Read me

Command line

```
java -heap -jar antmot.jar names pdb_path graph_build dist
min_size max_size min_intra_freq max_extra_freq minimality
arff_path motif_path
```

Example

```
java -Xmx1024m -jar antmot.jar test.txt ./pdb 1 4 3 7 0.5
0 false test.arff motifs_test.txt
```

Paramaters

Input

heap : java heap memory for example *Xmx1024m*
names : file containing pdb names in the format illustrated by figure 1
pdb_path : folder where the pdb files are saved
graph_build : method of graph building, values={1 , 2}, 1 for *AllAtoms* method and 2 for *CarbonAlpha* method.
dist : distance used by the method of graph building (graph_build)
min_size : minimum number of vertices in motifs
max_size : maximum number of vertices in motifs
min_intra_freq : minimum frequency of a motif within a given class
max_extra_freq : maximum frequency of a motif in an outer class
minimality : boolean parameter to stop building the motif if it satisfies *min_intra_freq* and *max_extra_freq*. This parameter is not yet implemented in our program, so the current and default value is false.

Output

arff_path : arff file used to perform classification with Weka workbench.
motif_path : file where motifs are saved (figure 2)

```
#Family_1
1BLX.pdb
1BYG.pdb
1CKI.pdb
1CM8.pdb
1FGK.pdb
#Family_2
1AXI.pdb
1B7Y.pdb
1BH6.pdb
1C7K.pdb
1C9B.pdb
1CF5.pdb
```

Figure1. File containing the names of concerned pdb files belonging to two families

```
t#Motif 321
v0 I
v1 R
v2 L
e 0 1 0
e 0 2 1
t#Motif 322
v0 L
v1 V
v2 K
v3 T
e 0 1 0
e 0 2 1
e 0 3 2
t#Motif 323
```

Figure2. Sample of an output file containing spatial motifs.