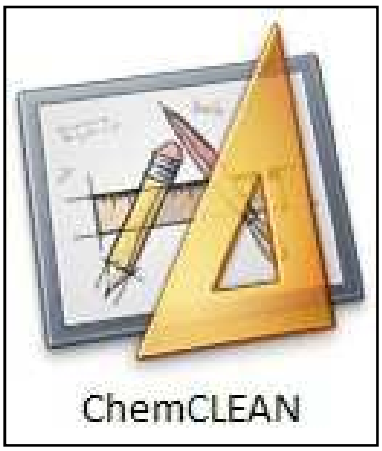
ChemCLEAN 1.0 User Manual

Development version



Department of Pharmacoinformatics

National Institute of Pharmaceutical Education and Research (NIPER), S.A.S. Nagar

ChemCLEAN

Installation:

Download the ChemCLEAN.msi file from the website.

Requirements for Installation:

1. Operating System should be Windows 7, XP, Vista
2. System should have .NET installed

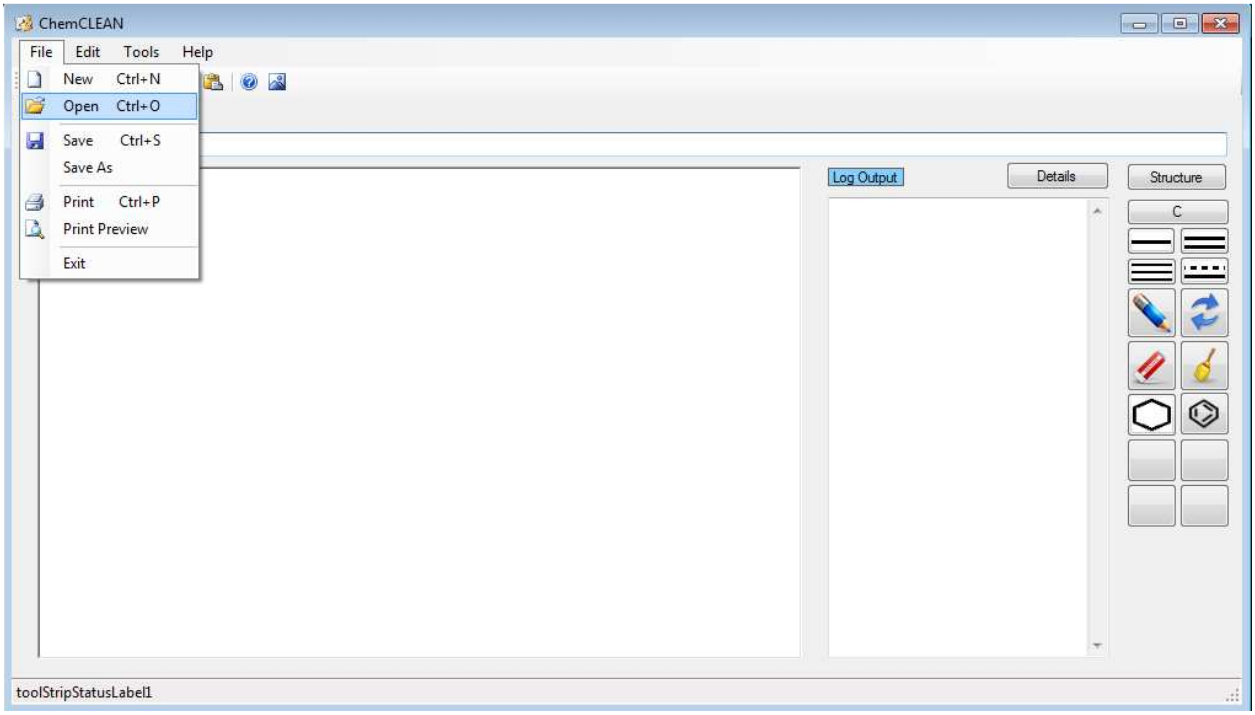
Status of the Tool:

As this ChemCLEAN (Version 1.0) tool is in a developing stage, so this includes the functionality related to structure cleanup of single ring system only. This tool can optimize aliphatic compounds and provides the connectivity table along with their atomic co-ordinates.

INPUT METHODS:

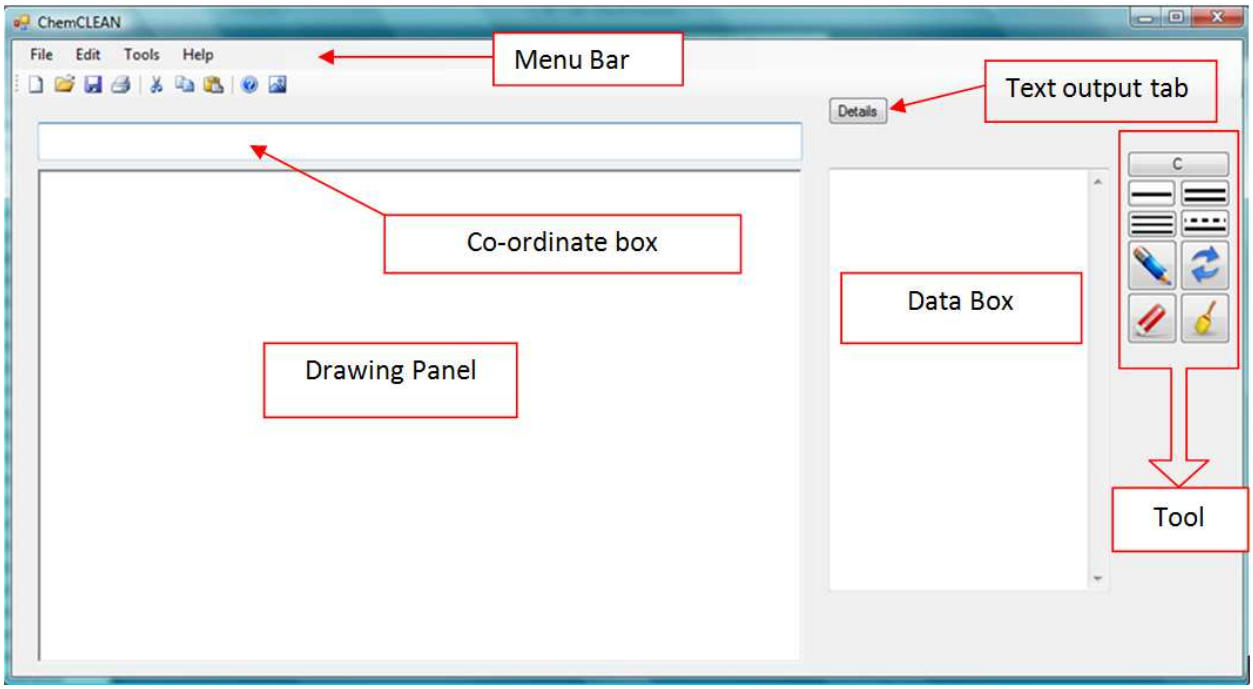
File Uploading:

- File can be uploaded in .mol or .mol2 format
- The uploaded molecule can be optimized using the options in tool bar



Drawing Panel:

Molecules can be drawn and edited using Drawing panel

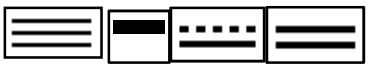


Tool Bar components

Details tab:

It is used for displaying the coordinates of the atom along with connectivity and Aromaticity of the atom in the data box. It displays connectivity and relational table in the data box.

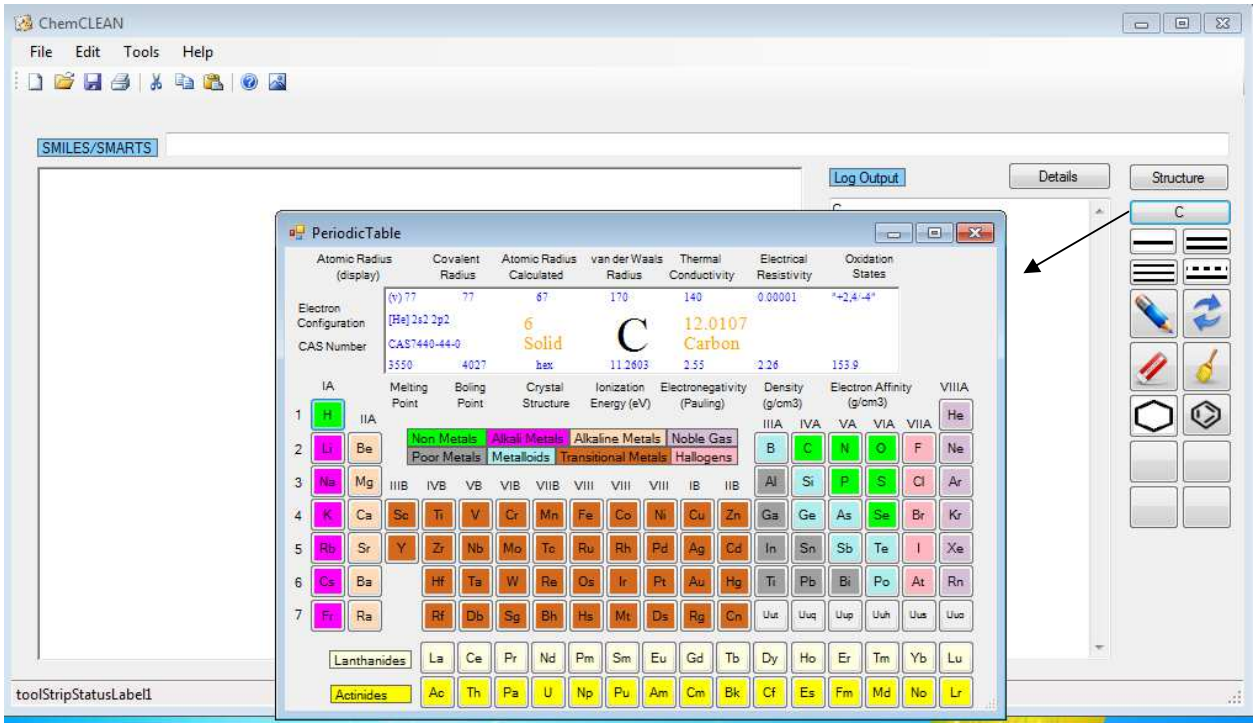
Bond:



Four kinds of bonds can be drawn like single, double, triple and aromatic by selecting through the bonds tab in the tool bar.

Atom:

Atom can be chosen for insertion into the structure from the tab for periodic table in the tool bar section.



Eraser:

Eraser can be used for the deletion of a bond or an atom from the structure drawn. When this tool is selected and then mouse click is made on any node then the atom and the bonds attached to the atom get deleted.

Trash:

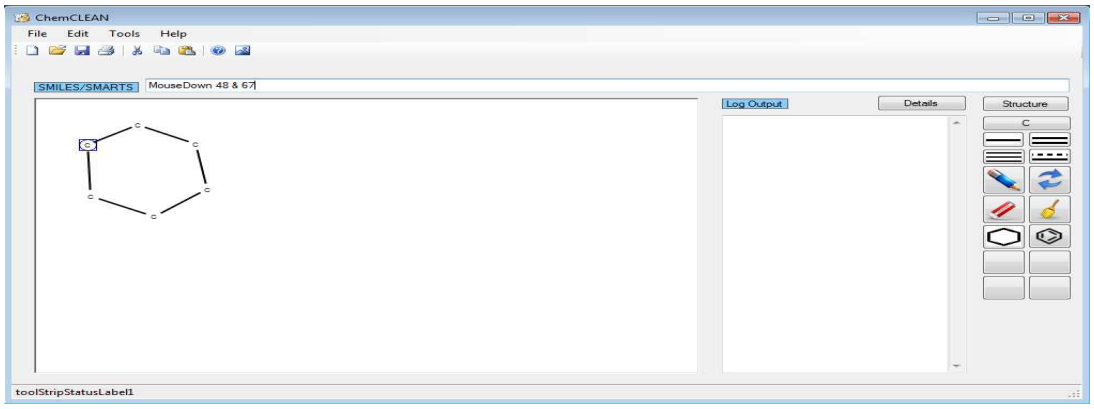
Trash tab is used to erase the whole structure at once and hence to make drawing panel empty for building structure again.

Pencil:

Pencil tab is used to draw the structure. Whenever we will draw a bond using pencil it will also display atom which is selected at that time from the periodic table. Every time when there is need to draw any structure or its fragment which is not in continuation then we have to select this tab.

Clean-up:

Clean-up tab can be used after the structure is completely built. It optimizes the geometry on the basis of constant bond length and the expected bond angle for that particular geometry. For *example :* Benzene



After optimization of the structure