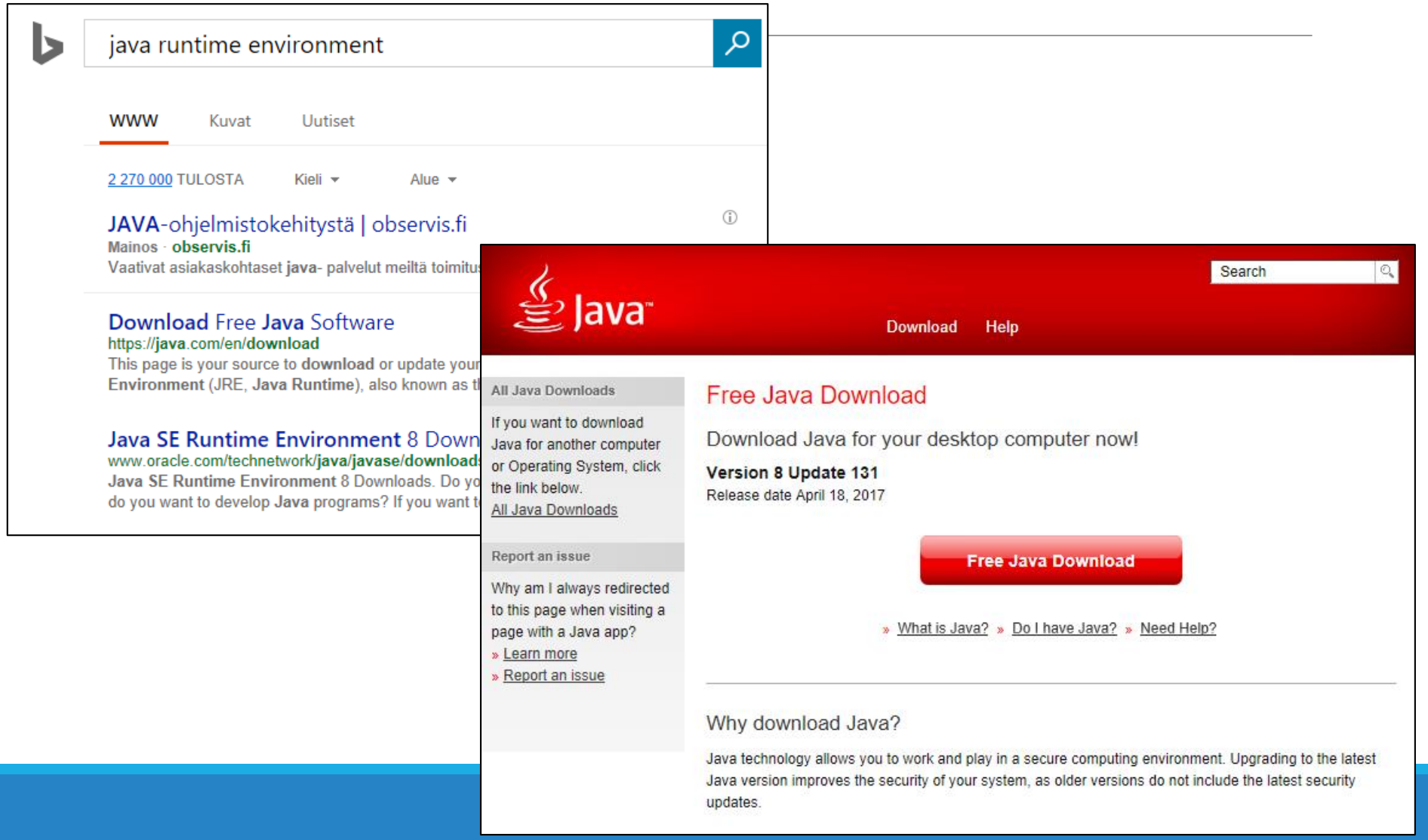
Asennuksen yhteydessä tarkistetaan Javan olemassaolo

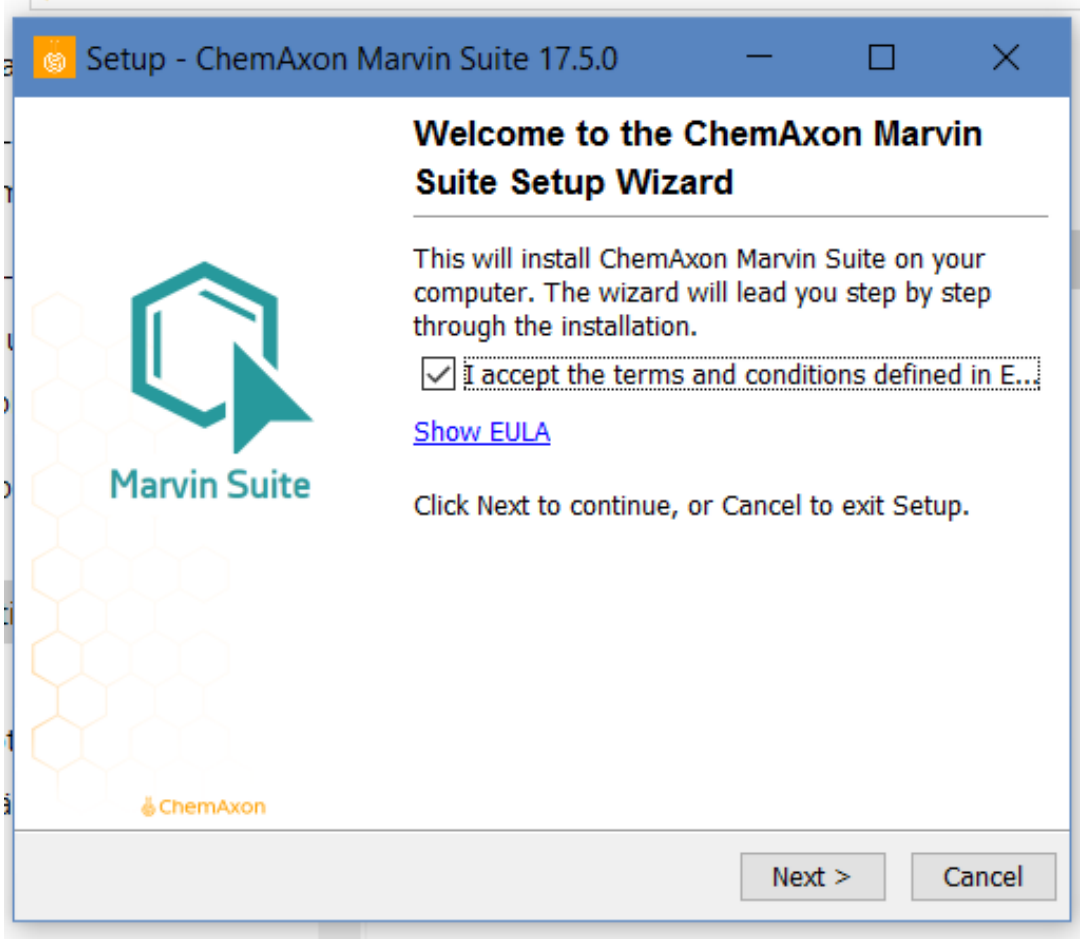


Javan asennus
(asennus vaatii admin –oikeudet)

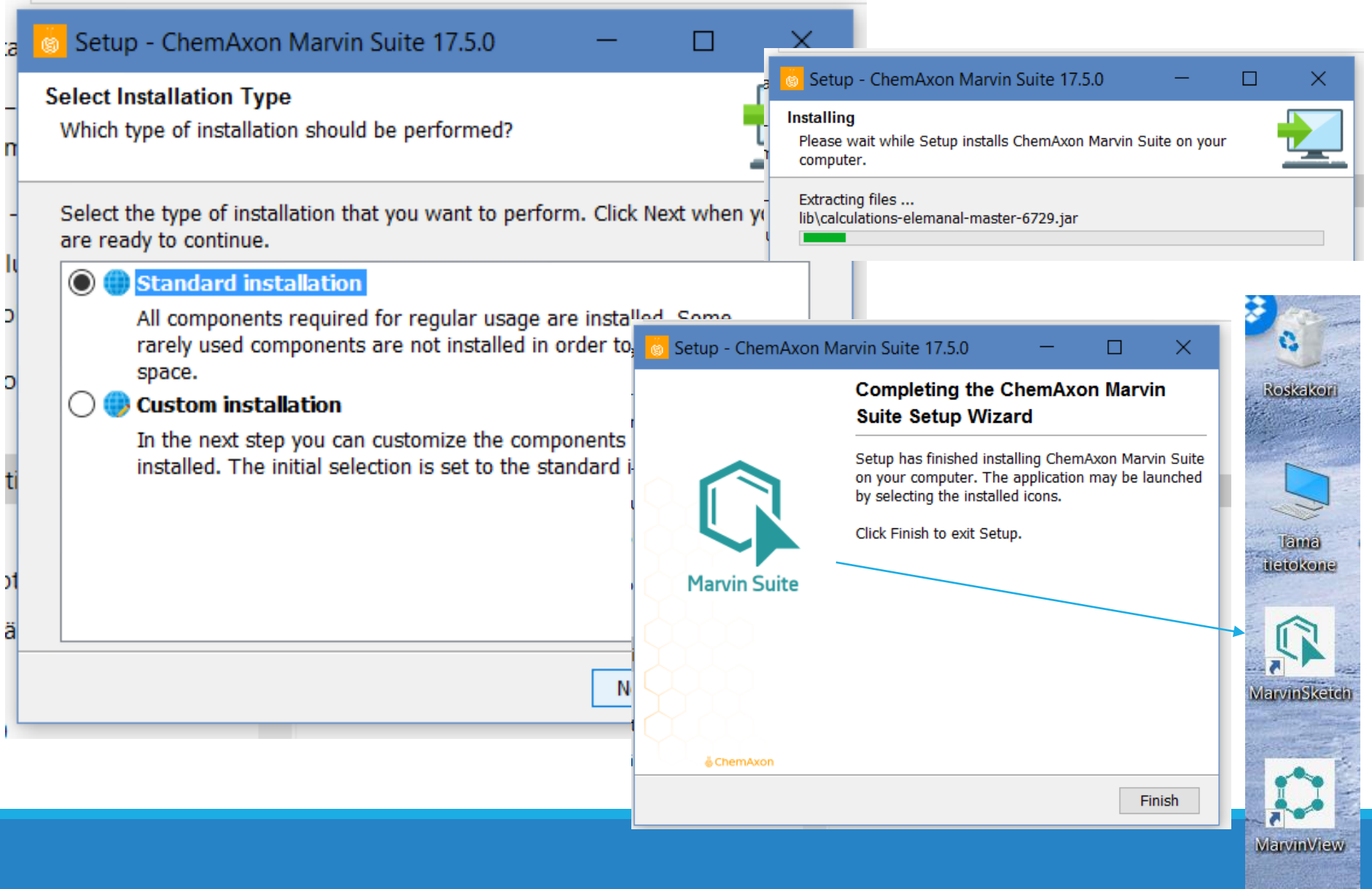


Marvin Suite -asennus

Kun Java-asennus on hoidettu, käynnistetään (Ladatut kansiosta) Marvin –ohjelman asennus



Marvin Suite –asennus 2



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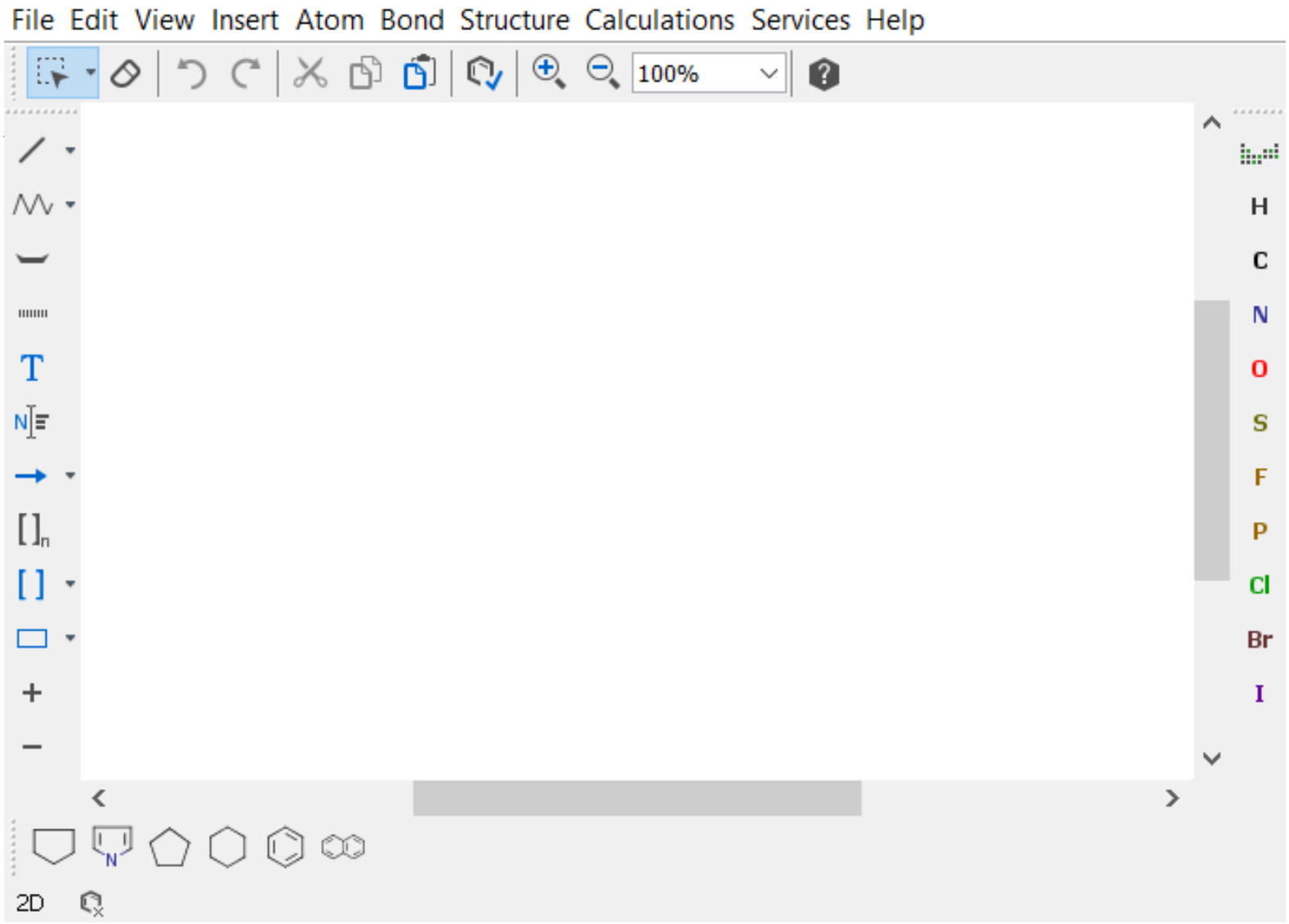

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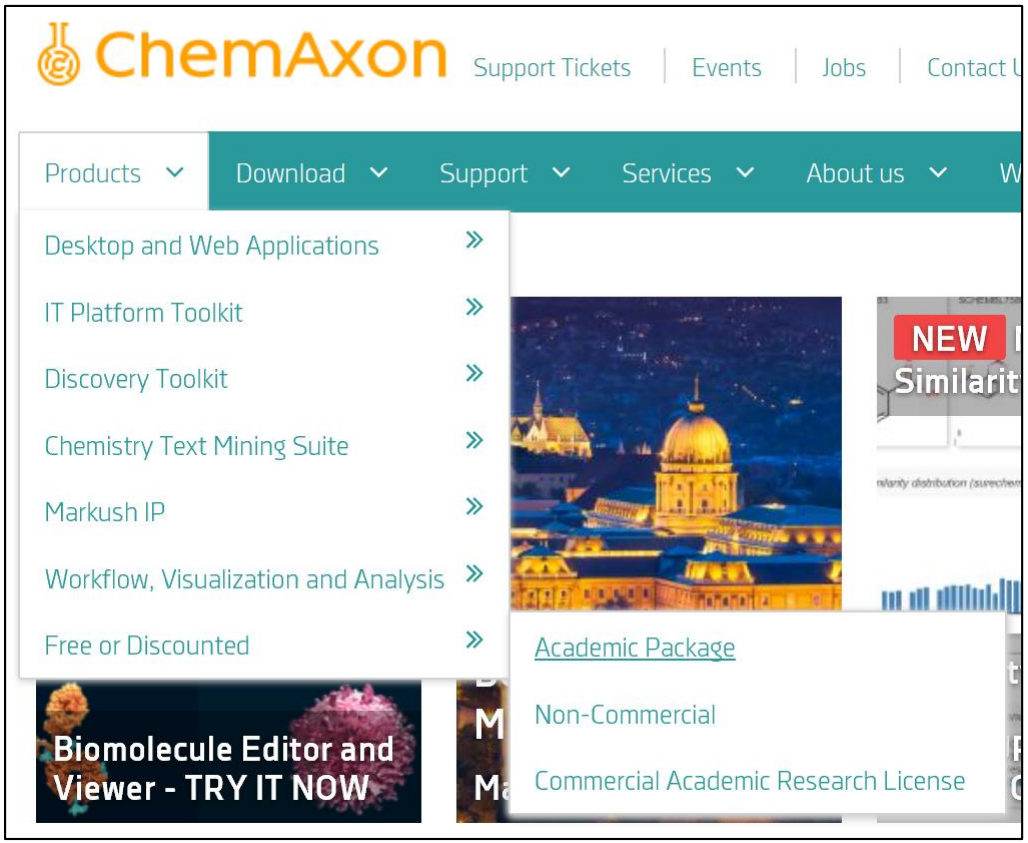
Lisenssiä haetaan erikseen ja kun sen on myönnetty, siitä tulee sähköpostiviesti.

Lisenssin myönnön jälkeen ko. tiedoston voi ladata sivustolta ja jakaa oppilaille.



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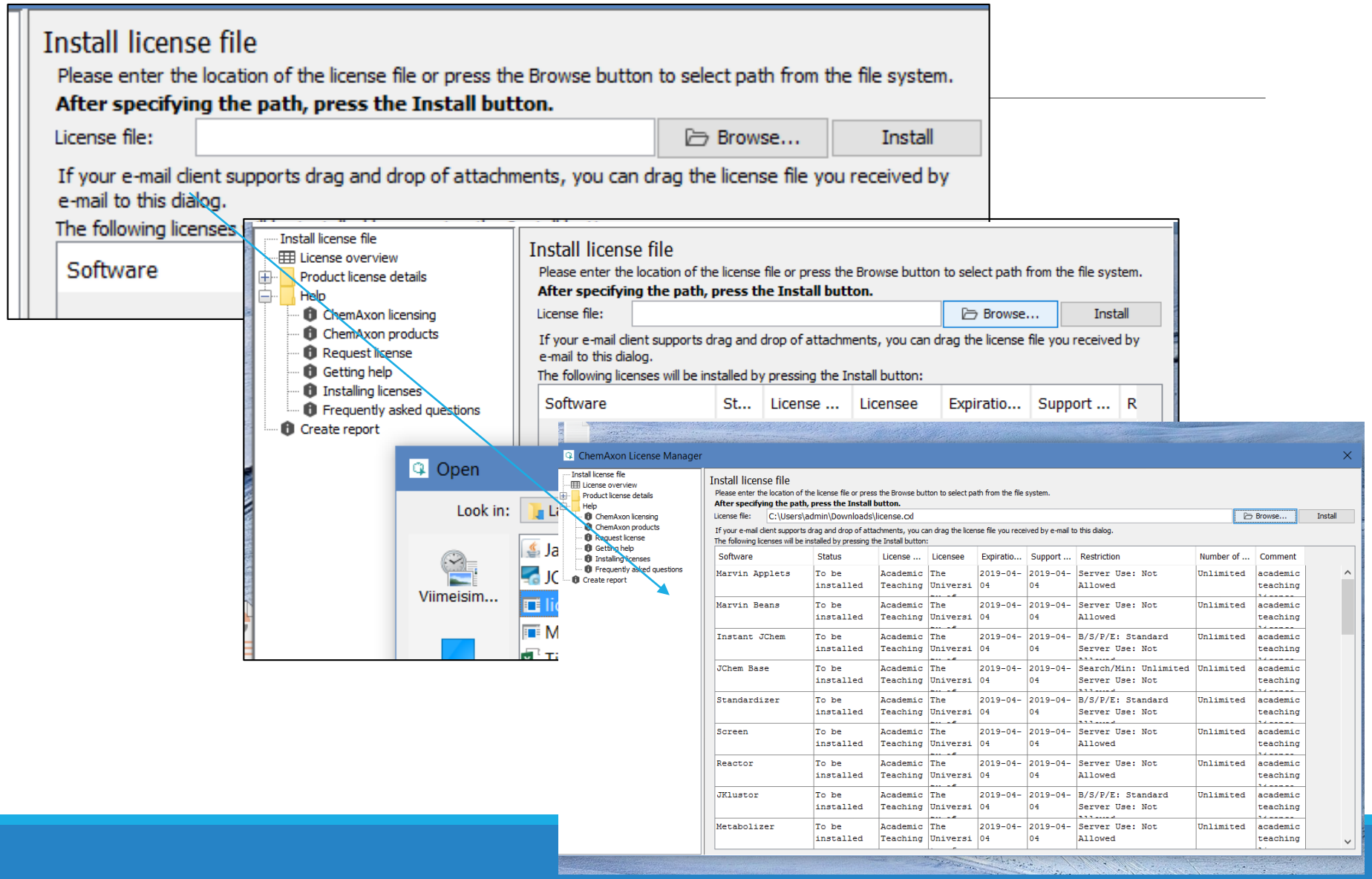
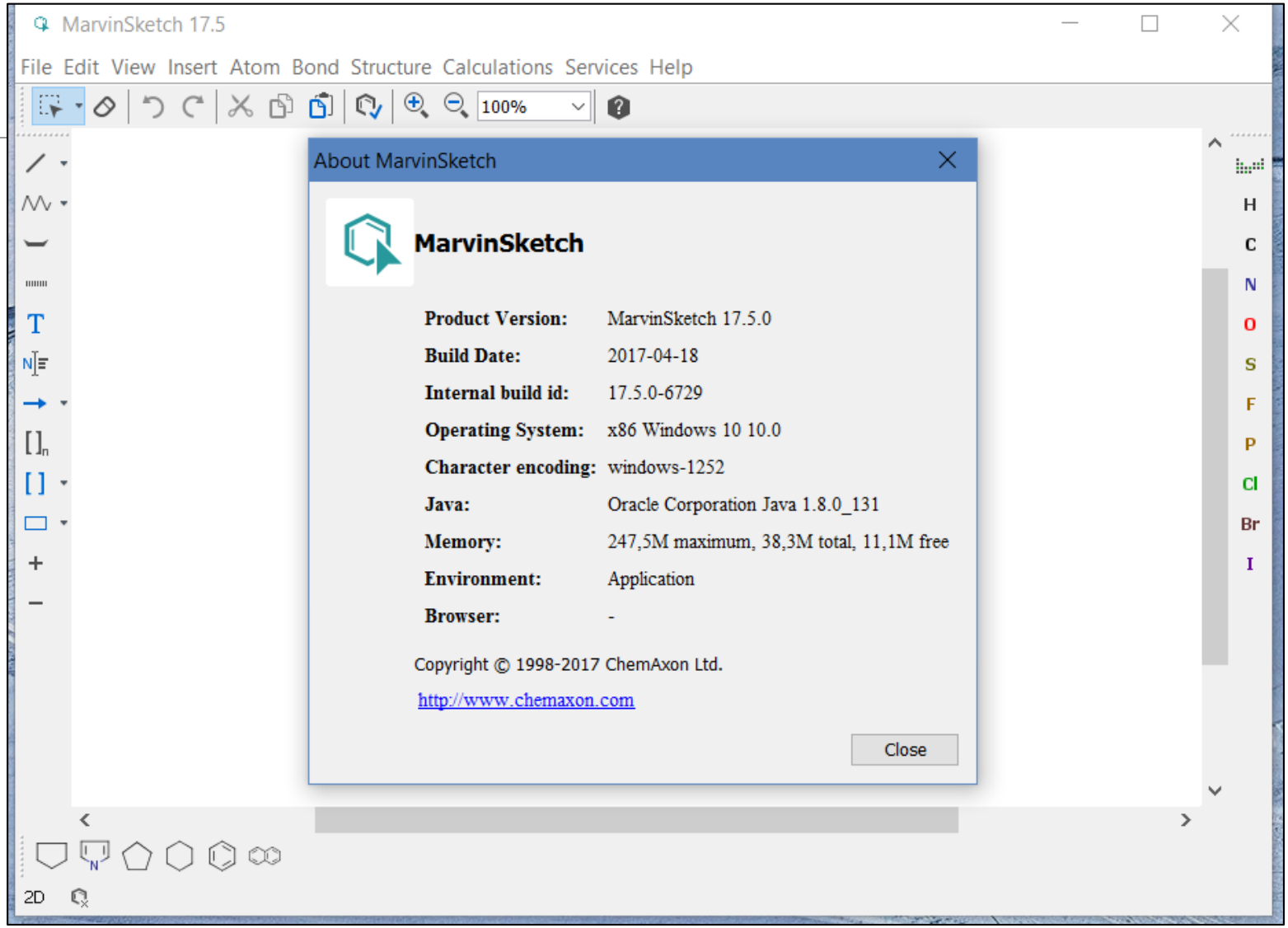


Asennus valmis



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MarvinSketch – ohjelman käyttö

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Mihin MarvinSketch ”taipuu”

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

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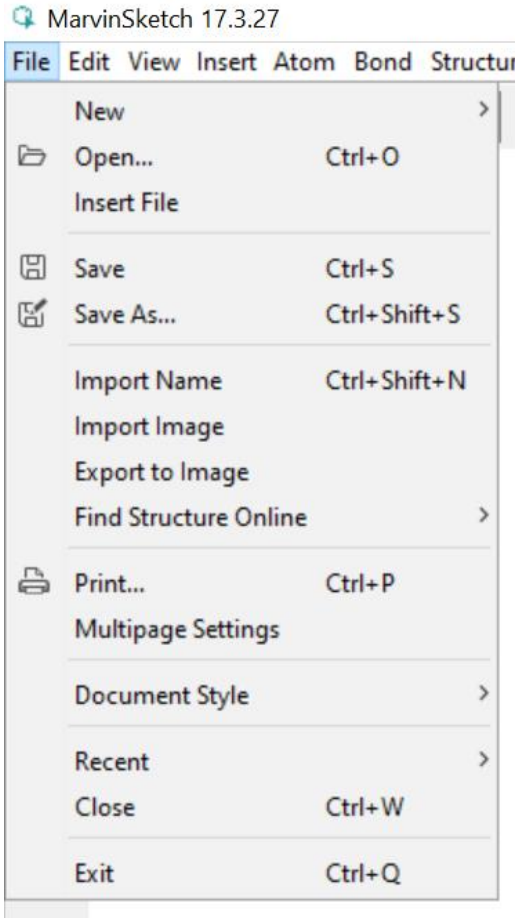
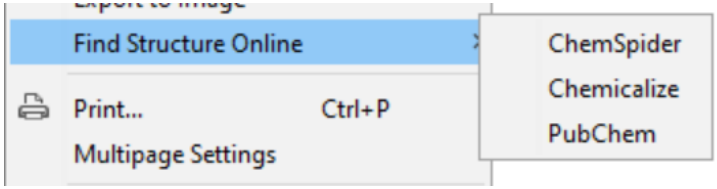
Valikot - **File**



ChemSpider – laaja datapankki, oma rakennekaavaeditori, ym.

Chemicalize - hyödyntää Marvin JS:ää, datapankki (kts. seuraava sivu)

PubChem -



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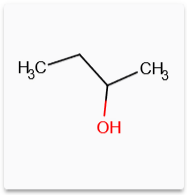
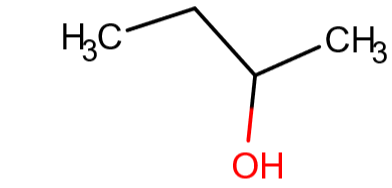


Calculation is free for this molecule, because it contains at most 12 heavy atoms.



Basic properties

Input	2-butanol
Molar mass	74.123 g/mol
Exact mass	74.073164942 Da
Formula	$C_4H_{10}O$
Composition	C (64.82%), H (13.6%), O (21.58%)
Lipinski's rule of five	✓

IDEA:
Empiirisen kaavan tehtävien tekemiseen!!

Structural properties

Atom count	15	Hydrogen bond donor count	1
Heavy atom count	5	Hydrogen bond acceptor count	1
Asymmetric atom count	1	Formal charge	0
Rotatable bond count	1	FSP3	1.00
Ring count	0	Topological polar surface area	20.23 $Å^2$
Aromatic ring count	0	Molar refractivity	21.95 cm^3/mol

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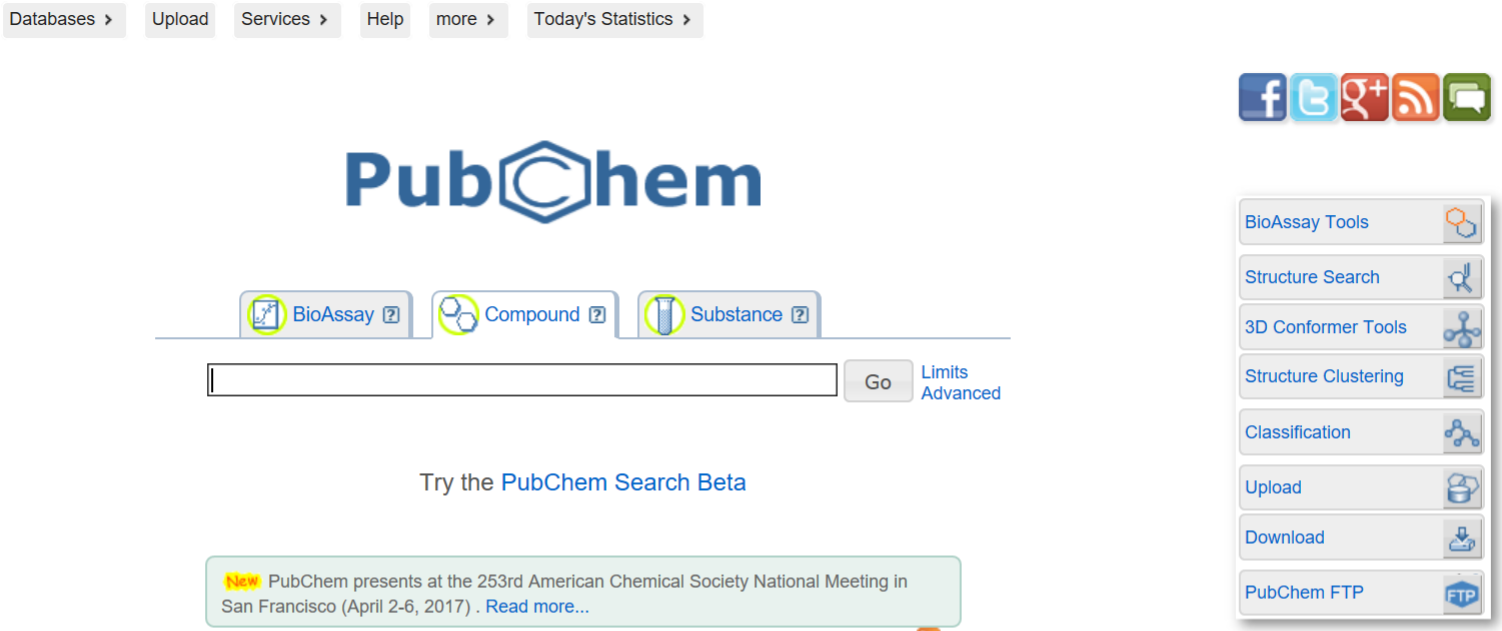
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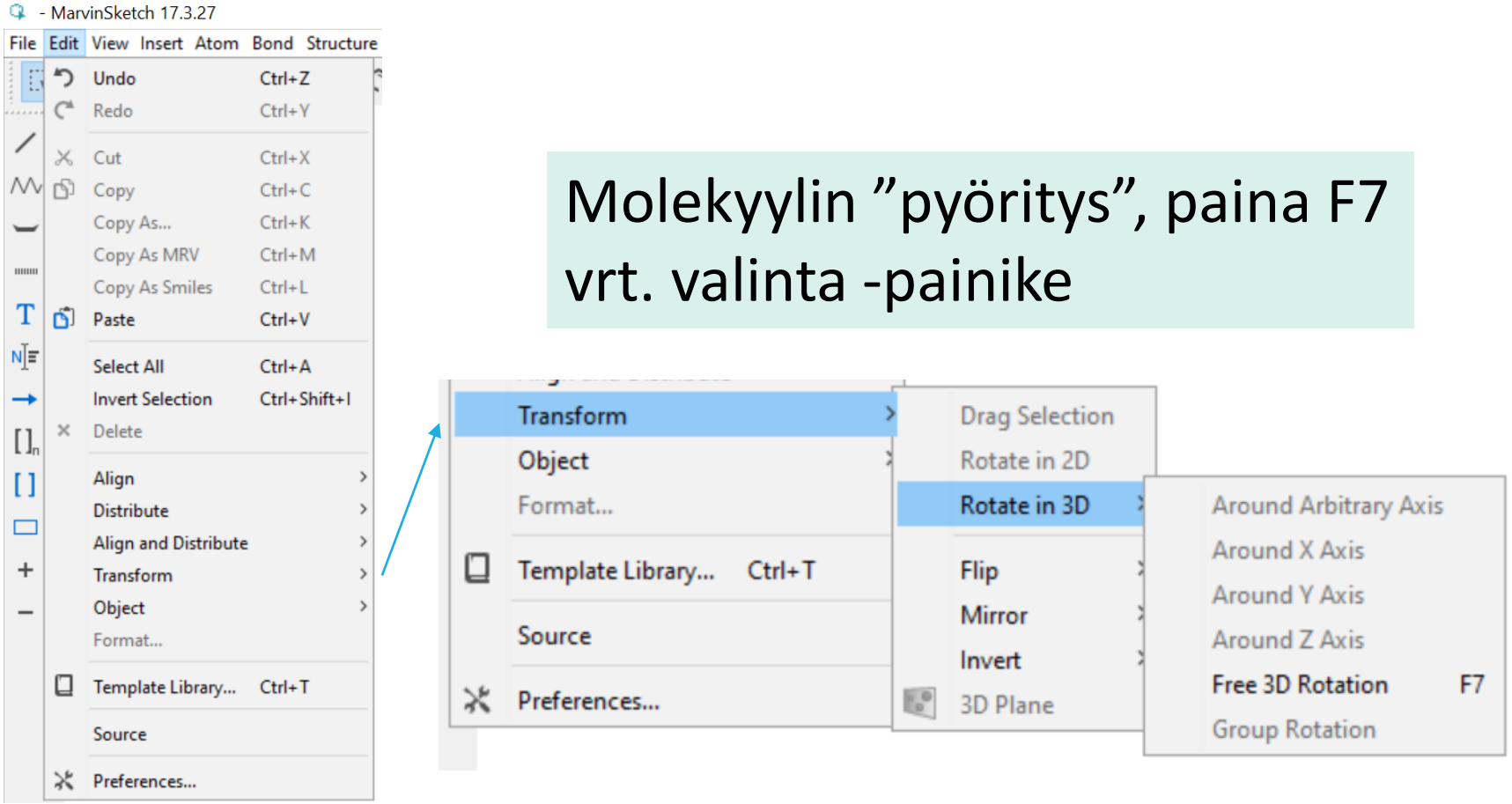
Valikot - **Edit**



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

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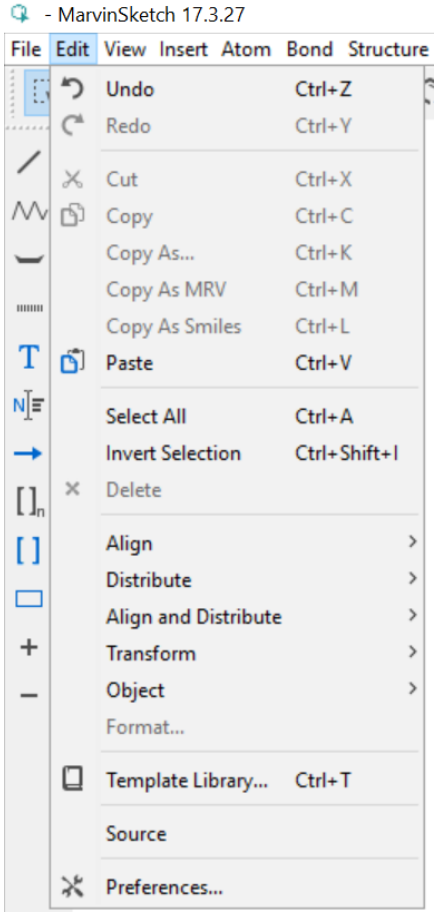
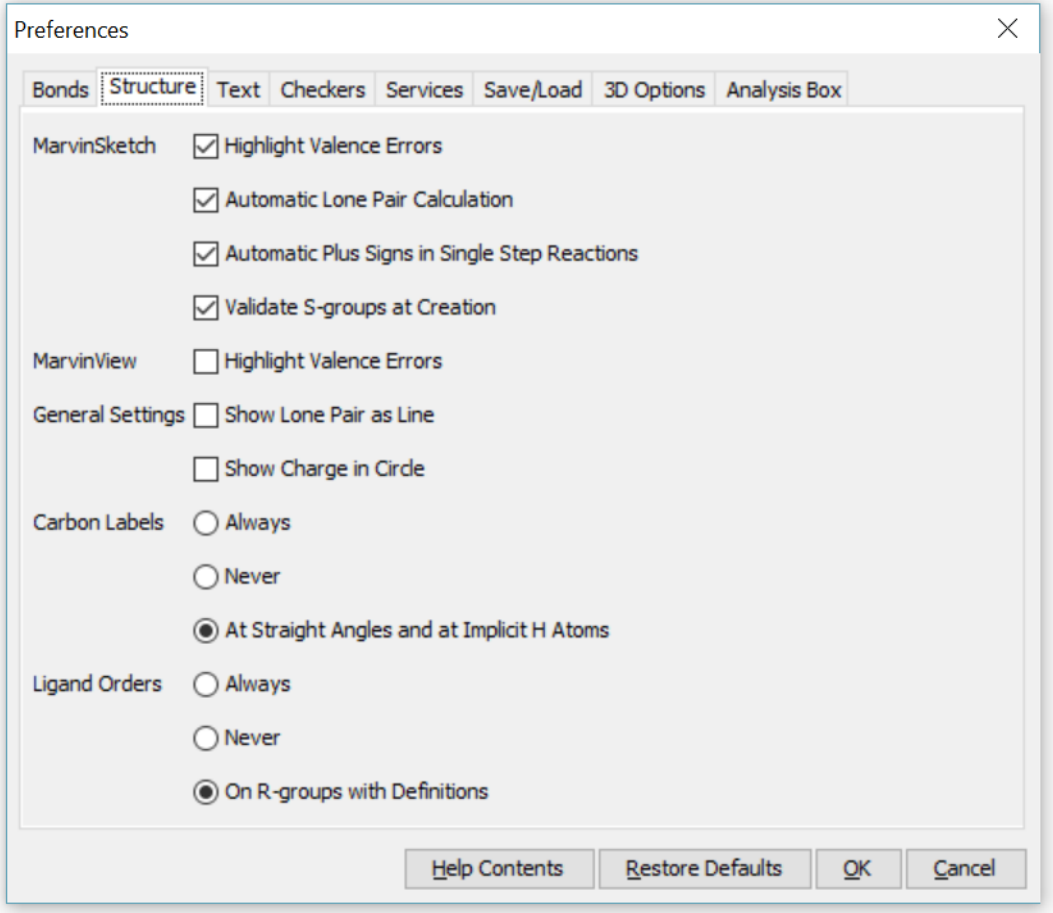
Valikot – Edit – **Preferences…**





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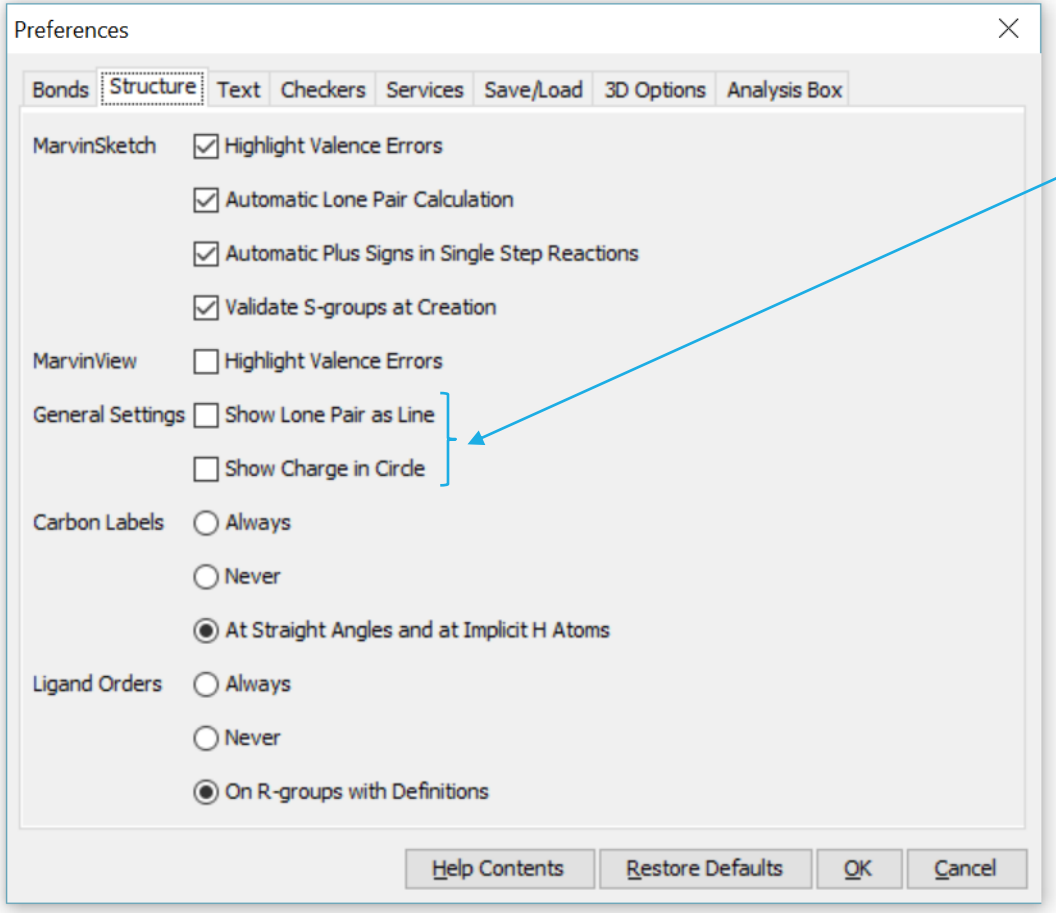
Vapaat elektroniparit näkyviin



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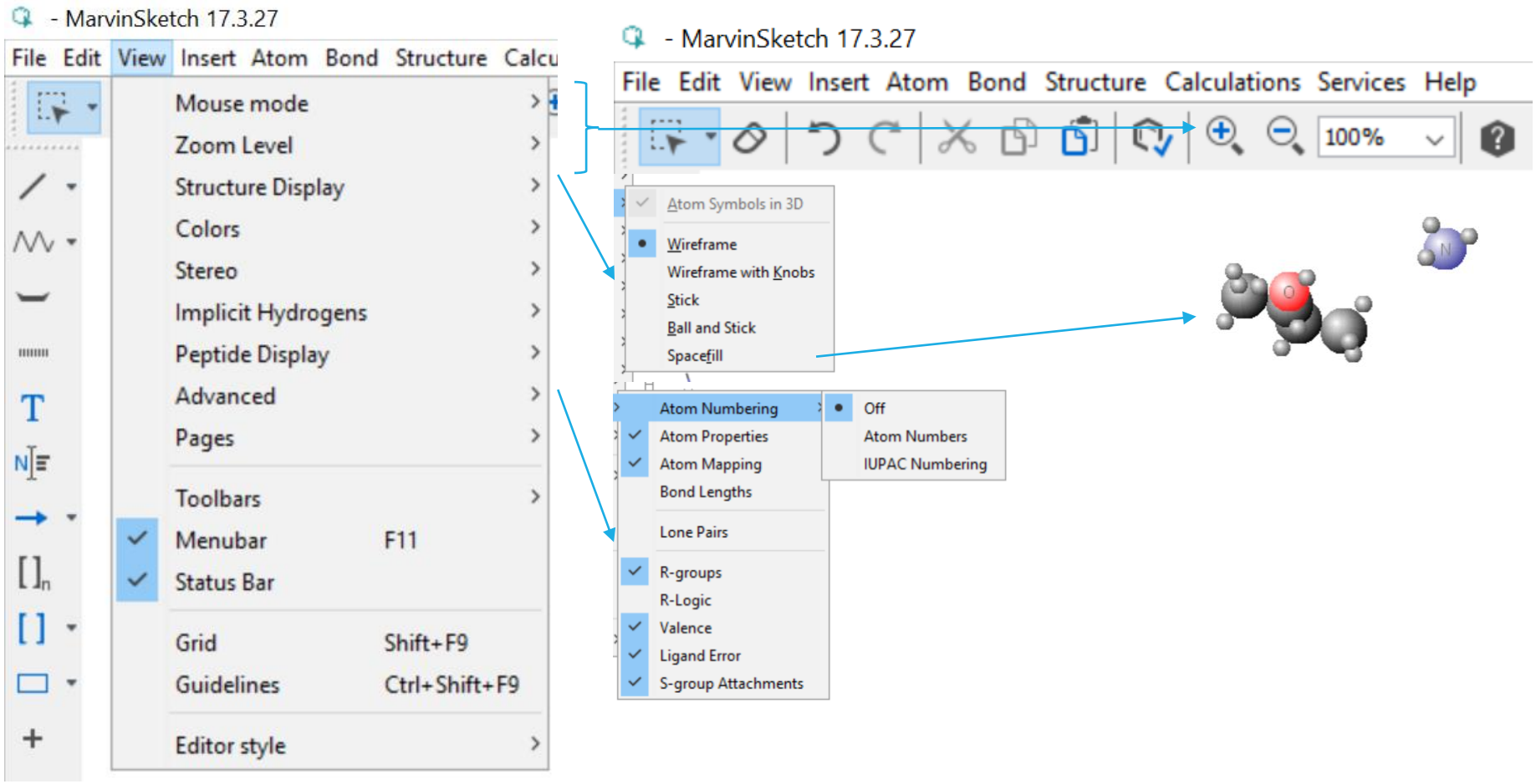
Valikot - **View**



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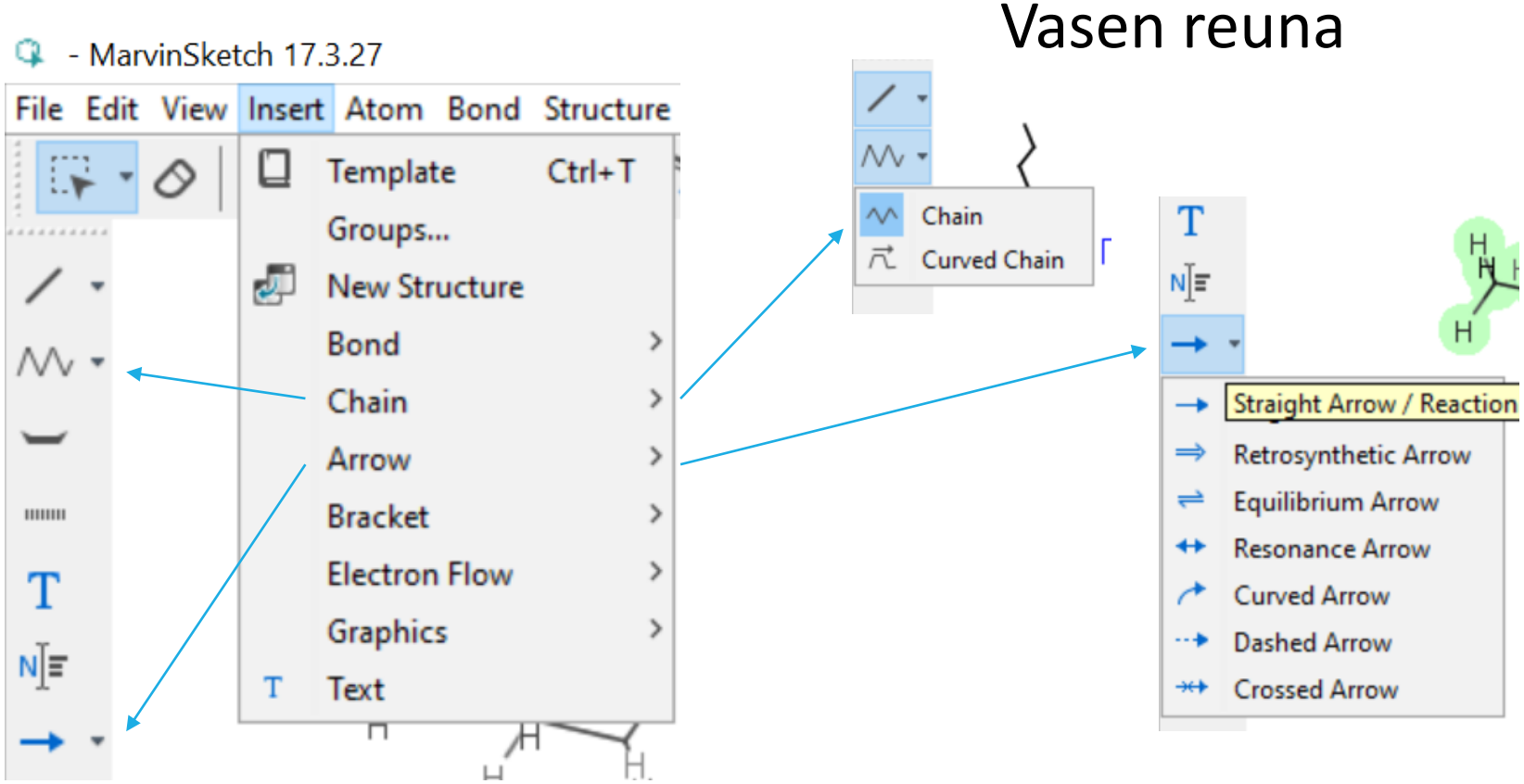
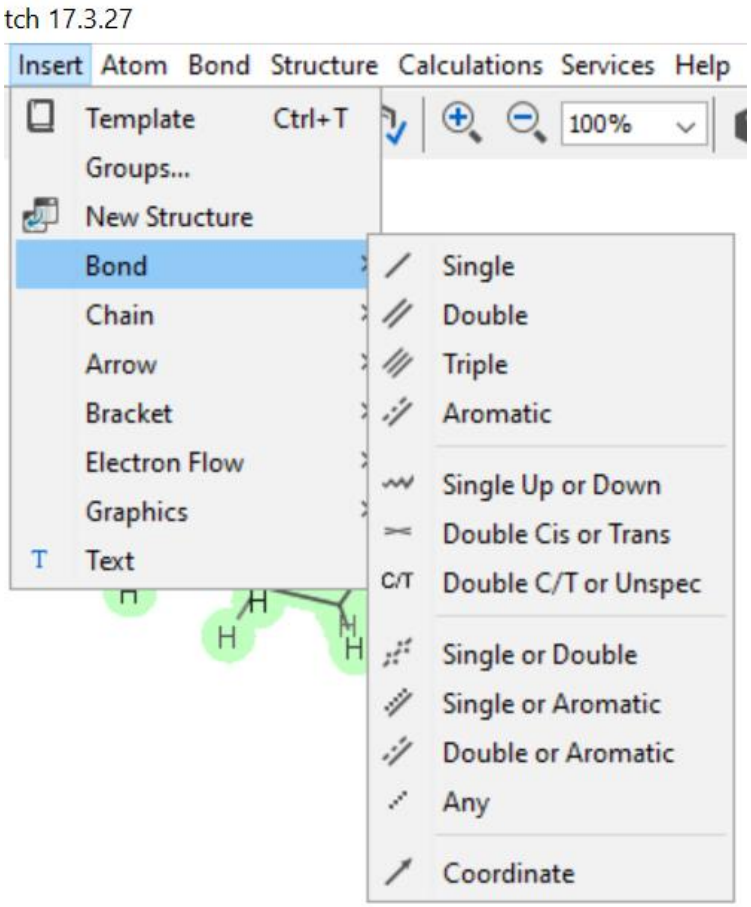
Valikot - **Insert**

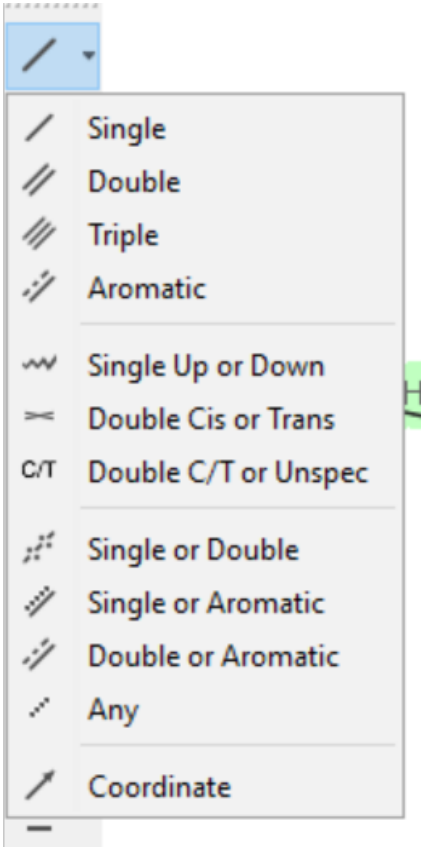


Vasen reuna

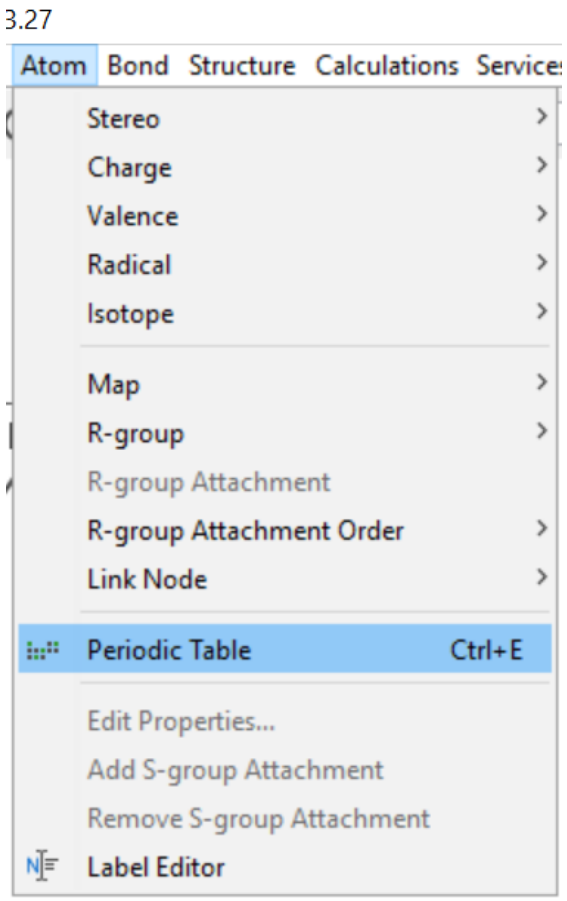
Bond - Pikavalikosta



Vasen reuna



Valikot - **Atom**



Oikea reuna

Valitse alkuaine

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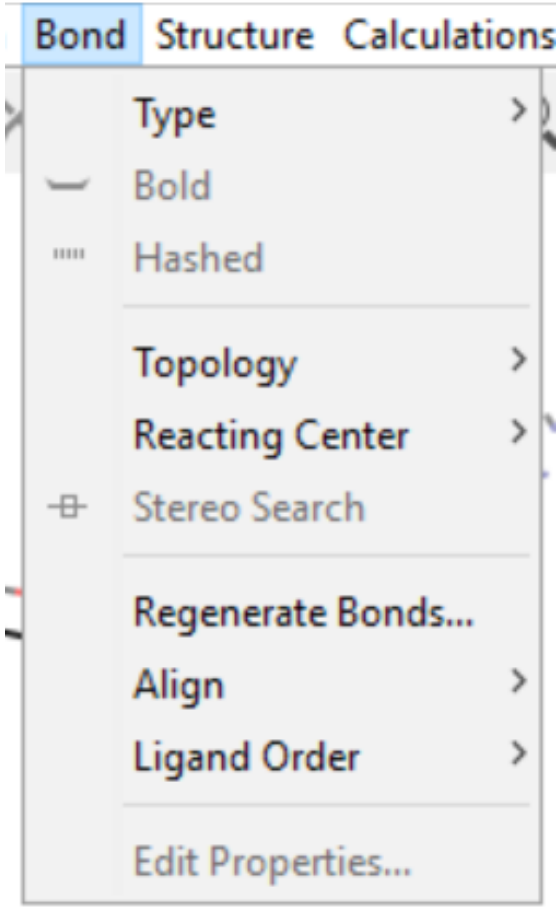
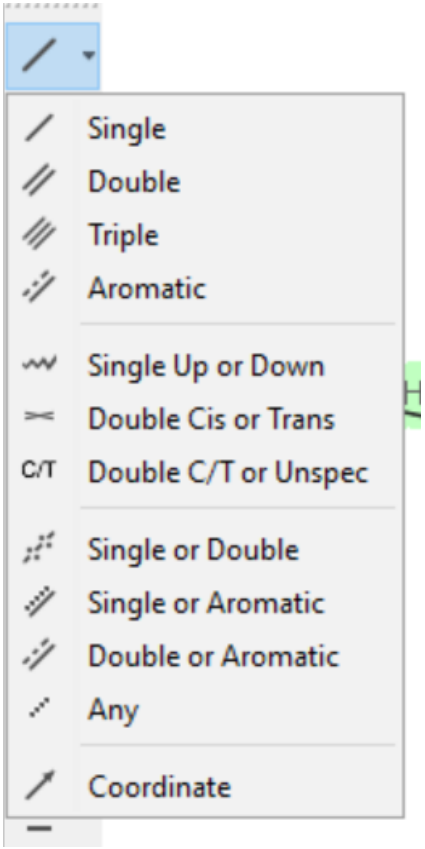
Valikot - **Bond**



Vasen reuna



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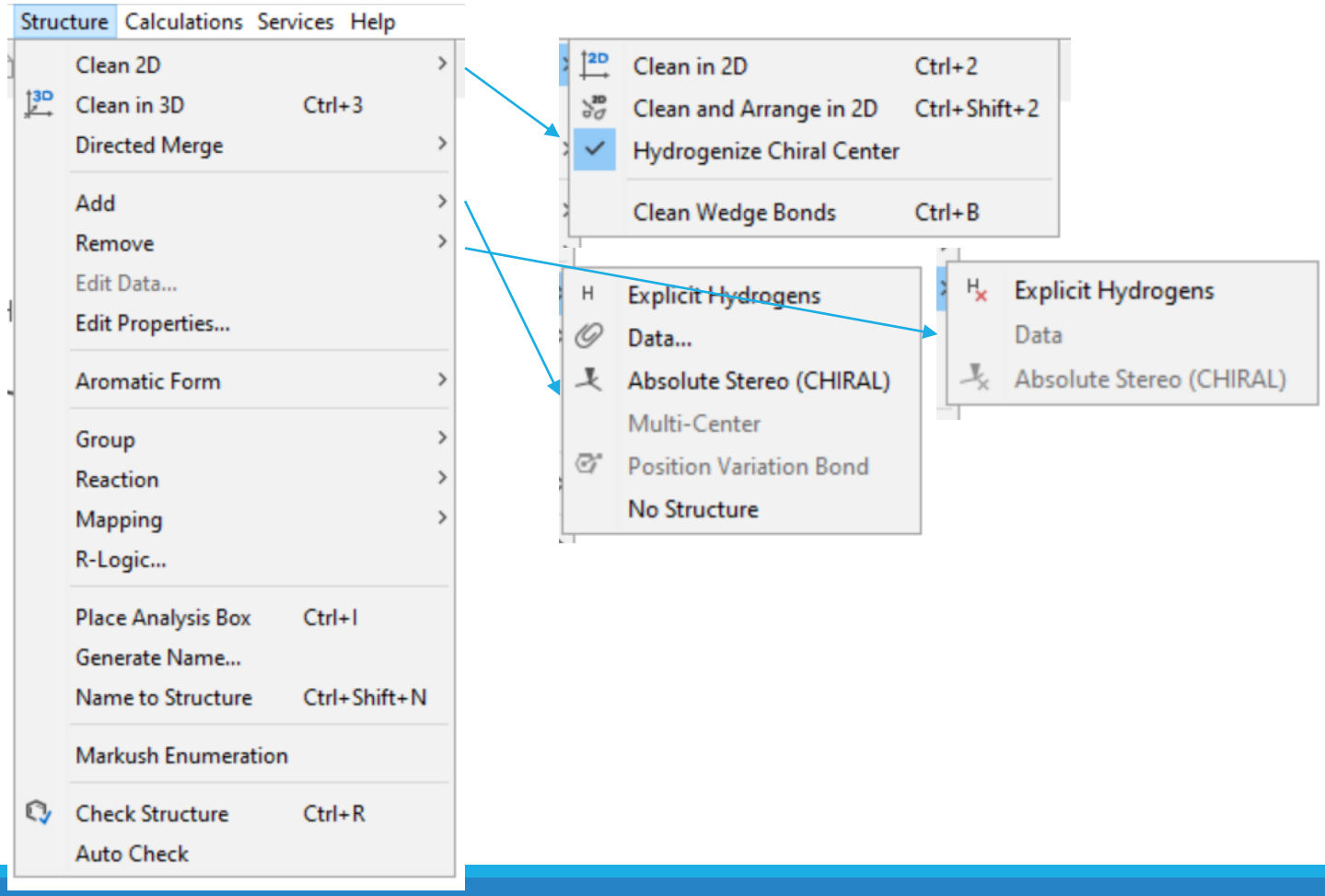
Valikot – **Structure**



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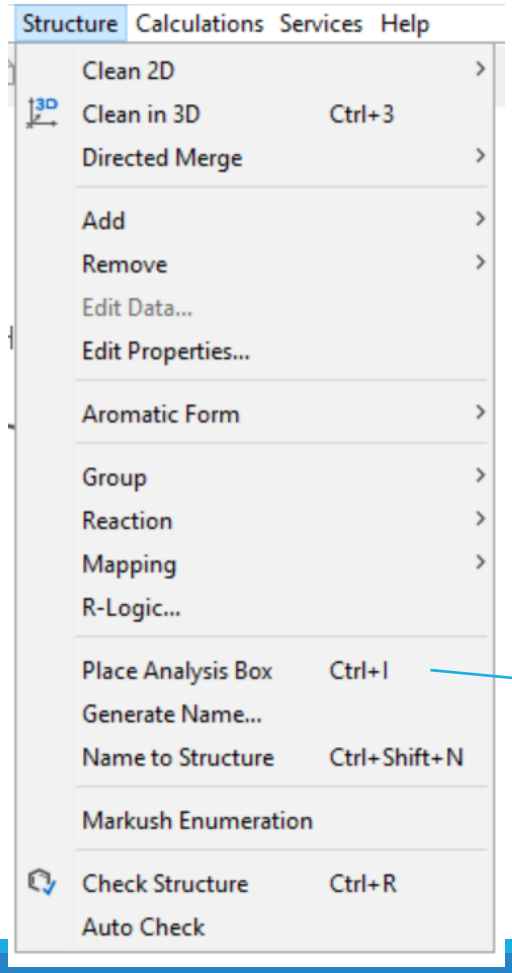
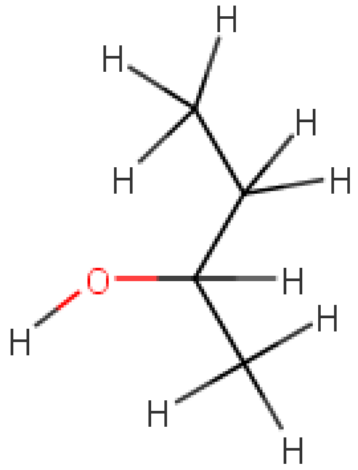
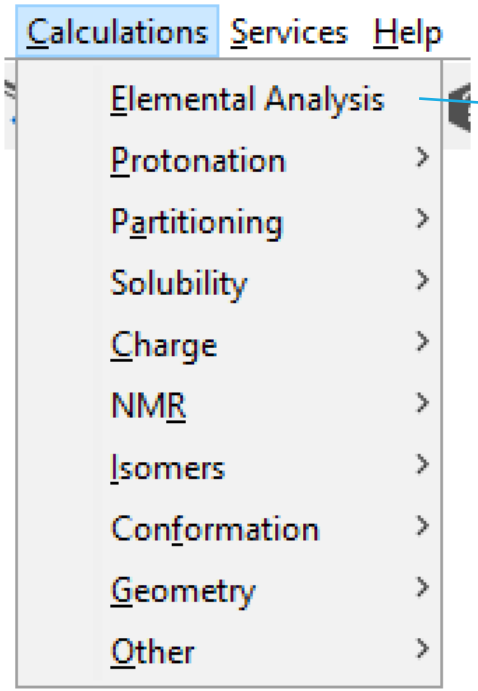
Valikot – **Structure**

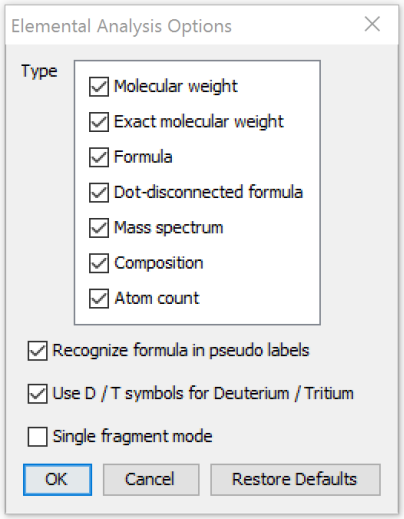


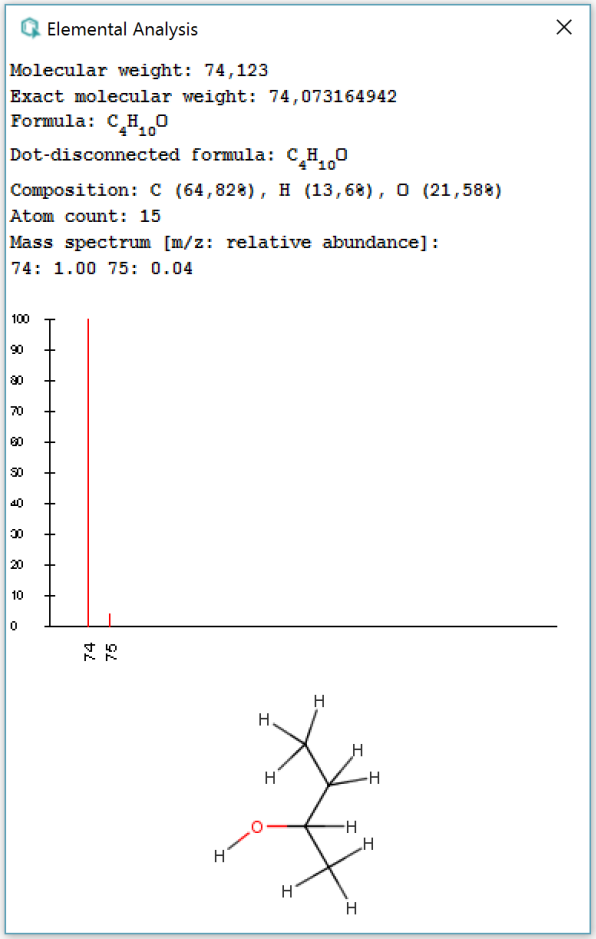


Name: butan-2-ol
Molecular weight: 74,12
Formula: $C_4H_{10}O$

Valikot – Calculations







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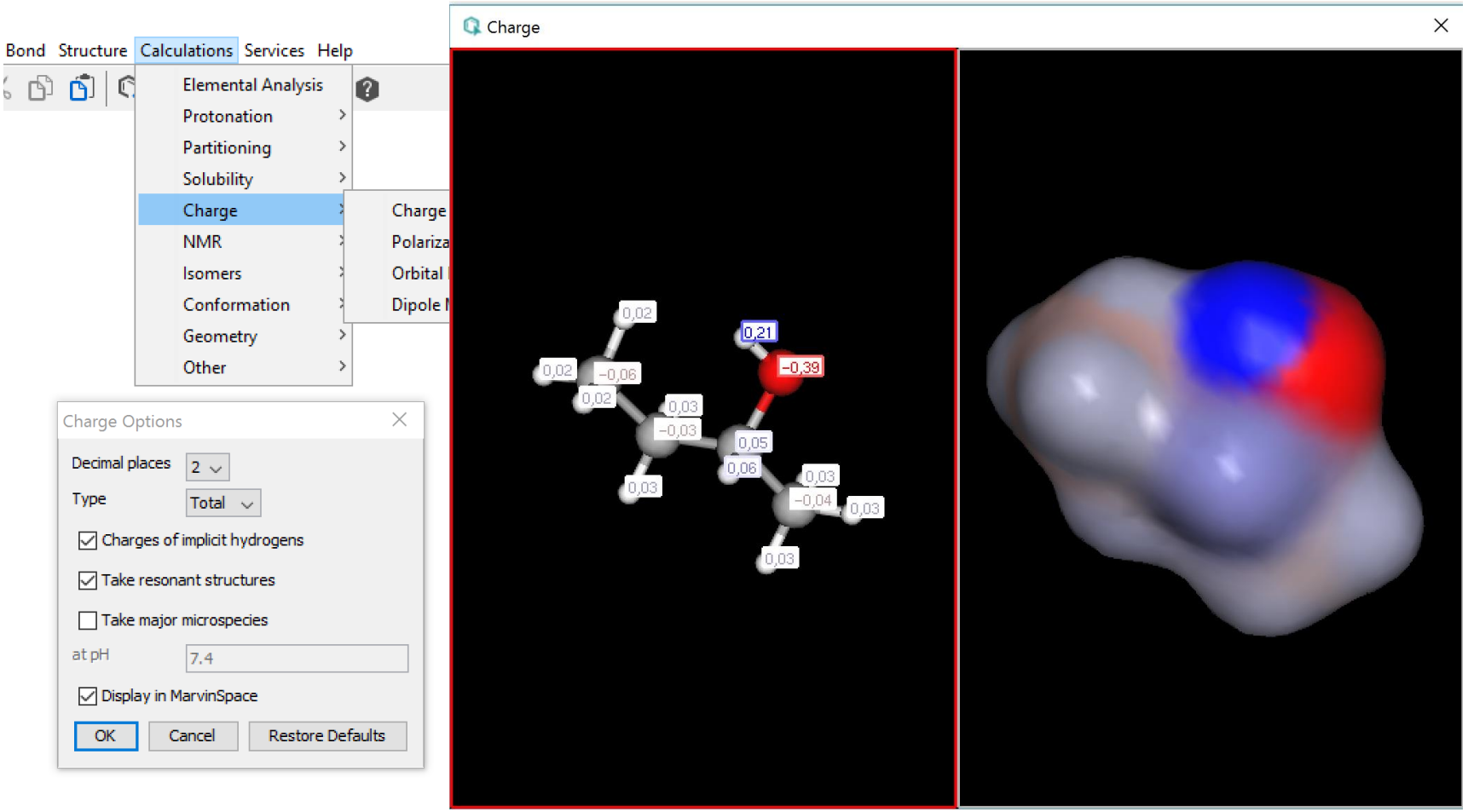
Valikot – Calculations - **Charge**



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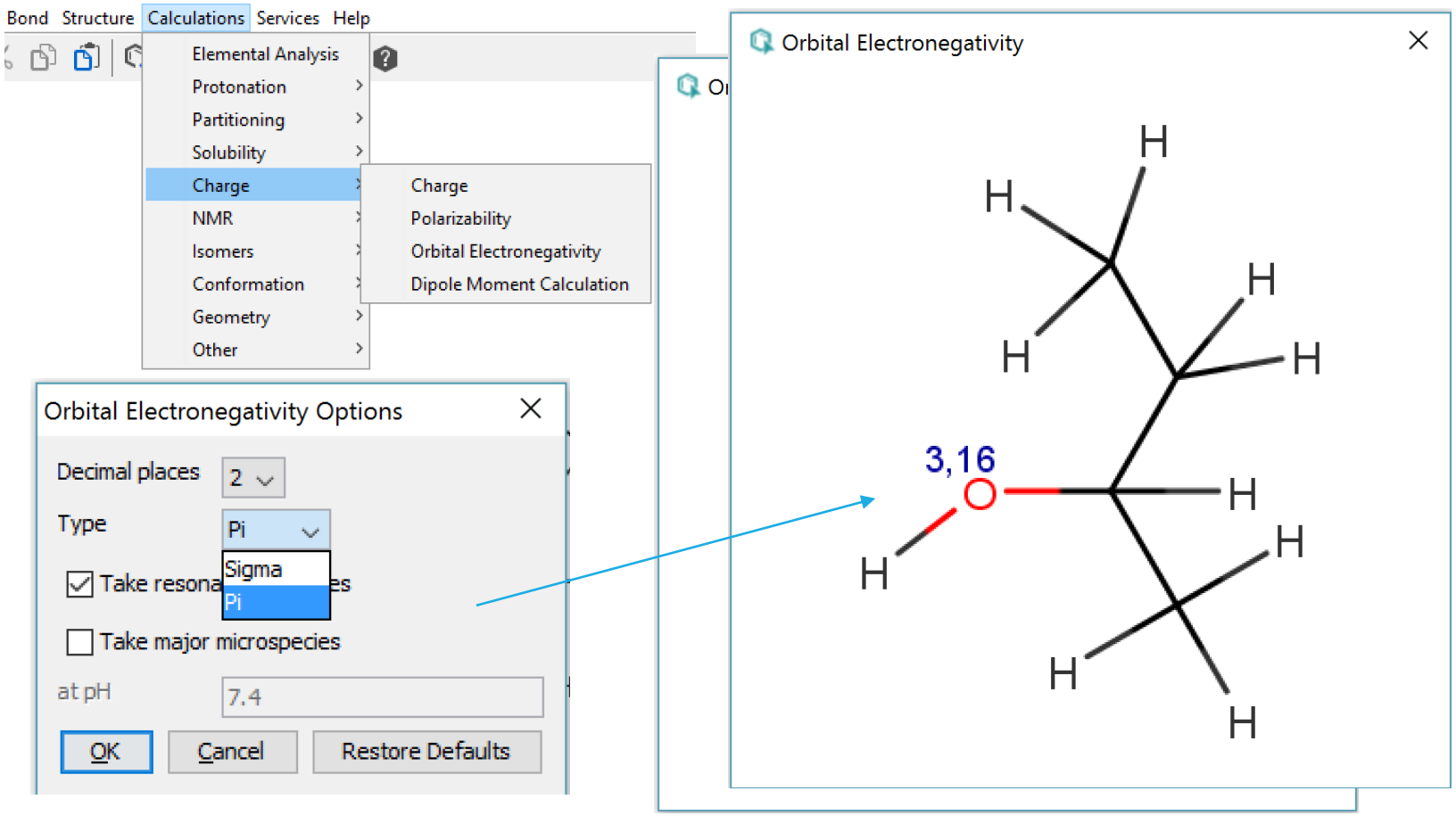
Valikot – Calculations - **Charge**



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Valikot – Calculations - **Charge**