NAME

PyMOLMutateNucleicAcids.py - Mutate nucleic acids

SYNOPSIS

PyMOLMutateNucleicAcids.py [--mutations <Spec1,Spec2,...>] [--overwrite] [-w <dir>] -i <infile> -o <outfile>

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

DESCRIPTION

Mutate nucleic acids in macromolecules. The mutations are performed using nucleic acids mutagenesis wizard available in PyMOL starting V2.2.

The supported input and output file format is: PDB (.pdb)

OPTIONS

-m, --mutations <Spec1,Spec2,...> [default: None]

Comma delimited list of specifications for mutating nucleic acids.

The format of mutation specification is as follows:

```
<ChainID>:<ResNum><BaseName>,...
```

A chain ID in the first specification of a mutation is required. It may be skipped in subsequent specifications. The most recent chain ID is used for the missing chain ID. The residue number corresponds to the residue to be mutated and must be present in the current chain. The base name represents the new base.

Examples:

```
A:9Thy, A:10Thy
A:9Thy,10Thy,11Thy
A:9Thy,10Thy,B:5Ade,6Ade
```

The base names must be valid for mutating nucleic acids. No validation validation is performed before mutating residues via nucleic acids mutagenesis wizard available in PyMOL. The current version of the wizard supports the following base names:

```
Adenine, Ade
Cytosine, Cyt
Guanine, Gua
Thymine, Thy
Uracil, Ura
```

-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 mutate a single residue in a specific chain and write a PDB file, type:

```
% PyMOLMutateNucleicAcids.py -m "A:9Thy" -i Sample9.pdb
  -o Sample9Out.pdb
```

To mutate multiple residues in a single chain and write a PDB file, type:

```
% PyMOLMutateNucleicAcids.py -m "A:9Thy,10Thy,11Thy" -i Sample9.pdb
  -o Sample9Out.pdb
```

To mutate multiple residues across multiple chains and write a PDB file, type:

```
% PyMOLMutateNucleicAcids.py -m "A:9Thy,10Thy,B:5Ade,6Ade"
  -i Sample9.pdb -o Sample9Out.pdb
```

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SEE ALSO

DownloadPDBFiles.pl, PyMOLMutateAminoAcids.py, PyMOLVisualizeMacromolecules.py

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