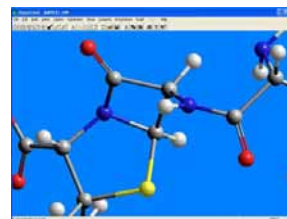


HyperChem 7 Student Edition

HyperChem 7.5 Student Edition a sophisticated molecular modeling environment that is known for its quality, flexibility, and ease of use. Uniting 3D visualization and animation with quantum chemical calculations, molecular mechanics and dynamics, HyperChem puts more molecular modeling tools at your fingertips than any other Windows program.



New HyperChem student version 7.5 will allow students to learn at their convenience and in the comfort of their own workspace. The student version contains features identical to those of the institutional version with the exception of the following atom size limitations:

* <i>Ab Initio</i> , DFT	12 atoms
*Semi-Empirical	36 atoms
*MM+	100 atoms
*Amber, Charmm, OPLS	1000 atoms

What is HyperChem 7.5?

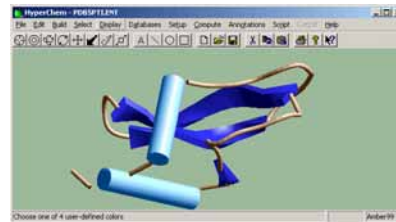


HyperChem 7.5 is the latest release of HyperChem the standard in Molecular Modeling Software for Windows. It introduces high-quality OpenGL rendering throughout, as well as significant enhancements to protein modeling and visualization. Secondary structures extracted from Protein Data Bank files can be rendered using a variety of cylinders, ribbons, and coils to quickly characterize complex topographies. Any atom can be individually rendered (ball and cylinder, CPK spheres, tubes, etc). Any of 16M colors are now available. Electron densities for large proteins can be rapidly computed. Release 7.5 restores HyperChem's premier position in PC graphics to go along with its traditional lead in ease of use and molecular modeling functionality.

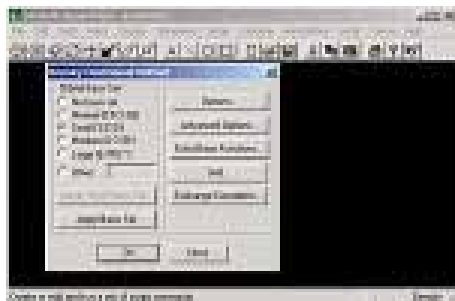
It is a Microsoft Windows application that runs in any of Windows 95, 98, NT, ME, 2000, and XP environments. It is the leading molecular modeling product for the popular Windows environment. Its ease of use along with its flexible licensing mechanisms make it popular for educational use by individual researchers, teachers, and students.

What is in HyperChem 7.5?

HyperChem 7.5 continues incorporate into a single, easy-to-use, Microsoft Windows application all important features of the “state of the art” in molecular modeling. Release 7.5 include many new scientific capabilities, new functional modules, and added improvements in ease of use.



Release 7.5 includes the calculations of Density Functional Theory (DFT). Existing users will find that DFT options bear a close resemblance to *ab initio* options; the two calculations can often be used interchangeably, with DFT expected to be more accurate (but more time consuming) in most cases. This capability gives HyperChem the four basic engines of chemical computation, molecular mechanics, semi-empirical, *ab initio*, and density functional.



HyperNMR has been directly incorporated into Release 7.5. Calculations of **NMR shielding and coupling** parameters can now be performed within HyperChem.

HyperChem Data, was also incorporated into Release 7.5. This module constitutes a database for HyperChem for input (molecules) and output (results). The database makes it easy to automate various kinds of HyperChem operations.. A database can be searched for 2D or 3D structure or for specific results. Users can create new databases or use the default database (10,000 molecules) that comes with HyperChem.



The Bio+ (Charmm) force field that comes with HyperChem has been extensively updated. The latest Charmm 27 parameter set is included as is the related force field that began with the Charmm 22 parameter set. This new force field is appropriate for protein simulations as well as nucleic acid simulations. A new semi-empirical method (**Typed Neglect of Differential Overlap TNDO**) was added with HyperChem 7.5. This method has parameters that depend upon an atom’s type rather than an atom’s atomic number. It thus incorporates ideas from molecular mechanics into the world of semi-empirical quantum mechanics leading to improved accuracy.

Other additions to HyperChem 7.5. included adding magnetic fields to the workspace, a new optimizer that included a capability for optimizing excited state geometries and MP2 geometries, a new rendering of aromatic rings, a general purpose drawing program that constituted additions to the annotation capabilities, interactive examination and editing of molecular mechanics parameters, addition of branched chains to the polymer builder, and new basis sets for *ab initio* and DFT calculations.