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ELFINv0

ELFIN is a tool developed for analysing and comparing three-dimensionally the electrostatic potential of proteins with a view to establish structural and/or evolutionary conclusions.

REQUIREMENTS, NOTES && TIPS

A) ELFIN uses output from **Adaptive Poisson-Boltzmann Solver (APBS)** software (DX files) as source of electrostatic potential data.

B) UPON COMPARING DIFFERENT PROTEINS, ALL PROTEINS MUST BE ALIGNED FIRST TO THE SAME TEMPLATE FOR MEANINGFUL RESULTS.

C) You need **tcl 8.5 version** for running this program as the associated tcl routine deals with dictionaries (new command "dict"). Such feature is not supported by early versions.

D) **Acrobat Reader** and **Gnome document viewer (Evince)** must be installed for visualizing output PDFs.
If you require a different PDF visualization software, just manually change the path of variables “VIEWER” and “ACROREAD” at the beginning of the main controller script *ELFIN.sh*, located at directory “*YOURHOMEDIR/ELFINvxx/bin/*”, being xx the ELFIN version you installed (i.e. *ELFINv0)*

E) *VMD – Visual Molecular Dynamics* software must be installed for spacial visualization of protein and cubes.

F) **OUTPUT** will show up at *Output/* folder and will include:

1. Three **PDF images** of the results (Heatmap, Contourn1 & Contourn2).
2. **Two tables** in flat format, containing the extracted data (coordinates, potential figures):
    a) One contains 3 dimensions (X, Y and POTENTIAL) and was used to generate the heatmap-like plot
    b) The other contains 4 dimensions (X, Y, Z and POTENTIAL)
3. A **VMD script** (.vmd) containing the saved state showing the 3D cube, if any. For loading up a vmd state, once ELFIN is finised, just run the following command in a terminal:

    $ vmd -e vmdstatefile.vmd

INSTALLATION & EXECUTION:

1. Unzip the package, open your terminal and type:

   $ bash intall.sh

   ELFIN is now installed and ready to be executed from a new terminal.

2. If you got the complete package, you'll find one DX/pqr sample in directory "Samples/" so you can play around a little

3. Now, use the following notation for interactive/non-interactive modes:

   For a guided **INTERACTIVE MODE** where you insert parameters step by step, add no arguments to:

   $ ELFIN

   and just follow-up...

   For **NON-INTERACTIVE MODE** (pass arguments in one command) you have 5 possible combinations of arguments:

   Customize your own patch:

   $ ELFIN dx prot ch coords refres dimx dimy dimz spac patchM cube plot

   Collect coordinates:

   Build A 3D patch around a certain atom:

   $ ELFIN dx prot ch coords coordM res1 atomname dimx dimy dimz spac plot

   Collect list of literal coordinates from 1 patch of all-atom residues:

   $ ELFIN dx prot ch coords coordM answ res1 res2 plot

   Collect list of literal coordinates from 2 different patches of all-atom residues:

   $ ELFIN dx prot ch coords coordM answ res1 res2 res3 res4 plot

   Electrostatic Surface analysis:

   $ ELFIN dx prot distsurf coords dimx dimy dimz spac patchM cube plot

   Dimer interface:

$ ELFIN dx prot coords dimx dimy dimz spac patchM cube plot

Description of <u>ARGUMENTS</u>:

dx

Name of DX file (i.e B2.dx)

prot

Name of structure file. Both PDBs and PQRs accepted (i.e B2.pqr)

ch

Chain ID (i.e A)

coords

Source of coordinates:
1 - Customize your own patch
2 - Residue coordinates collection
3 – Electrostatic surface
Value => 1 or 2

refres

ID of the residue you want to use as reference for building up the patch (i.e. 122)

dimx

Patch X dimension in angstroms (i.e. 6)

dimy

Patch Y dimension in angstroms (i.e. 6)

dimz

Patch Z dimension in angstroms (i.e. 6)

spac

Spacing used for building up the patch in angstroms (i.e. 0.6)

distsurf

Whenever “Electrostatic Surface” is called (*coords=3)*, distsurf

represents the distance of each surface patch to the centre of the structure.

patchM

Method for your path's geometry type:

1 - Line (1D)
2 - Slice (2D)
3 - Cube (3D)

Value => 1, 2 or 3

cube

If *patchmethod* is 3 (CUBE), you can activate visualizing your protein along with a cube of your selected dimensions containing the residues involved, over program execution.
Values => If true: YES | yes | y | 1; If false: NO | no | n | 0

Any other value or just leaving it empty will not produce any visualization. Also, unless no option stated, a VMD state will be saved to *Output/* folder, regardless of the option you choose (Y/N)

plot

Activate or deactivate an interactive visualization of the PDF image of your final results
Values => If true: YES | yes | y | 1; If false: NO | no | n | 0
Any other value or just leaving it empty will not produce any visualization.

coordM

Method for collecting coordinates, once you have picked "Residue coordinates collection" as source of coordinates:

1 - A 3D patch around a certain atom
2 - Literal coordinates of a residue/s

Value => 1 or 2

atomname

Atom ID used as reference for collecting coordinates (i.e. CA)

answ

Whether you'll process 1 or 2 different patches
Value => 1 or 2

res1: Residue ID of first patch's initial residue (i.e. 122)

res2: Residue ID of first patch's end residue (i.e. 130)

res3: Residue ID of second patch's initial residue (i.e. 150)

res4: Residue ID of second patch's end residue (i.e. 170)

UNISTALLING ELFIN:

For uninstalling ELFIN, just open your terminal and type:

$ cd $ELFINDIR

$ bash uninstall.sh