
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; Generation of fingerprints corresponding to atom neighborhoods, atom types, E-state indices, extended connectivity, MACCS keys, path lengths, topological atom pairs, topological atom triplets, topological atom torsions, topological pharmacophore atom pairs, and topological pharmacophore atom triplets; Generation of fingerprints with atom types corresponding to atomic invariants, DREIDING, E-state, functional class, MMFF94, SLogP, SYBYL, TPSA and UFF; Calculation of similarity matrices using a variety of similarity and distance coefficients; Calculation of physicochemical properties including rotatable bonds, van der Waals molecular volume, hydrogen bond donors, hydrogen bond acceptors, SLogP, TPSA and so on.

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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