

MarvinSketch

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KEMIAN JA MATEMATIIKAN LEHTORI

HELSINGIN YLIOPISTON VIIKIN NORMAALIKOULU

Sisältö

1. ...

KYSELY:

2. ...

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

3. ...

4. Ohjeet

5. Ohjelman käyttö

MarvinSketch – ohjelman käyttö

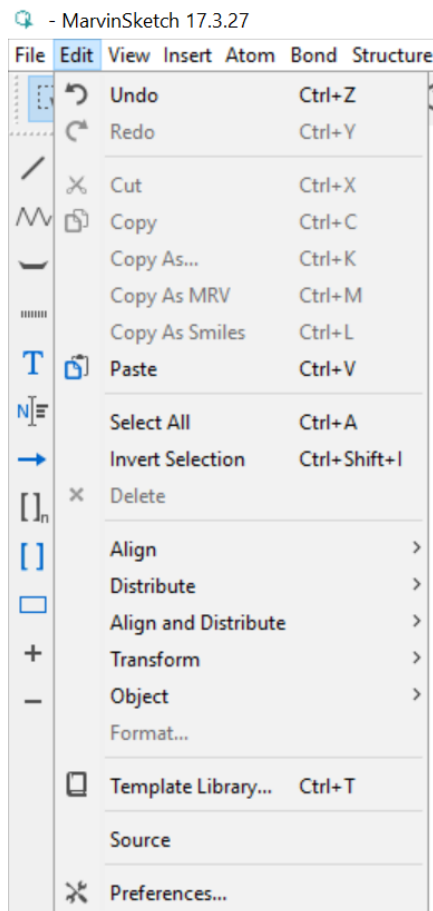
ABITTI-TIKUSSA MARVINSKETCH 17.3.27

LADATTAVISSA 18.3.0 (17.29.0 17-SARJAN VIIMEINEN)

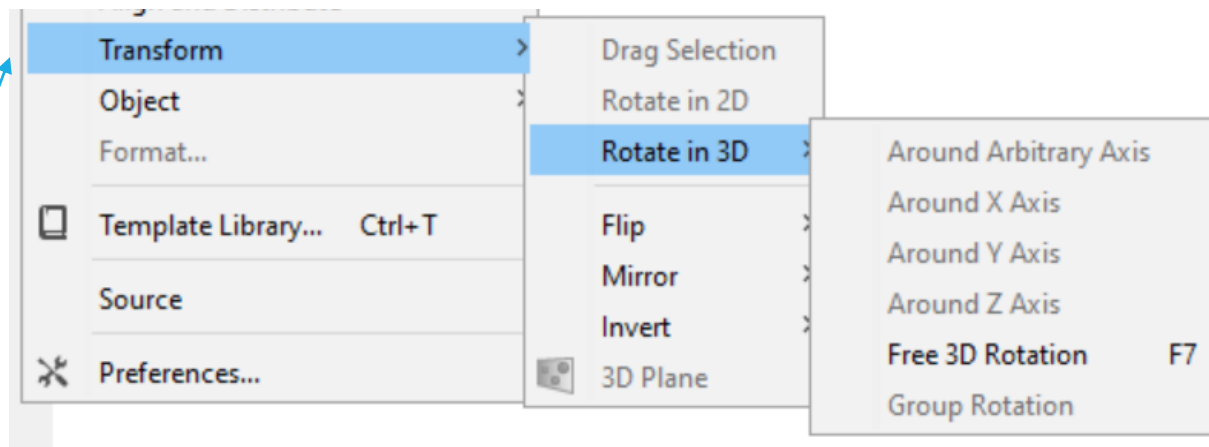
Mihin MarvinSketch ”taipuu”

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

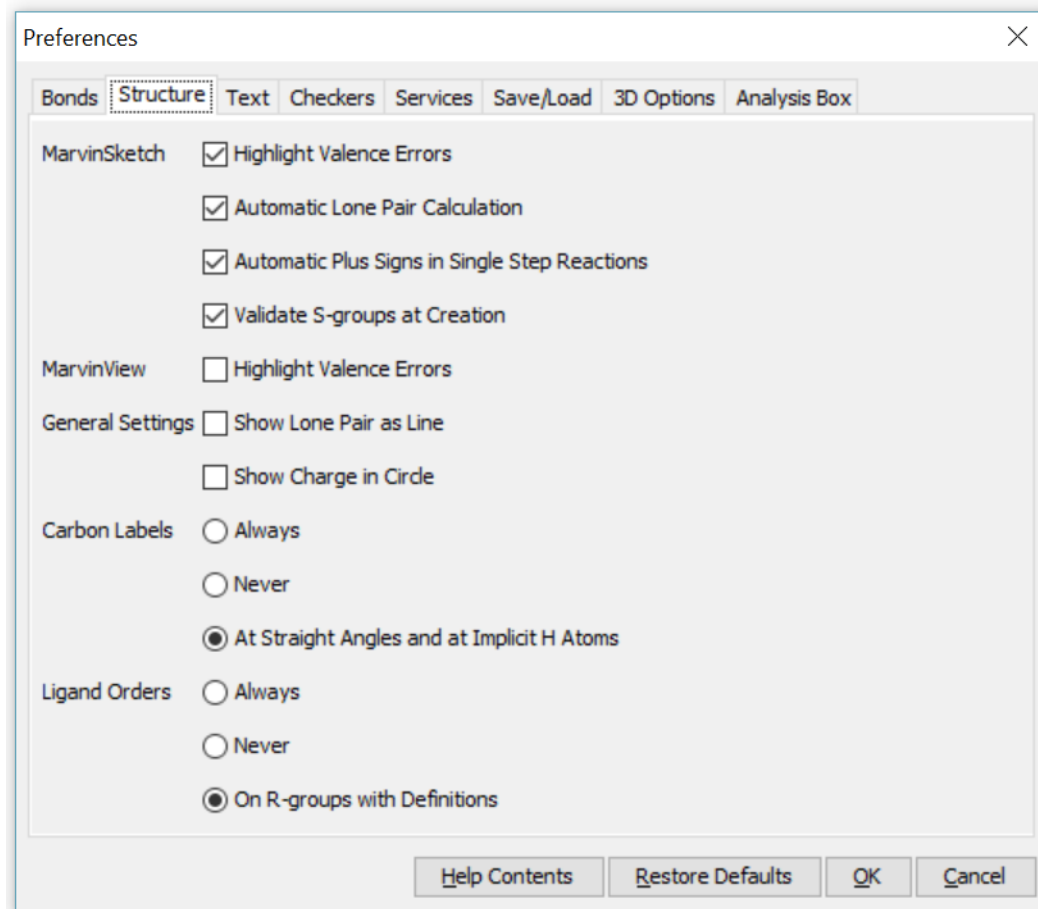
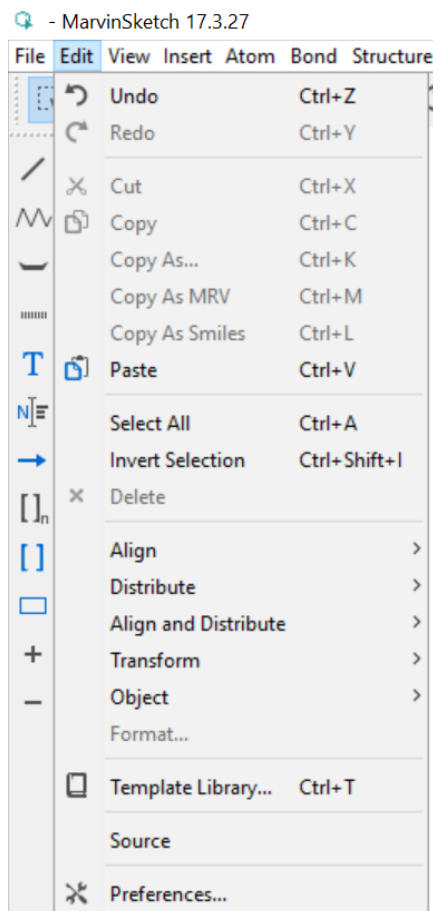
Valikot - Edit



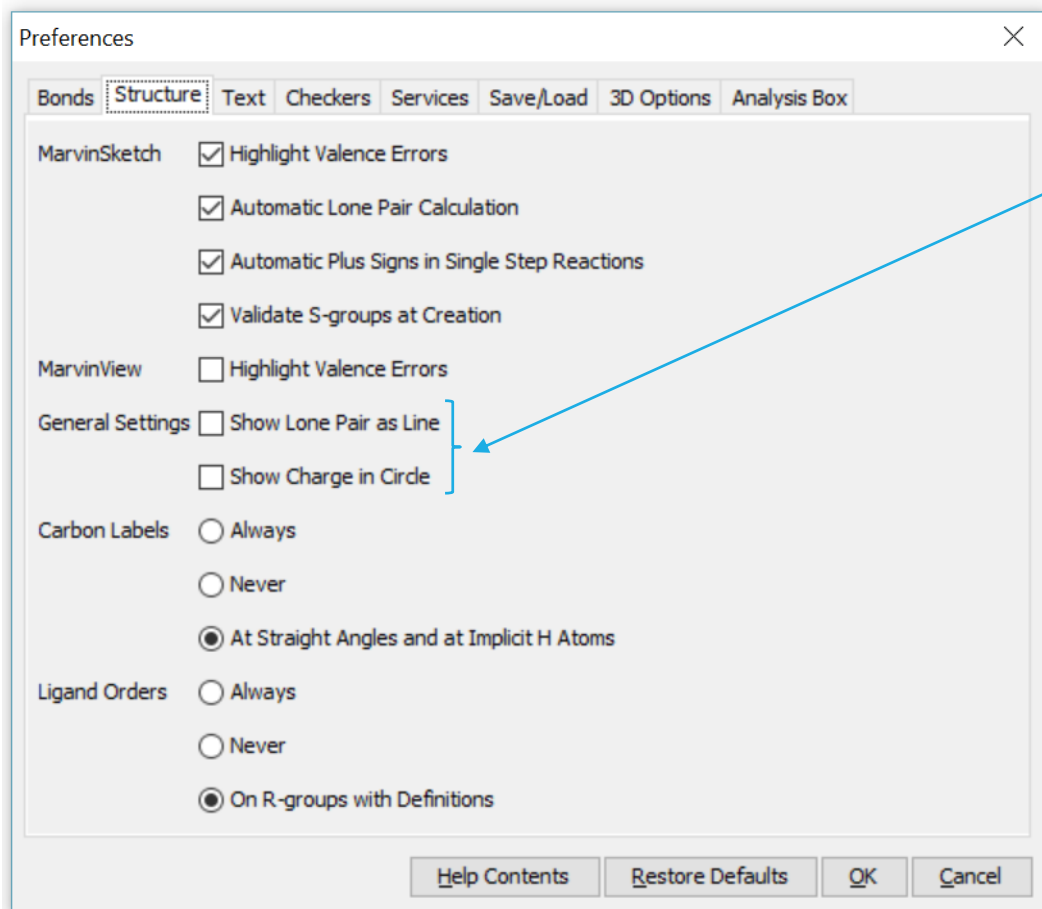
Molekyylin ”pyöritys”, paina F7 vrt. valinta -painike



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
- Colors
- Stereo
- Implicit Hydrogens
- Peptide Display
- Advanced
- Pages
- Toolbars
- Menubar F11
- Status Bar
- Grid Shift+F9
- Guidelines Ctrl+Shift+F9
- Editor style

MarvinSketch 17.3.27

File Edit View Insert Atom Bond Structure Calculations Services Help

- Atom Symbols in 3D
 - Wireframe
 - Wireframe with Knobs
 - Stick
 - Ball and Stick
 - Spacefill
- Atom Numbering
 - Off
 - Atom Numbers
 - IUPAC Numbering
- Atom Properties
- Atom Mapping
- Bond Lengths
- Lone Pairs
- R-groups
- R-Logic
- Valence
- Ligand Error
- S-group Attachments

100%

The image displays two screenshots of the MarvinSketch 17.3.27 software interface. The left screenshot shows the 'View' menu with 'Wireframe' selected. The right screenshot shows the 'View' menu with 'Wireframe' and 'Atom Numbering' selected, and a 3D ball-and-stick model of a molecule.

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 shown 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: C₄H₁₁NO

Valikot - Insert

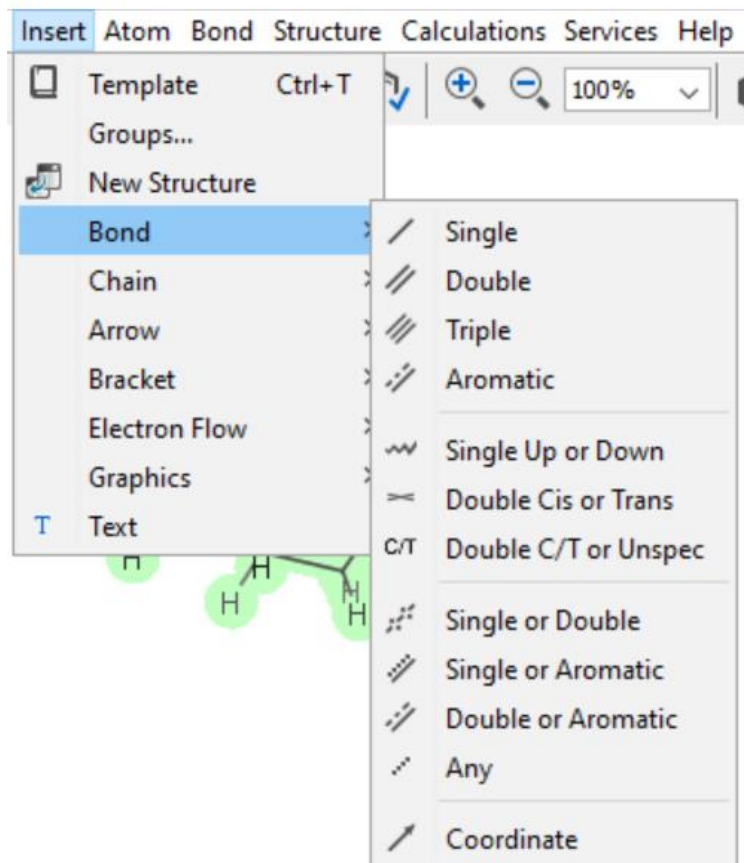
Vasen reuna

MarvinSketch 17.3.27

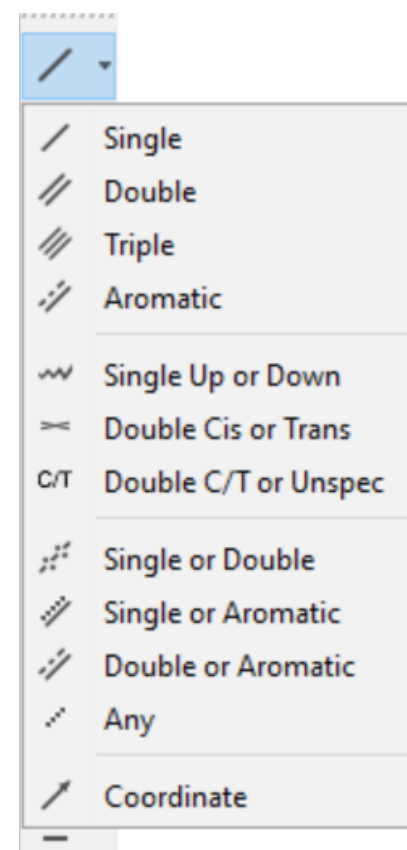
The image displays the 'Insert' menu in MarvinSketch 17.3.27. The menu is open, showing various options. The 'Chain' option is highlighted, and its sub-menu is shown, containing 'Chain' and 'Curved Chain'. The 'Arrow' option is also highlighted, and its sub-menu is shown, containing 'Straight Arrow /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

Bond - Pikavalikosta

tch 17.3.27



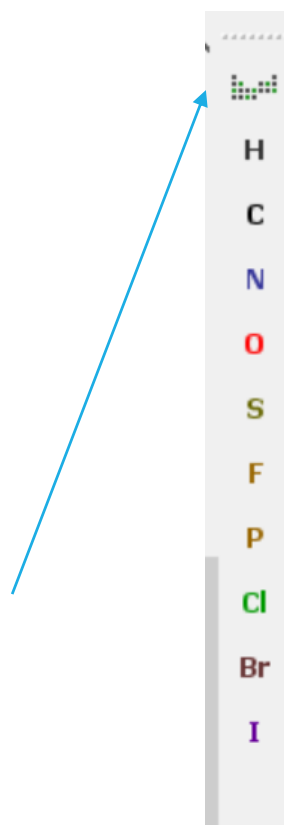
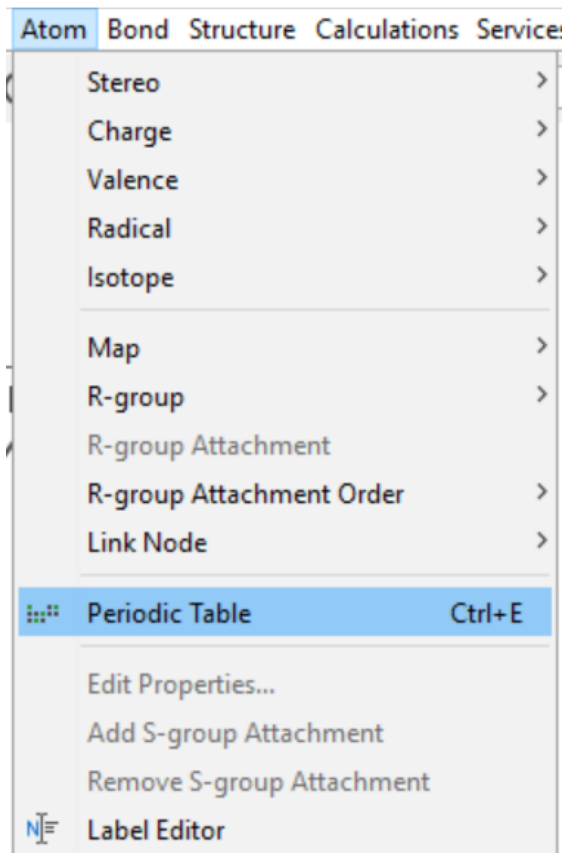
Vasen reuna



Valikot - Atom

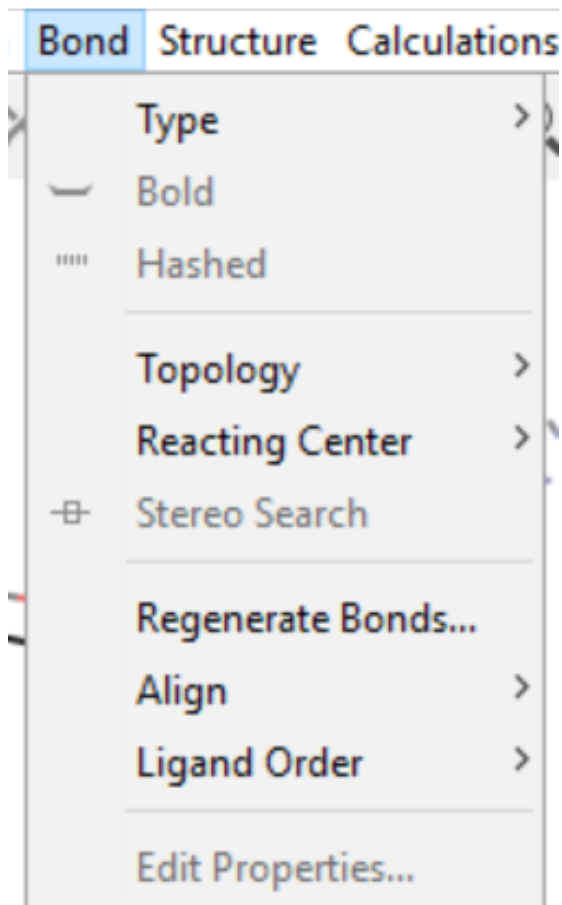
3.27

Oikea reuna

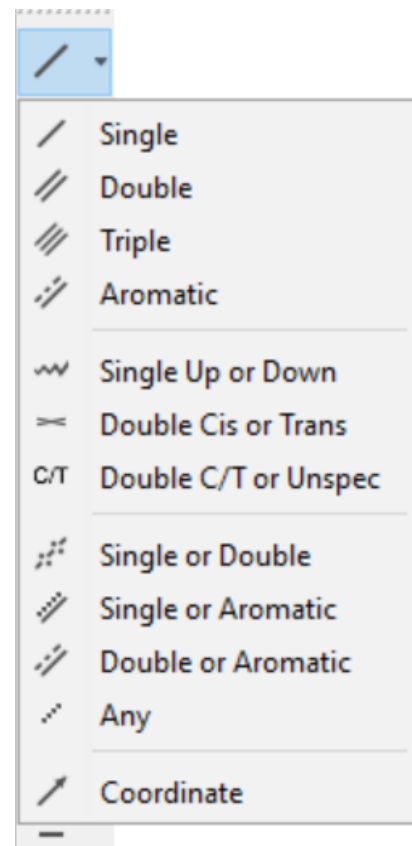


Valitse alkuaine

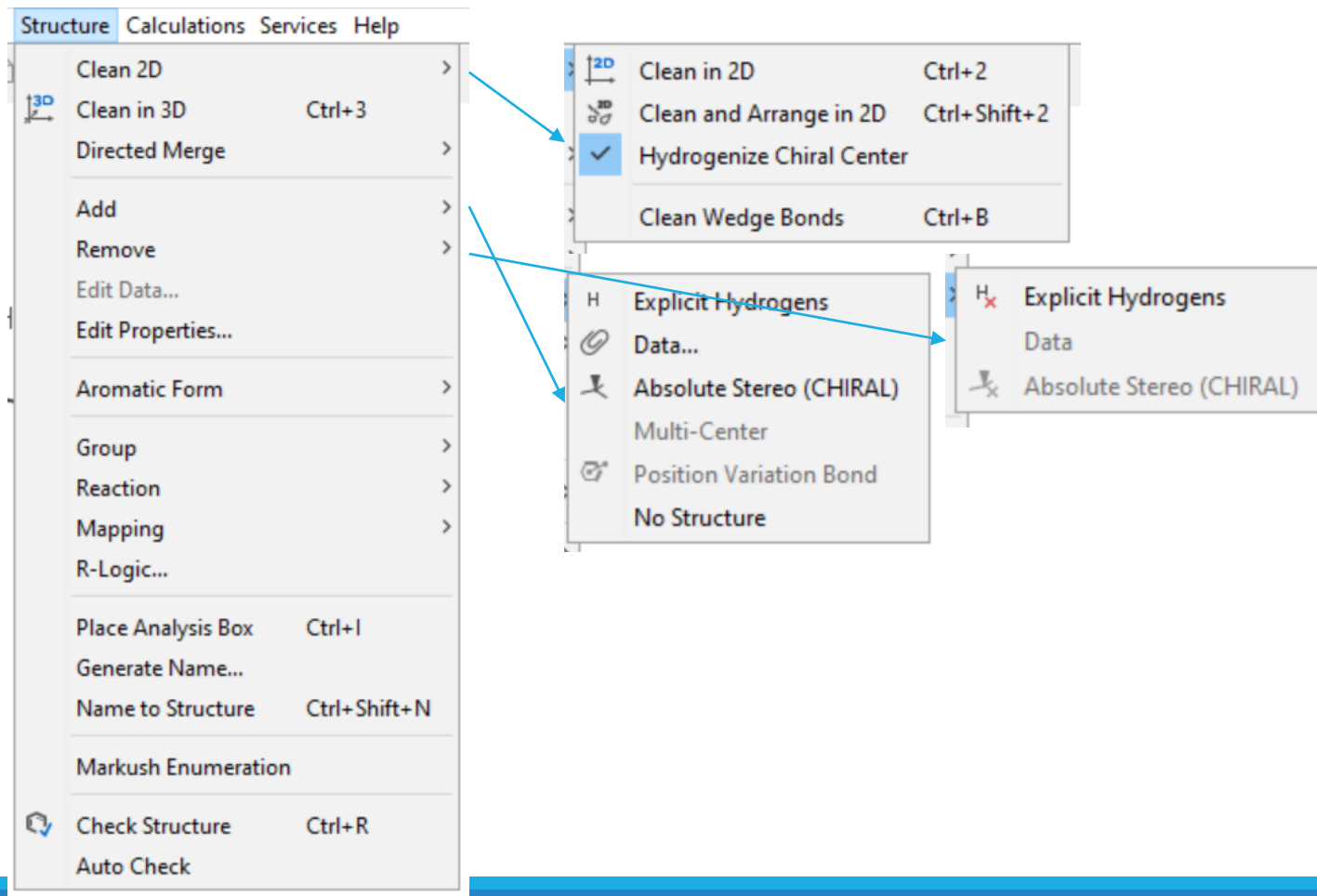
Valikot - Bond



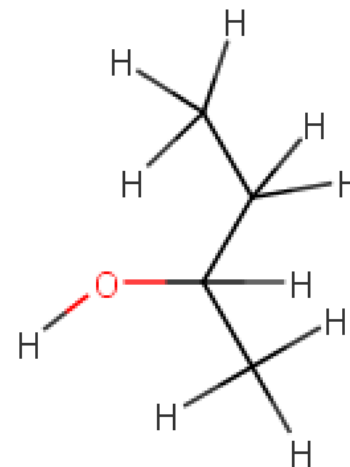
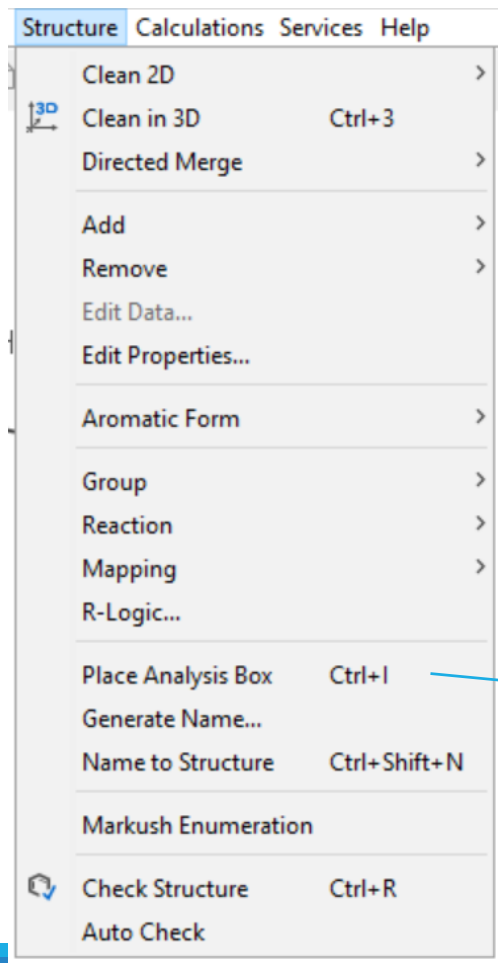
Vasen reuna



Valikot – Structure

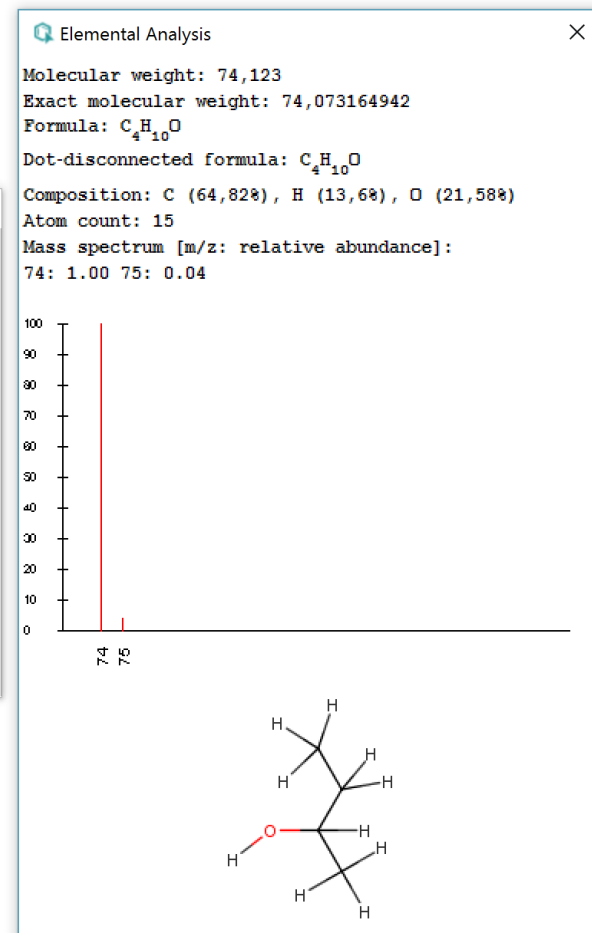
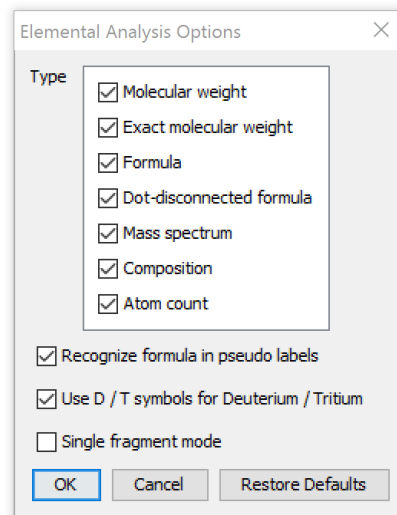
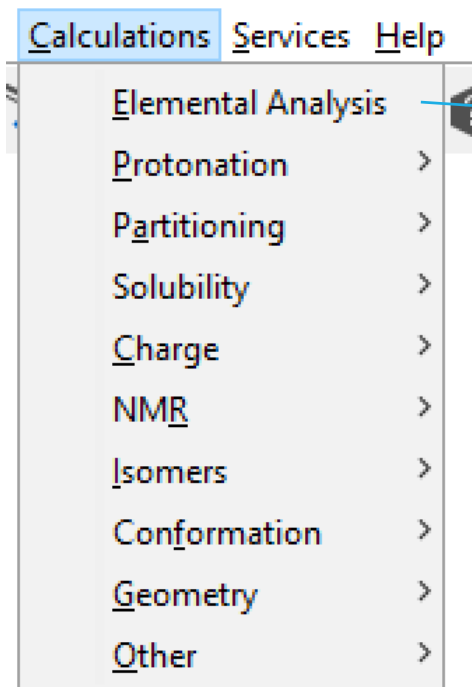


Valikot – Structure



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

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' and 'Polariza' (likely Polarization) options.

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 visible at the bottom of the dialog.

The main window, titled 'Charge', displays two views of a molecular structure. The left view shows a ball-and-stick model with partial charges labeled on the atoms: 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. The right view shows a 3D electrostatic potential map of the molecule, with blue representing positive charge and red representing negative charge.

Valikot – Calculations - Charge

The image displays a software interface for calculating orbital electronegativity. The main window shows a chemical structure of a branched alkane with a hydroxyl group. The oxygen atom is highlighted in red, and a blue arrow points to it from the 'Orbital Electronegativity Options' dialog box. The value '3,16' is displayed next to the oxygen atom in the main window.

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 structures
- Take major microspecies
- at pH: 7.4
- Buttons: OK, Cancel, Restore Defaults

Orbital Electronegativity Window:

- Chemical structure: CC(C)C(O)C
- Oxygen atom highlighted in red with value 3,16

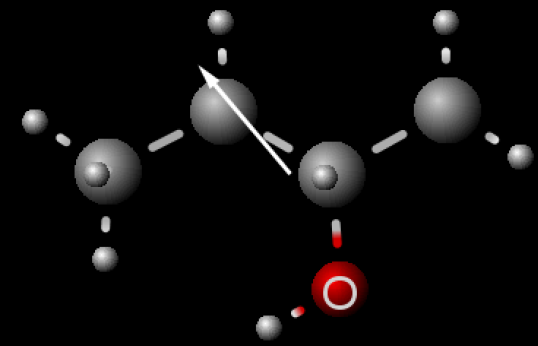
Valikot – Calculations - Charge

Bond Structure **Calculations** Services Help

- Elemental Analysis
- Protonation >
- Partitioning >
- Solubility >
- Charge**
- NMR
- Isomers >
- Conformation >
- Geometry >
- Other >

- Charge
- Polarizability
- Orbital Electronegativity
- Dipole Moment Calculation

Dipole Moment

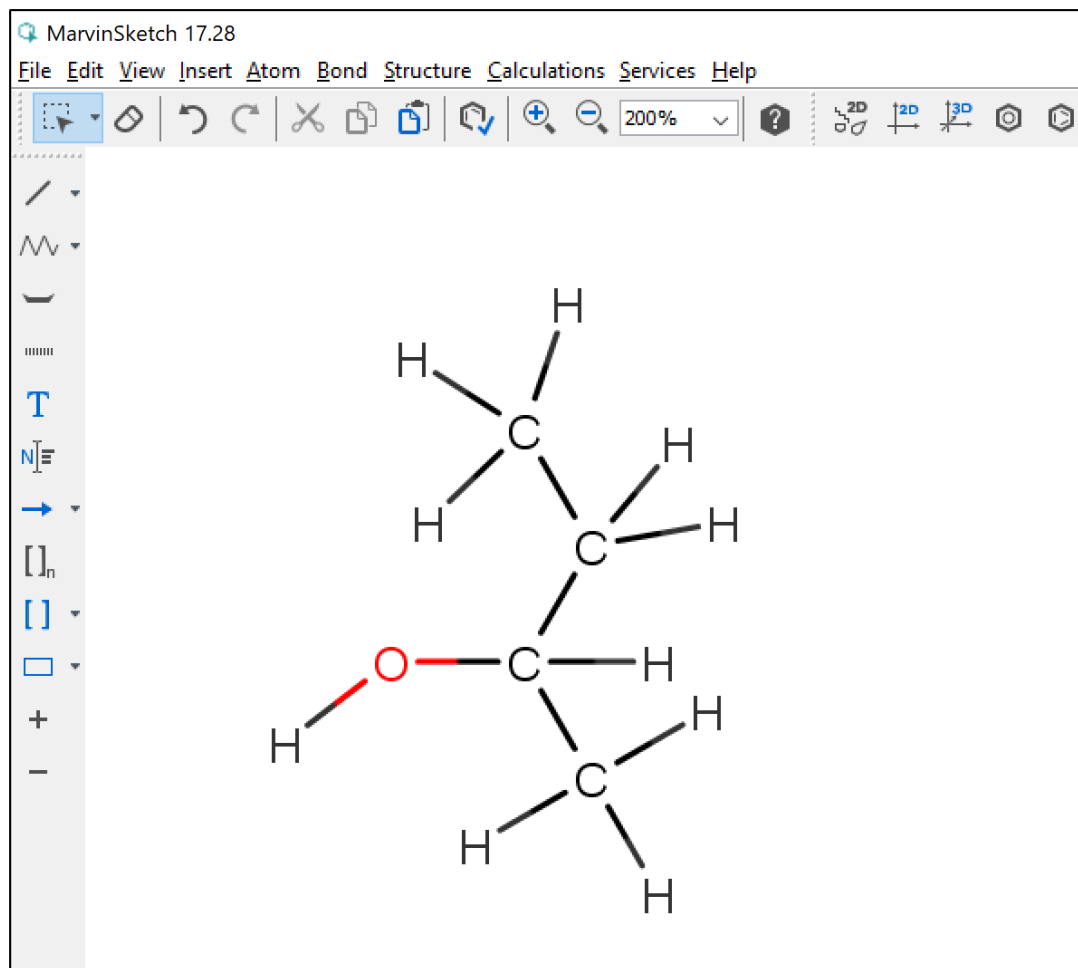


Dipole Moment information:
 Dipole: 1,65 Debye
 Dipole X: -0,94 Debye
 Dipole Y: 1,11 Debye
 Dipole Z: 0,78 Debye

MarvinSketch

Pedagogisia valintoja?

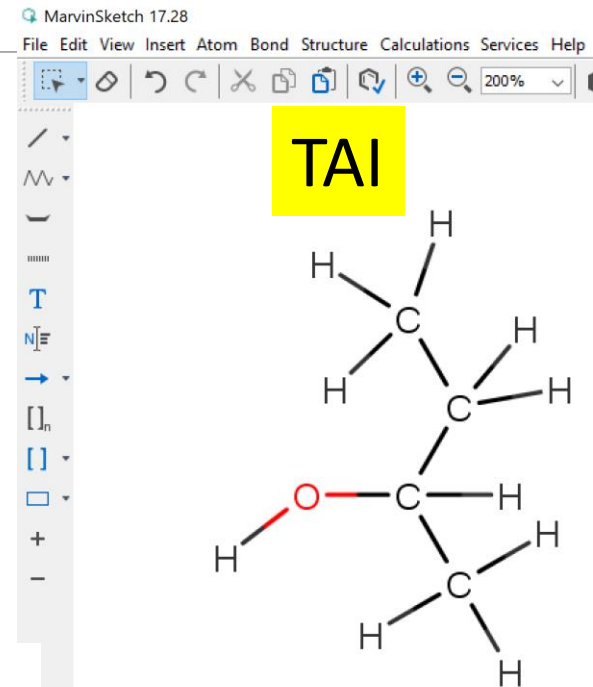
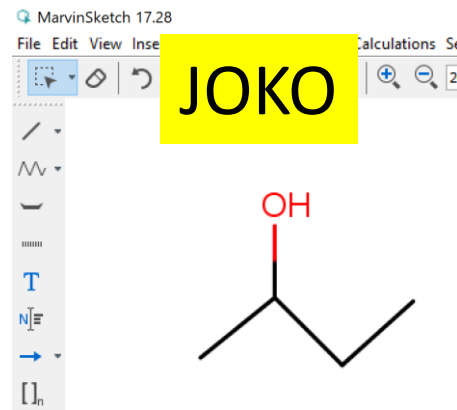
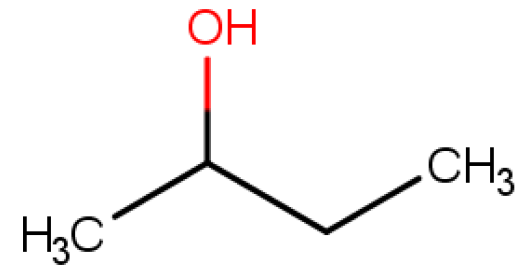
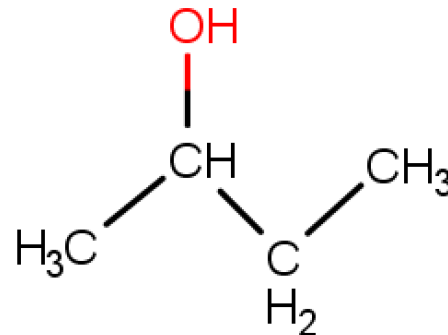
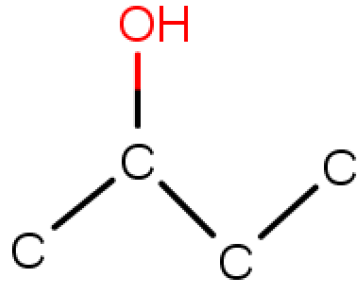
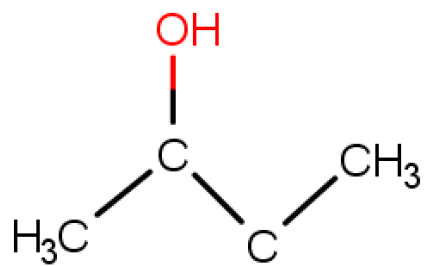
1. Viivakaava vai täydellinen rakennekaava?



AEEF Joko viivakaava tai täydellinen rakennekaava?

On valittava **joko viivakaava tai (täydellinen) rakennekaava**, kun piirretään orgaanisia molekyylejä!

Alla olevat EIVÄT KELPAA!

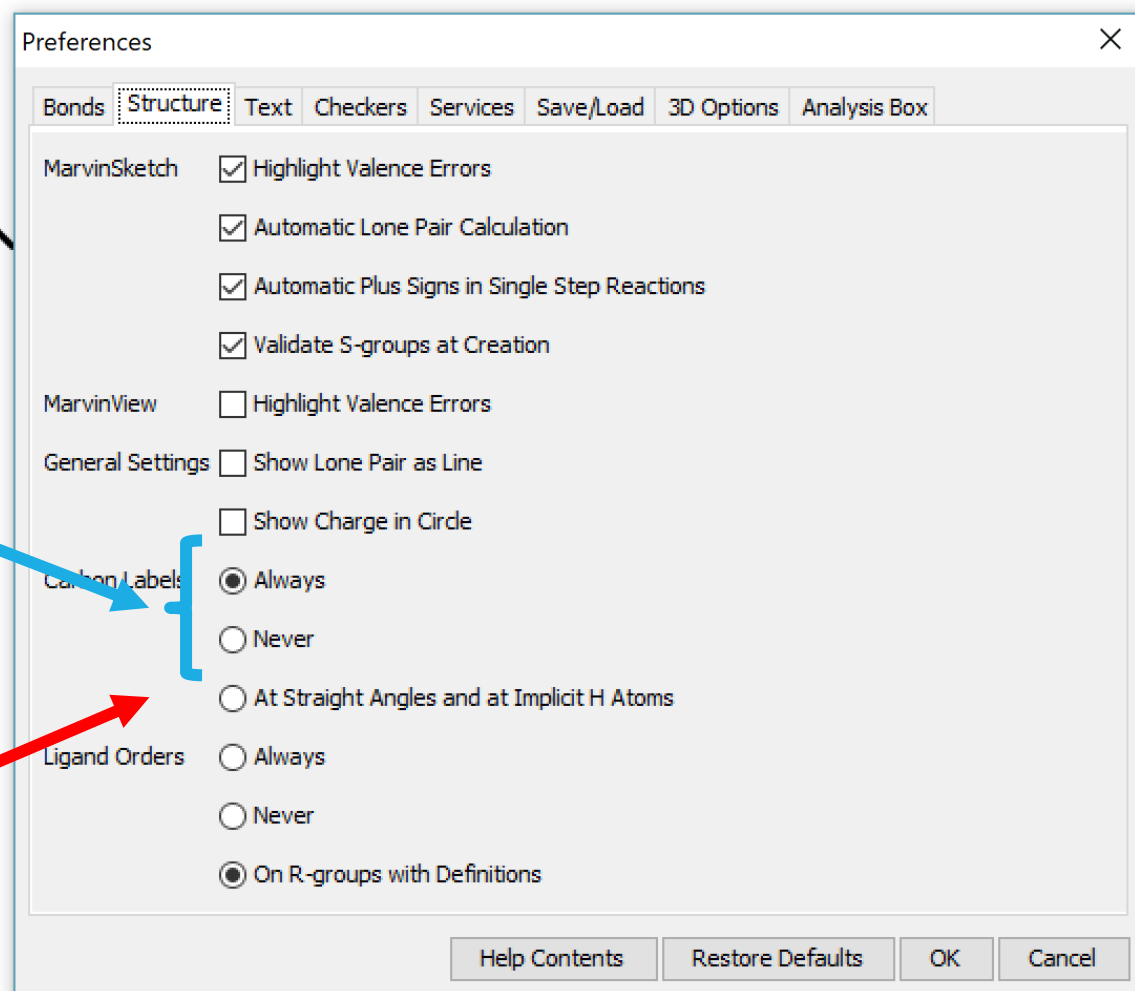


VAIHE 1: Hiilet näkeviin tai ei?

VAIHE1: Viivakaava tai täydellinen rakennekaava

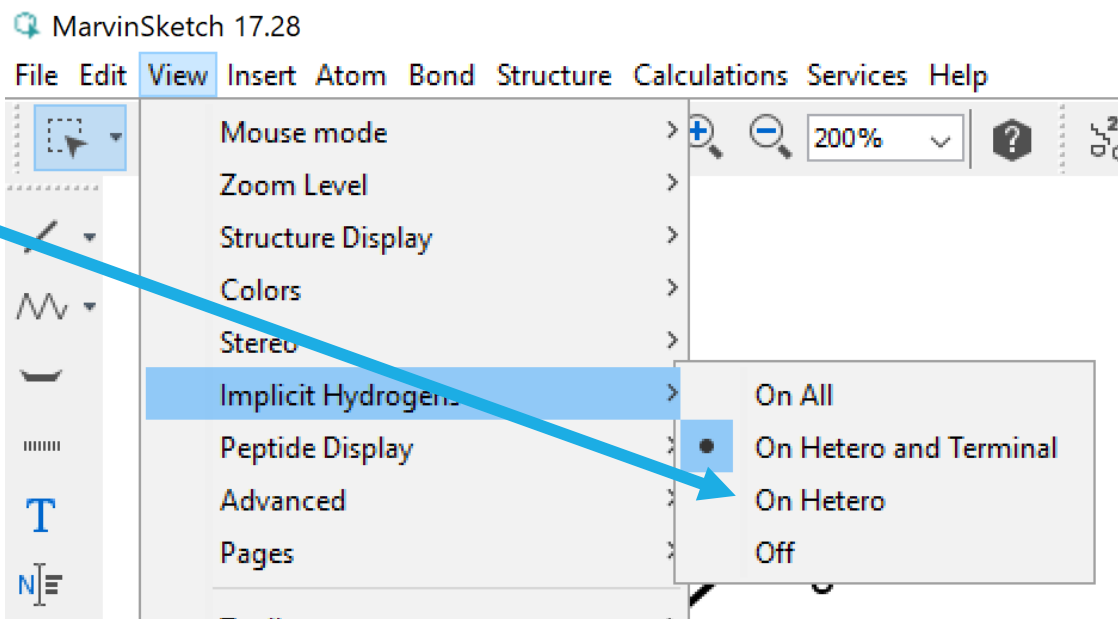
Valitaan se, **näytetäänkö hiilet lainkaan tai kaikki** (ei muita vaihtoehtoja käytetä!!!)

EI TÄTÄ



VAIHE 2: "Implisiittiset vedyt" pois

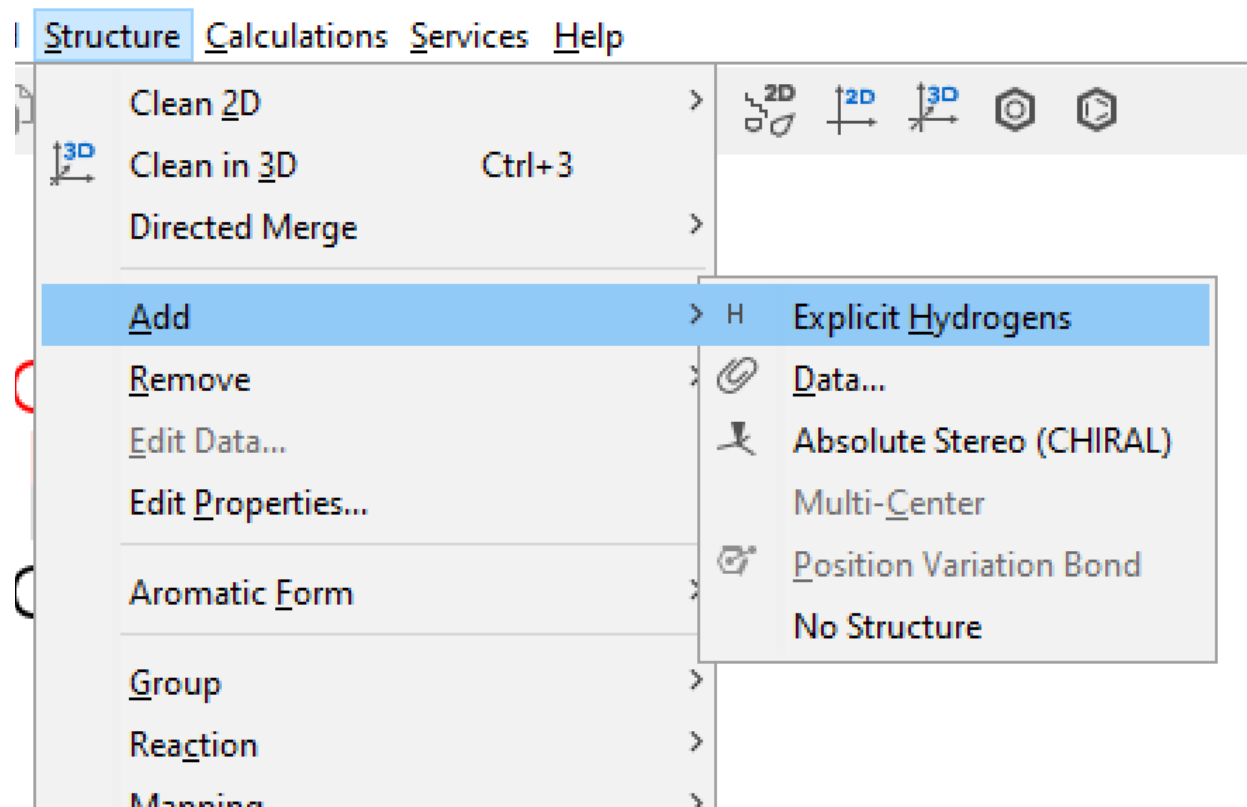
Varmistetaan vetyjen näkyminen **vain "heteroatomien"** yhteydessä (funktionaalinen ryhmä).



Vaihe 3: Jos täydellinen rakennekaava →

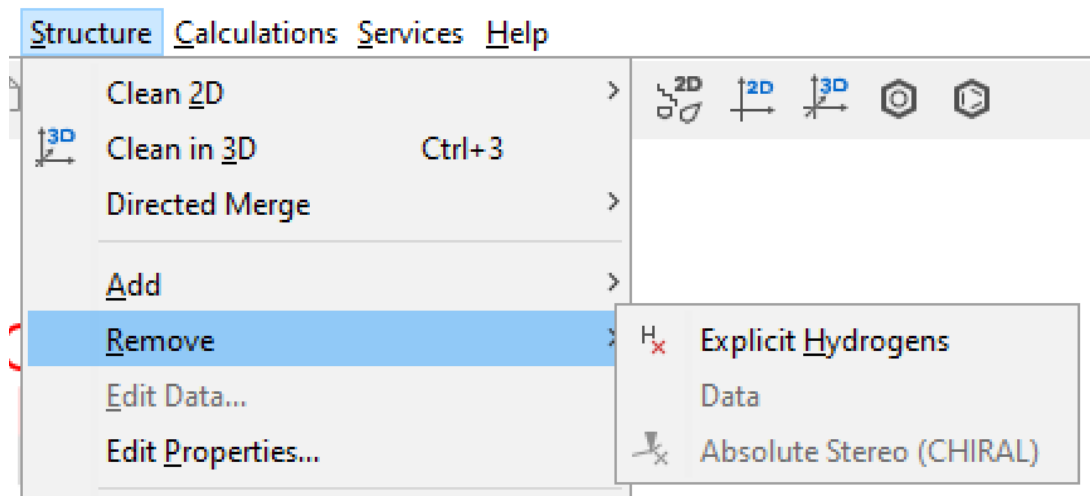
Täydelliseen rakennekaavaan valitaan "Carbon labels" ALWAYS (Preferences -kohdasta). JA

Structure-kohdasta **Add Explicit Hydrogens**



Paluu viivakaavaan?

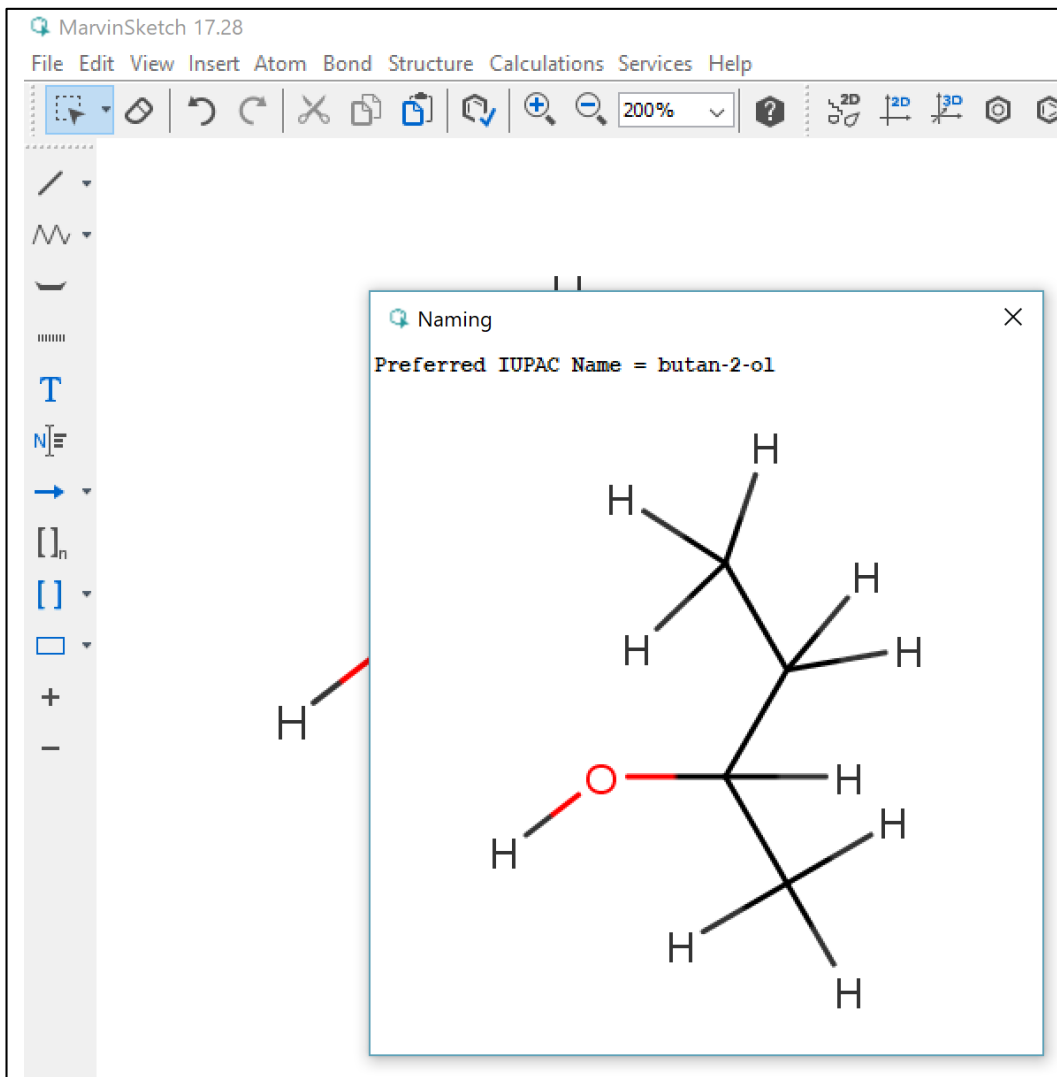
Jos haluaa palata viivakaavaesitysmuotoon. Poistetaan vedyt (viereinen kuva) ja poistetaan hiiliatomien merkinnät (Preferences –osiosta Carbon labels → Never)



MarvinSketch

Pedagogisia valintoja?

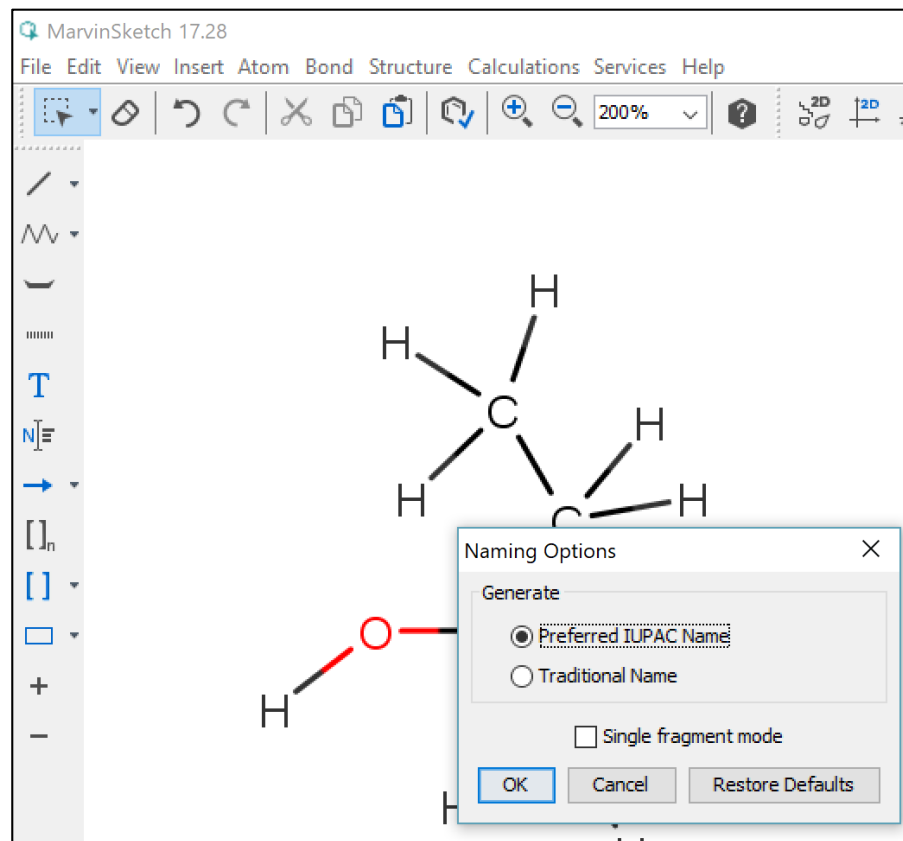
2. Nimeämisen opetus



MarvinSketch nimeää molekyylit (myös Abitti-versiossa)

Miten kurssilla opetetaan orgaanisten molekyylien nimeäminen? Miksi?

MarvinSketch tuottaa nimet ja toisinpäin – nimestä rakenteen.



3. Isomerian opetus

KE2 – LOPS2003

Keskeiset sisällöt

- alkuaineiden ominaisuudet ja jaksollinen järjestelmä
- **elektroniverhon rakenne ja atomiorbitaalit**
- hapetuslukujen määräytyminen ja yhdisteen kaava
- kemiallinen sidos, sidosenergia (→ KE3) ja aineen ominaisuudet
- **atomiorbitaalien hybridisoituminen ja orgaanisten yhdisteiden sidos- ja avaruusrakenne**
- isomeria

KE2 – LOPS15

Keskeiset sisällöt

- kemian merkitys hyvinvoinnin ja terveyden kannalta
- orgaanisten yhdisteiden, kuten hiilivetyjen, happi- ja typpiyhdisteiden, **rakenteiden mallintaminen ja kuvaaminen erilaisilla malleilla**
- **avaruusrakenne** ja isomeria
- orgaanisten yhdisteiden ominaisuuksien selittäminen rakenteen avulla
- ...
- aineen rakenteen analyysimenetelmät, kuten spektroskopia