
CABS Documentation

Release 2012

Andrzej Koliński

July 06, 2012

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class `pycabs.CABS` (*sequence, secondary_structure, templates_filenames, project_name*)
 CABS main class.

Parameters

- **sequence** (*string*) – one line sequence of the target protein
- **secondary_structure** (*string*) – one line secondary structure for the target protein
- **templates_filenames** (*list*) – path to 3D protein model templates in pdb file format which you want to use for modeling. C α numbering in templates must be aligned to target sequence
- **project_name** (*string*) – project_name and working directory name (uniq)

calcConstraints (*exclude_residues*=[], *other_constraints*=[])

Calculate distance constraints using templates 3D models.

Parameters

- **exclude_residues** (*list*) – indexes of residues without constrains
- **constrains** (*other*) – user-defined constrains as list of tuples: (residue_i_index, residue_j_index, constraint_strength)

convertPdbToDcd (*catdcd_path*='/home/hydek/pycabs/FF/catdcd')

This is only simple wrapper to CatDCD software (<http://www.ks.uiuc.edu/Development/MDTools/catdcd/>), could be usable since *.dcd binary format is few times lighter than pdb, and many python libraries (ProDy, MDAnalysis) use *.dcd as trajectory input format. Before use, download CatDCD from <http://www.ks.uiuc.edu/Development/MDTools/catdcd/> and modify catdcd_path.

createLatticeReplicas (*start_structures_fn*=[], *replicas*=20)

Create protein models projected onto CABS lattice, which will be used as replicas.

Parameters

- **start_structures_fn** (*list*) – list of paths to pdb files which should be used instead of templates models. This parameter is optional, and probably not often used. Without it script creates replicas from templates files.
- **replicas** (*integer*) – define number of replicas in CABS simulation. However 20 is optimal for most cases, and you don't need to change it in protein modeling case.

Note: If number of replicas is smaller than number of templates - program will create replicas using first *replicas* templates. If there is less templates than replicas, they are creating sequentially using template models.

rng_seed = None

seed for random generator

trafToPdb (*output_filename*='TRAF.pdb')

Convert TRAF CABS pseudotrajectory file format into multimodel pdb

class `pycabs.Calculate` (*output*)

Inherit if you want to process data used with `Monitor` class.

Parameters **output** (*array/list*) – output array with calculated results

processTrajectory (*data*)

Use it in *calculate* method if you parsing TRAF file, and want to calculate something on structure

Result Array of 1D model coordinates

exception `pycabs.Errors` (*value*)

Simple error messages

class `pycabs.Info` (*text*)

Simple message system

class `pycabs.Monitor` (*filename, calculate*)

Class for monitoring of CABS output data. You can run it and dynamically update output arrays with calculated results.

Parameters `calculate` (`Calculate`) – what to do with gathered data ?

daemon = `None`

if `True`, it will terminate when script terminates

run ()

Run monitor in background

terminate ()

Terminate monitor

`pycabs.parsePorterOutput` (*porter_output_fn*)

Porter (protein secondary structure prediction, <http://distill.ucd.ie/porter/>) output parser. Porter emailed output looks like:

```
IDVLLGADDGSLAFVPSEFSISPGEKIVFKNNAGFPHNIVFDEDSIPSGVDASKISMSEE
CEEEEECCCCCCECEEEEECCCCCEEEEECCCCCEEEEECCCCCCCCCHHHHCCCCC
```

```
DLLNAKGETFEVALSNKGEYSFYCSPHQGAGMVGKVTVN
CCECCCCCEEEEECCCCCEEEEECCCHHHHCCCEEEEEEC
```

Parameters `porter_output_fn` (*string*) – path to the porter output file

Returns tuple (sequence, secondary_structure)

`pycabs.parsePsipredOutput` (*psipred_output_fn*)

Psipred (protein secondary structure prediction, <http://bioinf.cs.ucl.ac.uk/psipred/>) output parser. Psipred output looks like:

```
> head psipred.ss
1 P C 1.000 0.000 0.000
2 K C 0.665 0.000 0.459
3 A E 0.018 0.000 0.991
4 L E 0.008 0.000 0.997
5 I E 0.002 0.000 0.998
6 V E 0.003 0.000 0.999
7 Y E 0.033 0.000 0.981
```

Parameters `psipred_output_fn` (*string*) – path to the psipred output file

Returns tuple (sequence, secondary_structure)

Contents:

```
from pylab import *
from matplotlib.patches import Ellipse
```

```
delta = 45.0 # degrees
```

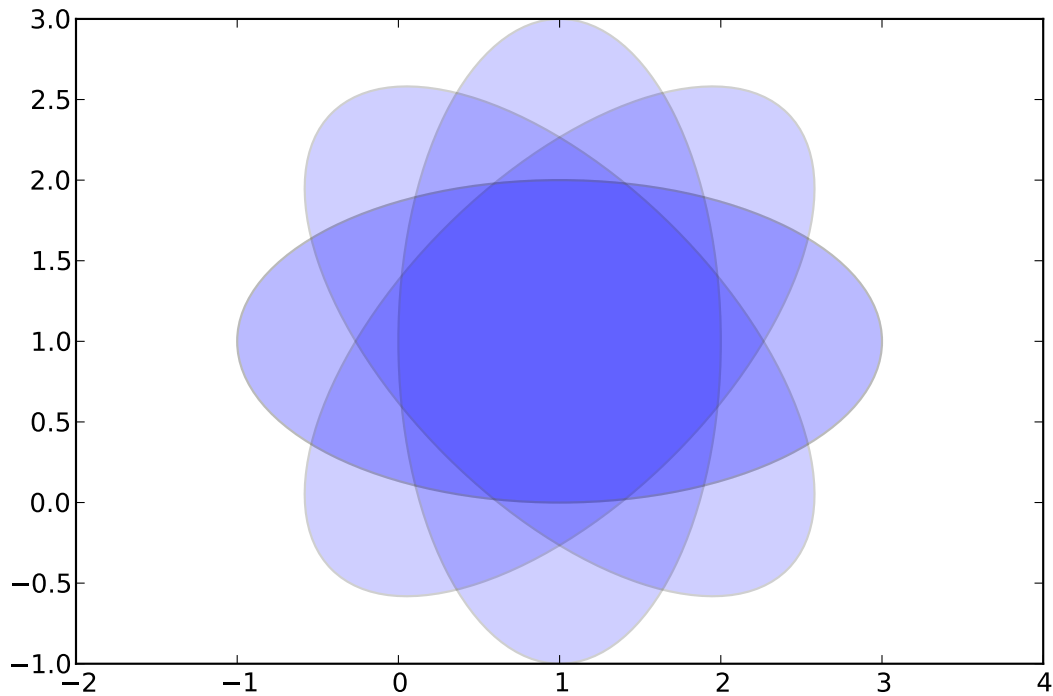
```
angles = arange(0, 360+delta, delta)
ells = [Ellipse((1, 1), 4, 2, a) for a in angles]

a = subplot(111, aspect='equal')

for e in ells:
    e.set_clip_box(a.bbox)
    e.set_alpha(0.1)
    a.add_artist(e)

xlim(-2, 4)
ylim(-1, 3)

show()
```



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