HyperChem Release 8.0 Feature Summary

Structure Input and Manipulation

Building molecules with HyperChem is simple: just choose an element from the periodic table, and click and drag with the mouse to sketch a structure as you would on paper, prior to applying the model builder to convert your 2D sketch to a 3D structure. Alternatively, select Hydrogen atoms and substitute them with a variety of substituents including your own custom substituent. If you make a mistake, just push the Undo button. Mouse control of rotation around bonds, stereochemistry, and "rubber banding" of bonds makes changing structures easy. Extensive selection, highlighting, and display capabilities make it easy to focus on areas of interest in complex molecules.

- Select, rotate, translate, and resize structures with convenient mouse-controlled tools. Modify settings to control operation of the tools.
- Convert rough sketches into full 3D structures with HyperChem's advanced model builder.
- Apply builder constraints easily: specify bond lengths, bond angles, torsion angles, or the bonding geometry about a selected atom.
- Specify atom type, formal charge, atomic charge, atomic mass, and custom atom labels.
- Build clusters and complex molecular assemblies; move individual atoms and molecules as easily as you move groups; automate molecular design with scripts; create complicated molecular systems.
- Just click to build peptides and nucleic acids from amino acid and nucleotide residue libraries; add counter ions or create zwitterions; inherit charges from templates for Amber, Charmm, and OPLS.
- Mutate residues and build large molecules incrementally (make changes at any point).
- Cut and paste protein segments for homology modeling; model proteins with over 100,000 atoms.
- Read protein sequences and create specific secondary structure as input to modeling calculations.
- Add a periodic box of pre-equilibrated water molecules for aqueous solvation studies. Periodic boundary conditions can be used with other solvent systems, or without solvents.
- Import structures from standard file formats: Protein Data Bank PDB, ChemDraw CHM, MOPAC Z-matrix, MDL MOL and ISIS Sketch, Tripos MOL2 files, and Cambridge Crystallographic files.
- Build molecular crystals from individual molecules; set crystal type and unit cell parameters.
- Create atomic crystals with a variety of sample unit cells, with or without periodic boundary conditions.
- Use a library of aldoses, ketoses, and derivatives to automate the building of polysaccharides from components; create your own sugar components as desired.
- Invoke the polymer builder to build straight or branched polymers from arbitrarily drawn monomers; specify all the structural parameters for monomer linkages or optionally randomize linkages.
- Input molecules directly from a database of your own creation or choose from over 10,000 molecules in HyperChem's database.
- Perform a Root-Mean-Square (RMS) fit of one molecule to another.
- Assign formal charges to atoms for display and for deciding on how many hydrogens the model builder will add (i.e. specify the valence).
- Create a custom component with one selected Hydrogen and store it away. Later use it as a substituent, R, anywhere you like or use common pre-defined substituents instead. Every option for creating your molecule is available.
- Made a mistake altering a structure of deleting some atoms? Just press Undo. Changed your mind? Press Redo.

Molecular Display

- Display structures using sticks, ball and stick, ball and cylinders, fused CPK spheres, or tubes; choose any rendering for any atom; switch easily between rendering styles; quickly center any selected portion of a molecule.
- Add a dot surface to any atom; choose your own stick width or the radius of balls, cylinders and tubes.
- Specify your own colors for simple, repetitive use; select from any of 16M colors.
- Show orbitals and electron densities as 2D contours or 3D isosurfaces.
- Display molecular electrostatic potential as 3D isosurface or as mapped onto electron density surface.
- Display protein backbones with optional display of sidechains; display high-quality secondary structure renderings such as a cylinder for a helix, a thick ribbon for a beta sheet or tubing for a random coil.
- Use selection to mix and match what is shown and how; distinguish atoms versus secondary structures.
- Highlight potential hydrogen bond interactions and render accordingly.
- Display dipole moment vectors or vectors representing the force on any or all atoms.
- Show aromatic rings via either of two user-selected methods.
- Produce ray-traced graphics from HyperChem structures; assign a variety of lights with different position and color.