index /home/mpastor/soft/eTAM/src/utils.py

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utils
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# -*- coding: utf-8 -*-
#
# Description eTAM utility functions
#
#
#
# Authors: Manuel Pastor (manuel.pastor@upf.edu)
#
# (c) PhI 2013
```

Modules

<u>os</u> <u>shutil</u>

Functions

lastVersion(verID)

Returns the path to the directory where the verID version of the model is located

If a value of -1 is provided, analyzes the "version0000" directories and returns the last one

nextVersion(

Returns the path to the directory where the verID version of the model is located

If a value of -1 is provided, analyzes the "version0000" directories and returns the last one

removefile(file)

Removes silently files or whole paths.

It checks the existence of the file in the argument and if it does not exists do not issue any error

splitSDF(molecules)

Splits a SDFile containing 1 to n molecules

Every molecule is written to a ""m0000000001.sdf"" file and the full list of names is returned in a list

writeError(error)

Print an error message

Data

opt = '/home/mpastor/soft/eTAM/opt/'
wkd = '/home/mpastor/soft/eTAM/src'