Whole-cell utilities Documentation

Release 0.0.23

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This package contains utilities that are useful to multiple whole-cell (WC) software components.

CHAPTER

ONE

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1.1 Installation

1.1.1 Prerequisites

First, install the third-party packages listed below. Detailed installation instructions are available in An Introduction to Whole-Cell Modeling.

- ChemAxon Marvin: optional to calculate major protonation states
  - Java >= 1.8
- Git
- OpenBabel: optional to calculate chemical formulae
- Pip >= 18.0
- Python >= 3.6

To use ChemAxon Marvin to calculate major protonation states, set `JAVA_HOME` to the path to your Java virtual machine (JVM) and add Marvin to the Java class path:

```
export JAVA_HOME=/usr/lib/jvm/default-java
export CLASSPATH=$CLASSPATH:/opt/chemaxon/marvinsuite/lib/MarvinBeans.jar
```

1.1.2 Latest release From PyPI

Run the following command to install the latest release from PyPI:

```
pip install wc_utils[all]
```

1.1.3 Latest revision from GitHub

Run the following command to install the latest version from GitHub:

```
pip install git+https://github.com/KarrLab/pkg_utils.git#egg=pkg_utils[all]
pip install git+https://github.com/KarrLab/wc_utils.git#egg=wc_utils[all]
```

1.2 About

1.2.1 License

The software is released under the MIT license

```
The MIT License (MIT)

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```

1.2.2 Development team

This package was developed by the Karr Lab at the Icahn School of Medicine at Mount Sinai in New York, USA.

1.2.3 Acknowledgements

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1.2.4 Questions and comments

Please contact the Karr Lab with any questions or comments.