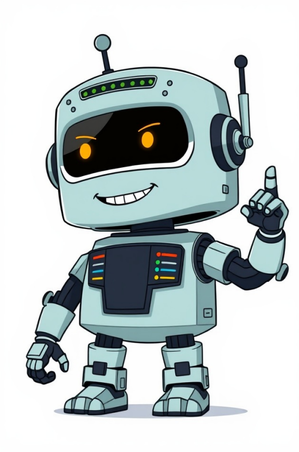
Click to verify



Enable Javascript inorder to use PubChem website. The pubchem 3d viewer consists of several interface elements that provide different views of 3D structures and organize acces to multiple commands and options in the program. The application window is split into three sections: the tabbed 3D Viewers on the left, the tabbed Controls section on the right and the Information section at the bottom of the application window. Toolbar Open... Open a new molecule file - loads a new molecule from one of the supported file formats. Note that the compounds loaded before this operation will be discarded. Add molecules into your environment - loads more molecules from files, but maintains the previously loaded conformers in the PC3D Viewer. Close molecule files - closes opened molecule files. Save... Save current molecules into a molecule file - saves current molecules into a PubChem 3D file. Save current overlay view as an image - saves current overlay view into an image file. Preferences - shows/hides Control Windows. Help - displays this page. Overlay Structure Viewer - allows users to see single molecular structure or to overlay multiple structures in a single coordinate system. This view is ideal for observing a single molecule in detail and/or for looking at structural overlap of different conformers to see similarities and differences in molecular structures. Tiled Structure Viewer - provides ability to show multiple molecules in different tiled sections of the viewer. This view is designed to browse multiple conformers and analyse overall 3D coverage of conformer space. Double clicking on any given conformer tile will show that particular conformer in an overlap view. Note, that this viewer is enabled only if multiple conformers are loaded into the PC3D Viewer. Control Windows Options - provides ability to customize the appearance of the graphical elements in molecular visualization and tune the behavior of the PC3D Viewer. Clicking (+) or (-) signs on the tree node allows access to preferences arranged hierarchicaly into three main groups: General - controls rendering options affecting the appearance of the molecule as a whole. Image Quality - higher values generate images of greater qualities, but may decrease the speed of keyboard and mouse rotations. Light Model - allows to use different lighting on the molecular scene. One may toggle the ambient light, emmisivitiy of atomic and bond surfaces, add or remove highlights and shininess. Background Color - specifies the color of the 3D viewer window not occupied by the molecule. Viewing Angle - controls the amount of perspecive in the projection. Higher values are equivalent to looking from the objective of an ultra-wide angle camera and show nearby objects scaled bigger and further objects appearing smaller. Smaller values of viewing angle turn the appearance of the molecule into flatter projection with less perspective scaling. Scale Strategy - toggles between different scaling modes of the molecule into the viewing area. User may chose not to scale, or scale only once at the loading time of the molecule, or to scale relative to the first conformer shown, or use all conformers for scaling. Orthogonal Projection - toggles between perspective and orthogonal modes of projection. In orthogonal mode objects appear at the same scale regardless of distance; in perspective mode further objects are scaled down. Shortcut 'O'-key. Hide Coordinate System - toggles the visibility of reference coordinate system. Shortcut 'C'-key. Hide Box - controls the visibility of virtual box containing the molecule. Shortcut 'X'-key. Transparent Conformers - toggles the transparency of conformer overlaps. Note, that the reference conformer (the first visible) is always shown opaque regardless of this flag. However, the following conformers are affected by this flag. Show Pharmacophores - toggles the visibility of pharmacophores. Shortcut 'G'-key. Show Mol-Info - toggles the visibility of molecular information in tiled structure viewer. Shortcut 'I'-key. Conformer Opacity - defines how transparent are the non-reference conformers. Lower values of opacity correspond to transluscent appearance and higher values make query conformers look more solid. Pharma Scale - determines the relative size of Pharmacophores. Atoms - includes options affecting the appearance of chemical elements in the drawing. Atom Scale - determines the relative size (radius) of atomic spheres. Atom Coloring - controls the color schema for rendering atoms: Element Specific - uses conventionally accepted coloring for elements: Carbons as Gray, Oxygens as Red, Nitrogens as Blue, etc... Conformer Specific - colors all atoms of molecules to the same color, specific to the particular conformer. Conformer colors are assigned at the loading time. These are predefined enumerated colors designed to best represent differences in conformer overlaps. Conformer Specific Carbon - carbons follow conformer specific coloring mode, all other atoms follow element specific schema. Black Carbon - renders carbons as black spheres, other atoms are colored according to their element specific color. Non Specific - colors all atoms in a single light gray. Atoms Invisible - toggles the visibility of atomic spheres. Shortcut 'A'-key. Symbols Inivisible - controls the visibility of atomic Symbols. Shortcut 'S'-key. All Same Size Atoms - dictates to render atomic spheres uniformly, not proportional to their covalent radii. Hide Hydrogen - toggles the visibility of Hydrogen atoms. Shortcut 'H'-key. Hide Carbons - toggles the visibility of carbon atoms. Shortcut 'Q'-key. Atom Info - toggles the information shown on atomic spheres. User may choose to show corresponding chemical element's symbol, periodic number of the element, the serial number of atoms in the conformer, the charge or the isotopic mass of the element. Bonds - consists of preferences influencing the appearance of bonds. Bonds Invisible - controls the visibility of bonds' cylinders. Shortcut 'B'-key.Conformer Colors and Coloring Modes Conformer colors are predefined enumerated colors designed to best represent differences in conformer overlaps. Conformer Specific Carbon - carbons follow conformer specific coloring mode, all other atoms follow element specific schema. Black Carbon - renders carbons as black spheres, other atoms are colored according to their element specific color. Non Specific - colors all atoms in a single light gray. Mimic Atom Coloring - makes the coloring of bonds similar to coloring of atoms, whatever the choice. Bond Info - selects the information shown on bonds. User may choose to see bond lengths or bond orders. Bond Width - determines the relative thickness of bonds cylinders. Log - is designed to provide information about the molecular structure, and about success or failure of operations performed. The content of this window can be copy/pasted, edited and manipulated manually to create a operation journal. Context Menu - organizes easy access to the most frequently used commands, provides shortcuts and brief description of commands' behavior. Commands are arranged into three main groups: Mouse Move Rotate Z - rotates around Z axis. Rotate X/Y - rotates around X and Y axes. Zoom - zooms in or out. Scroll - scrolls up or down in tile viewer. Commands Scale - toggles between different scaling modes of the molecule into the viewing area. User may chose not to scale, or scale only once at the loading time of the molecule, or to scale relative to the first conformer shown, or use all conformers for scaling. Align - operations aligning the molecule along predefined axes. User may chose to align the compounds along positive (+) or negative (-) direction of different principal axes of intertial coordinate system. Tile - commands toggling between overlay and tile viewer. Style - commands toggling the predefined rendering styles. Next - selects the next molecule in tile viewer. Previous - selects the previous molecule in tile viewer. Continous Rotation Mode - toggles continoutly rotations mode. In this mode the very last mouse rotation operation is repeated continoutly until the user stops either by pressing Escape or by using the shortcut 'T'-key again. Othogonal - toggles between perspective and orthogonal modes of projection. In orthogonal mode objects appear at the same scale regardless of distance; in perspective mode further objects are scaled down. Show/Hide Box Molecule Info Atoms Bonds Symbols Hydrogen Carbon Mesh Features The following file formats are supported by NCBI PubChem PC3D Viewer: PubChem Compound Files - PC3D Viewer supports generic NCBI PubChem molecule definition formats available for export at //pubchem.ncbi.nlm.nih.gov: PubChem Compound - provides one ore more conformer geometries for a single Compound object from PubChem databases. PubChem Compound files are available at PubChem compound summary pages for download. Note that some compounds do not have 3D geometries stored in PubChem databases. For such molecules this viewer will not be able to render a 3D image. While loading these files the 3D Viewer performs rotational and translational operations to the geometry of the molecule to align those with the intertial frame of reference where Z-axis corresponds to the highest rotational momentum and X-axis corresponds to the lowest. This aligns the molecules to appear flattest on the screen given the initial positioning of the viewport. At the same time molecules are shifted to the their geometrial center (not the center of mass) to create visually appealing, centered image of the chemical structure. PubChem Compounds (plural) - provides a list of multiple 3D structures from different Compound objects. Those objects are assumed to be aligned to each other by one of the conformer alignment routines at PubChem. While loading such files the viewer will not attempt to cross re-align such molecules, but will translate all those geomteries into an intertial coordinate system of the first compound in the list. Thus, the cross-alignment present in the PubChem Compounds (plural) object is preserved. PubChem Substance - provides one or more deposited structural records related to a single substance. Usually these geometries are not computed by PubChem tools, but are provided by PubChem depositors as a part of their initial deposition record. Note that all three native formats can be packaged into files with extensions .pc3d, .asn or .asnt. Native file types are registered by PC3D Viewer during installation on users PC as pc3d_compound. Corresponding MIME type is registered as chemical/x-pc3d. SDF Files - provides a single molecular geometry in a text ASCII format according to CTFile format description. For comprehensive coverage on this topic see the provider's documentation. SDF file may or may not contain bonding information in which case the bonding will be deduced from the coordinates of atoms and covalent radia of correspodning elements. Compressed Molecular Files - provides a compressed molecular file in gzip format. XYZ Model Files - provides a single mlecular geometry in a text ASCII formated file. Such file consists of a single header line with the number of atoms followed by an empty line, followed by coordinate input lines. Each coordinate line has the chemical symbol followed by three coordinates (x,y,z). Note, that XYZ files do not have bond information encoded in them, this is deduced from distances between atoms based on the covalent radia of participating elements. This, although usually a good approximation, is not always accurate for chemicals with non-covalent bonding. Rotation X,Y rotations around the viewers x,y coordinate axes can be achieved by simple mouse drags on a 3D viewer area. Moving the mouse vertically while left button is pressed will rotate the molecule around user's equatorial x axis creating an impression of molecule following after the drag. Correspondingly, the horizontal mouse movements will turn the molecule around user's axial y direction. Holding the Ctrl key while rotating the mouse pointer around the center of the view will perform a rotation of a molecule around viewing z axis. Again, an attempt is made to create impression of a molecule following mouse movements. To achieve similar rotation results user may press Left and Right arrows keys on keyboard for equatorial rotations, Up and Down for axial rotations and Home and End for rotations around the viewing direction. The rotations by keyboard are performed by a larger increment of 15 degrees. Moving dragging the mouse pointer around the 3D viewer area can be used to create more precise rotations. The molecular viewer allows for precise control over the molecule's orientation using the mouse and keyboard. By holding the left button and pressing the Shift key, the molecule will move in response to the mouse pointer's direction. This movement is centered around the center of rotation, which is distinct from the center of view. Scaling can be achieved by rolling the mouse wheel with the Ctrl key pressed. This operation zooms the molecule into or out of focus, simulating a scaling effect without altering its actual geometry. However, when using the autoscale mode continuously, this operation has no impact as the renderer automatically readjusts to fit the best view. In tile mode, these operations not only apply to the viewer under the mouse but extend to all other tiles, enabling users to inspect molecules displayed in smaller screens from identical viewpoints. By pressing and holding the Alt key during these actions, the effect is limited to the single molecule under the cursor. To align a molecule with predefined positions along the main axes of the coordinate system, users can press arrow keys while maintaining the Ctrl key. This allows alignment along positive or negative directions of the user's equatorial axis (Ctrl+Left or Ctrl+Right), axial direction (Ctrl+Up or Ctrl+Down), and viewing direction (Ctrl+Home or Ctrl+End). Navigating through multiple geometries loaded into PC3D Viewer can be achieved by pressing 'N' for next or 'P' for previous, making the next/previous molecule visible while hiding the currently displayed conformer. This feature enables users to sequentially observe the geometries of molecules. Selecting atoms using a left mouse button click provides information about the selected atom, including its coordinates. By selecting multiple atoms, users can view not only their positions but also distances, flat angles, and torsion angles between them. Notably, there is a limit of four atoms that can be selected simultaneously, with any additional selection causing the initial atom to be deselected. This page provides an overview of the Globally Harmonized System of Classification and Labeling of Chemicals (GHS), developed by the United Nations to standardize chemical regulations across countries. It covers GHS hazard statements, pictograms, signal words, hazard classes, categories, and precautionary statements. The safety guidelines for handling and storing hazardous materials are crucial to prevent accidents and ensure a safe working environment. The chemicals listed below fall under various categories of danger, ranging from highly flammable gases and liquids to corrosive substances. For those who come into contact with these dangerous materials, it's important to take the necessary precautions, such as wearing protective gear like gloves, goggles, and masks. It is also essential to follow proper storage procedures, including keeping them in well-ventilated areas and using appropriate containers to prevent leakage or spillage. Some of these hazardous substances can catch fire spontaneously if exposed to air, while others may react explosively even in the absence of air. This highlights the importance of handling each substance with extreme care. When working with flammable gases and liquids, it's also vital to ensure that there are adequate ventilation systems in place to prevent fires from starting due to incomplete combustion. There are substances listed here that can cause severe injuries if not handled properly. Some can cause burns or respiratory problems upon exposure, so proper training is necessary for those who will be working with these hazardous materials. To maintain a safe working environment and minimize the risk of accidents, it's essential to follow all safety guidelines and regulations set by relevant authorities. This substance is hazardous to the environment and human health. It may be harmful in contact with skin (Acute toxicity, dermal) and causes severe skin burns and eye damage. Prolonged exposure can lead to irritation and long-term harm. It is also toxic if inhaled (Acute toxicity, inhalation), and may cause respiratory problems, allergic reactions, or dizziness. Additionally, it may affect fertility, reproductive health, and development of the fetus. The substance is harmful to aquatic life with short-term effects, and may be toxic to water organisms through long-lasting exposure. It can also harm public health by destroying ozone in the upper atmosphere (Harms public health and the environment). This substance can cause fatal poisoning if ingested or if it comes into contact with the skin or respiratory system.Caution Advised for Handling and Use Due to Toxicity If you swallow this product, call a poison center/doctor immediately. Get medical help right away if you feel unwell. Get emergency medical help right now if you have swallowed it. Rinse your mouth with water and do not induce vomiting. If the substance gets on your skin, get medical help right away. Immerse in cool water or wrap in wet bandages. Brush off loose particles from skin. Gently wash with plenty of soap and water if it gets on your skin. Take off contaminated clothing immediately and rinse with water for several minutes. Take off all contaminated clothing and wash it before reuse. In case of fire: Stop the leak if it is safe to do so, use a special extinguishing agent if available. Evacuate the area and fight the fire from a distance due to the risk of explosion.