Cross-Alpha-Det

A python-based GUI software to detect cross-α amyloid candidates

Introduction

Cross-α amyloid like structures are a relatively new idea in protein chemistry and are formed by repeated α-helices, similar to cross-β sheets. There has been only one naturally occurring cross-α amyloid structure found and six others have been synthesized. It was found that the interactions mainly through hydrophobic groups, i.e. the hydrophobic residues are found to be close between the helices while the part exposed to solvent has been found to be hydrophilic. This concept led us to design a software which, on producing RCSB PDB ID, PDB File or Stride file, will give us the possible candidates which may form cross-α helix structures.

Installation

Currently, the source code works for Linux/Mac only. You will need the following packages:

- Python 3 (>=3.6)

- PyQt5

- PyInstaller

- Stride (http://webclu.bio.wzw.tum.de/stride/)

In case you are using **Anaconda** or **Miniconda** as your default python package, kindly note that you will have to go through **advanced options**.

Quick Installation

If you are a newbie and is not an expert in Linux/Mac, or you do not want to change the default options, then:

1. Download the file: **crossalphadet.tgz**

2. Open terminal and `cd` into the directory downloaded

3. Type in the following commands:

```
tar -xvzf crossalphadet.tgz
cd crossalphadet
sudo make pythoncomponents
make
sudo make install
```

Quick Uninstallation

For uninstalling, open terminal and `cd` into the source directory. Then type in the following commands:

```
make clean
sudo make uninstall
```

Advanced Options

The advanced installation has various options in the Makefile. Kindly find them with the description below. Note that if you wish to use the advanced options, kindly write them along with every make command you use.

- **PY**: This is the command/location of system Python3 interpretor.

- **PYINSTALLER**: This is the command/location of system PyInstaller.

- **BUILDDIR**: Location where the executable will be built. Default: ./bin.

- **INSTALLDIR**: Location for installing Cross-Alpha-Det files. Default: /opt/crossalphadet

- **LINKDIR**: Location of a directory where symbolic links for Cross-Alpha-Det and stride (if installed along with Cross-Alpha-Det) will be created. Default: /bin **LINKDIR** has to be some directory in your **PATH**, if you want to execute Cross-Alpha-Det from anywhere in terminal.

- **INSTALL_STRIDE**: If set to yes, stride will be installed from source (supplied with Cross-Alpha-Det). Default: yes If you set this to no, then it is your responsibility to **install a copy of stride** and provide the location in **PATH**.

- **INSTALL_PIP**: If set to yes, installs pip. Internet is required for this activity. Default: yes

- **INSTALL_PYINSTALLER**: If set to yes, installs PyInstaller using pip. Internet is required for this activity. Default: yes

- **INSTALL_PYQT5**: If set to yes, installs PyQt5 using pip. Internet is required for this activity. Default: yes

Anaconda/Miniconda users are suggested to use their **system python and pyinstaller (not Anaconda python or pyinstaller)** for installing crossalphadet. Kindly set the variables **PY** and **PYINSTALLER** accordingly.

There are five activities one can use in Makefile. Kindly find each activity below:

- **make** or **make crossalphadet**: This option build stride and Cross-Alpha-Det in **BUILDDIR**. Stride compilation is dependent on **INSTALL_STRIDE**. The option uses PyInstaller, hence appropriate value of **PYINSTALLER** has to be provided.

- **make pythoncomponents**: This option installs python components (pip, PyInstaller and PyQt5). Python location depends on **PY**, while installation of pip, PyInstaller and PyQt5 is dependent on **INSTALL_PIP**, **INSTALL_PYINSTALLER** and **INSTALL_PYQT5** respectively.

- **make install**: Installs Cross-Alpha-Det in **INSTALLDIR** and creates symbolic link of stride (if built) and Cross-Alpha-Det in **LINKDIR**. Must be run after building Cross-Alpha-Det in **BUILDDIR**.

- **make uninstall**: Removes Cross-Alpha-Det in **INSTALLDIR** and links created in **LINKDIR**.

- **make clean**: Removes complied Cross-Alpha-Det from **BUILDDIR**.

Using Cross-Alpha-Det

The GUI-based software, Cross-Alpha-Det, is incredibly easy to use. A screenshot of the interface has been given in Figure 1 and 2. There can be three starting points — an RCSB PDB ID, a PDB file or a stride file. There are a few adjustable parameters, discussed below.

- **Angle**: This is the angle for which possible sequences for hydrophilic residues will be generated. For example, if the angle is 95°, then if the helix is viewed laterally, 0-95° will contain hydrophilic residues, while 95-360° will contain hydrophobic residues.

- **Correlation**: This is the lower limit of the similarity function between the helix read and a helix of similar length generated.

- **Helix Length**: This function checks if the requested helix lie within the given range.

- **The Check Box**: On enabling, it checks if the minimum number of hydrophilic residues are met in order to at least cover a strip of the helix. In other words, it checks if the no of hydrophobic residues is at least (total residues/3.6).
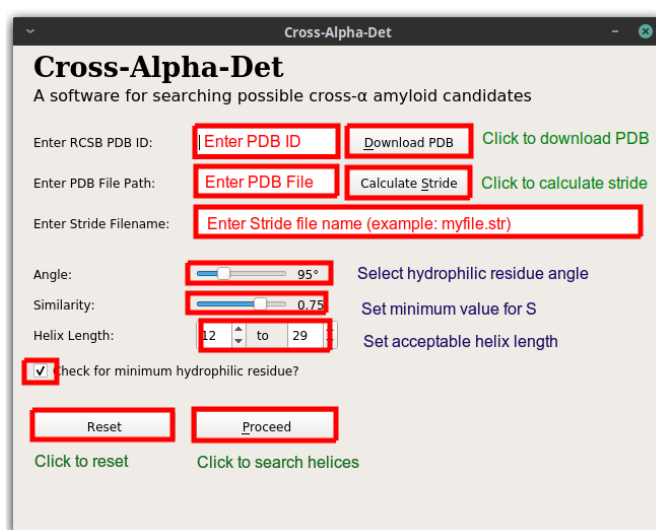

Figure 1: Screen shot of Cross-Alpha-Det with instructions.

The software, along with calculating the possible candidates, also calculated the propensity for each candidate, which gives one a rough idea about the stability of the helix. Helices with higher propensity value are considered to be less stable.

Contact Details

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