NAME

OpenMMPrepareMacromolecule.py - Prepare a macromolecule for simulation.

SYNOPSIS

OpenMMPrepareMacromolecule.py [--addHeavyAtoms <yes or no>] [--addHydrogens <yes or no>] [--addHydrogensAtpH <number>] [--addResidues <yes or no>] [--deleteHeterogens <All, AllExceptWater, WaterOnly, None>] [--ionPositive <text>] [--ionNegative <text>] [--ionicStrength <number>] [--listDetails <yes or no>] [--membrane <yes or no>] [--membraneParams <Name,Value,..>] [--overwrite] [--replaceNonStandardResidues <yes or no>] [--waterBox <yes or no>] [--waterBoxParams <Name,Value,..>] [-w <dir>] -i <infile> -o <outfile>

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

DESCRIPTION

Prepare a macromolecute in an input file for molecular simulation and and write it out to an output file. The macromolecule is prepared by automatically performing the following actions:

```
. Identify and replace non-standard residues
. Add missing residues
. Add missing heavy atoms
. Add missing hydrogens
```

You may optionally remove heterogens, add a water box, and add a lipid membrane.

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

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

OPTIONS

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

Add missing non-hydrogen atoms based on the templates. The terminal atoms are also added.

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

Add missing hydrogens at pH value specified using '-addHydrogensAtpH' option. The missing hydrogens are added based on the templates and pKa calculations are performed.

--addHydrogensAtpH <number> [default: 7.0]

pH value to use for adding missing hydrogens.

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

Add missing residues unidentified based on the PDB records.

--deleteHeterogens <All, AllExceptWater, WaterOnly, None> [default: auto]

Delete heterogens corresponding to non-standard names of amino acids, dna, and rna along with any ligand names. 'N' and 'UNK' also consider standard residues. Default value: WaterOnly during addition of WaterBox or Membrane; Otherwise, None.

The 'AllExceptWater' or 'None' values are not allowed during the addition of a water box or membrane. The waters must be deleted as they are explicitly added during the construction of a water box and membrane.

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

--ionPositive <text> [default: Na+]

Type of positive ion to add during the addition of a water box or membrane. Possible values: Li+, Na+, K+, Rb+, or Cs+.

--ionNegative <text> [default: Cl-]

Type of negative ion to add during the addition of a water box or membrane. Possible values: Cl-, Br-,

F-, or I-.

--ionicStrength <number> [default: 0.0]

Total concentration of both positive and negative ions to add excluding the ions added to neutralize the system during the addition of a water box or a membrane.

-l, --listDetails <yes or no> [default: no]

List details about missing and non-standard residues along with residues containing missing atoms.

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

Add lipid membrane along with a water box. The script replies on OpenMM method modeller.addMebrane() to perform the task. The membrane is added in the XY plane. The existing macromolecule must be oriented and positioned correctly.

A word to the wise: You may want to start with a model from the Orientations of Proteins in Membranes (OPM) database at http://opm.phar.umich.edu.

The size of the membrane and water box are determined by the value of 'padding' parameter specified using '--membraneParams' option. All atoms in macromolecule are guaranteed to be at least this far from any edge of the periodic box.

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

A comma delimited list of parameter name and value pairs for adding a lipid membrane and water.

The supported parameter names along with their default values are are shown below:

```
lipidType, POPC  [ Possible values: POPC, POPE, DLPC, DLPE,  DMPC,
    DOPC or DPPC ]
membraneCenterZ, 0.0
padding, 1.0
```

A brief description of parameters is provided below:

```
lipidType: Type of lipid to use for constructing the membrane.
membraneCenterZ: Position along the Z axis of the center of
    the membrane in nanomertes.
padding: Minimum padding distance to use in nanomertes. It's used
    to determine the size of the membrane and water box. All atoms
    in macromolecule are guaranteed to be at least this far from
    any edge of the periodic box.
```

-o, --outfile <infile>

Output file name.

--overwrite

Overwrite existing files.

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

Replace non-standard residue names by standard residue names based on the list of non-standard residues available in pdbfixer.

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

Add water box.

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

A comma delimited list of parameter name and value pairs for adding a water box.

The supported parameter names along with their default values are are shown below:

```
mode, Padding  [ Possible values: Size or Padding ]
size, None  [ Possible value: xsize ysize zsize ]
padding, 1.0
shape, cube  [ Possible values: cube, dodecahedron, or octahedron ]
```

A brief description of parameters is provided below:

```
mode: Specify the size of the waterbox explicitly or calculate it
    automatically for a macromolecule along with adding padding
    around macromolecule.
size: A space delimited triplet of values corresponding to water
    size in nanometers. It must be specified during 'Size' value of
```

```
            'mode' parameter.
        padding: Padding around macromolecule in nanometers for filling
            box with water. It must be specified during 'Padding' value of
            'mode' parameter.
```

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To prepare a macromolecule in a PDB file by replacing non-standard residues, adding missing residues, adding missing heavy atoms and missing hydrogens, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py -i sample11.pdb -o Sample11Out.pdb
```

To run the first example for listing additional details about missing atoms and residues, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --listDetails -i Sample11.pdb
  -o Sample11Out.pdb
```

To run the first example for deleting all heterogens including water along with performing all default actions, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --deleteHeterogens All -i Sample11.pdb
  -o Sample11Out.pdb
```

To run the first example for deleting water only heterogens along with performing all default actions, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --deleteHeterogens WaterOnly
  -i Sample11.pdb -o Sample11Out.pdb --ov
```

To run the first example for adding a water box by automatically calculating its size, along with performing all default actions, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --waterBox yes -i Sample11.pdb
  -o Sample11Out.pdb
```

To run the previous example by explcitly specifying various water box parameters, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --waterBox yes
  --waterBoxParams "mode,Padding, size, none, padding, 1.0, shape, cube"
  -i Sample11.pdbi -o Sample11Out.pdb
```

To run the first example for adding a water box of a specific size along with performing all default actions, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --waterBox yes
  --waterBoxParams "mode,Size, size, 7.635 7.077 7.447"
  -i Sample11.pdbi -o Sample11Out.pdb
```

To add a lipid membrane around a correctly oriented and positioned macromolecule, along with performing all default actions, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --membrane yes
  -i Sample11.pdbi -o Sample11Out.pdb
```

To run the previous example by explcitly specifying various membrane parameters, and generate a PDB file, type:

```
% OpenMMPrepareMacromolecule.py --membrane yes
  --membraneParams "lipidType, POPC, membraneCenterZ, 0.0, padding, 1.0"
  -i Sample11.pdb -o Sample11Out.pdb
```

AUTHOR

Manish Sud(msud@san.rr.com)

SEE ALSO

InfoPDBFiles.pl, ExtractFromPDBFiles.pl, PyMOLExtractSelection.py, PyMOLInfoMacromolecules.py, PyMOLSplitChainsAndLigands.py

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