AUTOMATIC APPROACH TO THE MOLECULAR DYNAMICS INVESTIGATIONS ALL OF THE 400 NATURAL DIPEPTIDES

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Molecular dynamics research automatic methods are discussed in terms of original molecular dynamic software package MoDyp 1.13 build 1a developed on Biophysics and Bioengineering departments of Moscow State University [1]. Automatic molecular dynamics investigations for characteristics of a large number of chemically homological molecular series is very important in terms of comparison analysis and database creations in molecular design researches.

The molecular dynamics investigation software package is introduced as a sequence of execution modules that covers most significant molecular design and molecular dynamic simulation research tasks. This package is developed mostly for Win32 operation platform under IBM PC compatible architecture. In case there are portable modules that were successfully tested and now using under MIPS (IRIX 6.5.9), SPARC (Sun Solaris 6), Itanium (Win64), x86 and AMD Athlon (Linux Red Hat 7.0+).

The most usable and highlighted features of this package are:

- TCL like scripting language controls all modules execution flow coexists with a full-functional graphical windowed interface that helps perform a different class of tasks for beginners as power users.
- Many standard types of files are supported: ENT (PDB) and HIN (HyperChem) as molecular geometry files, AMBER Force Field as force field parameter files, DCD (CHARMm, NAMD, X-PLOR) as trajectory files.
- Most common and standard molecular dynamics simulation algorithms are present in coexistence with original algorithms like relaxation and collision thermostat.
- On-fly molecular statistics calculations are implemented to interactive control a molecular dynamics simulation process. It provides a backward interactive control under simulation by force field parameters fitting.
- Software Development Kit (SDK) is also helps user to make own utilities for molecular trajectory analysis. In one package are already exist many utilities and examples written by this software libraries.
- Text mode trajectory scanning and querying utilities helps present results in a portable universal text format. This text formatted result in files containing that data which is wanted by user only. For example only one or two torsion angels dependence of time.
- There are MatLab R11+ toolbox exists for high level trajectory analysis and computations.
- Also this package provides an extended interface with HyperCube HyperChem molecular editor by Microsoft Windows DDE.

Automatic molecular dynamics simulations of the 400 natural dipeptides (all combinations of 20 natural amino acids) have been performed by using an extended MoDyp package scripting. In fact the common time of one trajectory calculation with 20 on-fly statistics takes about 3 hours on the AMD Athlon 1100MHz. The calculation main parameters are: 10^7 integration steps per trajectory, 1fs integration step. Thermostats that were used is a combination of the Berendsen thermostat and the original collision thermostat under temperature 2500K. Cut-off distance was assumed on 20Å length of pair interactions. Full-qualified atom models were used for natural dipeptides, which contain all hydrogen atoms. As force field constants an AMBER96 force field files were used.

Automatic cluster analysis of the trajectories performed by MoDyp package tools and libraries was done. Methods of auto- and cross-correlation functions, 3D probability distributions of the significant torsions angels φ, ψ, χ in the amino acids were proposed. Some of the amino acids dramatically influence on the dynamic behavior of the dipeptides and significantly transforms a topology of the dipeptides potential energy surfaces.

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