Naccess V2.1.1 - Atomic Solvent Accessible Area Calculations

Naccess is a stand alone program that calculates the accessible area of a molecule from a PDB (Protein Data Bank) format file. It can calculate the atomic and residue accessiblities for both proteins and nucleic acids. It runs on most Linux/Unix systems including cygwin under windows.

Naccess calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule. Such 3-dimensional co-ordinate sets (PDB files) are available from RCSB. The program uses the Lee & Richards (1971, J. Mol. Biol., 55, 379-400) method, whereby a probe of given radius is rolled around the surface of the molecule, and the path traced out by its centre is the accessible surface. Typically, the probe has the same radius as water (1.4 Angstroms) and hence the surface described is often referred to as the solvent accessible surface. The calculation makes successive thin slices through the 3D molecular volume to calculate the accessible surface of individual atoms, and hence is an approximation - thinner slices improves the accuracy.

Naccess can be run with:

- user-defined probe size
- user-defined residues (amino, nucleic and heteroatom)
- user-defined atomic radii
- user-defined "standard state" residue accessibilities
- with/without hetatoms, hydrogens, waters

and produces

- a file of atomic accessible areas
- a file of summed absolute and relative residue accessible areas
- a calculation log file

You need

- A Linux/Unix-based system
- A Fortran 77 compiler (e.g. g77 or gfortran)

The program is written in (fairly) standard FORTRAN 77, and runs on most Unix platforms (including most linuxes, cygwin and people have got it working on macs). The program itself is controlled by a C-Shell script. It does not require vast amounts of memory and is reasonably fast. You will need a Unix system and a Fortran compiler to install the program.

Applications

Accessiblities are widely used in the macromolecular modelling community, and Naccess can be used to calculate both atomic and residue accessible surfaces, for amino and nucleic acids. The output from the program can also be read in by 2 programs available from the Biomolecular Structure and Modelling Unit at UCL:-

HBPLUS .. which calculates hydrogen bonds, hydrogen atom positions and can suggest optimal conformations for Asn, Gln and His sidechains. [Written by Ian McDonald].

LIGPLOT .. which automatically generates schematic diagrams of protein-ligand interactions for a given PDB file. [Written by Andrew Wallace & Roman Laskowski].

Category
Software/Bioinformatics

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