## NAME

PyMOLCalculateProperties.py - Calculate physicochemical properties

## SYNOPSIS

PyMOLCalculateProperties.py [--addHydrogens <yes or no>] [--chainIDs <First, All or ID1,ID2...>] [--list] [--keepInorganics <yes or no>] [--keepLigands <yes or no>] [--keepSolvents <yes or no>] [--mode <All or Name1,Name2,Name3,...>] [--overwrite] [--precision <number>] [--quiet <yes or no>] [-w <dir>] -i <infile1,infile2,infile3...> -o <outfile>

PyMOLCalculateProperties.py -l | --list

PyMOLCalculateProperties.py -h | --help | -e | --examples

## DESCRIPTION

Calculate physicochemical properties for macromolecules. The properties may be calculated for the complete complex or a specified list of chain IDs. Ligands, inorganics, and solvents may be optionally excluded during the calculation of properties.

The supported input file format are: PDB (.pdb), mmCIF (.cif)

The supported output file formats are: CSV (.csv), TSV (.tsv, .txt)

## OPTIONS

-a, --addHydrogens <yes or no> [default: yes]

Add hydrogens before calculating physiochemical properties.

-c, --chainIDs <First, All or ID1,ID2...> [default: All]

List of chain IDs to use for calculating physicochemical properties. Possible values: First, All, or a comma delimited list of chain IDs. The default is to use all chain IDs in input file.

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infiles <infile1,infile2,infile3...>

A comma delimited list of input files. The wildcards are also allowed in file names.

--keepInorganics <yes or no> [default: yes]

Keep inorganic molecules during calculation of physiochemical properties. The inorganic molecules are identified using inorganic selection operator available in PyMOL.

--keepLigands <yes or no> [default: yes]

Keep ligand molecules during calculation of physiochemical properties. The ligand molecules are identified using organic selection operator available in PyMOL.

--keepSolvents <yes or no> [default: yes]

Keep solvent molecules during calculation of physiochemical properties. The solvent molecules are identified using solvent selection operator available in PyMOL.

-l, --list

List available property names without performing any calculations.

-m, --mode <All or Name1,Name2,Name3,...> [default: All]

Comma delimited lists of physicochemical properties to calculate. Default: 'All'. The following properties may be calculated for macromolecules:

```
CenterOfMass,MolecularWeight,MolecularSurfaceArea
SumOfFormalCharges,SumOfPartialCharges,SolventAccessibleSurfaceArea
```

-o, --outfile <outfile>

Output file name for writing out calculated values. Supported text file extensions: csv, tsv or txt.

--overwrite

Overwrite existing files.

-p, --precision <number> [default: 3]

Floating point precision for writing the calculated property values.

-q, --quiet <yes or no> [default: yes]

Do not print information during the calculation of properties.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

## EXAMPLES

To calculate all available properties for all chains in input file along with all ligands, inorganics and solvents after adding hydrogens and write out a CSV file containing calculated values and PDB IDs, type:

```
% PyMOLCalculateProperties.py  -i Sample3.pdb -o Sample3Out.csv
```

To calculate specified properties for all chains in input file along with all ligands, inorganics and solvents after adding hydrogens and write out a CSV file containing calculated values and PDB IDs, type:

```
% PyMOLCalculateProperties.py  -m "MolecularWeight,CenterOfMass"
  -i Sample3.pdb -o Sample3Out.csv
```

To calculate all available properties for chain E in input file without including ligands, inorganics and solvents, and addition of hydrogens, and write out a TSV file containing calculated values and PDB IDs, type:

```
% PyMOLCalculateProperties.py  --addHydrogens no -c E --keepLigands
  no --keepInorganics  no --keepSolvents no -i Sample3.pdb -o
  Sample3Out.tsv
```

To calculate all available properties for all chains in multiple files along with all ligands, inorganics and solvents after adding hydrogens and write out a CSV file containing calculated values and PDB IDs, type:

```
% PyMOLCalculateProperties.py  -i "Sample3.pdb,Sample4.pdb,Sample5.pdb"
  -o SampleOut.csv
```

## AUTHOR

Manish Sud(msud@san.rr.com)

## SEE ALSO

PyMOLCalculateRMSD.py, PyMOLSplitChainsAndLigands.py, PyMOLVisualizeMacromolecules.py

## COPYRIGHT



The functionality available in this script is implemented using PyMOL, a molecular visualization system on an open source foundation originally developed by Warren DeLano.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.