Visualizing molecular structures for analysis of NMR spectra

Start in ChemDraw

NOTE: Chemdraw for ND will ask about URL: https://notredame.signalsresearch2.revvitycloud.com

1. Make a molecule in ChemDraw
2. Select it
3. Copy to clipboard in SMILES format: `Edit:Copy As:SMILES`

Load a molecule in Avogadro and optimize geometry

Avogadro manuals are here: https://avogadro.cc/docs/

1. Start a new document: `File:New`
2. `Build:Insert:SMILES`
3. Paste from clipboard (Cmd-V or Ctrl-V), click OK
4. Set view parameters: `Display Settings`, check `Ball and Stick`
5. Right-click to deselect the atoms
6. Optimize molecular geometry by energy minimization: `Extensions:Optimize Geometry`

Parameters of geometry optimization are set in `Extensions: Molecular Mechanics: Setup force field`. For more details on force fields and optimization see https://avogadro.cc/docs/optimizing-geometry/molecular-mechanics/

Distance measurements in Avogadro

1. Rotate the molecule to see both atoms of interest with `Select Tool`
2. Press `Click to Measure` button in the toolbar
3. Click first atom, click second atom
4. Read the distance on the bottom of the screen
5. Clicking on the same atom again removes it from the selection