**3DIGARS**

**Supplementary Material**

3DIGARS software and the related material can be downloaded free of cost from the internet at: <http://cs.uno.edu/~tamjid/Software/3DIGARS/3DIGARS.zip>

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**Prerequisite for 3DIGARS software**: Please have **java (JDK and JRE)** installed in your machine to run this program.

* Download 3DIGARS-Sup-Material.zip
* Unzip the file “3DIGARS-Sup-Material.zip”, you will find the folder with name “3DIGARS-Sup-Material” which looks like Figure1 below.

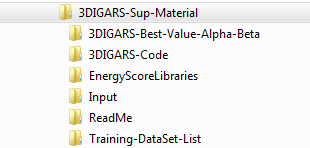


Figure 1: Directory content structure

* 3DIGARS-Code
  + - ThreeDimEnergy.java => main program file
    - BufferReaderAndWriter.java => supporting file to the program
* Input
  + - 3DIGARSTrainDataFasta.txt => fasta file containing protein id and sequences of training data (program needs this file as input)
    - 3DIGARSTrainDataPDB => directory contains the PDB structure files (required if you want to generate energy score libraries on your own)
* 3DIGARS-Best-Value-Alpha-Beta
  + - Alpha-Beta-BestValue-3DIGARS.txt => contains best value of 3D alpha and 3D beta generated by 3DIGARS Genetic Algorithm program
* Training-DataSet-List
  + - 3DIGARS-Train-PDB-List.txt => contains list of PDB ID's used by 3DIGARS
* Before running the code do following:
  + Requirements to run 3DIGARS program (run without generating energy scores libraries):
    - Fasta file “3DIGARSTrainDataFasta.txt” should be under same directory where program files are placed
    - 3DIGARSTrainingDataPDB directory contains training dataset which should also be under same directory where program files are placed. **Note that the program will not work if PDB structure files are not provided. Copy whole directory 3DIGARSTrainingDataPDB and put it inside your working directory.**
    - Copy three library files which you can find inside EnergyScoreLibraries to your working directory
  + Requirements to run 3DIGARS program (run by first generating energy scores libraries):
    - Fasta file “3DIGARSTrainDataFasta.txt” should be under same directory where program files are placed
    - 3DIGARSTrainingDataPDB directory contains training dataset which should also be under same directory where program files are placed. **Note that the program will not work if PDB structure files are not provided. Copy whole directory 3DIGARSTrainingDataPDB and put it inside your working directory.**
    - Open the code file (ThreeDimEnergy.java) with any editor and uncomment (remove “//”) from line number 124. This line of code will generate energy score libraries within your working directory.
  + Compiling and Running Java files
    - Compile the program:
      * You will need jdk to run the program.
      * navigate to the directory where you copied 3DIGARS code and all the required Input files.
      * javac \*.java => this command will compile all the java files in the current directory
    - Execute the progam:
      * use command "java ThreeDimEnergy fileNameWithDirectory" to execute the main file ThreeDimEnergy.class. Note: You will need to provide full path and file name of your structure file along with the execute command.
* Output
  + This program prints the file name and the energy score corresponding to the file name that you provided separated by “\t” tab character.

!!! Cheers !!!