hmatrix

Generated by Doxygen 1.8.5

Contents

Chapter 1

File Index

1.1 File List

Here is a list of all files with brief descriptions:

Chapter 2

File Documentation

2.1 hmatrix.cpp File Reference

```
#include <iostream>
#include <fstream>
#include <string>
#include <vector>
#include <cstdlib>
#include <map>
#include <iomanip>
#include <cmath>
```

Functions

- void load_hb_data (vector< vector< char > > &hinter, string hb_dat_file="hb.dat")

- int load_ms_data (vector< string > &resName, vector< vector< int > > &resinter, vector< vector< char > > &hinter, string ms_dat_file="ms.dat")

- void output_hb_txt (vector< string > &resName, vector< vector< int > > &resinter, int totalState, float threshold=0.001, string hb_txt_file="hb.txt")

- int main ()

2.1.1 Function Documentation

2.1.1.1 void load_hb_data (vector< vector< char > > & *hinter,* string *hb_dat_file =* `"hb.dat"`)

Load hbond info between every two conformers from "hb.dat", which is a binary file. The first 4 bytes is an integer indicating the number of conformers, followed by n∗n matrix. The matrix element (i, j) being 1 means there is hbond between conformer i and conformer j, with conformer i being the donor and conformer j the accepter. 0 means no hbond between conformer i and j.

Parameters

hinter	the matrix stores the hbond info between every two conformers.
hb_dat_file	the name of the binary file which saves the hbond info between every two conformers.

2.1.1.2 int load_ms_data (vector< string > & *resName,* vector< vector< int > > & *resinter,* vector< vector< char > > & *hinter,* string *ms_dat_file =* `"ms.dat"`)

Load all the microstates from file ms.dat, which is a binary file. The first 4 bytes is an integer giving the number of key residues whose microstates are saved. Followd by the names of the key residues in a format like ASPA0085. Then comes a set of microstate records, which have the conformer id number of the chosen conformer of each residue in each microstate.

Parameters

resName	the names of key residues whose microstates are saved and only which are shown in the hbond network.
resinter	the number of hbonding between two residues among all the microstates.
hinter	the matrix stores the hbond info between every two conformers, in which the element is either 0 or 1.
ms_dat_file	the name of the binary file which saves all the microstates.

2.1.1.3 int main ( )

2.1.1.4 void output_hb_txt (vector< string > & *resName,* vector< vector< int > > & *resinter,* int *totalState,* float *threshold =* `0.001`*,* string *hb_txt_file =* `"hb.txt"`)

Write the probability of hbond between two residues into file "hb.txt".

Parameters

resName	the names of key residues whose microstates are saved and only which are shown in the hbond network.
resinter	the number of hbonding between two residues among all the microstates.
totalState	the number of all the microstates.
threshold	the hbond connection is written if the probability is larger or equal to this threshold.
hb_txt_file	the name of the text file which outputs the probability of hbonding between two residues.