

MarvinSketch

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Kemian ja matematiikan lehtori

Helsingin yliopiston Viikin normaalikoulu

Sisältö

1. ...
2. ...
3. ...
4. Ohjeet
5. Ohjelman käyttö

MarvinSketch – ohjelman käyttö

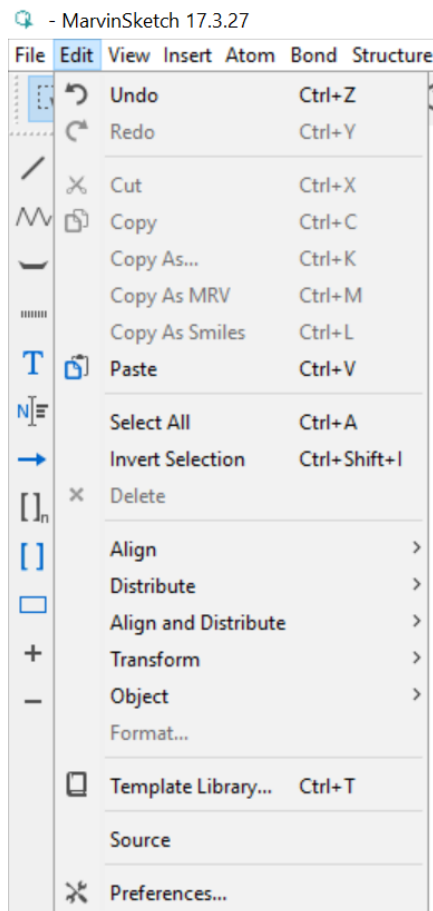
ABITTI-TIKUSSA MARVINSKETCH 17.3.27

LADATTAVISSA 18.21.0 (17.29.0 17-SARJAN
VIIMEINEN)

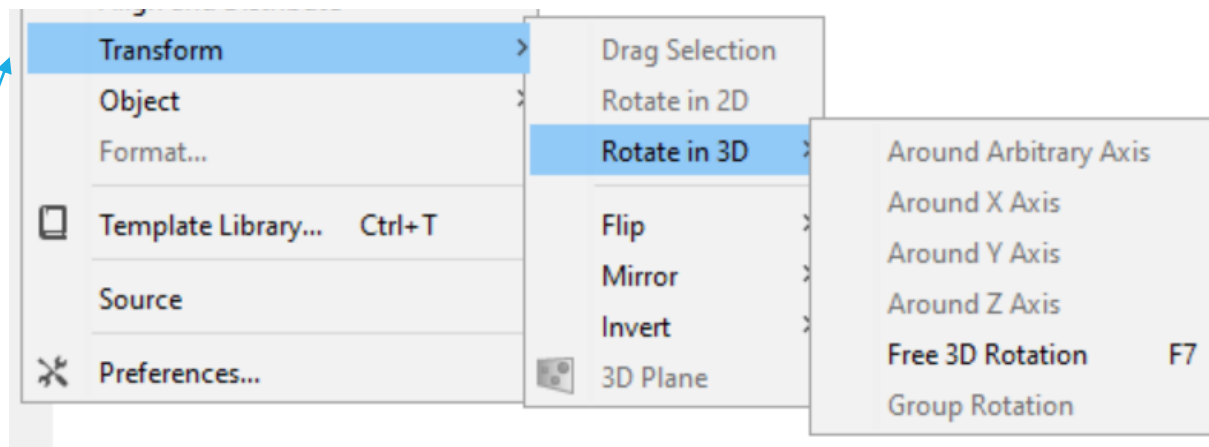
Mihin MarvinSketch ”taipuu”

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

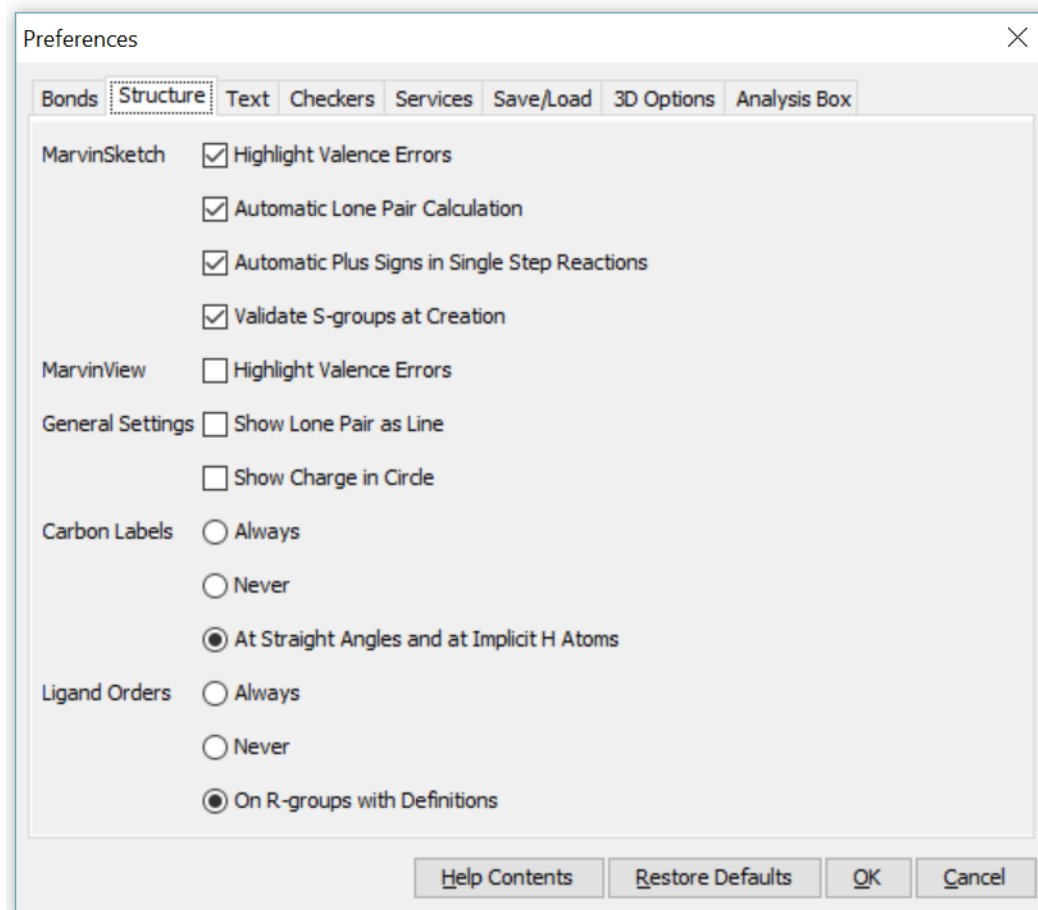
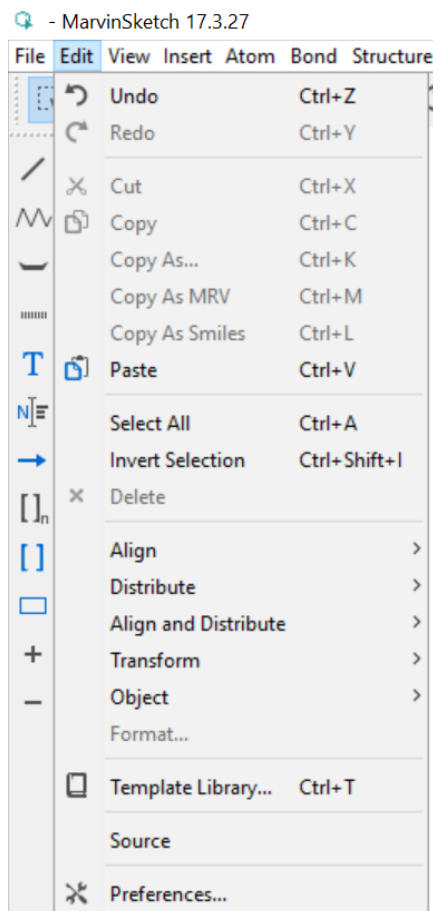
Valikot - Edit



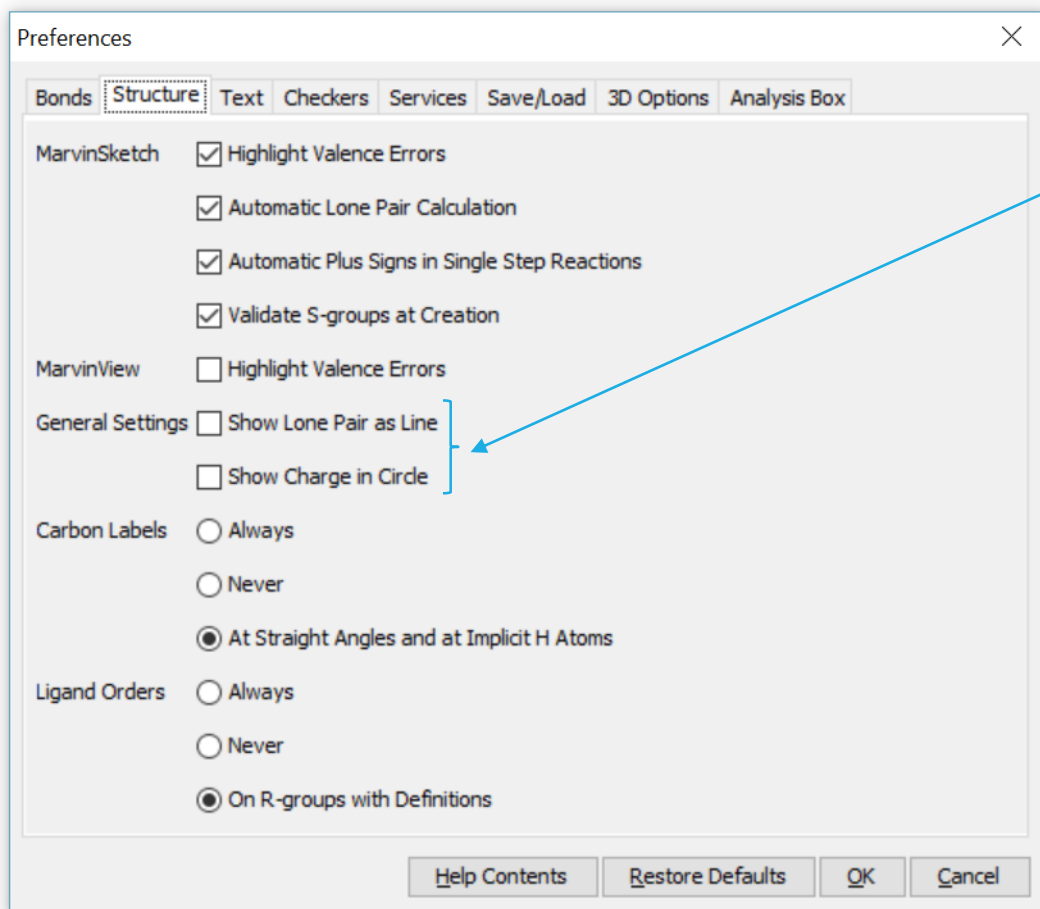
Molekyylin ”pyöritys”, paina F7 vrt. valinta -painike



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

Atom Symbols in 3D

- Wireframe
- Wireframe with Knobs
- Stick
- Ball and Stick
- Spacefill

Atom Numbering

- Off
- Atom Numbers
- IUPAC Numbering

File Edit View Insert Atom Bond Structure Calculations Services Help

100%

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: 1.47
- C-C: 1.55
- C-C: 1.56
- C-O: 1.43
- C-C: 1.55

Name: 3-aminobutan-2-ol
Molecular weight: 89,14
Formula: C₄H₁₁NO

Valikot - Insert

Vasen reuna

MarvinSketch 17.3.27

The screenshot displays the MarvinSketch 17.3.27 interface. The 'Insert' menu is open, showing the following options:

- Template (Ctrl+T)
- Groups...
- New Structure
- Bond >
- Chain >
- Arrow >
- Bracket >
- Electron Flow >
- Graphics >
- Text

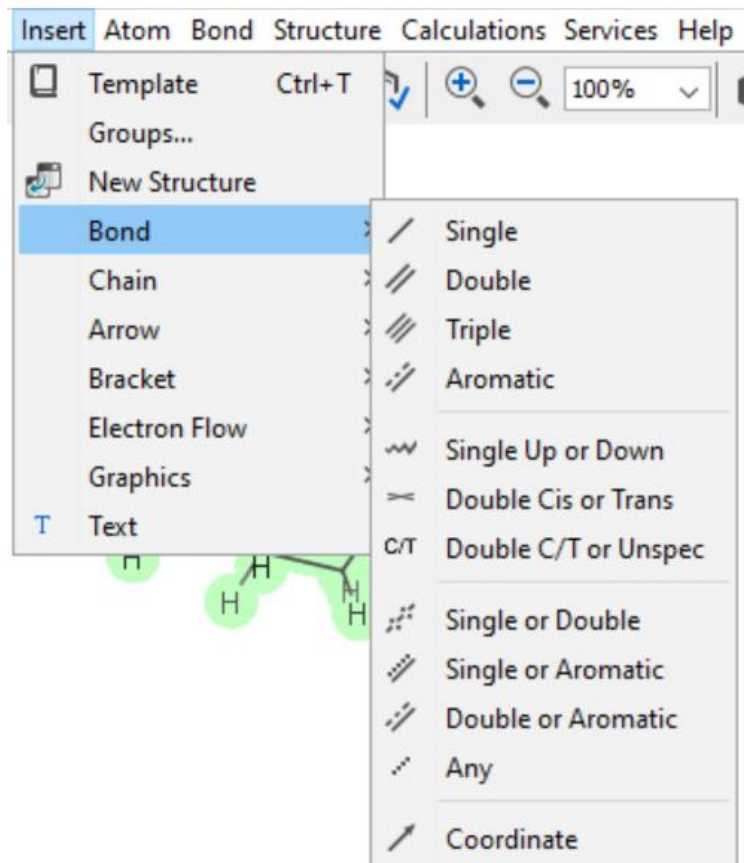
Blue arrows indicate the following sub-menus:

- The 'Chain' option in the main menu points to a sub-menu containing 'Chain' and 'Curved Chain'.
- The 'Arrow' option in the main menu points to a sub-menu containing:
 - Straight Arrow / Reaction
 - Retrosynthetic Arrow
 - Equilibrium Arrow
 - Resonance Arrow
 - Curved Arrow
 - Dashed Arrow
 - Crossed Arrow

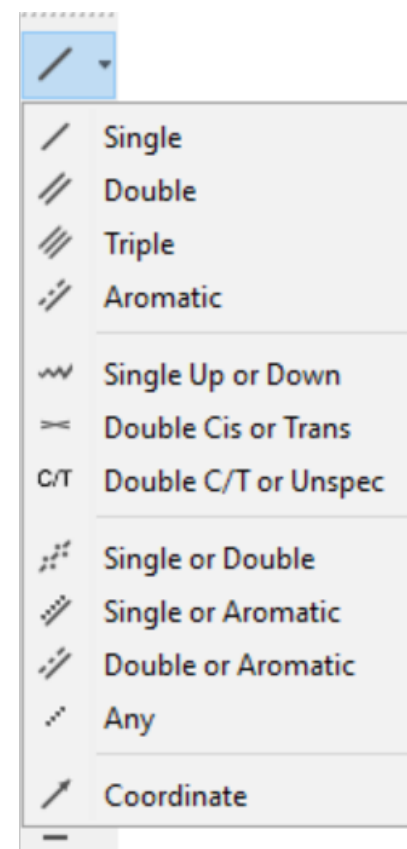
A small chemical structure is visible in the background, showing a carbon atom bonded to three hydrogen atoms.

Bond - Pikavalikosta

tch 17.3.27



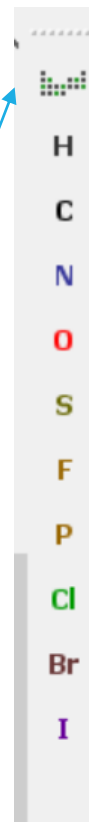
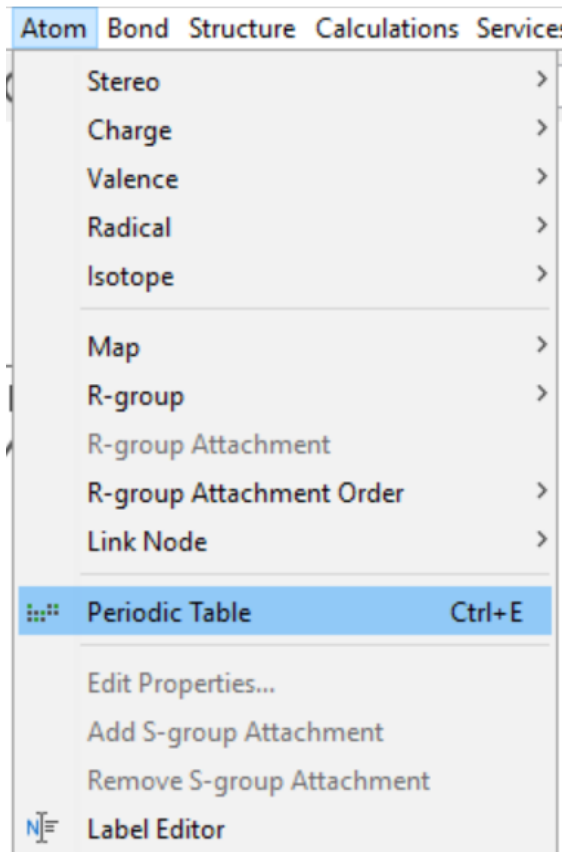
Vasen reuna



Valikot - Atom

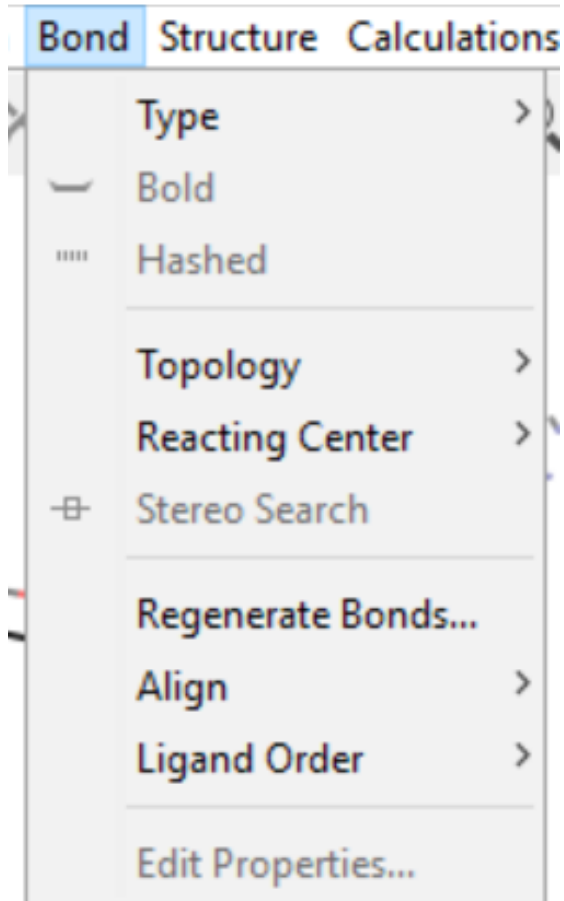
3.27

Oikea reuna

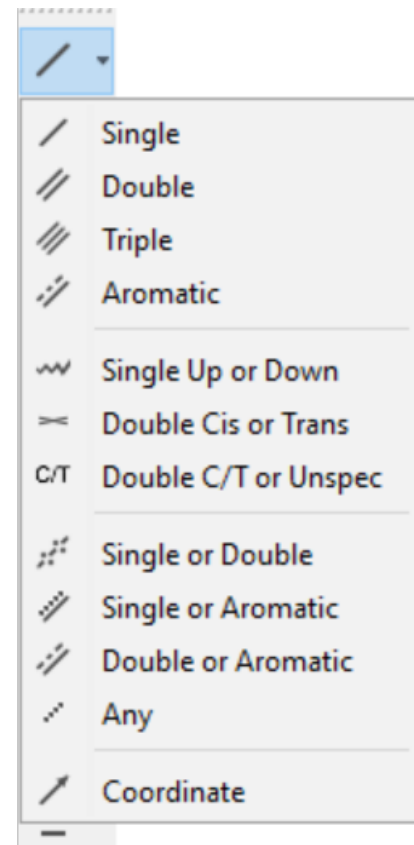


Valitse alkuaine

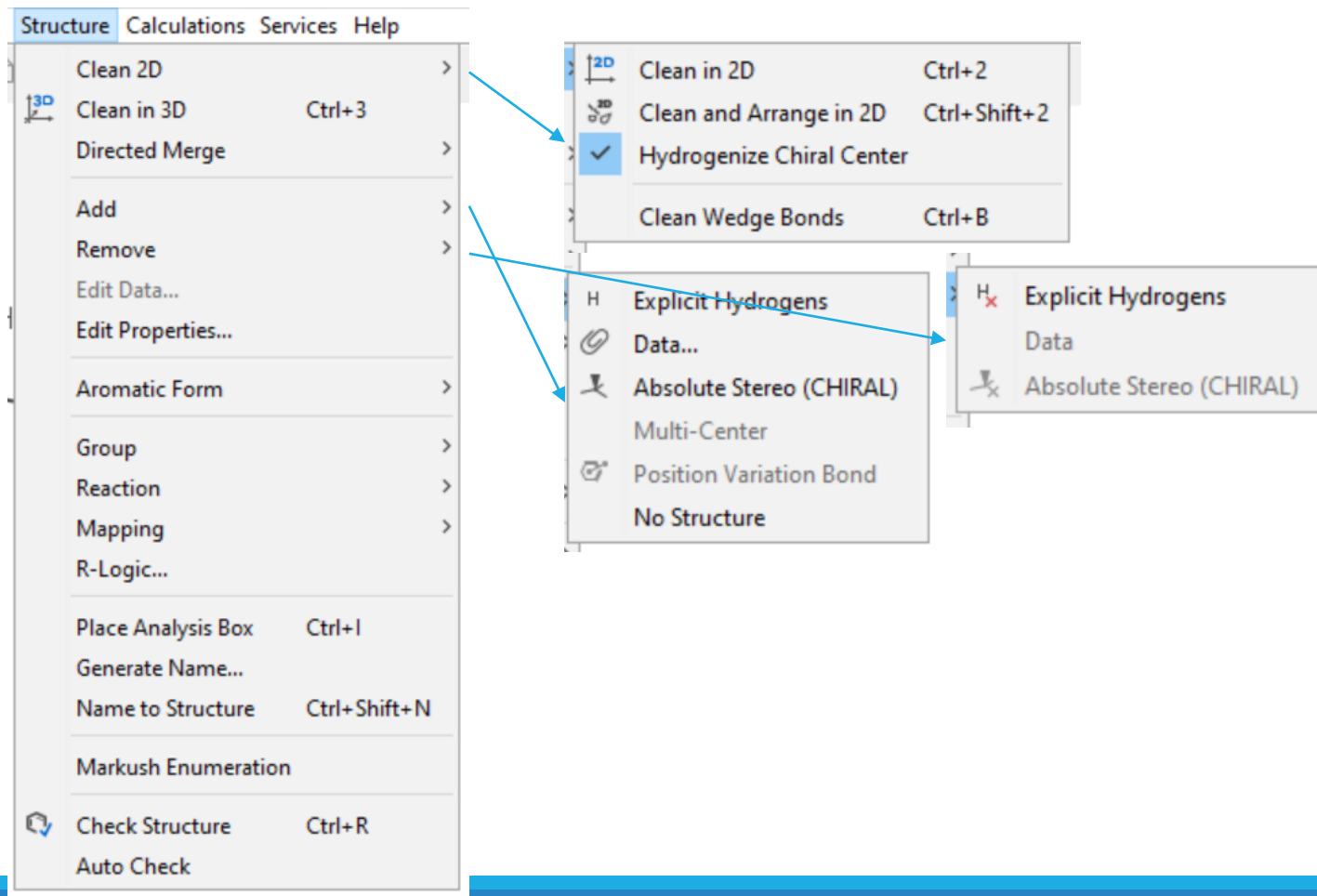
Valikot - Bond



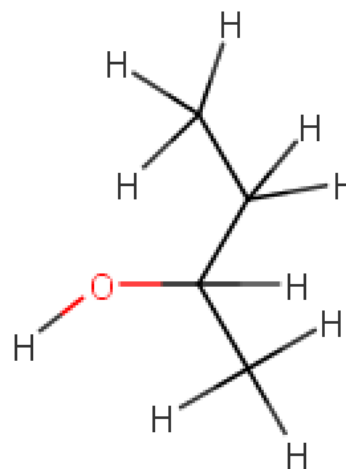
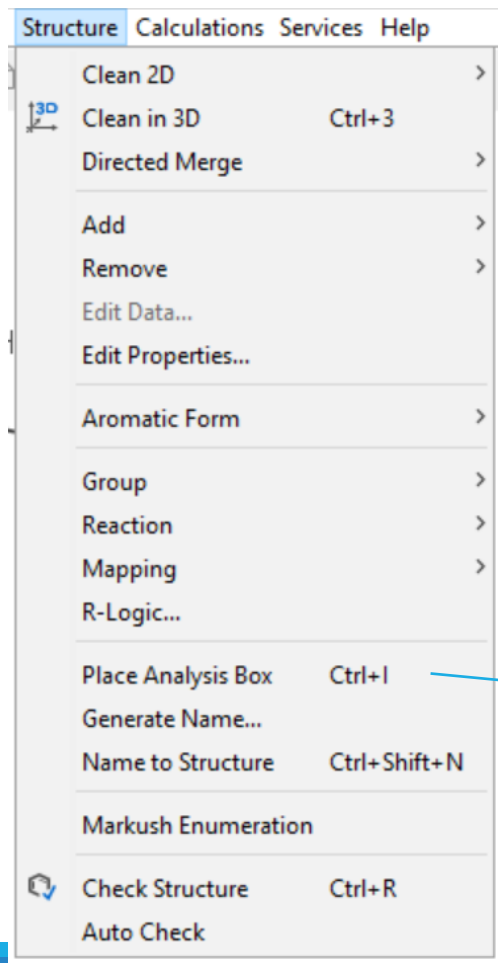
Vasen reuna



Valikot – Structure

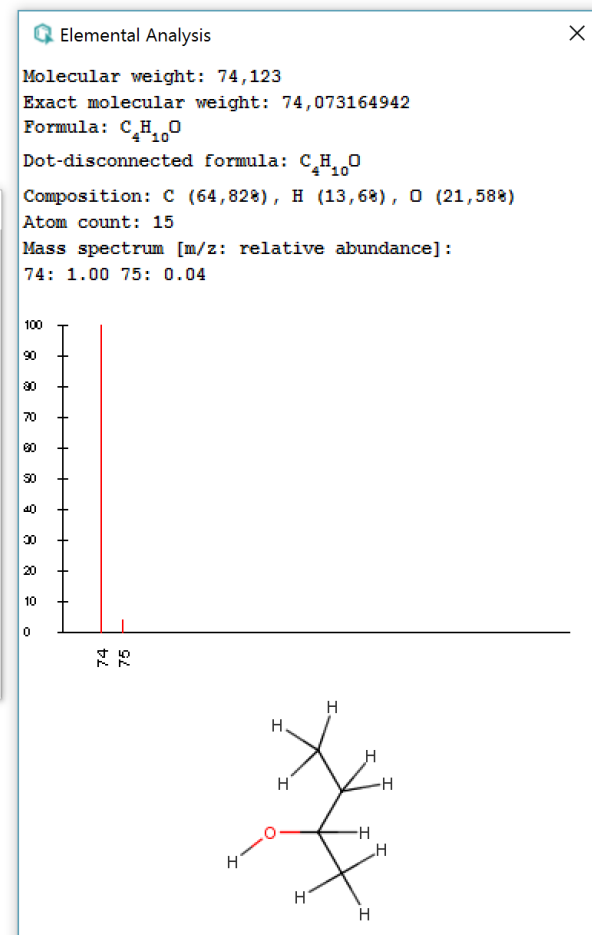
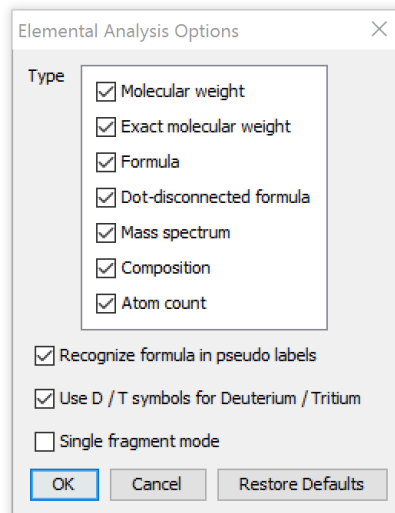
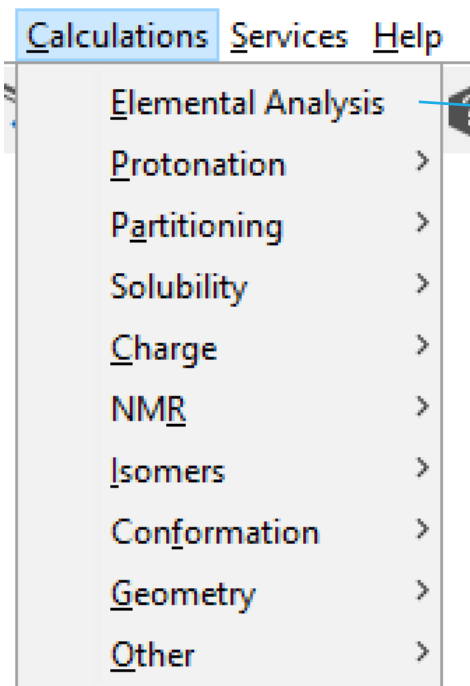


Valikot – Structure



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 '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 options: Charge, Polariza, Orbital, and Dipole I. Below the menu, the 'Charge Options' dialog box is open, showing settings for decimal places (2), type (Total), and checkboxes for 'Charges of implicit hydrogens', 'Take resonant structures', 'Take major microspecies', and 'Display in MarvinSpace'. The 'at pH' field is set to 7.4. Buttons for 'OK', 'Cancel', and 'Restore Defaults' are at the bottom.

The 'Charge' dialog box shows the following options:

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

Buttons: OK, Cancel, Restore Defaults

The main window shows a 3D ball-and-stick model of a molecule with partial charges displayed 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, a 3D electrostatic potential map of the molecule is shown, with blue representing positive charge and red representing negative charge.

Valikot – Calculations - Charge

The image shows the AEEF software interface. 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 options: Charge, Polarizability, Orbital Electronegativity, and Dipole Moment Calculation.

The 'Orbital Electronegativity Options' dialog box is open, showing settings for Decimal places (2), Type (Pi), Take resonance (checked), Take major microspecies (unchecked), and at pH (7.4). The 'OK' button is highlighted.

The 'Orbital Electronegativity' window displays a chemical structure of a branched alkane with a highlighted oxygen atom. The oxygen atom is labeled with the value 3,16, indicating its orbital electronegativity.

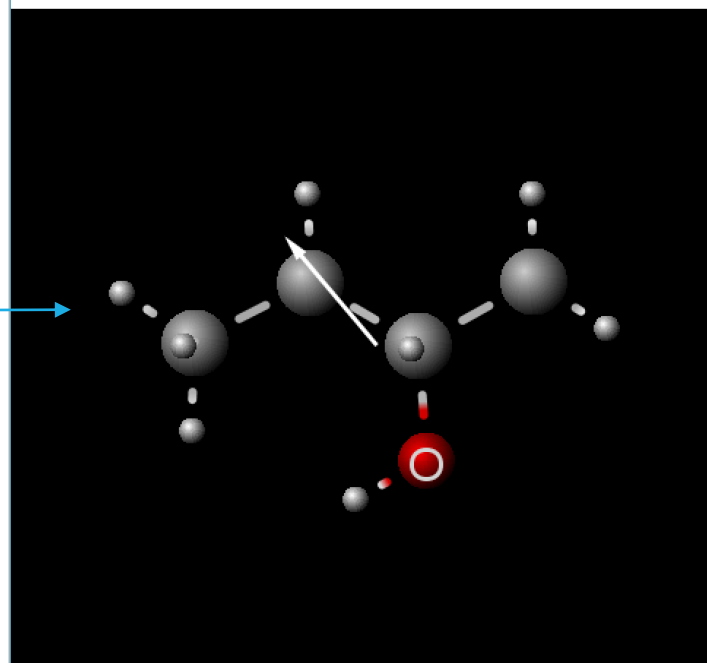
Valikot – Calculations - Charge

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

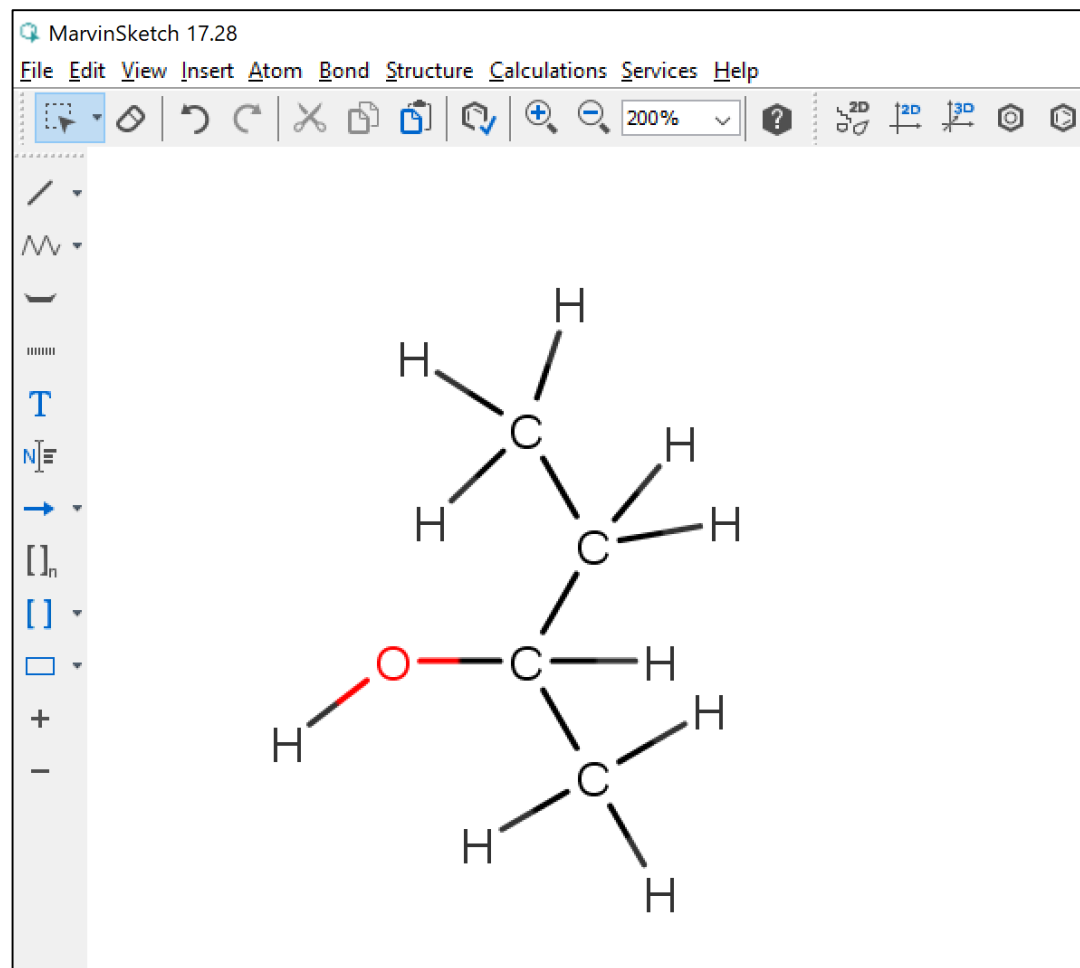


Dipole Moment information:
 Dipole: 1,65 Debye
 Dipole X: -0,94 Debye
 Dipole Y: 1,11 Debye
 Dipole Z: 0,78 Debye

MarvinSketch

Pedagogisia valintoja?

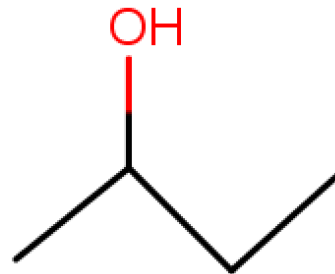
1. Viivakaava vai täydellinen rakennekaava?



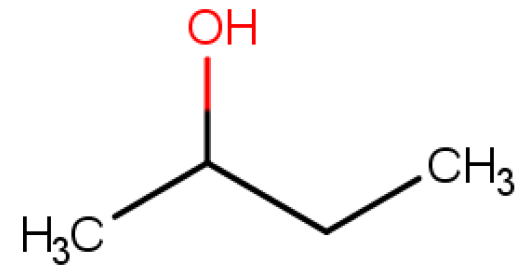
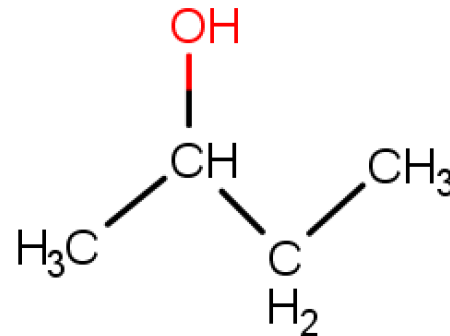
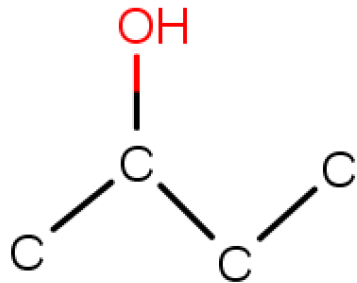
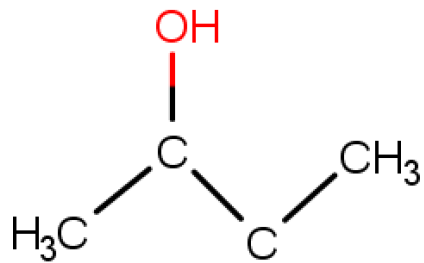
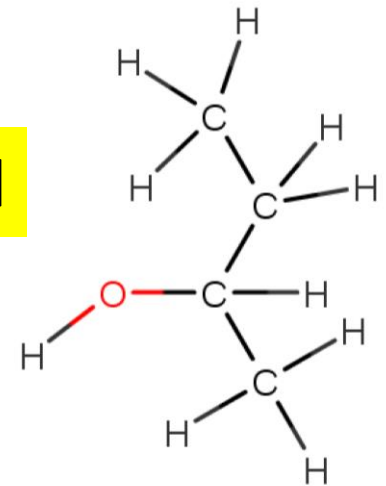
AEEF Joko viivakaava tai täydellinen rakennekaava?

Joko viivakaava tai täydellinen rakennekaava

JOKO



TAI

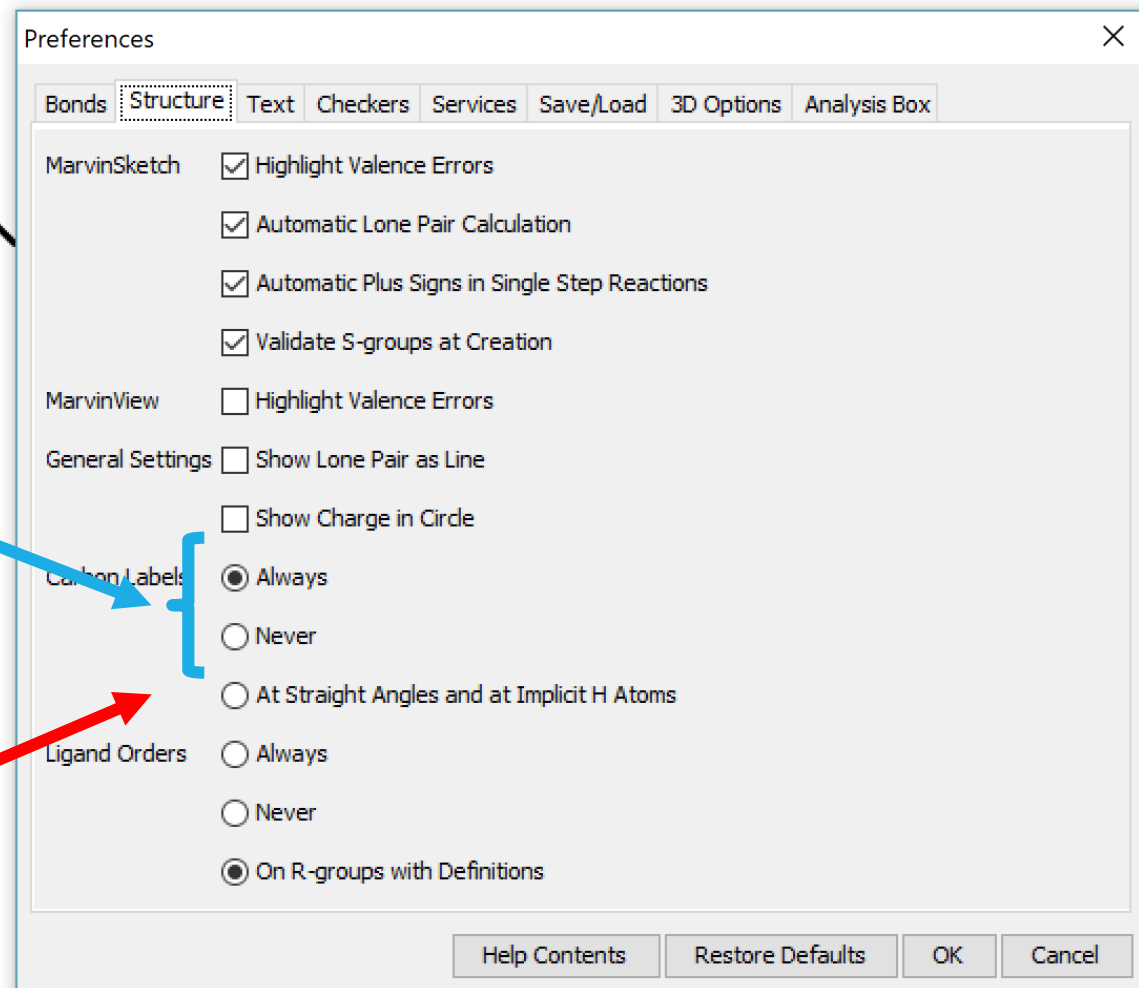


VAIHE 1: Hiilet näkeviin tai ei?

VAIHE1: Viivakaava tai täydellinen rakennekaava

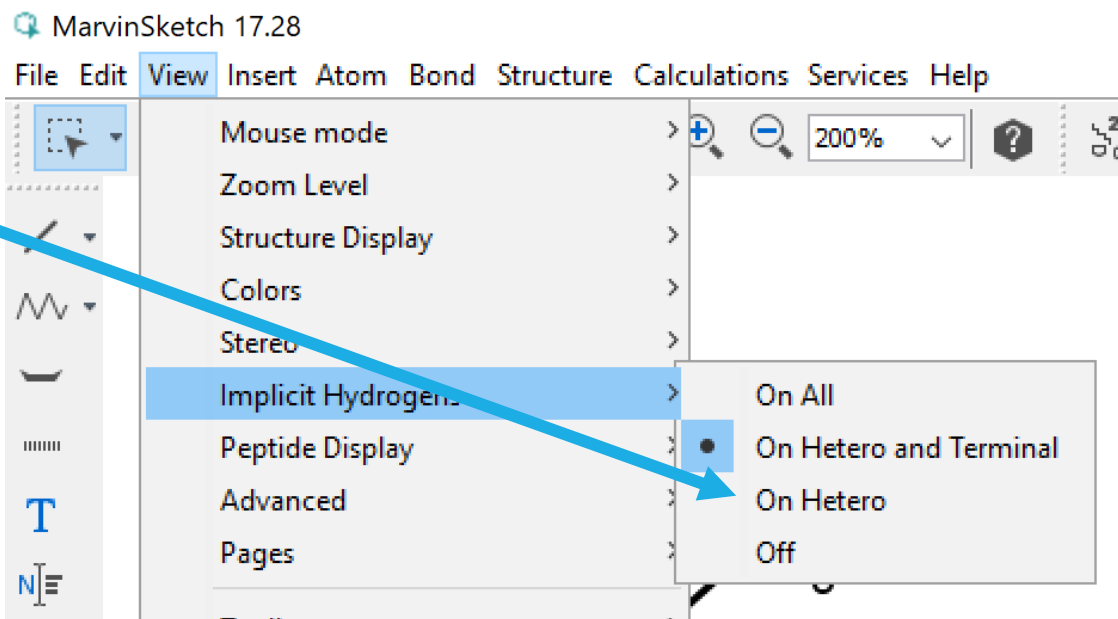
Valitaan se, **näytetäänkö hiilet lainkaan tai kaikki** (ei muita vaihtoehtoja käytetä!!!)

EI TÄTÄ



VAIHE 2: "Implisiittiset vedyt" pois

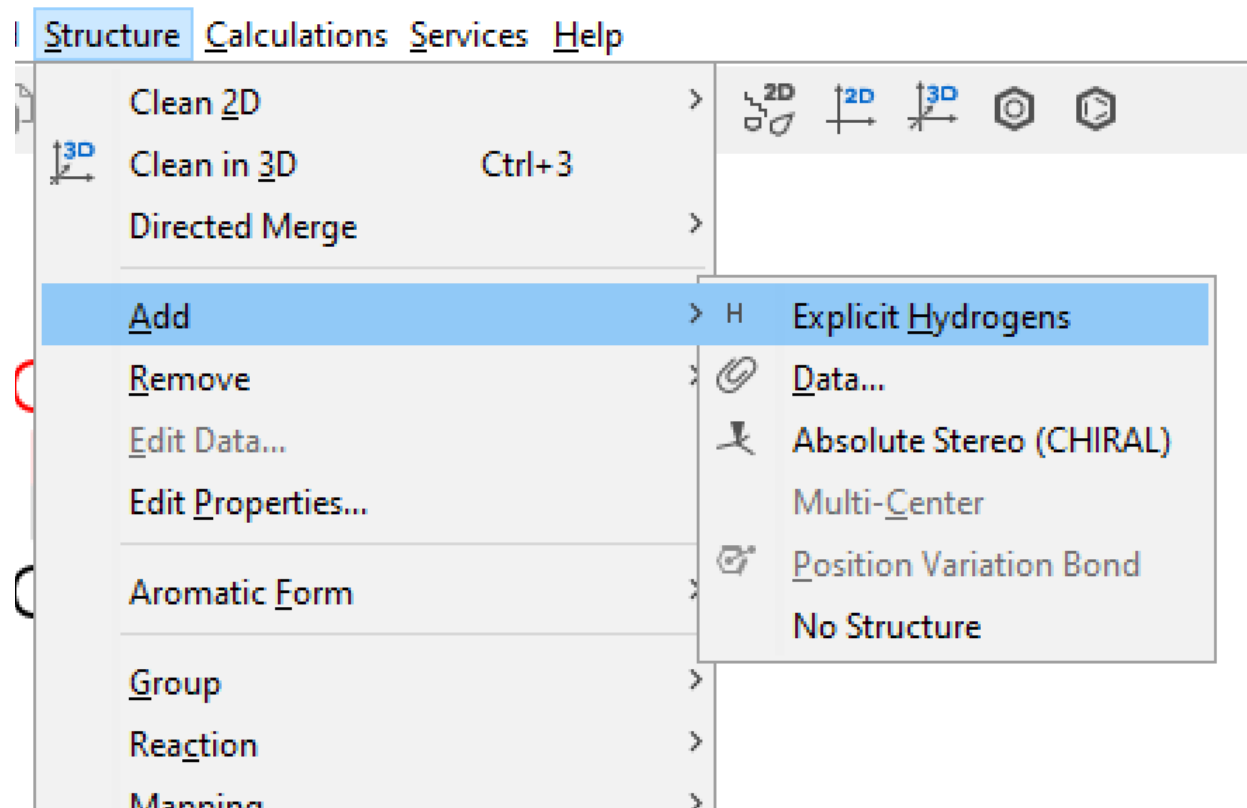
Varmistetaan vetyjen näkyminen **vain "heteroatomien"** yhteydessä (funktionaalinen ryhmä).



Vaihe 3: Jos täydellinen rakennekaava →

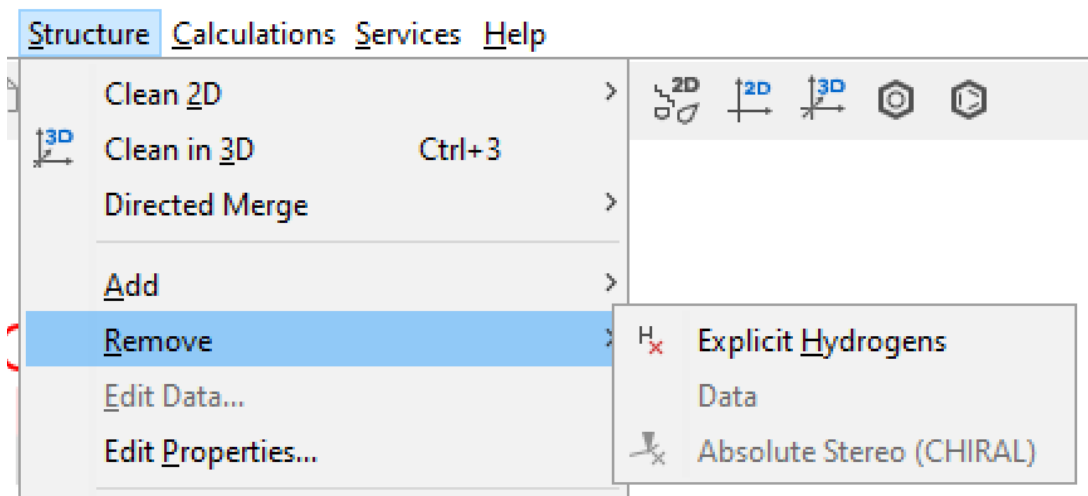
Täydelliseen rakennekaavaan valitaan "Carbon labels" ALWAYS (Preferences -kohdasta). JA

Structure-kohdasta **Add Explicit Hydrogens**



Paluu viivakaavaan?

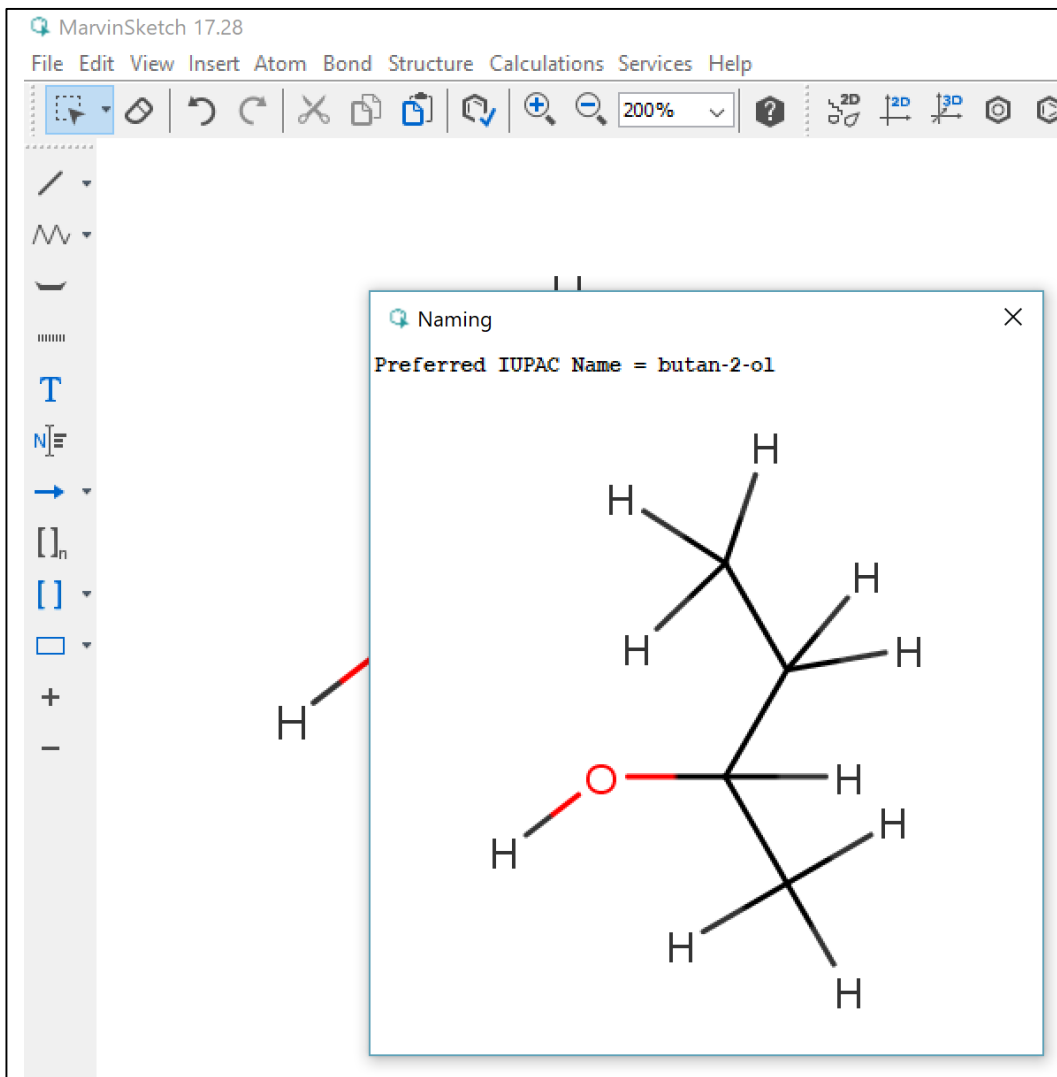
Jos haluaa palata viivakaavaesitysmuotoon. Poistetaan vedyt (viereinen kuva) ja poistetaan hiiliatomien merkinnät (Preferences –osiosta Carbon labels → Never)



MarvinSketch

Pedagogisia valintoja?

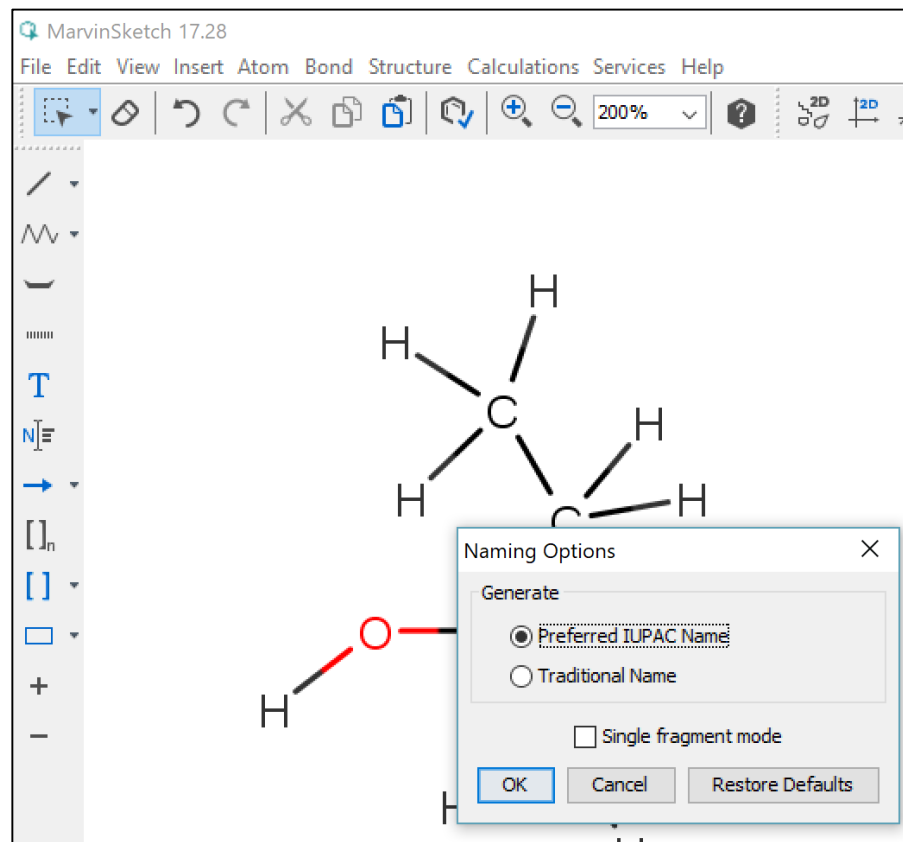
2. Nimeämisen opetus



MarvinSketch nimeää molekyylit (myös Abitti-versiossa)

Miten kurssilla
opetetaan orgaanisten
molekyylien
nimeäminen? Miksi?

MarvinSketch tuottaa
nimet ja toisinpäin –
nimestä rakenteen.



View Inset Atom Bond Structure Calculations Services Help

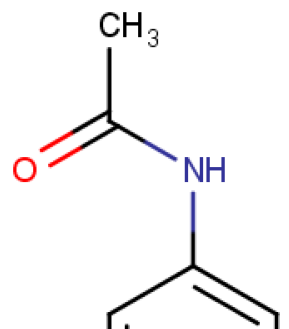
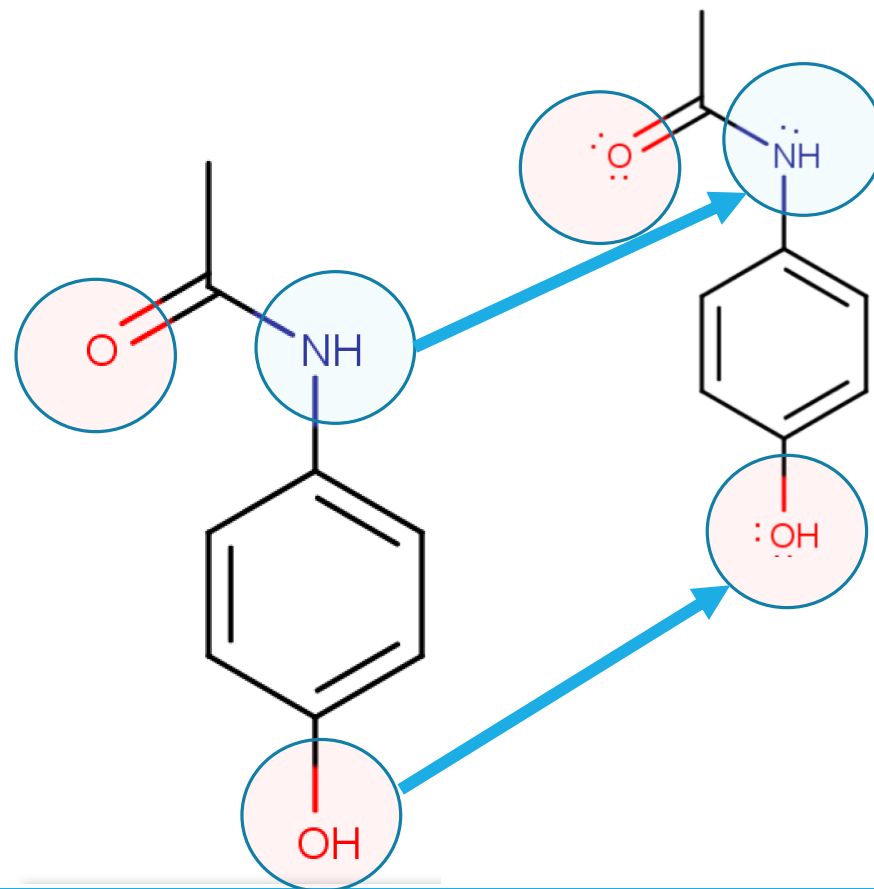
Mouse mode > [Icons] 200% [?]

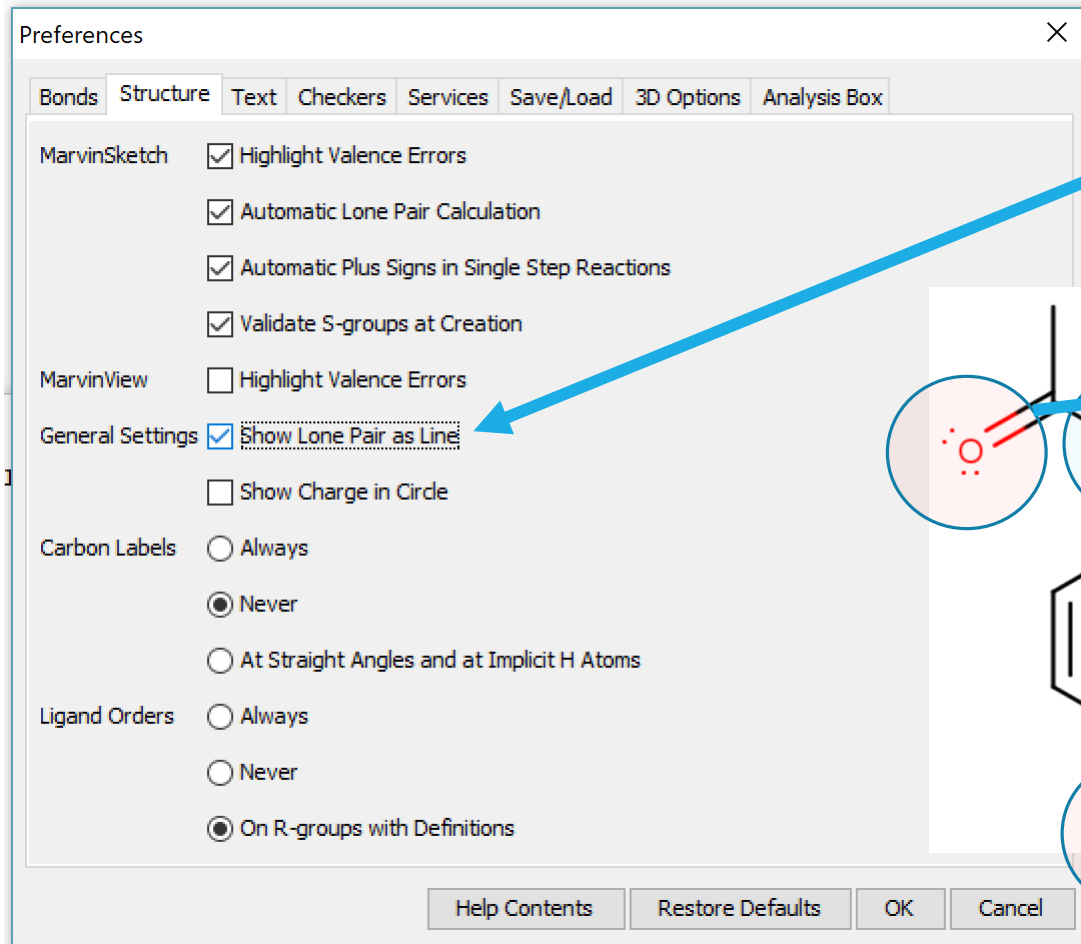
- Zoom Level >
- Structure Display >
- Colors >
- Stereo >
- Implicit Hydrogens >
- Peptide Display >
- Advanced >
 - Atom Numbering >
 - Atom Properties ✓
 - Atom Mapping ✓
 - Bond Lengths
 - Lone Pairs
 - R-groups ✓
 - R-Logic
 - Valence ✓
 - Ligand Error ✓
 - S-group Attachments ✓
- Pages >
- Toolbars >
- Menubar F11 ✓
- Status Bar ✓
- Grid Shift+F9
- Guidelines Ctrl+Shift+F9
- Editor style >

VALITSE

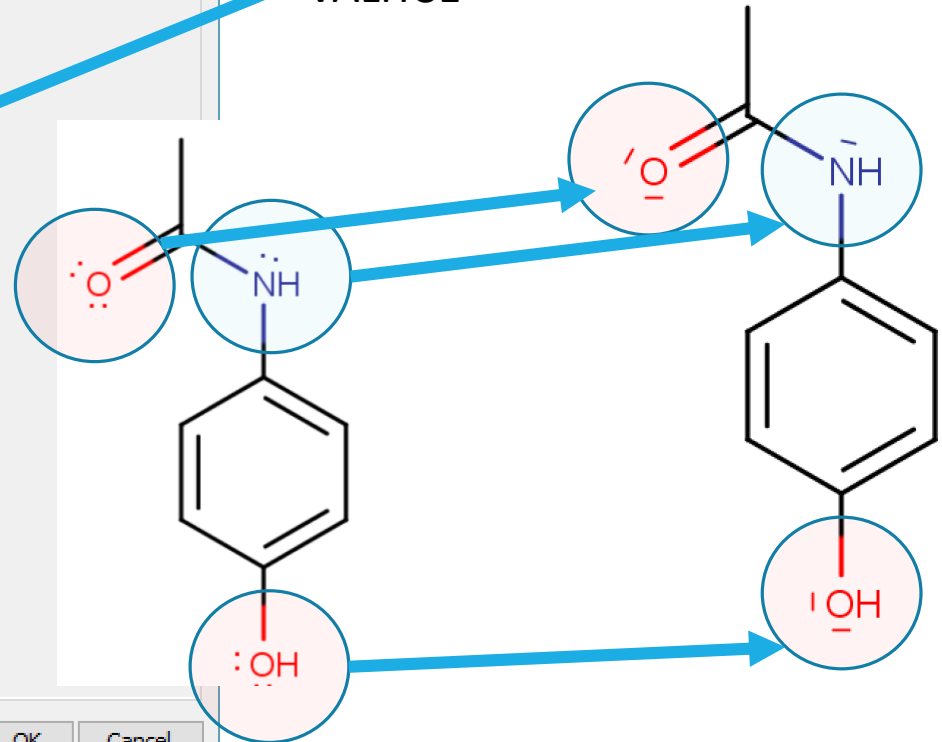
Naming

Preferred IUPAC Name = N-(4-hydroxyphenyl)acetamide



VALITSE



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