

mm_envir
V.1.0.3

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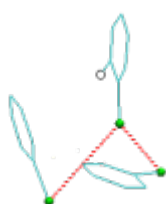
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Chapter 1

mm_envir



1.1 Introduction

About this program:

- Program that searches environment for chosen molecule by geometric criterion

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License:

- GPL

1.2 How to use

Usage:

```
mm_envir -i INPUT -c X,Y,Z -o OUTPUT [ -n NUM_OF_MOLECULE ] [ -r RADIUS ]  
[ -l LOGFILE ] [ -q ] [ -h ]
```

Parameters:

-i	- input file name
-c	- cell size (float), A
-o	- output file name
-n	- number of molecule for search (integer). Default is 1
-r	- radius of environment (float). Default is 6.0
-l	- log enable
-q	- quiet enable
-h	- show this help and exit

Chapter 2

Install

2.1 Requirements

The application mm_envir requires the following external stuff:

- cmake \geq 2.8
- gcc \geq 4.8

2.2 How to install

2.2.1 Linux

```
* mkdir build && cd build
* cmake -DCMAKE_INSTALL_PREFIX=/usr -DCMAKE_BUILD_TYPE=Release ../
* make
* make install
*
```

2.2.2 Windows

```
* create project file using 'cmake'
* compile project
*
```

You may also download compiled executable file for Win_x86.

Chapter 3

Changelog

V.1.0.3 (2013-08-30)

- Bug fixes

V.1.0.1 (2013-07-27)

- initial release

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

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Chapter 5

File Documentation

5.1 src/add_main.c File Reference

```
#include <stdio.h>
#include "messages.h"
```

Functions

- int [error_checking](#) (const float *cell, const char *input, const char *output)
function that checks errors in input variables
- int [print_message](#) (const int quiet, FILE *std_output, const int log, FILE *f_log, const int mode, const char *str)
function that prints message in log and stdout
- int [set_defaults](#) (float *cell, char *input, int *log, int *num_of_mol, char *output, int *quiet, float *rad)
function that sets default values of variables

5.1.1 Function Documentation

5.1.1.1 int [error_checking](#) (const float * *cell*, const char * *input*, const char * *output*)

function that checks errors in input variables

```
* error\_checking (cell, input, output);
*
```

Parameters

<i>cell</i>	massive of cell size
<i>input</i>	input file name
<i>output</i>	output file name

Returns

- 11 - error in 'cell'
- 12 - error in 'input'
- 13 - error in 'output'
- 0 - exit without errors

5.1.1.2 int print_message (const int *quiet*, FILE * *std_output*, const int *log*, FILE * *f_log*, const int *mode*, const char * *str*)

function that prints message in log and stdout

```
* print_message (quiet, stdout, log, f_log, 0, str);
*
```

Parameters

<i>quiet</i>	status of quiet-mode
<i>std_output</i>	stdout
<i>log</i>	status of log-mode
<i>f_log</i>	log file
<i>mode</i>	number of message in "messages.c"
<i>str</i>	additional text in message

Returns

0 - exit without errors

5.1.1.3 int set_defaults (float * *cell*, char * *input*, int * *log*, int * *num_of_mol*, char * *output*, int * *quiet*, float * *rad*)

function that sets default values of variables

```
* set_defaults (cell, &from, input, &log, &max_depth, &num_of_inter, output, &to,
*               &type_inter, &quiet);
*
```

Parameters

<i>cell</i>	massive of cell size
<i>input</i>	mask of trajectory files
<i>log</i>	status of log-mode
<i>num_of_mol</i>	number of molecule
<i>output</i>	output file name
<i>quiet</i>	status of quiet-mode
<i>rad</i>	radius of environment sphere

Returns

0 - exit without errors

5.2 src/coords.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
```

Functions

- int [reading_coords](#) (const int mode, const char *filename, const int type_inter, const int *label_atom, const float *cell, int *num_mol, int *num_atoms, int *true_label_mol, int *label_mol, int *type_atoms, float *coords, char *ch_type_atoms)

function that reads coordinates from special file format

5.2.1 Function Documentation

5.2.1.1 `int reading_coords (const int mode, const char * filename, const int type_inter, const int * label_atom, const float * cell, int * num_mol, int * num_atoms, int * true_label_mol, int * label_mol, int * type_atoms, float * coords, char * ch_type_atoms)`

function that reads coordinates from special file format

```
* reading_coords (0, filename, type_inter, label_atom, cell, &num_mol, &num_atoms,
*               true_label_mol, label_mol, type_atoms, coords, ch_type_atoms);
*
```

Parameters

<i>mode</i>	mode of reading; '1' is statgen, '2' is envir or frad, '3' is agl
<i>filename</i>	input file name
<i>type_inter</i>	number of needed atoms (number of needed molecules)
<i>label_atom</i>	massive of needed atom types (massive of needed molecules)
<i>cell</i>	massive of cell size
<i>num_mol</i>	number of molecules
<i>num_atoms</i>	number of atoms
<i>true_label_mol</i>	massive of true numbers of molecule for atoms
<i>label_mol</i>	massive of numbers of molecule for atoms
<i>type_atoms</i>	massive of atom types
<i>coords</i>	massive of coordinates
<i>ch_type_atoms</i>	massive of char atom types

Returns

- 1 - file \$filename does not exist
- 2 - unknown mode
- 0 - exit without errors

Work blocks

reading file

translation

free memory

5.3 src/envir_search.c File Reference

```
#include <math.h>
```

Functions

- `int search_envir (const int num_of_mol, const int num_mol, const float *centr_coords, const double rad, int *needed_mol, int *num_needed_mol)`

function that searchs environment

5.3.1 Function Documentation

5.3.1.1 `int search_envir (const int num_of_mol, const int num_mol, const float * centr_coords, const double rad, int * needed_mol, int * num_needed_mol)`

function that searches environment

```
* search_envir (number_of_molecule, num_mol, centr_coords, rad, needed_mol,
*               &num_needed_mol);
*
```

Parameters

<i>num_of_mol</i>	number of molecule
<i>num_mol</i>	number of molecules
<i>centr_coords</i>	massive of centered coordinates
<i>rad</i>	radius of environment sphere
<i>needed_mol</i>	massive of number of needed molecules
<i>num_needed_mol</i>	number of needed molecules

Returns

0 - exit without errors

5.4 src/main.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "add_main.h"
#include "coords.h"
#include "envir_search.h"
#include "messages.h"
#include "print_struct.h"
#include "set_center.h"
```

Functions

- `int main` (int argc, char *argv[])

5.4.1 Function Documentation

5.4.1.1 `int main (int argc, char * argv[])`

Returns

- 1 - error in error_checking
- 2 - input file does not exist
- 3 - memory error
- 4 - unknown flag
- 0 - exit without errors

5.5 src/messages.c File Reference

```
#include <stdio.h>
#include <time.h>
```

Functions

- int `message` (const int *log*, const int *mode*, const char **text*, FILE **output*)
function that prints messages to output

5.5.1 Function Documentation

5.5.1.1 int `message` (const int *log*, const int *mode*, const char * *text*, FILE * *output*)

function that prints messages to output

```
* message (log, mode, text, output);
*
```

Parameters

<i>log</i>	equal to 1 if print to logfile
<i>mode</i>	number of message
<i>text</i>	additional text
<i>output</i>	output file (may be stdout)

Returns

- 1 - unknown mode
- 0 - exit without errors

5.6 src/print_struct.c File Reference

```
#include <stdio.h>
```

Functions

- int `print_structure` (const char **output*, const int *num_needed_mol*, const int **needed_mol*, const int *num_atoms*, const int **label_mol*, const char **ch_type_atoms*, const float **coords*)
function that prints structure to pdb file

5.6.1 Function Documentation

5.6.1.1 int `print_structure` (const char * *output*, const int *num_needed_mol*, const int * *needed_mol*, const int *num_atoms*, const int * *label_mol*, const char * *ch_type_atoms*, const float * *coords*)

function that prints structure to pdb file

```
* print_structure (output, num_needed_mol, needed_mol, num_atoms, label_mol,
*                   char_type_atoms, coords);
*
```

Parameters

<i>output</i>	output file name
<i>num_needed_mol</i>	number of needed molecules
<i>needed_mol</i>	massive of number of needed molecules
<i>num_atoms</i>	number of atoms
<i>label_mol</i>	massive of numbers of molecule for atoms
<i>ch_type_atoms</i>	massive of char atom types
<i>coords</i>	massive of coordinates

Returns

0 - exit without errors

5.7 src/set_center.c File Reference

Functions

- int [set_center](#) (const int num_atoms, const int num_mol, const int *label_mol, const float *coords, float *centr_coords)

function that searchs center mass of molecules

5.7.1 Function Documentation

5.7.1.1 int set_center (const int num_atoms, const int num_mol, const int * label_mol, const float * coords, float * centr_coords)

function that searchs center mass of molecules

```
* set_center (num_of_atoms, num_of_molecules, label_molecules, coords, centr_coords);
*
```

Parameters

<i>num_atoms</i>	number of atoms
<i>num_mol</i>	number of molecules
<i>label_mol</i>	massive of numbers of molecule for atoms
<i>coords</i>	massive of coordinates
<i>centr_coords</i>	massive of centered coordinates

Returns

0 - exit without errors

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