Pyshifts User Guide

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January 16, 2017

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1 Introduction

1.1 Overview

PyShifts is a PyMol based graphical analysis tool that utilize chemical shifts to assess the global quality of NMR structures of RNA. Pyshifts takes structure and measured chemical shifts file as input, using various predictors to predict chemical shifts for the structure (or different states in an ensemble if input is an ensemble), comparing it to measured chemical shifts, analyze and visualize difference. Or, it can take external predicted chemical shifts, comparing it to measured chemical shifts and visualize difference.

Codes and resources are freely available at out github site. For more information on theoretical basis as well as our promising test results, see manuscript.

Pyshifts is tested on Mac OS X El Captain, the following manual uses Mac OS X as example.

1.2 Copyright Notice

2 Installation

2.1 Requirements

Pyshifts is a plugin in PyMOL, an open source Python-enhanced molecular graphics tool. Python of version 2.7.10 and PyMOL are REQUIRED for Pyshifts.

2.2 Installation guide

1. Python

   Python version of 2.7.10 (and 2.7.10 only), which is freely available at https://www.python.org/downloads/release/python-2710/.

   If your current Python version is not 2.7.10, and you prefer not to change it, you can use the following commands to create a Python 2.7.10 environment temporarily for Pyshifts:

   ```
   conda create -n pyshifts python=2.7.10
   source active pyshifts
   ```

   After each use of Pyshifts, use

   ```
   source deactivate pyshifts
   ```

   to go back to your normal Python settings.

2. PyMOL

   You can obtain PYMOL at sourceforge https://sourceforge.net/projects/pymol/.

3. Adding Pyshifts to PyMOL

   Download or clone this git repository. Open PyMOL and then go to "Plugin"→"Plugin manager"→"Install new plugin", and choose the Pyshifts.py file in your local Pyshifts repository. For this step PyMOL need to be run with the Tcl/Tk interface, read more on PyMOL wiki https://pymolwiki.org/index.php/Plugins.

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