
NAME

RDKitConvertFileFormat.py - Convert between molecular file formats

SYNOPSIS

```
RDKitConvertFileFormat.py [--infileParams <Name,Value,...>] [ --outfileParams <Name,Value,...> ] [
--overwrite] [-w <dir>] -i <infile> -o <outfile>
```

```
RDKitConvertFileFormat.py -h | --help | -e | --examples
```

DESCRIPTION

Convert between molecular file formats.

The supported input file formats are: Mol (.mol), SD (.sdf, .sd), SMILES (.smi, .txt, .csv, .tsv), MOL2 (.mol2), PDB (.pdb)

The supported output file formats are: SD (.sdf, .sd), SMILES (.smi), PDB (.pdb)

OPTIONS

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

--infileParams <Name,Value,...> [default: auto]

A comma delimited list of parameter name and value pairs for reading molecules from files. The supported parameter names for different file formats, along with their default values, are shown below:

```
SD, MOL: removeHydrogens,yes,sanitize,yes,strictParsing,yes
MOL2: removeHydrogens,yes,sanitize,yes
SMILES: smilesColumn,1,smilesNameColumn,2,smilesDelimiter,space,
        smilesTitleLine,auto,sanitize,yes
PDB: removeHydrogens,yes,sanitize,yes
```

Possible values for smilesDelimiter: space, comma or tab.

-o, --outfile <outfile>

Output file name.

--outfileParams <Name,Value,...> [default: auto]

A comma delimited list of parameter name and value pairs for writing molecules to files. The supported parameter names for different file formats, along with their default values, are shown below:

```
SD: compute2DCoords,auto,kekulize,yes,forceV3000,no
SMILES: smilesKekulize,no,smilesDelimiter,space, smilesIsomeric,yes,
        smilesTitleLine,yes,smilesMolName,yes,smilesMolProps,no
```

Default value for compute2DCoords: yes for SMILES input file; no for all other file types.

--overwrite

Overwrite existing files.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To convert a SD file into a isomeric SMILES file, type:

```
% RDKitConvertFileFormat.py -i Sample.sdf -o SampleOut.smi
```

To convert a SD file into a non isomeric SMILES file, type

```
% RDKitConvertFileFormat.py --outfileParams "smilesIsomeric,no"
-i Sample.sdf -o SampleOut.smi
```

To convert a SMILES file into a SD file along with calculation of 2D coordinates, type:

```
% RDKitConvertFileFormat.py -i Sample.smi -o SampleOut.sdf
```

To convert a MDL MOL file into a PDB file, type:

```
% RDKitConvertFileFormat.py -i Sample.mol -o SampleOut.pdb
```

To convert a CSV SMILES file with column headers, SMILES strings in column 1, and name in column 2 into a SD file containing 2D coordinates, type:

```
% RDKitConvertFileFormat.py --infileParams "smilesDelimiter,comma,
smilesTitleLine,yes,smilesColumn,1,smilesNameColumn,2" -i Sample.csv
-o SampleOut.sdf
```

AUTHOR

Manish Sud(msud@san.rr.com)

SEE ALSO

RDKitDrawMolecules.py, RDKitRemoveDuplicateMolecules.py, RDKitSearchFunctionalGroups.py,
RDKitSearchSMARTS.py

COPYRIGHT

Copyright (C) 2024 Manish Sud. All rights reserved.

The functionality available in this script is implemented using RDKit, an open source toolkit for cheminformatics developed by Greg Landrum.

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.