Pocket-Match(version2.0) README file:
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These programs/scripts generate all-to-all Pocket-Match(PM) pocket-comparison scores for given pocket-descriptor input-files (cabbage format).

USAGE:

1) enter the '**Pocketmatch_v2.0**' directory on terminal:

```
$ cd PocketMatch_v2.0
```

2) Create '**alpha-files**'. A sampling of PDB-format pockets is provided in the '**Sample_pockets**' folder:

```
$ cd alpha-file_maker
$ bash Step0-cabbage.sh Sample_pockets
```

to explore other options, simply type:

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

3) Run pocketmatch of generated alpha_file (**outfile.cabbage**)

```
$ cd ../
$ ./Step3-PM_serial alpha-file_maker/outfile.cabbage
```

4) interpret output:

```
$ cat PocketMatch_score.txt              #this file contains the similarity score.
$ cat PocketMatch_pairs.txt|fold -64     #this file contains pairings of similar residues.
```

5) Altering the code: If you are unsatisfied with the speed of Pocketmatch (**./Step3-PM_serial)**, then you can turn off the 'sphinx module' (it generates the '**PocketMatch_pairs.tx**t' file). This is how you can do it:

```
$ #TURN OFF SPHINX MODULE
$ sed -i s/"#define SUMA_TOGGLE 1"/"#define SUMA_TOGGLE 0"/ Step3-PM_serial.c
$ gcc4.4 -o Step3-PMserial Step3-PMserial.c -lm -m32

$ #TURN ON SPHINX MODULE
$ sed -i s/"#define SUMA_TOGGLE 0"/"#define SUMA_TOGGLE 1"/ Step3-PM_serial.c
$ gcc4.4 -o Step3-PMserial Step3-PMserial.c -lm -m32
```

ONLINE HELP:
If you still have unresolved issues, e-mail me at ***1337deepesh@gmail.com***
I may or may not reply.

UPDATE (Tuesday 12 May 2015 05:55:36 PM IST):
All programs were written on a 32-bit machine. If you're using a 64-bit maching and want to re-compile any programs, then use these commands:

```
$ gcc4.4 -o Step2-compressor Step2-compressor.c
$ gcc4.4 -o Step3-PMserial Step3-PMserial.c -lm -m32
```

NOTE:
The MPI version has not been tested on 64-bit operating systems and is **NOT GUARANTEED TO WORK**. I strongly recommend using the serial version on multiple processors instead.

CITATION:
Nagarajan, D., & Chandra, N. (2013, February). PocketMatch (version 2.0): A parallel algorithm for the detection of structural similarities between protein ligand binding-sites. In *Parallel Computing Technologies (PARCOMPTECH), 2013 National Conference on* (pp. 1-6). IEEE.