NAME

PyMOLExtractSelection.py - Extract selection from a macromolecule

SYNOPSIS

PyMOLExtractSelection.py [--overwrite] [--selectionAppend <yes or no>] [-w <dir>] -i <infile> -o <outfile> -s <selection>

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

DESCRIPTION

Extract data corresponding to a PyMOL selection specification from a macromolecule in an input file and write it out to an output file.

The selection specification must be a valid PyMOL specification. No validation is performed.

The supported input file format are: PDB (.pdb) and CIF (.cif)

The supported output file formats are: PDB (.pdb) and CIF (.cif)

OPTIONS

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

-o, --outfile <infile>

Output file name.

-s, --selection <PyMOL SelectionSpec>

Selection specification for extracting data from a macromolecule in an input file. The selection specification must be a valid PyMOL specification. No Validation is performed.

The specified selection specification is optionally appended to PyMOL object name for input file.

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

Append specified selection specification to PyMOL object name for input file before creating PyMOL object for a specified selection specification. The PyMOL object name for input file is <InfileRoot>.

You may choose to explicitly specify PyMOL object name in the selection specification instead of automatically appending it to the selection.

--overwrite

Overwrite existing files.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To extract all data corresponding to chain E in a macromolecule and write out to a PDB file, type:

```
% PyMOLExtractSelection.py -i Sample3.cif -o Sample3Out.pdb -s "chain E" --ov
```

To extract only polymer chain data for chains E and I in a macromolecule and write out to a PDB file, type:

```
% PyMOLExtractSelection.py -i Sample3.cif -o Sample3Out.pdb
  -s "((chain E) or (chain I)) and polymer" --ov
```

To extract only polymer chain data for chain E in a macromolecule and write out to a PDB file, type:

```
    % PyMOLExtractSelection.py -i Sample3.pdb -o Sample3Out.pdb
      -s "(chain E) and polymer" --ov
```

To extract only polymer chain data for chain E in a macromolecule by explicitly ignoring non-polymer chain data and write out to a CIF file, type:

```
    % PyMOLExtractSelection.py -i Sample3.pdb -o Sample3Out.cif
      -s "(chain E) and (not organic) and (not solvent) and
      (not inorganic)" --ov
```

To extract solvent data corresponding to chain E in a macromolecule and write out to a PDB file, type:

```
    % PyMOLExtractSelection.py -i Sample3.pdb -o Sample3Out.pdb
      -s "(chain E) and solvent" --ov
```

To extract ligand data corresponding to chain E in a macromolecule and write out to a PDB file, type:

```
    % PyMOLExtractSelection.py -i Sample3.pdb -o Sample3Out.pdb
      -s "(chain E) and organic" --ov
```

To extract binding pocket residues with 5.0 of ligand ID ADP in chain E and write out a PDB file, type:

```
    % PyMOLExtractSelection.py -i Sample3.pdb -o Sample3Out.pdb
       --selectionAppend no -s "(byresidue (Sample3 and chain E)
      within 5.0 of (Sample3 and chain E and organic and resn ADP))
      and polymer" --ov
```

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SEE ALSO

PyMOLAlignChains.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.

This file is part of MayaChemTools.