pyvol Documentation

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CONTENTS

PyVOL is a python library packaged into a *PyMOL* GUI for identifying protein binding pockets, partitioning them into sub-pockets, and calculating their volumes. PyVOL can be run as a PyMOL plugin through its GUI or the PyMOL prompt, as an imported python library, or as a commandline program. Visualization of results is exclusively supported through PyMOL though exported surfaces are compatible with standard 3D geometry visualization programs.

CHAPTER

ONE

INSTALLATION

PyVOL can be installed into any python environment; however, for most users direct installation into PyMOL will be easiest.

1.1 Installation into PyMOL

PyVOL is distributed as a GUI and a backend. Installation into PyMOL uses PyMOL's plugin manager to install the GUI and then the GUI to install the backend. The GUI is installed through the plugin manager through loading the zipped GUI file:

```
https://github.com/rhs2132/pyvol/blob/master/pyvolgui.zip
```

This creates a new `PyVOL` menu entry under plugins. The third tab of the GUI allows installation of PyVOL from PyPI along with all available dependencies. For more information, especially on Windows, see the installation page.

CHAPTER

TWO

RUNNING PYVOL

2.1 Quick Start

From within PyMOL, the simplest binding pocket calculation is simply run at the PyMOL prompt with:

```
pocket protein_selection
```

The two parameters that most dramatically affect calculations are the maximum and minimum radii used to respectively define the exterior surface of the protein and the boundary of the binding pocket itself. In practice, the minimum radius does not need to be changed as its default (1.4) is broadly useful. The maximum radius does often need to be adjusted to find a suitable value using the max_rad parameter:

```
pocket protein_selection, min_rad=1.4, max_rad=3.4
```

2.2 Further Examples

For extensive explanations and documentations of the GUI and command line interfaces, see the examples page.

CHAPTER

THREE

MODULE DOCUMENTATION

For full documentation of the code, see the modules page.

3.1 Installation

PyVOL distribution is hosted by PyPI and accessed through pip. PyVOL can consequently be installed into any python environment. For convenience, the PyMOL GUI contains an installer.

3.1.1 Detailed Installation into PyMOL

PyVOL is distributed as a GUI and a backend. Installation into PyMOL uses PyMOL's plugin manager to install the GUI and then the GUI to install the backend. The GUI is installed through the plugin manager through loading the zipped GUI file:

```
https://github.com/rhs2132/pyvol/blob/master/pyvolgui.zip
```

This creates a new `PyVOL` menu entry under plugins. The third tab of the GUI allows installation of PyVOL from PyPI along with all available dependencies. On Linux and MacOS, MSMS is automatically installed from the platform-limited bioconda channel. MSMS installation instructions are otherwise below.

3.1.2 Manual Installation

PyVOL minimally requires biopython, MSMS, numpy, pandas, scipy, scikit-learn, and trimesh in order to run. PyVOL is available for manual installation from github or through PyPI. Most conveniently:

```
pip install bio-pyvol
```

3.1.3 MSMS Installation

MSMS can be installed on MacOS and Linux using the bioconda channel:

```
conda install -c bioconda msms
```

Otherwise MSMS must be installed manually by downloading it from MGLTools and adding it to the path. PyMOL distributions from Schrodinger have MSMS included; however, it must still be added to the path manually. The executable is located at:

```
<pymol_root_dir>/pkgs/msms-2.6.1-2/bin/msms
```

3.1.4 Updating

PyVOL can be updated via the command line:

```
pip update bio-pyvol
```

If using the PyMOL GUI, the third tab has a button labeled `Check for Updates` that will query PyPI to detect whether an update is available. If one is available, that button changes to `Update PyVOL` and permits updating with a single click.

3.1.5 Uninstallation

PyVOL can be uninstalled via the command line:

```
pip uninstall bio-pyvol
```

If using the PyMOL GUI, the third tab has a button labeled `Uninstall PyVOL` that will remove the PyVOL backend. Afterwards, selecting uninstall on the plugin within the PyMOL plugin manager will the GUI.

CHAPTER

FOUR

INDICES AND TABLES

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