

\*\*\*\*\*INTRODUCTION\*\*\*\*\*

This tool is designed for predicting the distance of unknown structure from its native without using its native form in terms of RMSD, GDT and TM, therefore it named as D2N. Principle of prediction is based on universal properties of protein structure such as area, energy, and secondary structure and CB arrangement. User has to submit a protein file in PDB format and D2N gives score of RMSD, GDT and TM.

\*\*\*\*\*INSTALLATION\*\*\*\*\*

=====STEP 1. Prerequisite tools and software=====

- a) This tool can run only on linux machine.
- b) Naccess: <http://www.bioinf.manchester.ac.uk/naccess/>
- c) Psipred: [http://bioinf.cs.ucl.ac.uk/software\\_downloads/](http://bioinf.cs.ucl.ac.uk/software_downloads/)
- d) AMBER: <http://ambermd.org/>
- e) Stride: <http://webclu.bio.wzw.tum.de/stride/>
- f) R statistical software

=====STEP 2. Download D2N=====

- a) Download tool (FILE: web\_donloadable\_D2N.tar.gz) from <http://www.scfbio-iitd.res.in/software/d2n.jsp>
- b) Uncompressed file in home directory
- c) Place following directories/file/executable/scripts in home directory  
all\_Model energy\_minimization\_short\_step  
CB\_CB.exe first\_resi.exe sequencenumber.exe  
d2n.sh final\_result.sh run\_energy.sh  
run\_merge\_features.sh run\_polar\_area.sh run\_residue\_length.sh  
tleap1.sh  
exseq.sh run\_area.sh run\_euclidian\_distance.sh run\_pair\_number.sh  
run\_process\_pdb.sh run\_secondary\_structure.sh trial.sh  
run\_merge\_features\_area.sh  
one\_file.pl s1.cmd tleap1.sh  
singlecode test-result-4.RData testUsingRandomForest\_new\_area.R  
testUsingRandomForest.R

=====STEP 3. Set Path=====

- a) Set the path of Naccess in run\_area.sh
- a) Set the path of Naccess in run\_polar\_area.sh
- b) Set the path of runpsipred in run\_secondary\_structure.sh
- c) Set the path of Stride in run\_secondary\_structure.sh

\*\*\*\*\*STEP3. RUN D2N\*\*\*\*\*

- a) Make a sub directory (ex:TEST) in directory web\_donloadable\_D2N (extracted in step 2(a) & (b))
- b) Copy a query protein model in TEST
- c) Remove multiple chain entry, HETATM record, HEADERS from protein file
- c) run d2n script:  
sh d2n.sh TEST

\*\*\*\*\*STEP 4. RESULT\*\*\*\*\*

Result File: patch\_result  
Result File (HTML): result\_d2n.html (open in browser)