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

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

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