

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, molecular complexity and so on; Similarity searching using fingerprints.

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

Manish Sud<msud@san.rr.com>

Copyright & License

Copyright (C) 2017 Manish Sud. All rights reserved.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License. Please see GNULICENSE.txt file for additional information.