

Pocket-Match(version 2.1) README file:

Deepesh Nagarajan, 2015, NSC lab.

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REVISIONS MADE IN VERSION 2.1:

- 1) Sphinx module has been made disabled. Users complained that the Sphinx module caused memory overflows (segfaults) even when not used, and no one used it anyway.
- 2) The MPI version (**Step3-PM_MPI.c**) is obsolete and has been removed.
- 3) A program for the pairwise comparison of 2 datasets has been included.
- 4) A makefile has been included for easy compilation.

This folder contains the following data (**files/executables/directories**).

Dependencies are listed hierarchially:

```
cabbage-file_maker
  Sample_cabbage-files
    1g64.pdb.cabbage ... 4djd.pdb.cabbage
  Sample_pockets
    1g64.pdb ... 4djd.pdb
  Step0-cabbage.sh
    Step0-cabbage_core.cpp (Step0-cabbage_core)
    Step0-cabbage_core.h
    Step0-PDBclass.h
    Step0-cabbage_decoder.cpp (Step0-cabbage_decoder)
    Step0-END-FILE.c (Step0-END-FILE)
```

README

README.odt

README.pdf

PocketMatch.pdf (note: cabbage files are called alpha-files in the paper).

Step3-PM_typeA.c (Step3-PM_typeA) -> use for comparisons inside a dataset

Step3-PM_typeB.c (Step3-PM_typeB) -> use for comparisons between 2 datasets

Step3-PM.h

Installation:

All executables should work out-of-the-box. If not, use the makefile:

```
$ make
```

The end-user workflow is as follows:

- 1) Make 1 or 2 directories full of pockets in the **PDB format**.
 - Make sure to stick to **80** characters per line.
 - There should be **no DNA/RNA** molecules in the ATOM coordinates
 - (Recommended) Make sure that pocket files contain all atoms of pocket residues (backbone and sidechain). Hydrogen atoms are not necessary.
 - Rigidly stick to the PDB convention. I have not written any error-detection modules.

2) Enter the 'cabbage-file_maker' directory:

```
$ cd PocketMatch_v1.2/cabbage-file_maker
$ ls
outfile.cabbage      Step0-cabbage_core.cpp      Step0-cabbage.sh
Sample_cabbage-files  Step0-cabbage_core.h        Step0-END-FILE
Sample_pockets        Step0-cabbage_decoder        Step0-END-FILE.c
Step0-cabbage_core    Step0-cabbage_decoder.cpp    Step0-PDBclass.h
```

3) Run the script '**Step0-cabbage.sh**' WITHIN this folder. '**Sample_pockets**' are provided as an example here, but you will need to use your own pockets.

```
$ bash Step0-cabbage.sh Sample_pockets/
```

An '**outfile.cabbage**' should be generated

4) Exit the 'cabbage-file_maker' directory:

```
$cd ..
```

5) Run pocketmatch. There are two executables: '**Step3-PM_typeA**' and '**Step3-PM_typeB**'.

-for input pockets [A, B, C], '**Step3-PM_typeA**' gives the following comparisons: [A-B, A-C, B-C].

-for input pockets [A, B, C], [1, 2, 3] '**Step3-PM_typeB**' gives the following comparisons: [A-1, A-2, A-3, B-1, B-2, B-3, C-1, C-2, C-3].

Run the executables as follows:

```
$ ./Step3-PM_typeA outfile.cabbage
$ ./Step3-PM_typeB outfile.cabbage outfile.cabbage
```

4) The Pocket-match output will appear in a file called 'PocketMatch_score.txt'.

This is the format:

input file X:		input file Y:		
3som.pdb		4djd.pdb		
P-min_OP	P-max_OP	A	B	C
0.522222	0.509485	3321	3240	1692

Note: A,B,C are for debugging only, however:

$P\text{-min_OP} = C/A$ | $P\text{-max_OP} = C/B$

Usually, I only consider the P-max score. The P-min score is too 'optimistic', but can be useful if comparing similarly sized pockets.

Online help:

If you still have unresolved issues, e-mail me at **1337deepesh@gmail.com**

I may or may not reply.