
IDSS - Version 1.0

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This program implements the IDSS (Inner Distance Shape Signature) algorithm for retrieval of flexible proteins

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System Requirements

Source code was written to perform the IDSS for retrieval of flexible proteins, as well as visualize the results.

The code was developed and tested using Microsoft Visual C++ 2005 on a Windows XP system.

REQUIRED INSTALLATIONS:
    -Microsoft Visual C++ 2005
    -MICROSOFT FOUNDATION CLASS (MFC) LIBRARY
    -OpenGL

Protein data set

The Database of Macromolecular Movements (MolMovDB) is a set of known proteins with conformational changes in different crystallographic structures.

Web site: http://www.molmovdb.org/cgi-bin/browse.cgi

The database is a collection of data and software pertaining to flexibility in protein and RNA structures, which can be found at: (http://www.molmovdb.org/).

Packages

The executable package contains two folder and one tutorial.

1) IDSS_win32exe

The executable program IDSS.exe and four MRC files used in our paper.

2) BenchmarkProtein

The Database for Testing the IDSS.
Web site: http://molmovdb.org/cgi-bin/sets.cgi

Reference: N. Echols, D. Milburn, and M. Gerstein. MolMovDB: Analysis and visualization of conformational change and structural flexibility. Nucleic Acids Research, 31(1):478--482, 2003.

Operation
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1. Uncompress BenchmarkProtein.zip into the system root directory C:\
2. Execute IDSS.exe
3. Open a MRC file.
   Menu: File --> Open a MRC file.
4. Compute IDSS of flexible proteins
   Menu: Inner Distance --> Compute Inner Distance,
5. Optionally, retrieve the similar protein in the database.
   Menu: Retrieve --> ID Retrieve

Mouse:
 Left: rotation
 Right: Zoom in/out

Menu --> Display for assistant display