

QUANTA is a molecular graphics analysis program

Integrated X-ray crystallography, modeling, and simulation tools in an easy to use interface

QUANTA Modeling Environment

QUANTA is a molecular graphics analysis program that integrates a range of computational methods through a consistent interface. Throughout the pharmaceutical and biotechnology industry, the discovery process relies on the ability to develop molecular level hypotheses based on laboratory and computational experiments. When scientists generate models that explain a particular process or activity, these models provide mechanistic understanding of the chemical system being studied. From this understanding, scientists gain new insight that leads the way to new chemicals and better models.

Generating Initial Models

The interaction with computational chemistry starts with the generation of the initial model of the system to be studied. QUANTA provides a suite of molecule builders to make this a simple and reliable process.



A secondary structure ribbon diagram of GP120

Starting with ChemNote, a 2D structure-sketching tool, you can simply draw the relevant molecules just as you might draw a paper sketch of the structure. You can specify the various chemical attributes such as element type, bond order, relational or absolute stereochemistry. You can also use chemical templates as starting points or as additions to the working molecule. Once the full 2D structure is complete, you can convert it automatically into a reasonable 3D model.

A full featured 3D editor is also available to refine or augment existing models. This allows you to experiment with new structures or test hypotheses in areas of chemistry that may not be accessible experimentally.

QUANTA also provides several other molecular editors. These include a sequence editor, which can be customized for various types of synthetic and biological polymers, together with a variety of specialized editors, which are incorporated into QUANTA as optional modules. You can also import your initial model from standard sources, such as PDB or Cambridge formats, or from other modeling packages.

Unfortunately, not all data formats contain all the necessary information to continue a study of the imported molecular system. Charges, atom and bond types, and even 3D coordinates may be missing. The *Split and Clean* tool in QUANTA streamlines the process of 'cleaning up' the imported system. *Split and Clean* first divides the system up into protein, solvent, DNA, and other components. *Split and Clean* then allows you to clean up the individual components. You can cap proteins, add or remove different hydrogen representations, and highlight incomplete or disordered sidechains. *Split and Clean* will also automatically attempt to identify and type atoms and bonds in any small molecule that is present. Atoms and bonds in nucleic acids are also typed according to standard dictionaries, and hydrogens are added where appropriate.

Molecular Visualization

Once you have created a model of a molecular system, the ability to flexibly visualize various aspects of the molecular system is extremely important. Visual examination often provides key insights to properties such as a protein's function. Key features include:

- The ability to specify color based on:
 - Element or monomer type
 - Atom-based properties such as electronic charge or polarity
 - Monomer properties such as hydrophobicity
 - Molecule-based properties such as solvent accessibility or electronic field
 - Simulation derived properties such as forces of atoms or velocities from molecular dynamics simulations
- Graphical styles, including stick drawings, ball and stick, full spheres, dot surfaces, solid surfaces, and transparency, for displaying molecules to give you more information about the molecules in question

QUANTA supports both interactive stereo viewing and stereo plot generation.

With this broad range of viewing capabilities, QUANTA allows you to better perceive 3D shapes and structures and assist in those application areas where 3D visualization is essential, such as docking or comparing multiple molecules.

X-Ray Crystallography

QUANTA provides a complete environment for all stages of crystallographic model-building and refinement. Protein-ligand experiments can be carried out using X-BUILD (previously available as X-LIGAND), while *de novo* map tracing and model-building experiments can be performed

with X-AUTOFIT (which now also includes X-POWERFIT). X-SOLVATE can be used for efficient water-picking. After model building, the transition to reciprocal-space refinement using powerful CNX protocols can be made seamlessly through an updated QUANTA/CNX interface.

The Simulation Process

While a great deal of insight can be gained through the simple 3D visualization of a molecular system, it is simulation that provides understanding. Through its simulation engine, CHARMM, QUANTA provides a rich set of capabilities for the set up, execution and analysis of simple to very complex simulation strategies. Many of these capabilities use features of CHARMM, the well-known molecular mechanics and dynamics program originally developed in the laboratory of Dr. Martin Karplus at Harvard University. Over twenty research laboratories around the world continue to extend this molecular simulations engine by contributing to the development of CHARMM.

Through a transparent interface from QUANTA, CHARMM provides well-validated energy and force field calculations, which form the core of a broad range of simulation capabilities, including evaluation of conformational energies, local minima, transition barriers, and time-dependent dynamics.

Components of Molecular Modeling

- ChemNote 2D structure building; 3D Molecular Editor; Biopolymer Sequence Builder
- Full Molecular Mechanics and Molecular Dynamics simulations through CHARMM
- Exhaustive and Stochastic Conformational Search
- ChemTable, spreadsheet-like data storage and manipulation

Components of Molecular Modeling (Continued)

- Read and generate structural data in all standard file formats, including PDB, Cambridge, MOPAC, and MDL
- Read and generate sequence data in all standard file formats (GCG, PIR, SWISSPROT)
- Automatically split up and clean an input molecule to rapidly identify correct atom typing and hydrogen representation
- Molecular Surface Generation including Connolly electrostatic potential, solvent accessibility, and Van der Waals surfaces

Complementary Software

- X-AUTOFIT (includes X-POWERFIT functionality)
- X-BUILD (includes X-LIGAND functionality)
- X-SOLVATE
- CHARMm
- CNX
- MODELER

System Requirements:

QUANTA runs on Linux and SGI workstations.

Dial Box is supported for QUANTA on both the Linux and SGI IRIX platforms.

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