

Vdisplay v1.0

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OVERVIEW

Vdisplay is a 3D graphics program for viewing molecular and atomic properties, including properties computed with VeraChem software. Vdisplay 1.0 reads molecules in SDfile or MOLfile format (See http://www.mdl.com/solutions/white_papers/ctfile_formats.jsp).

In the current version, atoms can be labeled by atom number, element, and formal charge and, if the input file contains this information, by stereo parity. Partial atomic charges computed using VeraChem's Vcharge can also be displayed.

We welcome comments and suggestions. Please send them to support@verachem.com

GETTING STARTED

Simply double-click the Vdisplay icon and then select a SD or MOL file to view when prompted. When more than one molecule is loaded, you can step through the molecules by using your keyboard's arrow keys or the arrow buttons at the top right of the Vdisplay toolbar. Alternatively, you can jump to a specific molecule by clicking on its name in the "molecules loaded" list at the bottom of the Vdisplay window.

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INTERFACE

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Vdisplay's interface is divided into four main sections:

1. Menu/Toolbar along the top
2. 3D Graphics Window – the main application window
3. Control Panel at the left of the main application
4. Molecule Panel at the bottom of the 3D Graphics window

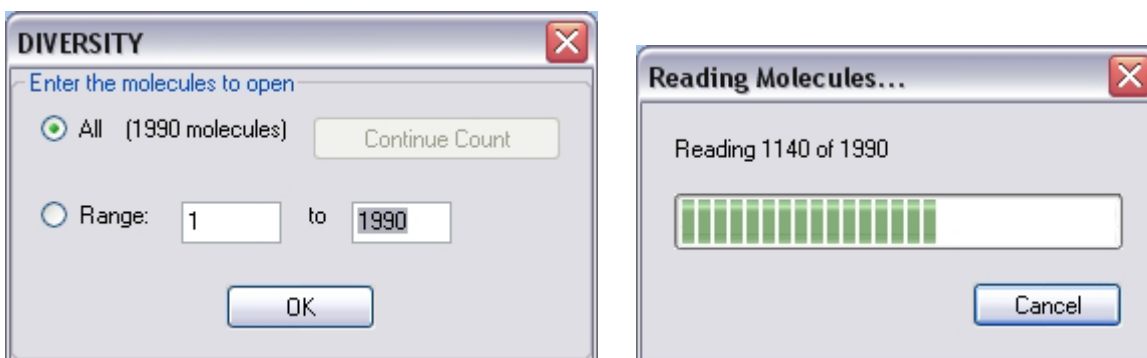
These are illustrated and described below.

The screenshot displays the Vdisplay v1.0 software interface. The window title is "Vdisplay v1.0 - DIVERSITY.sdf". The interface is divided into four main sections:

- {Menu/Toolbar}**: Located at the top, it includes a menu bar (File, View, Help) and a toolbar with buttons for "A-A+", navigation arrows, and zoom controls.
- {3D Graphics Window}**: The central area showing a 3D ball-and-stick model of a complex organic molecule. The text "Labeling: Element" is visible at the top left of this window.
- {Control Panel}**: Located on the left side, it contains several sections:
 - Labels**: Includes a "Label" dropdown menu set to "Element", a "Label All" button, and "Measure" options for "dist.", "angle", and "dih." with checkboxes.
 - View**: Includes "Set Origin..." and "Center" buttons, an "Auto Spin" button, a "Show Fog" checkbox, and sliders for "Fog Density" and "Fog Position".
 - Mouse**: Includes "Commands" (Click: Select-None-Menu; Shift Click: Select-None-Menu; Drag: Rotate-Move-Scale) and "Options" (Quick Select checked).
- {Molecule Panel}**: Located at the bottom, it includes a "Molecules Loaded:" list with entries 479, 1004, 1011, 1012 (selected), and 1013. It also has a "Name:" field with "1012" and a "Number:" field with "4". Below these are fields for "> <CAS_RN>" (5394-35-4) and "> <NSC>". Buttons for "Add", "Remove", and "Remove All" are at the bottom.

File Menu

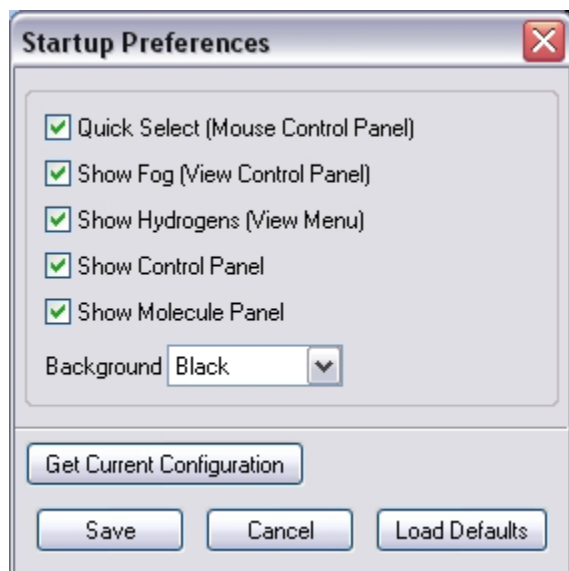
Open... – Opens a Load Molecules file browser. When a file is opened, Vdisplay counts the molecules it contains, up to the first 5000, and displays a dialog box with the number of molecules next to the “All” button. If there are more than 5000 molecules, then “>5000 molecules” is shown, but you may complete the count by selecting “Continue Count”. It is only necessary to continue the count if you would like to know the number of molecules in the file; clicking “All” will load all molecules in the file, regardless of whether or not a full count has been done. To load a range of molecules, type the limits into the Range fields. Leave the “to” field blank to load all molecules from the first listed up to the end of the file. Once loading has begun, clicking on “Cancel” stops the loading process but keeps the molecules already loaded.



After molecules have been loaded, they are listed in the Molecules Loaded list box in the Molecule Panel. The molecule name shown here is the first word of the first line of the molecule’s listing in the MOL file or SDfile. If this name field is blank in the file, the molecular name is listed in Vdisplay as <filename>_mol_<index> where <filename> is the name of the file without the .mol or .sdf extension and <index> is the number of the molecule in the file. For example if the 5th molecule in a file named sample.sdf did not have a name the molecule would be listed as “sample_mol_5”. If a new molecule name repeats one already in use, it is modified by addition of a numerical suffix. For example, if there are multiple molecules named “methyl”, the first will be listed at methyl, the next as methyl(2), the next as methyl(3), etc.

Startup Preferences... – Opens a window allowing the program’s startup configuration to be changed and saved. Each option is discussed below.

- “Get Current Configuration” fills out the preferences with the options currently set in the application.
- “Save” saves the preferences as filled out for use when the application is opened again.
- “Cancel” closes the “Startup Preferences” window without saving changes to the preferences.
- “Load Defaults” restores Vdisplay's default preferences.



Quit – Closes the application.

View Menu

Show Hydrogens – Toggles the display of hydrogens. Turning hydrogens off may make it easier to view the overall molecular structure and some atom labels, especially for complicated molecules.

Hide All Panels – Toggles the display of the “Molecule” and “Control” panels.

Show Molecule Panel – Toggles the display of the Molecule panel.

Show Control Panel – Toggles the display of the Control panel.

Help Menu

Shows this documentation and information about Vdisplay and VeraChem LLC.

Toolbar Buttons

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Six shortcut buttons are provided on the right hand side of the menu/toolbar:



Decrease or increase, respectively the size of the font used for labels in the 3D Graphics window.



Display previous molecule in Molecules Loaded list (= UpArrow).



Display next molecule in Molecules Loaded list (= DownArrow).



Center the molecule and set the center of rotation to the atom closest to the center of geometry of the molecule.



Select the atom to be used as the center for rotation of the molecule. The next atom selected will be used as the center.

3D GRAPHICS WINDOW

This window displays the current molecule along with status information bars on the top and bottom. The top status bar shows the currently selected labeling option. The left side of the lower status bar shows helpful hints and the right side shows the atom-selection option that is currently active.

How to move the molecule:

Rotate: hold left mouse button down and drag.

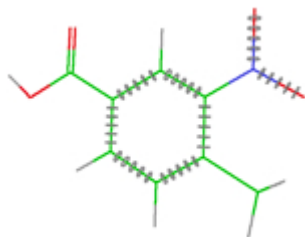
Translate: hold middle mouse button down and drag. (Moves molecule without rotating it)

Zoom: hold right mouse button down and drag up to zoom out and down to zoom in.

To make the molecule rotate continuously, use Auto Spin in the View sub-panel of the Control Panel.

Right click menu: All the functions in the Control Panel and Molecule Panel are accessible with a right mouse click on the background of the 3D Graphics Window. This is useful when one has hidden these panels in order to have a larger viewing area. This menu options are as follows:

Mouse	shows Mouse sub-panel in a separate window
View	shows View sub-panel in a separate window
Labels	shows Labels sub-panel in a separate window
Molecule List	shows Molecules Loaded list in a separate window
Full Screen	toggles the display of both the Molecules and Control panels
Show Molecule Panel	toggles the display of the Molecule panel.
Show Control Panel	toggles the display of the Control panel.
Remove Molecule	removes selected molecule from the Molecules Loaded list
Remove All	removes all molecules from the Molecules Loaded list
Load Molecule	brings up the Load Molecules browser.



Note: The MOL/SDfile format allows for ambiguous bond orders such as “single or double”. Vdisplay marks bonds with ambiguous bond orders as shown here

CONTROL PANEL

The Control Panel contains three sub-panels: Labels, View and Mouse, as described below. Each sub-panel can be closed by clicking on its main sub-panel button. A sub-panel can also be separated from the main window by right clicking on its main sub-panel button; to return the sub-panel to the Control Panel, just close it by clicking on the small “x” in its upper right corner.

Labels

Atoms can be labeled by Atom Number, Element, Formal Charge, MOLfile Atom Parity, and (if displaying the results of [Vcharge](#)) Partial Charge. An individual atom can be labeled by left-clicking on it and all atoms can be labeled by clicking on Label All. All labels can be cleared by clicking on the Clear All button, and clicking on the Clear Last button removes the label from only the last item labeled.

The Label All button is a toggle: when it is on, molecules will continue to be labeled as one changes the label type or moves from one molecule to another.

Atom-atom distances, angles and dihedrals, can be measured by clicking on the “dist”, “angle” and “dih.” buttons, respectively, and then clicking on the two, three or four atoms of interest.

Note: If you prefer not to have atoms labeled or selected by a simple left-click, you can deselect Quick Select in the Mouse sub-panel (see below). Shift-left-click then becomes the labeling/selection method. This option can also be made your personal default via File... Startup Preferences.

View

- Set Origin – allows selection of the atom used as the center of rotation (i.e. the “origin”).
- Center – centers the molecule and resets the center of rotation to the atom closest to its center of geometry.
- Auto Spin – rotates the molecule continuously about a vertical axis.
- +/- toggle – reverses the direction of the Auto Spin rotation.
- Show Fog – turns 3D depth-cuing fog off/on. Note that if Show Fog is off the Fog Density and Fog Position sliders are disabled.

Fog Density – modifies the density of the fog. To increase the fog density, move the slider to the right.

- Fog Position – moves the position of the fog. Slide right to move the fog toward the viewer, left to move it back.
- Background – changes the background color of the 3D Graphics window. Current options are Black (default), White and Light Grey.

Mouse

The Commands box displays a reminder of how the mouse functions when the cursor is over the 3D Graphics Window. In the screen shot shown above, for example “Select--None--Menu” is displayed below “Click”. This means that clicking the left mouse button will select an atom, clicking the middle mouse button will do nothing, and clicking on the right mouse button will bring up the right-click menu (see above).

Quick Select – Controls the method of selecting an atom. When QuickSelect is active, a left mouse click will select an atom. When QuickSelect is not active, selecting an atom requires a Shift-left-click. This option avoids accidentally selecting atoms while scaling, translating, or rotating the molecule. The current status of Quick Select is displayed in the right portion of the lower status bar, and Startup Preferences in the File menu can be used to save your preferred selection mode.

MOLECULE PANEL

Use the Up-Arrow and Down-Arrow keys to step between molecules in the list if the mouse focus is in either the 3D Graphics window or the Molecules Loaded list. To find and select a molecule by name, type its name as listed in the Molecules Loaded list into the Name field above the information box. The wild cards ‘*’ and ‘?’ may be used, where ‘*’ matches any non-specified characters and ‘?’ matches any single character. You can also select a molecule entering its index (order number) in the Number field and hitting Enter.

An information box below the Name and Number fields contains information from the data block section of the MOL/SDFfile, including any generated by VeraChem software. For example, if the SDfile read into Vdisplay came from a Vcharge run, any warning or error messages for each molecule will be displayed here.

Add

Clicking on the Add button below the Molecules Loaded list brings up a file browser (see File → Open, above)

Remove

Selecting a molecule in the Molecules Loaded list and clicking the “Remove” button removes (unloads) the molecule from Vdisplay.

Remove All

Removes (unloads) all molecules from Vdisplay.