

mm\_envir

V.1.1.0

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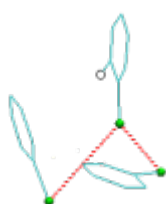
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# Chapter 1

## mm\_envir



### 1.1 Introduction

#### About this program:

- Program that searches environment for chosen molecule by geometric criterion

#### Developer:

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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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