

Introduction

MayaChemTools is a growing collection of Perl scripts, modules, and classes to support day-to-day computational discovery needs.

The current release of MayaChemtools provides command line scripts for the following tasks: Manipulation of SD, CSV/TSV, Sequence/Alignments, and PDB files; Analysis of data in SD, CSV/TSV, and Sequence/Alignments files; Information about data in SD, CSV/TSV, Sequence/Alignments, PDB, and fingerprints files; Exporting data from Oracle and MySQL tables into text files; Properties of periodic table elements, amino acids, and nucleic acids; Elemental analysis; Fingerprints generation; Similarity matrix calculation

Review the documentation for further details.

Installation

1. Add <YOUR MAYACHEMTOOLS DIR>/bin to your PATH environment variable.
2. And check to make sure PATH doesn't contain multiple entries for MayaChemTools package, and all *.pl files in <YOUR MAYACHEMTOOLS DIR>/bin are executable.

That's it. And you're all set to try out the various scripts.

Caveats

All output files generated by MayaChemTools package contain UNIX style new line character; you can modify it using ModifyNewLineChar.pl script.

Dependencies

Perl v5.8 or higher. Additional Perl modules required to use database scripts: DBI, DBD-mysql and/or DBD-Oracle.

Supported Platforms

Whatever Perl supports: www.cpan.org/ports/. It includes support for various flavors of UNIX, LINUX, Windows, and Mac operating systems running on all kinds of hardware platforms.

Perl Download

www.cpan.org

Feedback

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