Reference manuals

Avogadro

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Avogadro

http://avogadro.openmolecules.net/wiki/Main_Page

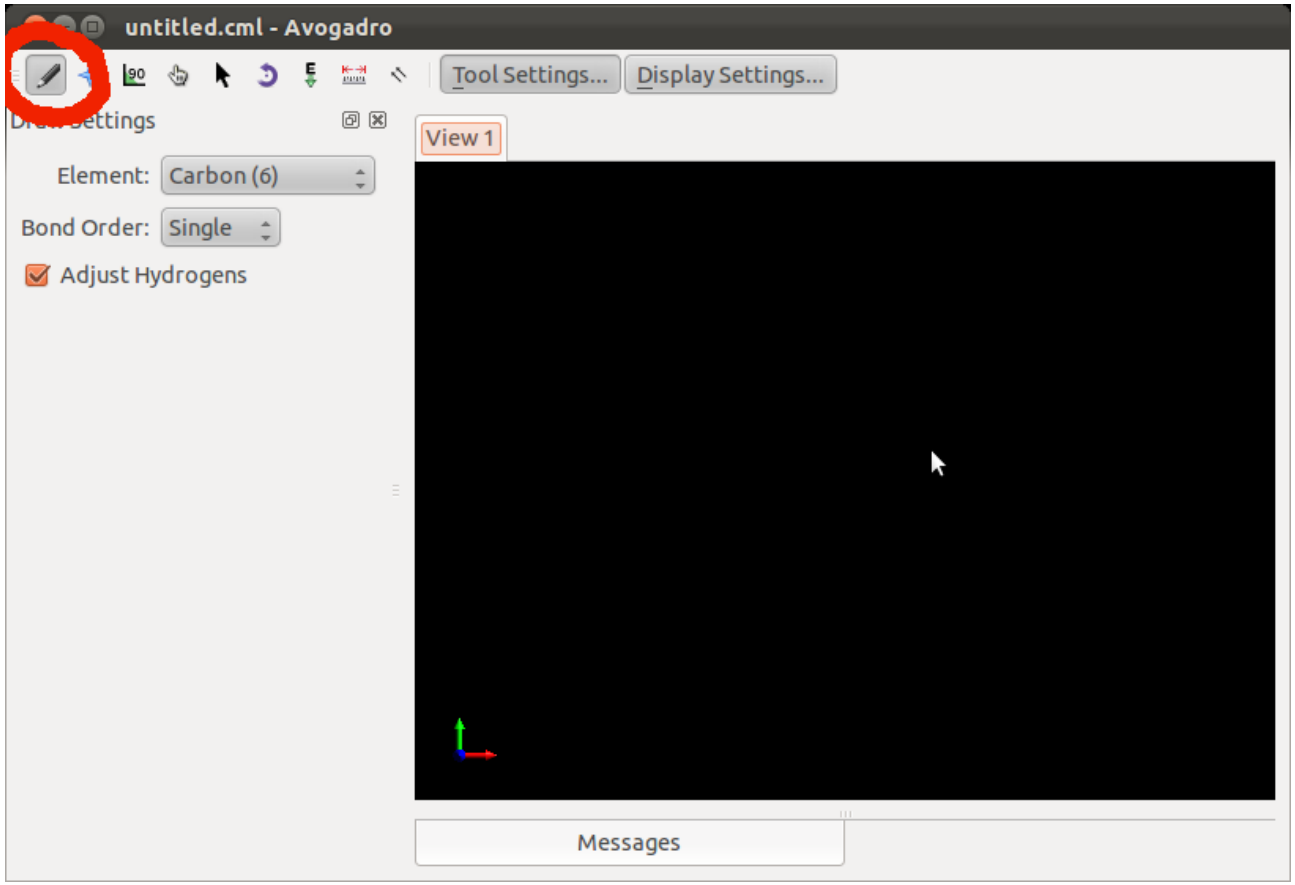
Program for construction and visualization of molecules. Freely available for MS Windows and Linux.

Functionality overview: https://www.youtube.com/watch?v=xdmLoBlLmqs

Building a model

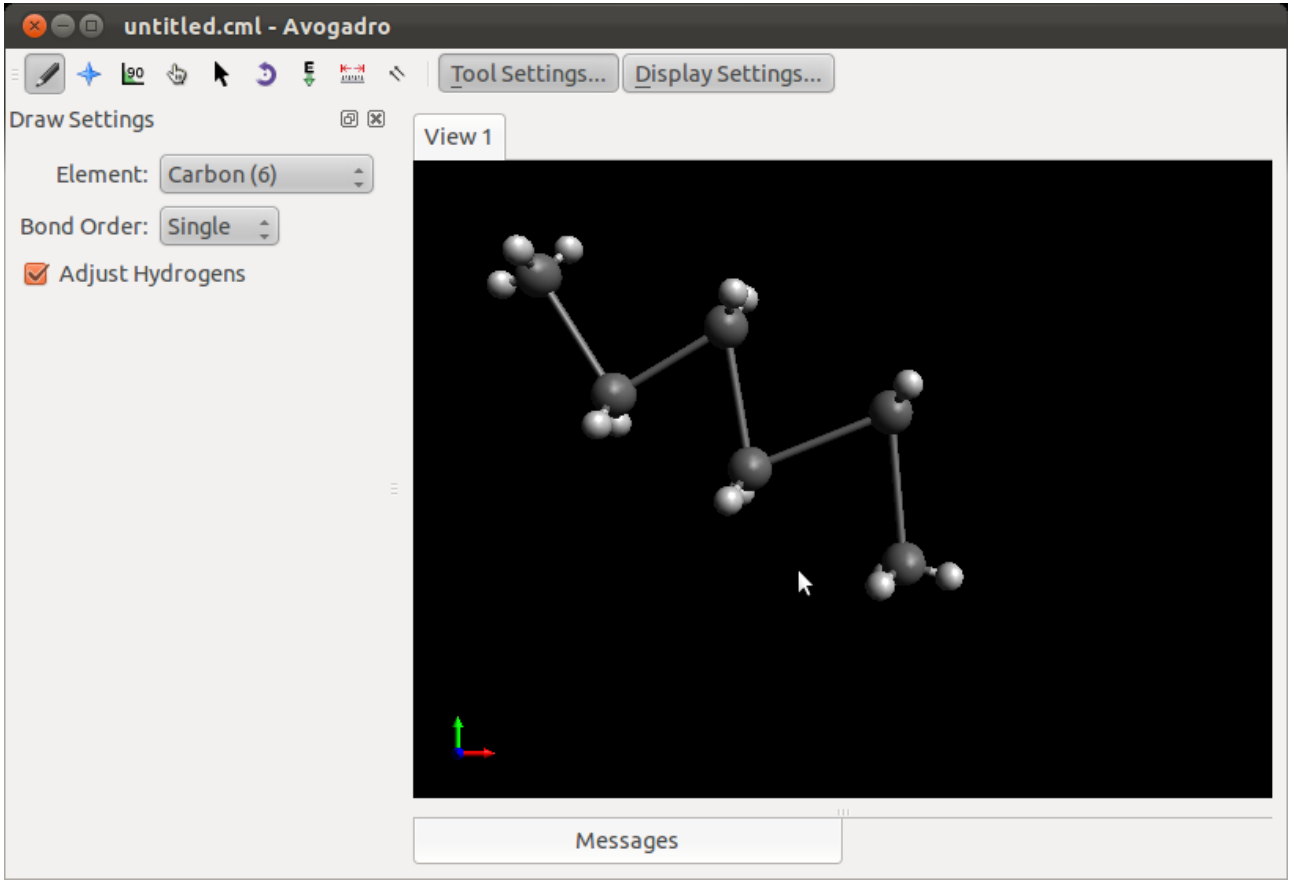
Building a model

You can use the **Avogadro** program to build a 3D model of the reactant and the product. It is a freely distributed program that can be used both under the MS Windows operating system and under Linux clones (e.g., Ubuntu).



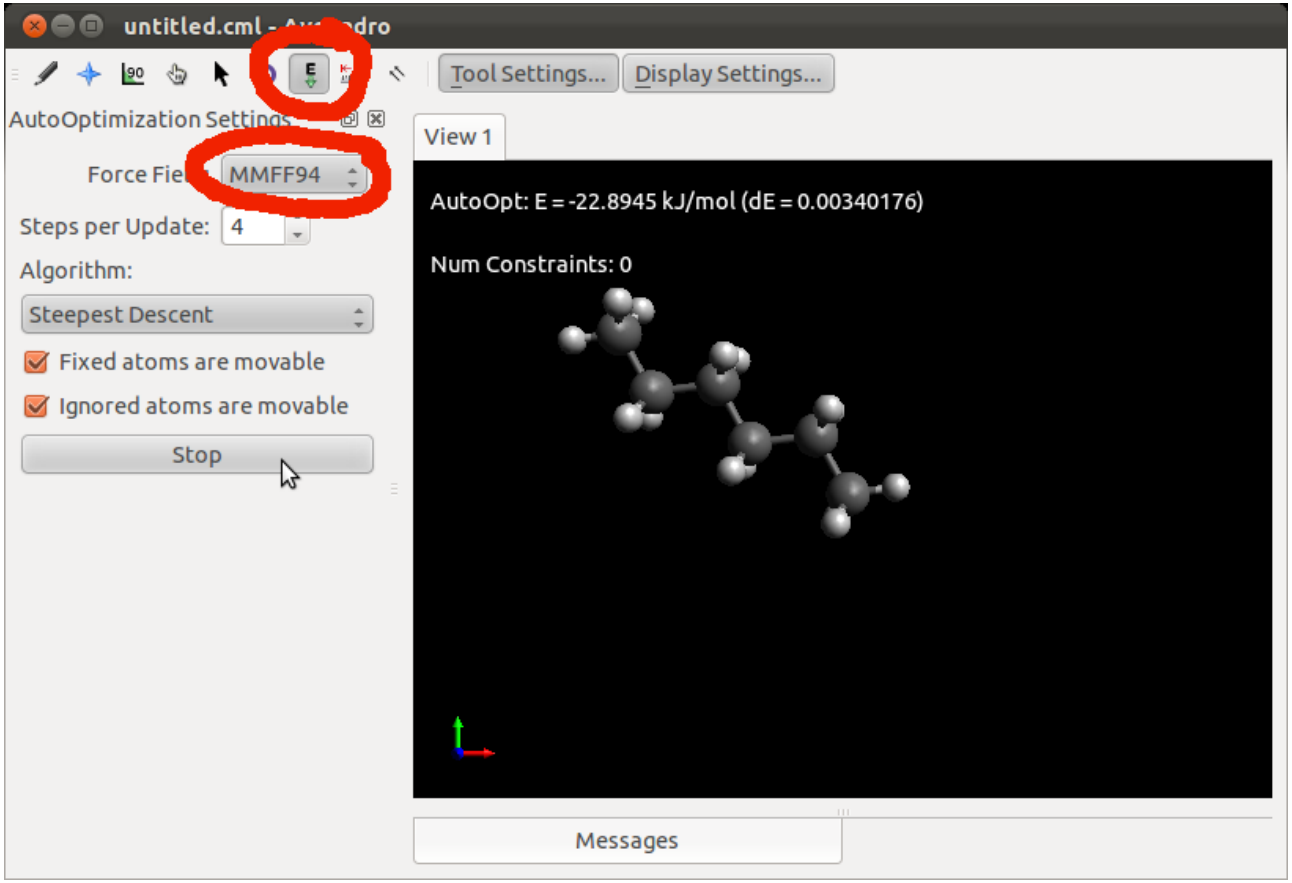
Model draft

When building a molecule, the bond lengths, angles and other parameters of the molecule are not optimal. This is due to the way structures are edited in the Avogadro program. The draft model must therefore be modified by optimizing the geometry before further use.



Model optimization

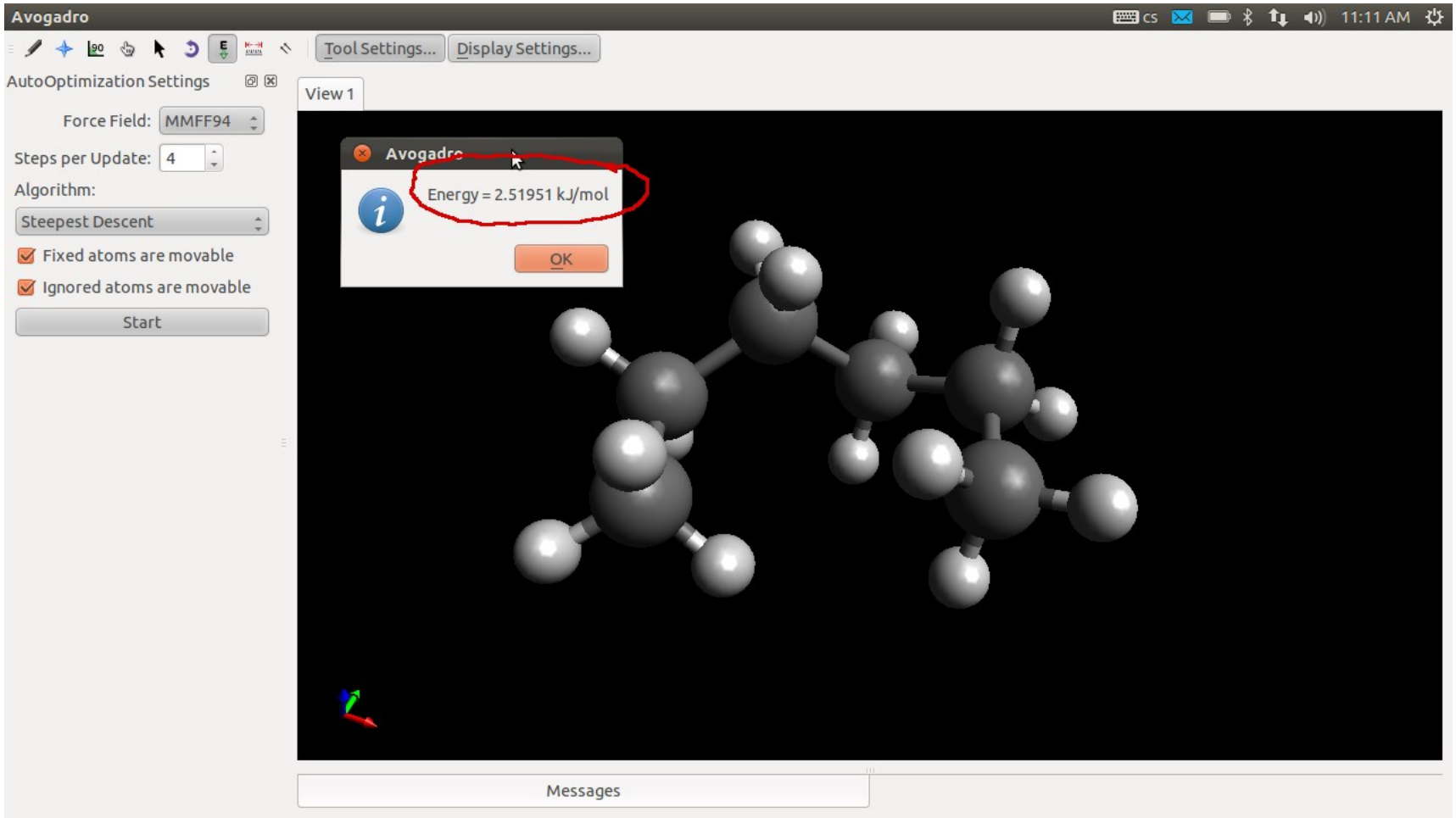
The program uses molecular mechanics (MM) methods to optimize geometry. For it to function properly, you must correctly define bond orders in the structure. Because MM is an empirical method, you must also choose the type of parameterization. In our case, we will use the force field MMFF94.



Searching for the global minimum

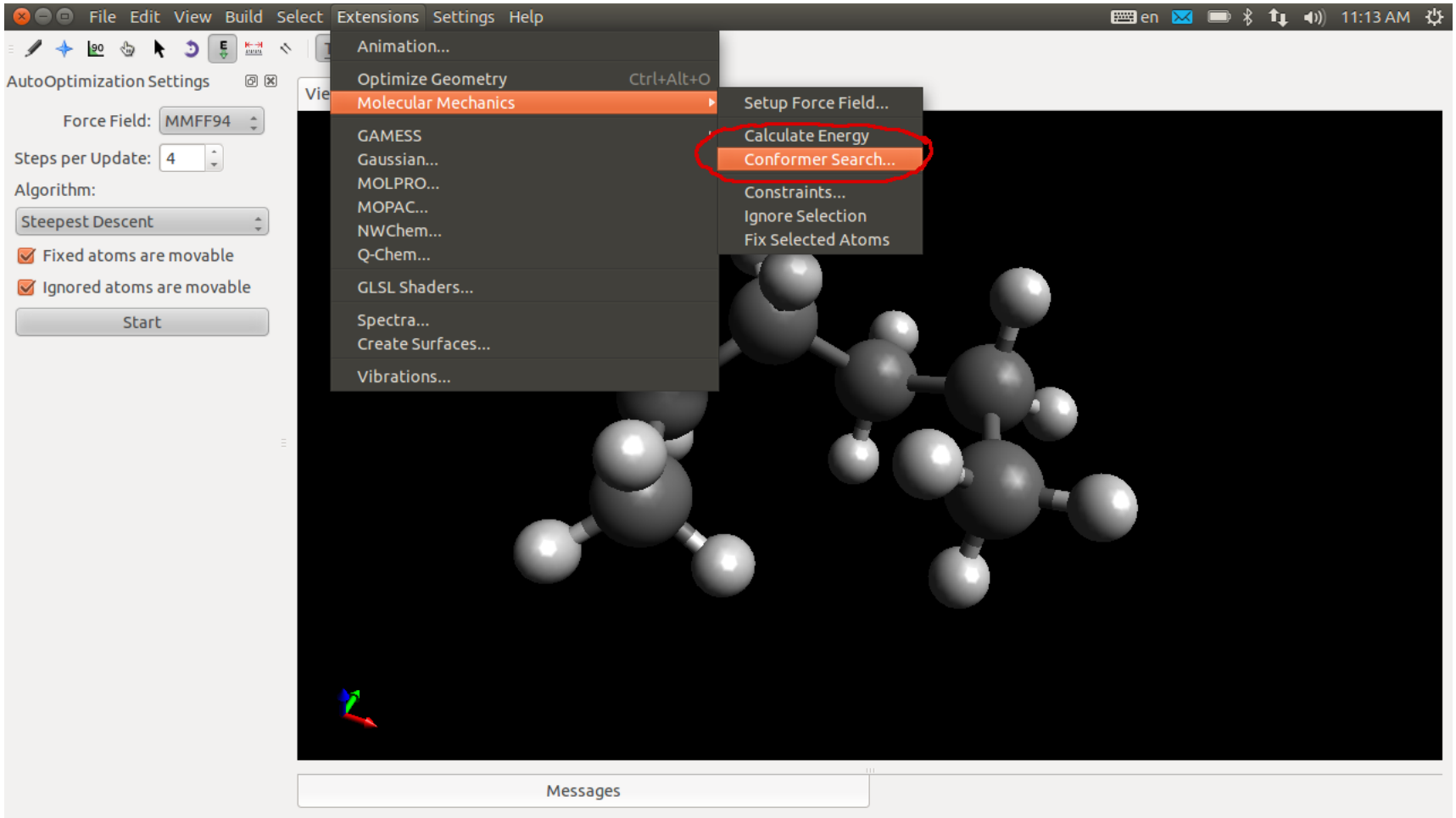
Finding the most stable geometry, I

Default optimized geometry of the hexane has energy 2.5 kJ/mol (MMFF94). It is a local minimum on the potential energy surface, which is not the lowest.



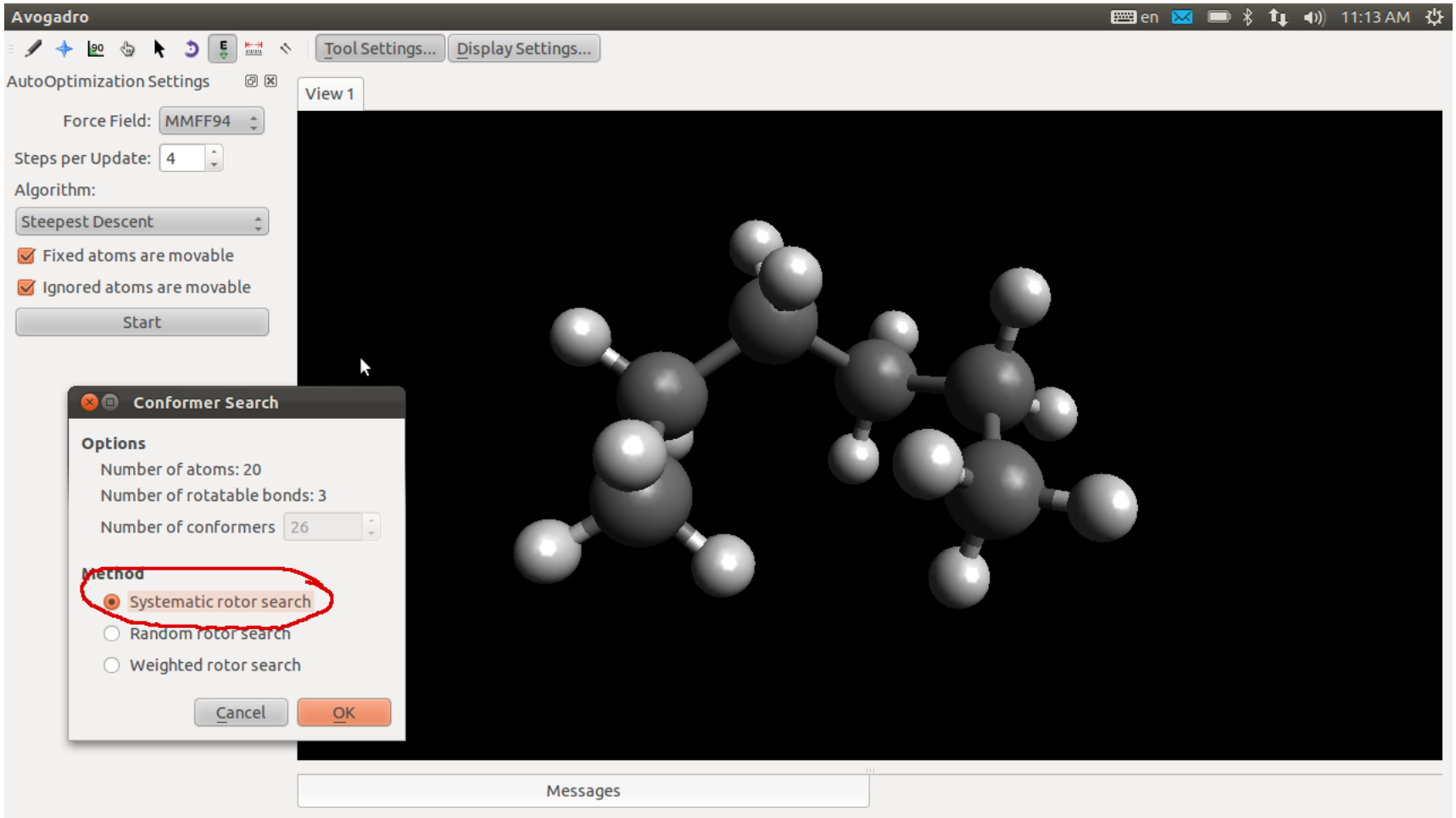
Finding the most stable geometry, II

Avogadro contains methods for finding the most stable conformer (structures).



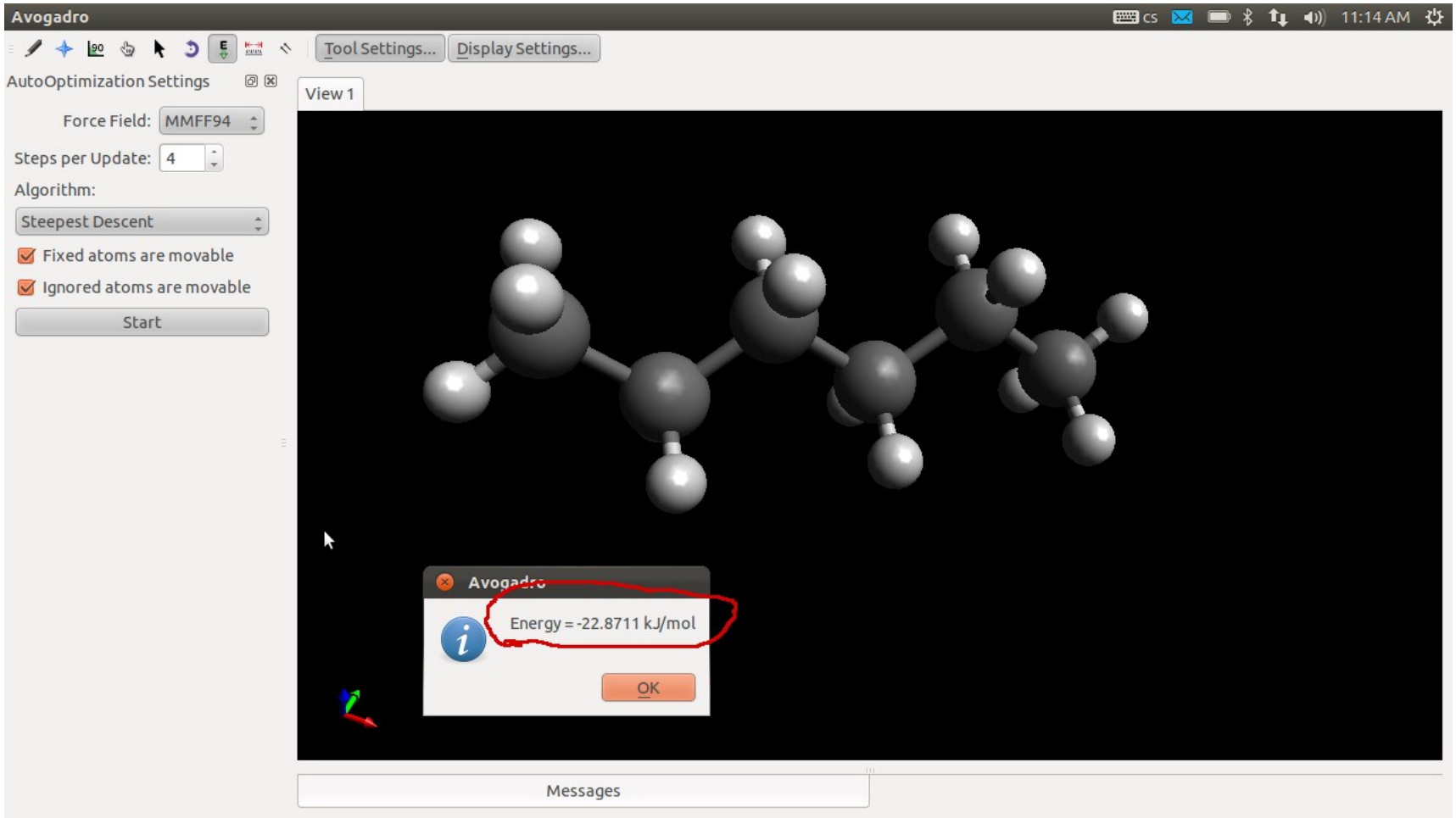
Finding the most stable geometry, III

To find the most stable conformer we will use the systematic search method.



Finding the most stable geometry, IV

The most stable hexane conformer has energy -22.9 kJ/mol (MMFF94). The geometry of the found structure should be optimized again.



Vibration visualization

Vibration visualization

Load **soubor.log**, containing results of vibration analysis, into Avogadro program. A summary of individual normal vibration frequencies can be found in the menu **Extensions->Vibrations.**