

# BIOPOLYMER BUILDING AND ANALYSIS IN DISCOVERY STUDIO

The complex 3D structure of biopolymers, such as peptides, proteins and nucleic acids, are critical to their biological functions. One of the key factors that dictate the structure of a macromolecule is the electrostatic interactions among polymer residues. DS Biopolymer not only allows you to create and modify biopolymers from their basic residues building blocks, but also allows you to calculate a molecule's electrostatic properties, including the effects of bulk solvent and ionic strength, thereby providing crucial data for rationalizing differences in the activity of macromolecules.

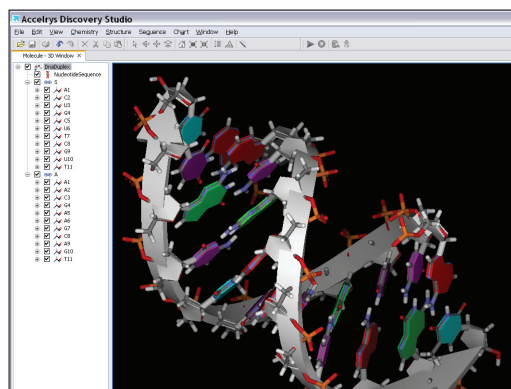
## THE DISCOVERY STUDIO RESEARCH ENVIRONMENT

DS Biopolymer is part of the Discovery Studio® research environment, which is a comprehensive suite of modeling and simulation solutions. Because Discovery Studio is built on SciTegic®'s Pipeline Pilot, Accelrys' scientific operating platform, these modules are extensively integrated with many other powerful software applications that will allow you to carry out such tasks as aligning sequences, creating protein homology models, building and analyzing pharmacophore models, examining receptor ligand interactions, performing molecular mechanics, and much more.

## FEATURES

### Building and Editing Macromolecular Structures

With DS Biopolymer, you can rapidly build and modify peptides, proteins and nucleic acid (DNA and RNA) structures.



*DS Biopolymer was used to create and type a DNA duplex in preparation for minimization and molecular dynamics.*

- Peptide and Protein Structure
- Polypeptide structures can be easily constructed and edited by appending, replacing, or deleting residues.
- You have the ability to set charges or radii of atoms in your structure and create neutral or charged N- or C-termini.
- You can create secondary structures by imposing a variety of standard helices or beta strands to a desired range of residues.

- Any desired nonstandard turn can be imposed by specifying the two relevant pairs of phi and psi angles.
- DS Biopolymer can also fix any protein structural errors, such as incomplete side chains, or improper connectivity and bond order.
- Included are tools that allow you to generate protein reports and create hydrophobicity plots.

## NUCLEIC ACID STRUCTURE

You rapidly can create single-, double-, and triple-stranded DNA molecules in A-, B-, or Z-form using standard helix parameters.

Single- or double-stranded RNA and DNA-RNA hybrid molecules in A-form can be constructed with standard helix parameters.

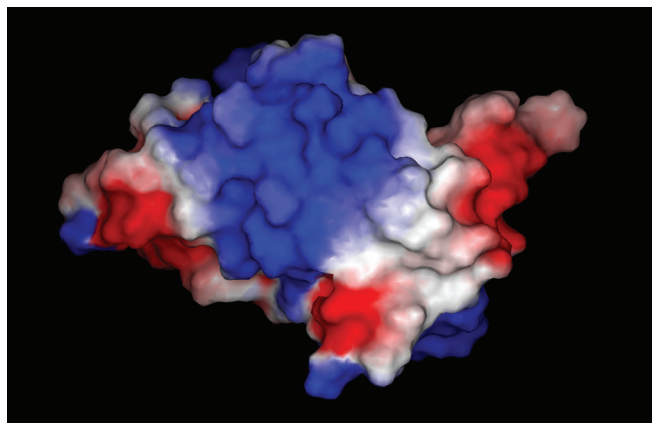
You can further modify your structure with tools for ligating two nucleic acid molecules together, and for adding caps and primes to the 5' end.

### Electrostatic Analysis

DelPhi, a powerful and versatile Poisson-Boltzmann electrostatics simulation engine for calculating electrostatic potentials and solvation energies of both small- and macro- molecules, is available within DS Biopolymer. Shape and electrostatic properties often determine the function of small- and macro-molecules. DS Biopolymer provides sophisticated tools for examining such properties, without resorting to inappropriate dielectric models or including explicit solvent. The effects of the presence or absence of solvent are taken into account, both of which may result in a different calculation for the electrostatic potential of a macromolecule.

- The electrostatic potential changes that occur upon mutation of protein residues can be studied with DS Biopolymer
- High resolution calculations are possible using focusing methods.

- By treating macromolecules and solvent as separate dielectric domains, DelPhi can rigorously account for the effect of molecular shape on solvation, substrate binding, and electrostatic interactions.
- The total electrostatic energy for a set of charges, including the total solvation energy of each charge and between charges, is accounted for.
- DelPhi calculations can reproduce experimental results where Colulombic models fail.
- The powerful visualization capabilities of Discovery Studio allow you to view electrostatic potential grids generated by DelPhi as solid, triangle or quad mesh, or volume isosurfaces. This enables you to evaluate the shape and the extent of electrostatic potentials in and around a protein.



*The Poisson-Boltzmann electrostatic potentials displayed on the protein surface indicated areas of positive (blue), neutral (white) and negative (red) regions.*

### X-ray Analysis Tools

DS Biopolymer provides tools that allow you to automatically fit your protein models and ligands into electron density maps of a specified protein-ligand complex.

To learn more about Discovery Studio, go to [accelrys.com/discovery-studio](http://accelrys.com/discovery-studio)

## REFERENCES:

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2. Nicholls, A., and Honig, B., J. Comp. Chem., 1991, 12, 435.
3. Sharp, B., Nichols, A., Friedman, R., and Honig, B., Biochemistry, 1991, 30, 9686.