Package 'modygliani'

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Type Package

Title MOlecular DYnamics GLobal ANalysis

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Description RMSD and Internal Energy analysis of NAMD and YASARA Molecular Dynamics output files. Allows to comparison of different dynamics per different complexes. Input files have to be ASCII files tab separated.

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RoxygenNote 5.0.1

NeedsCompilation no

Repository CRAN

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R topics documented:

`modygliani` *modygliani: MOlecular DYnamics GLobal ANalysis*

Description

Modygliani performs a fitting of the RMSD trajectories. Internal energies are analyzed on the basis of the RMSD fitting. This process is iterated as many times as the number of files provided. Modygliani allows for the comparison of different trajectories. See the references for further information. Example input files are in 'inst/extdata/'.Example output files are stored in 'inst/extdata/output'.

Usage

```
modygliani(path, names, tauGuess, miniRMSD, maxiRMSD, miniEne, maxiEne, YFlag,
  title, colors)
```

Arguments

path	A string containing the path to the properly formatted ASCII files. NAMD file style have to be composed of 3 columns including time, RMSD and Energy. Yasara styles are as the standard output.
names	A vector of strings containing the names of the peptides/proteins to compare. The number of files to analyze have to correspond to the length of this vector and vice versa. File names cannot contain an extension.
tauGuess	A numerical value containing the time constant that is guessed by the user. tayGuess is a useful parameter when fitting fails. If tauGuess is to 0, Modygliani guesses tau in order to attempt fittings.
miniRMSD	A numerical value corresponding to the minimum value of RMSD
maxiRMSD	A numerical value corresponding to the maximum value of RMSD
miniEne	A numerical value corresponding to the minimum value of Energy
maxiEne	A numerical value corresponding to the maximum value of Energy
YFlag	A 1|0 numerical value. The values are 1 for Yasara dynamics and 0 for NAMD
title	A string containing the title of the charts
colors	A vector of strings containing color shades, see the example for further details

Author(s)

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References

Belmonte, L. Rossetto, D. Forlin, M. Scintilla, S. Bonfio, C. Mansy, S. S. "Cysteine containing dipeptides show a metal specificity that matches the composition of seawater" Phys. Chem. Chem. Phys., 2016, DOI: 10.1039/C6CP00608F

Examples

```
## fitting and comparison of four different MD trajectories
names <- c("fe_CG","co_CG","ni_CG","zn_CG") # file names
colors<- c("gray0","gray25","gray50","gray75")
path <-"inst/extdata/"
modygliani(path, names, 0, 0, 8, -200, 250, 0, "Modygliani example on NAMD trajectories", colors)
```

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