

How to use ALAscanApp

ALAscanApp.py

The utility will create hot constellations and calculate ddG for them from a PDB file. Hot constellations will only be formed from the 'ligand'. The PDB file must have at least two chains and no non-standard amino acids.

It has two modes, auto and manual. In manual mode the constellations are space separated. Each constellation is composed by comma separated residue numbers. Each residue number must be preceded by the chain ID it belongs to. Residues can belong to different chains as long as the chains are part of the ligand.

e.g.

If we have two constellations, one from chain 'C' with residues 6 and 7 and the second one from chain 'D' with residues 10, 12 and 17.

C6,C7 D10,D12,D17

By default the script runs silently and shows the plots at the end of the calculations. This behaviour can be toggled from a general perspective or from the used mode.

Finally, it writes the plot data into a comma separated values (csv) file and the calculations' results into a json file.

The csv file can be used to plot the data with other plotting programs and the json file to replot the data using the [replotAlaScan.py](#) script.

If the number of hot constellations created in the auto mode exceeds the '**MaxAutoNumber**'. We will calculate '**MaxAutoNumber**' of them. The rest will be written to a file, so they can be calculated using the manual mode. Alternatively the '**MaxAutoNumber**' could be increased in initialisation file '**.alascanapp.ini**'.

There are three ways to run the script.

- a. Giving the full path.
- b. Creating a symbolic link into the PATH and calling [ALAscanApp.py](#) like an ordinary command.
- c. Invoking the python interpreter with the full path of the script.

We will assume that you got the file [alaScanApp-dist.tar.gz](#) unpacked and uncompressed in your home directory creating the following directory structure.

```
/HOME/alaScanApp-dist  
/HOME/alaScanApp-dist/alaScanApp.tar.gz  
/HOME/alaScanApp-dist/setup_utils.py  
/HOME/alaScanApp-dist/ccpCode  
/HOME/alaScanApp-dist/ccpCode/getSD  
/HOME/alaScanApp-dist/ccpCode/colourBySD  
/HOME/alaScanApp-dist/ccpCode/dividePDB  
/HOME/alaScanApp-dist/ccpCode/BUDE-1.2.9.tar.gz  
/HOME/alaScanApp-dist/ccpCode/comp_utils.sh
```

We are also assuming that you ran 'setup_utils.py', it was done successfully and we also have this additional directory structure.

```
/HOME/alaScanApp-dist/alaScanApp  
/HOME/alaScanApp-dist/alaScanApp/ALAscanApp.py  
/HOME/alaScanApp-dist/alaScanApp/replotAlaScan.py
```

The final assumption is that you have '/HOME/bin' in your PATH.

Invoking the Script

- a.
>/HOME/alaScanApp-dist/alaScanApp/ALAscanApp.py -h
- b.
>ALAscanApp.py -h
- c.
>python /HOME/alaScanApp-dist/alaScanApp/ALAscanApp.py -h

To use option b. we need to link the script to the path first.

```
>cd /HOME/bin  
>ln -s /HOME/alaScanApp-dist/alaScanApp/ALAscanApp.py  
>ln -s /HOME/alaScanApp-dist/alaScanApp/replotAlaScan.py
```

From now on we will use option b. in our examples.

Usage:

ALAscanApp.py [options] [auto | manual] [options]

To see general help:

`>ALAscanApp.py -h`

To see auto mode help:

`>ALAscanApp.py auto -h`

To see manual mode help:

`>ALAscanApp.py manual -h`

To automatically create hot constellations and calculate ddG for them.

`>ALAscanApp.py auto -p pdb_id.pdb -r A -l B -z 3 -d 10.5`

Where options are:

-p pdb_id.pdb is the PDB file e.g.: 1r8u.pdb

-r A for using chain 'A' as the receptor.

-l B for using chain 'B' as the ligand and the chain to create hot constellations from.

-z 3 Size of the constellations, number of residues.

-d 10.5 Residues with a ddG of 10.5 or more will be used.

To manually calculate ddG for given hot constellations.

`>ALAscanApp.py manual -p pdb_id.pdb -r A -l B -c B345,b348,b349 b352,b353,b354`

Where options are:

-p pdb_id.pdb is the PDB file e.g.: 1r8u.pdb

-r A for using chain 'A' as the receptor.

-l B for using chain 'B' as the ligand and the chain that hot constellations are from.

-c B345,b348,b349 b352,b353,b354 are the hot constellations.

Two constellations from chain B

First one with residues 345, 348 and 349

Second one with residues 352, 353 and 354

To turn off the showing the plots:

Use option **-t**

```
>ALAscanApp.py auto -p pdb_id.pdb -r A -l B -z 3 -d 10.5 -t
```

or

```
>ALAscanApp.py -t auto -p pdb_id.pdb -r A -l B -z 3 -d 10.5
```

To turn on verbose output, not running silently.

Use option **-v**

```
>ALAscanApp.py auto -p pdb_id.pdb -r A -l B -z 3 -d 10.5 -v
```

or

```
>ALAscanApp.py -v auto -p pdb_id.pdb -r A -l B -z 3 -d 10.5
```

To replot the alanine scanning results.

```
>replotAlaScan.py -j pdb_id_auto_timestamp_scan.json
```

Where:

-j pdb_id_auto_timestamp_scan.json is the json file created by ALAscanApp for pdb_id.pdb file in auto mode at timestamp.