NAME

PyMOLConvertLigandFileFormat.py.py - Convert between ligand file formats

SYNOPSIS

PyMOLConvertLigandFileFormat.py.py [--overwrite] [-w <dir>] -i <infile> -o <outfile>

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

DESCRIPTION

Convert between ligand file formats.

The supported input and output file formats are: MDLMOL (.mol), MOL2 (.mol2), and PDB (.pdb).

OPTIONS

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

-o, --outfile <outfile>

Output file name.

--overwrite

Overwrite existing files.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To convert MDLMOL file format to MOL2 file format, type:

```
% PyMOLConvertLigandFileFormat.py -i caffeine.mol -o caffeine.mol2
```

To convert MDLMOL file format to PDB file format, type:

```
% PyMOLConvertLigandFileFormat.py -i caffeine.mol -o caffeine.pdb
```

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SEE ALSO

PyMOLConvertPMLToPSE.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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