simuAnalysis MANUAL

NAME

simuAnalysis, a python based tool for simple calculations over the results from atomistic (XTC files) and coarse-grain (PBD files) protein dynamic simulations.

The package calculates RG and residue distance for both atomistic and coarse grain, and additionally, it calculates Length Scaling Exponent (LSE), and estimated FRET measurements.

A configuration file must be concluded in the input directory.

COMMANDS

First attribute needs to be either ‘coarse’ or ‘atomistic’

-f <path>

Directory path withholds the simulation’s results. For ‘coarse’ any parent directory will be enough. (obligatory, ‘atomistic’, ’coarse’)

-seqName <sequence name>

Sequence name of which its atomistic simulations are quested to be analyzed. (obligatory, ‘atomistic’)

-start <frame number>

Simulation time point in which to begin the analysis should be given as an integer. (‘atomistic’, ’coarse’)

-end <frame number>

Simulation tie point in which to end the analysis should be given as an integer. (‘atomistic’, ’coarse’)

-out <path>

Directory path to save the analysis output. (‘atomistic’, ’coarse’)

-runMode <analysis type>

Either ‘full’ for default analysis of atomistic simulation (RG, residue distance), or ‘calcLSE’ to create a graph with fitted Flory exponent to the observed results. (‘atomistic’)

-calcFRET <Boolean>

‘True’/’T’/’TRUE’ to calculate estimated FRET measurements, or ‘False’/’F’/’FALSE’ (default). (‘atomistic’)