# LabBlouinTools

API Documentation

November 24, 2014

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# 1 Package labblouin

Bioinformatic python utilities modules, and libraries for use with Lab Blouin applications.

## 1.1 Modules


- **FASTAnet**: A simple parser and writer for FASTA sequence files that uses a rich object hierarchy. *(Section 2, p. 3)*
- **IO**: Different shortcut functions for dealing with file systems. *(Section 3, p. 6)*
- **Ordination**: Ordination is a class designed to compute and plot ordination methods such as PCA and MDS. *(Section 4, p. 8)*
- **PDBnet**: PDBnet is a collection of Python objects intended to model and contain PDB protein data. *(Section 5, p. 10)*
- **RegExpress**: Prosite pattern generator. *(Section 6, p. 26)*
- **SeqMask**: Get the amino acid sequence from a landmark file, align this profile to more sequences if required using muscle, and mask the membership vector into this alignment. *(Section 7, p. 27)*
- **expresso**: An (incomplete) parsing library for output from the T-Coffee Expresso executable. *(Section 8, p. 29)*
- **homology** *(Section 9, p. 30)*
- **homstrad**: A library to manage interfacing with the Homstrad database raw files. *(Section 10, p. 33)*
- **loadingBar** *(Section 11, p. 36)*
- **logfile** *(Section 12, p. 37)*
- **mdsa**: A library to manage interfacing with the MDSA database raw files (http://dna.cs.byu.edu/mdsas/index.shtml). *(Section 13, p. 39)*
- **memEfficient** *(Section 14, p. 41)*
- **passToqsub** *(Section 15, p. 45)*
- **pdbCompare** *(Section 16, p. 46)*
- **pfam** *(Section 17, p. 47)*
- **plotGM**: this will plot a gm of a 2D shape *(Section 18, p. 49)*
- **psub**: Run as many of a input set of jobs/commands as there are cores at any given time (i.e. *(Section 19, p. 50)*
- **sabmark** *(Section 20, p. 51)*
- **scop** *(Section 21, p. 53)*
- **svm** *(Section 22, p. 55)*
- **timer** *(Section 23, p. 56)*

# 2 Module labblouin.FASTAnet

A simple parser and writer for FASTA sequence files that uses a rich object hierarchy.

## 2.1 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `None` |

## 2.2 Class FASTAsequence

### 2.2.1 Methods

**__init__**(*self*, *name*, *seq*)

Initialize this object. Provide a name for the sequence and the sequence itself as parameters.

**__iter__**(*self*)

Iterate through a sequence in a pseudo-line-by-line manner as if it was read in a FASTA file.

**__hash__**(*self*)

**__eq__**(*self*, *o*)

**__ne__**(*self*, *o*)

**count**(*self*, *item*)

Return the number of characters in the sequence equal to input string.

**removeGaps**(*self*)

Modify the sequence so gaps are removed and return it.

**toUpper**(*self*)

Modify the sequence so it is uppercase and return it.

**toLower**(*self*)

Return a lowercase version of the sequence, also changing it in the structure.

**__len__**(*self*)

**__str__**(*self*)

## 2.3 Class FASTAstructure

### 2.3.1 Methods

**___init___**(*self*, *filein*=`''`, *uniqueOnly*=`True`, *curate*=`False`)

A file to be read is optional. If uniqueOnly is set to false, multiple duplicate sequences are allowed; otherwise, duplicates are ignored and their aliases are recorded in sequence Names. If curate is triggered, will remove special characters from names.

**getSequenceNames**(*self*)

**getSequences**(*self*)

**getSequenceByName**(*self*, *n*)

**getStrictlyUngappedPositions**(*self*, *seqInds*=`None`)

Acquire the positions of all strictly ungapped sites. If parameter is set, expects a list of what sequences (by index) you are checking. Defaults to all sequences.

**readFile**(*self*, *fin*)

Read a file in. Return this FASTA object.

**read**(*self*, *fast*)

Read the contents of a FASTA file.

**writeFile**(*self*, *fout*)

Write the information currently contained in the FASTAstructure to a file as a FASTA-formatted file.

**addSequence**(*self*, *name*, *seq*)

Add a sequence to the FASTA object.

**renameSequence**(*self*, *oldname*, *newname*)

Renames a given sequence.

**removeSequence**(*self*, *name*)

Remove a sequence from the FASTA object and return it; or return None if it was not found.

**reorderSequences**(*self*, *iterable*)

Reorder all sequences by an iterable sequence of their names.

**removeGaps**(*self*)

Remove the gaps for all sequences.

**allUpper**(*self*)

Change all sequences to uppercase.

**allLower**(*self*)

Change all sequences to lowercase.

**__iter__**(*self*)

Iterate through the FASTA by going through its sequences.

**__len__**(*self*)

Return the number of sequences in the FASTA object.

**__str__**(*self*)

Return the FASTA object as FASTA file text content.

# 3 Module labblouin.IO

Different shortcut functions for dealing with file systems.

IO Python Library / 2012 / Alex Safatli

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E-mail: safatli@cs.dal.ca Dependencies: -

## 3.1 Functions

**getFileName**(*path*)

Returns a filename of a given path.

**getFolderName**(*path*)

Returns the directory name of a given path.

**makeFolder**(*folder_name*)

Makes a folder (if does not already exist). Returns path.

**moveFile**(*origin*, *target*)

Moves a file. Returns path.

**copyFile**(*origin*, *target*)

Copies a file. Returns path.

**removeFile**(*origin*)

Removes a file.

**getFilesInFolder**(*folder*, *ext*)

Returns a list of all full file paths for a given extension in a given folder.

## 3.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

# 4 Module labblouin.Ordination

Ordination is a class designed to compute and plot ordination methods such as PCA and MDS. It is intended as a helper function to PDBnet, but have the functionality to work with gm files.

This file is based on Nelle Varoquaux <nelle.varoquaux@gmail.com> code plotmds.py, available at http://scikit-learn.org/stable/auto_examples/manifold/plot_mds.html, and recomendations in stackoverflow by Jaime Fernandez (http://numericalrecipes.wordpress.com/)

Dependencies: SKlearn, PDBnet

Author: Jose Sergio Hleap email: jshleap@dal.ca

## 4.1 Variables

| Name | Description |
|---|---|
| colors | **Value:** `['b', 'r', 'k', 'g', 'y', 'm', 'c', '#E0EEEE', '#D02090',...` |
| hexa | **Value:** `['#E0EEEE', '#D02090', '#EEC591', '#838B8B', '#6CA6CD', '...` |
| __package__ | **Value:** `'labblouin'` |

## 4.2 Class ORD

A class for the most popular ordination methods using PDBnet instaces or gm files.

### 4.2.1 Methods

**__init__**(*self*, *prefix*, *data*, *fastafile*=`None`, *n_comp*=`2`)

**PrepData4PDBnet**(*self*, *data*)

Load the data to the class assuming is a PDBnet instance file

**LoadDataGMfile**(*self*, *data*)

Load the data to the class assuming is a GM file

**dict2array2matrix**(*self*, *dict*)

Giving an upper-triangle distance matrix in a dictionary, returns a distance-like array

**Store**(*self*)

**MDS**(*self*, *options*, *typeof*=`'classic'`, *dist*=`False`, *groups*=`None`)

Perform Multidimensional Scaling wither classic (PCoA) or non-metric. If you have the upper triangle of a distance matrix as a dictionary, pass the dictionary as dist.

**PCA**(*self*, *options*, *groups*=`None`)

Performs a principal coordinate analysis of the data

**Plot**(*self*, *options*, *groups*=`None`)

Plot the components from an ordination method of the class ORD. If the number of components is greater than 3, it will plot the first three components. Components has to be a n x k numpy array of eigenvectors, where n is the observations/individuals and k the components. The option groups allow to pass a list (of the same lenght of the arrar, that is a lenght of n).

**PlotXDA**(*self*, *membership*, *options*, *group_labels*=`None`)

Plots a Linear Discriminant Analysis (LDA) or a Quadratic Discriminan Analysis (QDA) with confidence ellipses at std (standard deviations)

**ellipse**(*self*, *singlegroupx*, *singlegroupy*, *std*=`2`, *color*=`'k'`)

Create an ellipse given points with x coordinates in singlegroupx and singlegroupy

**pointsInEllipse**(*self*, *Xs*, *Ys*, *ellipse*)

Tests which set of points are within the boundaries defined by the ellipse. The set of points are defined in two arrays Xs and Ys for the x-coordinates and y-coordinates respectively

**getEllipses**(*self*, *stds*)

will populate the ellipses attribute

**LDA**(*self*, *membership*, *options*, *group_labels*=`None`)

Perform a Linear discriminant analysis of the data and plot it. Membership must be an array of integers of the same lenght of the number of observations in the data.

**QDA**(*self*, *membership*, *options*, *group_labels*=`None`)

# 5 Module labblouin.PDBnet

PDBnet is a collection of Python objects intended to model and contain PDB protein data.

PDBnet Copyright (C) 2012 Christian Blouin Contributions by Alex Safatli and Jose Sergio Hleap Major Refactoring (2014) done by Alex Safatli and Jose Sergio Hleap

E-mail: cblouin@cs.dal.ca, safatli@cs.dal.ca, jshleap@dal.ca Dependencies: Scipy, BioPython, FASTAnet (contained in LabBlouinTools)

**Version:** 1.0.2

**Authors:** Christian Blouin, Jose Sergio Hleap, Alexander Safatli

## 5.1 Variables

| Name | Description |
|---|---|
| PDB_LARGE_FILE_SIZE | **Value:** `100000000` |
| aa | **Value:** `{'ALA': 'A', 'ARG': 'R', 'ASN': 'N', 'ASP': 'D', 'CYS': '...` |
| aa_names | **Value:** `{'A': 'ALA', 'C': 'CYS', 'D': 'ASP', 'E': 'GLU', 'F': 'PH...` |
| aa_lists | **Value:** `{'ALA': ['N', 'CA', 'C', 'O', 'CB'], 'ARG': ['N', 'CA', '...` |
| __package__ | **Value:** `'labblouin'` |

## 5.2 Class PDBatom

object
└ **labblouin.PDBnet.PDBatom**

**Known Subclasses:** labblouin.PDBnet.PDBterminator

ATOM in a PDB protein structure.

### 5.2.1 Methods

**__init__**(*self*, *serial*, *name*, *x*, *y*, *z*, *oc*, *b*, *symbol*, *charge*)

Construct an atom in a PDB protein structure.

Overrides: object.__init__

**fixname**(*self*)

Ensures the name of this atom fits within 4 characters.

**___str___**(*self*)

Express this atom as a single line in a PDB file (see PDB format).

Overrides: object.___str___

**GetPosition**(*self*)

Get the 3-dimensional coordinate of this atom in space.

**DistanceTo**(*self*, *atom*)

Acquire the distance from this atom to another atom.

### *Inherited from object*

___delattr___(), ___format___(), ___getattribute___(), ___hash___(), ___new___(), ___reduce___(), ___reduce_ex___(), ___repr___(), ___setattr___(), ___sizeof___(), ___subclasshook___()

#### 5.2.2 Properties

| Name | Description |
|---|---|
| charge | |
| name | |
| occupancy | |
| parent | |
| serial | |
| symbol | |
| tempFactor | |
| x | |
| y | |
| z | |
| *Inherited from object* ___class___ | |

## 5.3 Class PDBterminator

object

labblouin.PDBnet.PDBatom

**labblouin.PDBnet.PDBterminator**

A placeholder class that represents a terminating ATOM-like line in the PDB file.

### 5.3.1 Methods

**___init___**(*self*, *chaininst*)

Construct an atom in a PDB protein structure.

Overrides: object.___init___ extit(inherited documentation)

**___str___**(*self*)

Express this atom as a single line in a PDB file (see PDB format).

Overrides: object.___str___ extit(inherited documentation)

***Inherited from labblouin.PDBnet.PDBatom(Section 5.2)***

DistanceTo(), GetPosition(), fixname()

***Inherited from object***

___delattr___(), ___format___(), ___getattribute___(), ___hash___(), ___new___(), ___reduce___(), ___reduce_ex___(), ___repr___(), ___setattr___(), ___sizeof___(), ___subclasshook___()

### 5.3.2 Properties

| Name | Description |
|---|---|
| charge | |
| lastatom | |
| lastreschain | |
| lastresind | |
| lastresname | |
| name | |
| occupancy | |
| parent | |
| serial | |
| symbol | |
| tempFactor | |
| x | |
| y | |
| z | |
| *Inherited from object* ___class___ | |

## 5.4 Class PDBresidue

A residue (collection of ATOM fields) in a PDB protein structure.

### 5.4.1 Methods

**__init__**(*self*, *index*=`None`, *name*=`''`)

Construct a residue (collection of atoms) in a PDB protein structure.

**GetAtoms**(*self*)

**AddAtom**(*self*, *atom*)

Add a PDBatom structure to this residue.

**GetCA**(*self*)

Get the alpha-carbon found in this residue as a PDBatom.

**Centroid**(*self*)

Calculate the centroid of this residue. Return this as a PDBatom.

**InContactWith**(*self*, *other*, *thres*=`4.5`)

Determine if in contact with another residue.

**__int__**(*self*)

**__str__**(*self*)

## 5.5 Class PDBchain

object
└
**labblouin.PDBnet.PDBchain**

**Known Subclasses:** labblouin.PDBnet.PDBmodel

A PDB chain (collection of protein residues).

### 5.5.1 Methods

**__init__**(*self*, *name*)

x.__init__(...) initializes x; see help(type(x)) for signature

Overrides: object.__init__ extit(inherited documentation)

**GetResidues**(*self*)

Acquire all of the residues in this chain. Note that if this is a large file, this will force the object to load all of these residues into memory from the file.

**IterResidues**(*self*)

Iteratively yield all of the residues in this chain. Note that if this is a large file, this will force the object to load all of these residues into memory from the file.

**GetResidueByIndex**(*self*, *index*)

Alias for acquiring a residue from this instance using [] operator.

**GetAtoms**(*self*)

Get all comprising atoms in this chain in order of residues.

**GetIndices**(*self*)

Acquire all of the indices for residues present in this chain.

**AddIndexOfResidue**(*self*, *index*)

Add an index for a residue to this chain. Will generate own residue information if called upon (forces lazy evaluation).

**AddResidue**(*self*, *resid*)

Add a residue to this chain.

**AddResidueByIndex**(*self*, *index*)

Add a residue to this chain by its index in the PDB. The residue object will automatically be constructed from the file.

**RemoveResidue**(*self*, *resid*)

Remove a residue from this chain.

**GetPrimaryPropertiesFromBioPython**(*self*)

Use BioPython to populate this class with attributes.

**AsFASTA**(*self*)

Return the string representing this chain's FASTA sequence.

**WriteAsPDB**(*self*, *filename*)

Write this single chain to a file as a PDB.

**SortByNumericalIndices**(*self*)

Sort all internal items by a numerical index.

**pop**(*self*, *s*)

Pop a residue.

**update**(*self*, *o*)

Add residues from another chain.

**__str__**(*self*)

str(x)

Overrides: object.__str__ extit(inherited documentation)

**__getitem__**(*self*, *i*)

Force the object to load the residue if not present in this structure.

**__len__**(*self*)

**__iter__**(*self*)

***Inherited from object***

__delattr__(), __format__(), __getattribute__(), __hash__(), __new__(), __reduce__(), __reduce_ex__(), __repr__(), __setattr__(), __sizeof__(), __subclasshook__()

#### 5.5.2 Properties

| Name | Description |
|---|---|
| indices | |
| name | |
| parent | |
| residues | |
| structure | |
| *Inherited from object*<br>__class__ | |

## 5.6 Class PDBmodel

object
labblouin.PDBnet.PDBchain
**labblouin.PDBnet.PDBmodel**

A PDB model (a special kind of chain).

### 5.6.1 Methods

**__init__**(*self*, *name*)

x.__init__(...) initializes x; see help(type(x)) for signature

Overrides: object.__init__ extit(inherited documentation)

**GetResidues**(*self*)

Acquire all of the residues in this model. Note that if this is a large file, this will force the object to load all of these residues into memory from the file.

Overrides: labblouin.PDBnet.PDBchain.GetResidues

**IterResidues**(*self*)

Iteratively yield all of the residues in this model. Note that if this is a large file, this will force the object to load all of these residues into memory from the file.

Overrides: labblouin.PDBnet.PDBchain.IterResidues

**GetChains**(*self*)

**GetChain**(*self*, *name*)

**GetChainByName**(*self*, *name*)

**GetChainNames**(*self*)

**NewChain**(*self*, *ch*)

Create a new PDBchain, add it to this model, and return it.

**AddChain**(*self*, *chain*)

Add a PDBchain (chain) to this model.

**AddResidue**(*self*, *resid*)

Add a residue to this model.

Overrides: labblouin.PDBnet.PDBchain.AddResidue

**__getitem__**(*self*, *i*)

Force the object to load the residue if not present in this structure.

Overrides: labblouin.PDBnet.PDBchain.__getitem__ extit(inherited documentation)

**__str__**(*self*)

str(x)

Overrides: object.__str__ extit(inherited documentation)

***Inherited from labblouin.PDBnet.PDBchain(Section 5.5)***

AddIndexOfResidue(), AddResidueByIndex(), AsFASTA(), GetAtoms(), GetIndices(), GetPrimaryPropertiesFromBioPython(), GetResidueByIndex(), RemoveResidue(), SortByNumericalIndices(), WriteAsPDB(), __iter__(), __len__(), pop(), update()

***Inherited from object***

__delattr__(), __format__(), __getattribute__(), __hash__(), __new__(), __reduce__(), __reduce_ex__(), __repr__(), __setattr__(), __sizeof__(), __subclasshook__()

### 5.6.2 Properties

| Name | Description |
|---|---|
| chainNames | |
| chains | |
| indices | |
| name | |
| residues | |
| structure | |
| *Inherited from labblouin.PDBnet.PDBchain (Section 5.5)*<br>parent | |
| *Inherited from object*<br>___class___ | |

## 5.7 Class PDBstructure

object
└
**labblouin.PDBnet.PDBstructure**

A PDB protein structure (a collection of chains/models).

### 5.7.1 Methods

**___init___**(*self*, *filein=''*)

x.___init___(...) initializes x; see help(type(x)) for signature

Overrides: object.___init___ extit(inherited documentation)

**GetChainNames**(*self*)

**GetModelNames**(*self*)

**GetChain**(*self*, *ch*)

Get a chain by name.

**GetModel**(*self*, *mod*)

Get a model by name.

**NewChain**(*self*, *name*)

Construct and add a new chain by name to the PDB. Returns the chain.

**NewModel**(*self*, *name*)

Construct and add a new model by name to the PDB. Returns the model.

**RemoveChain**(*self*, *name*)

Remove a chain from the structure (by name). Returns the chain.

**RemoveModel**(*self*, *name*)

Remove a model from the structure (by name). Returns the chain.

**AddChain**(*self*, *chainname*, *chain*)

Add a chain as a list of residues to the PDB.

**AddModel**(*self*, *modelname*, *model*)

Add a model as a list of residues to the PDB.

**AddResidueToChain**(*self*, *chain*, *res*)

Add a residue to a chain. Deprecated; use chain class function.

**AddResidueToModel**(*self*, *model*, *res*)

Add a residue to a model. Deprecated; use model class function.

**AddRemark**(*self*, *remark*)

Add a remark (note/comment) to the structure/PDB file.

**GetRemarks**(*self*)

Return all remarks from the PDB as a list of strings.

**CheckComplete**(*self*)

For every chain, check to see if every residue is complete (see aa_list dictionary).

**view**(*self*, *istrajectory*=`False`)

View the structure in a Pymol window. Requires an installation of Pymol.

**ViewStructure**(*self*)

**WriteFile**(*self*, *filename*)

Write this PDB structure as a single PDB file.

**read**(*self*, *filename*)

Alias for ReadFile().

**ReadFile**(*self*, *filename*)

Read a PDB file. Populate this PDBstructure.

**ChainAsFASTA**(*self*, *chain*)

Return the chain as a FASTA. Deprecated; use chain class function.

**ModelAsFASTA**(*self*, *model*)

Return the model as a FASTA. Deprecated; use chain class function.

**tmscore**(*self*, *fasta*, *chains*=`None`, *native*=`None`, *CA*=`True`)

Get the TMscore between two chains. Requires a FASTA alignment and a value for the length of the native structure (e.g., for a pairwise alignment, the length of the structure used as a reference before alignment was done). The latter is computed by assuming the first of both provided chains is the native structure; otherwise, uses a provided chain name (native input).

**gdt**(*self*, *fasta*, *chains*=`None`, *distcutoffs*=`[1, 2, 4, 8]`, *CA*=`True`)

Get the GDT score between two chains. Requires a FASTA alignment.

**rmsd**(*self*, *fasta*, *chains*=`None`, *CA*=`True`)

Get the RMSD between chains. Requires a FASTA alignment.

**rrmsd**(*self*, *fasta*, *chains*=`None`, *CA*=`True`)

Get the RRMSD between chains. Requires a FASTA alignment. See Betancourt & Skolnick, "Universal Similarity Measure for Comparison Protein Structures".

**GetAverage**(*self*, *chains*=`None`, *newname*=`None`)

Acquire a new chain or model corresponding to an average of all present chains or models specified.

**RadiusOfGyration**(*self*, *chains*=`None`)

Acquire the radius of the gyration of the entire, or a portion of, the PDB protein molecule.

**GetAllCentroid**(*self*, *chain*)

Populates the centroids of all residues.

**IndexSeq**(*self*, *chain*, *fst*)

Store in residues the correct index to the fasta. Requires a 1-to-1 correspondance at least a portion of the way through. Deprecated; use GetFASTAIndices().

**GetFASTAIndices**(*self*, *thing*, *fst*)

Given a PDBchain, find 1-to-1 correspondances between it and a FASTA sequence.

**IterAllResidues**(*self*)

Produce an iterator to allow one to iterate over all possible residues.

**gm**(*self*, *fasta*, *chains*=`None`, *CA*=`False`, *typeof*=`'str'`)

```
Acquire Geometric Morphometric data corresponding to the
(x,y,z) coordinates between all homologous residue positions.
Requires a FASTA alignment. Options include using alpha-carbon
positions. By default, uses centroids of residues. Returns a list
of labels and a list of coordinates as raw GM data. The typeof
        option provides an option for coordinate output; they are returned
        as a semicolon-delimited string (str) or as a numpy 2d array (matrix).
```

**WriteGM**(*self*, *fasta*, *gm*, *chains*=`None`, *CA*=`False`)

Write the information present in this PDB between multiple chains as a Geometric Morphometric text file. This file will be formatted such that individual lines correspond to chains and semi-colons separate the (x,y,z) coordinates between all homologous residue positions. Requires a FASTA alignment. Options include using alpha-carbon positions. By default, uses centroids of residues.

**WriteLandmarks**(*self*, *fasta*, *lm*, *chains*=`None`)

Write the information present in this PDB between multiple chains as a landmark text file. This file will be formatted such that the file is partitioned in sections starting with chain names and individual lines in these correspond to homologous residue positions denoted by homologous position, residue number, and residue name tab-delimited. Requires a FASTA file.

**FDmatrix**(*self*, *fasta*, *chains*=`None`, *scaled*=`True`)

Compute the form difference matrix (FDM) as explained in Claude 2008. It relates to the identification of the most influential residue, with respect to the overall shape/structure. If the scaled option is True, will return an scaled list (from -1 to 1) of the of lenght equal to the number of residues. Otherwise will return the raw FDM, rounded so it can be included in a PDB. The scaled version is better for vizualization. By default the FDM is computed far all chains, but a subset can be passed to the chains option.

**Map2Protein**(*self*, *outname*, *lis*, *chain*, *fasta*)

Map a list of values (lis), that must have a lenght equal to that of the number of residues in the PDB to be mapped (chain). If a list of list is provided, the first list will be mapped as the beta factor and the second as occupancy

**Contacts**(*self*, *chain*=`'ALL'`, *thres*=`4.5`)

Compute the contact map of all chains or a chain.

**WriteContacts**(*self*, *filename*)

Write contact map.

**__iter__**(*self*)

Returns all PDBchains as an iterator.

**__len__**(*self*)

Returns the length of the protein.

**__str__**(*self*)

As a string, outputs structure in the PDB format.

Overrides: object.__str__

***Inherited from object***

__delattr__(), __format__(), __getattribute__(), __hash__(), __new__(), __reduce__(), __reduce_ex__(), __repr__(), __setattr__(), __sizeof__(), __subclasshook__()

#### 5.7.2 Properties

| Name | Description |
|---|---|
| chains | |
| contactmap | |
| filepath | |
| handle | |
| ismodel | |
| models | |
| mutation | |
| orderofchains | |
| orderofmodels | |
| organism | |
| remarks | |
| taxid | |
| *Inherited from object*<br>__class__ | |

### 5.8 Class PDBfile

object
└
**labblouin.PDBnet.PDBfile**

#### 5.8.1 Methods

**__init__**(*self*, *fi*)

x.__init__(...) initializes x; see help(type(x)) for signature

Overrides: object.__init__ extit(inherited documentation)

**isLargeFile**(*self*)

Return whether or on the PDB file this object represents is incredibly large.

**close**(*self*)

Close the file.

**read**(*self*)

Acquire all remarks, and the indices of all models and residues. Returns remarks, and biological source information as a tuple (remarks, organism, taxid, mutant).

**readResidue**(*self*, *chain*, *res*, *model*=`-1`)

Parse a residue from the PDB file and return a PDBresidue.

**hasModels**(*self*)

**getModelNames**(*self*)

**getChainNames**(*self*)

**iterResidueData**(*self*)

Yield the model number, chain name, and residue number for all residues present in this PDB file, not necessarily in order.

**getResidueNamesInChain**(*self*, *ch*)

***Inherited from object***

__delattr__(), __format__(), __getattribute__(), __hash__(), __new__(), __reduce__(), __reduce_ex__(), __repr__(), __setattr__(), __sizeof__(), __str__(), __subclasshook__()

#### 5.8.2 Properties

| Name | Description |
|---|---|
| chains | |
| fileHandle | |
| filePath | |
| memHandle | |
| modelIndices | |
| residueIndices | |
| size | |
| *Inherited from object*<br>__class__ | |

*continued on next page*

| Name | Description |
| --- | --- |

# 6 Module labblouin.RegExpress

Prosite pattern generator. Will turn an alignment into a regular expression

## 6.1 Functions

**check_if_is_align**(*dictionary_fasta*)

will check the read fasta to see if is an alignment

**read_fasta**(*prefix*)

Wll read the fasta, place sequences in a dictionary. Will break if not an alignment

**strip_gaps**(*matrix*)

given an alignment matrix, strip out the gap columns

**reg_express_col**(*col*)

given a column of an alignment, return the string corresponding to the regular expression of such column

**reg_express**(*fastas*, *l*)

will create a matrix with the alignment, discard columns with gaps, and create a regular expression similar to prosite

## 6.2 Variables

| Name | Description |
|---|---|
| aa | **Value:** `{'A': 'Ala', 'C': 'Cys', 'D': 'Asp', 'E': 'Glu', 'F': 'Ph...` |
| allaa | **Value:** `set(['A', 'C', 'D', 'E', 'F', 'G', 'H', 'I', 'K', 'L', 'M...` |
| __package__ | **Value:** `'labblouin'` |

# 7 Module labblouin.SeqMask

Get the amino acid sequence from a landmark file, align this profile to more sequences if required using muscle, and mask the membership vector into this alignment.

## 7.1 Functions

**InferSingleLettterCode**(*threlettercode*)

Convert the amino acid three letter code, into a single letter code

**InferSeqs_landmarks**(*prefix*)

Given a landmark file, return a dictionary with the name as key and the sequence as value

**dict2fasta**(*outfilename*, *dic*)

Convert the dictionary return by InferSeqs_landmarks fuction and writes a fasta file. The dictionary should have the seq name as key and a string as value containing the sequence

**fasta2dict**(*fastafilename*)

convert a fasta file into a python dictionary, being the keys the name of the sequence and the values the sequence itself, in a list

**Mem2List2tuple**(*prefix*)

Read the membership vector, and returns a list and a dictionary with tupples for each module, indicating the indexes

**str2list**(*string*)

returns a list of a string that have no spaces between elements

**MaskAln**(*fastafilename*, *modulename*, *mem*, *tuples*)

Strip the module in an alignment (fasta) file

**modseq2Fasta**(*prefix*, *modseq*, *names*)

## 7.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

# 8 Module labblouin.expresso

An (incomplete) parsing library for output from the T-Coffee Expresso executable. expresso Python Library / Summer 2013 / Alex Safatli

E-mail: safatli@cs.dal.ca Dependencies: -

## 8.1 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `None` |

## 8.2 Class expressoParser

Parses Expresso output.

### 8.2.1 Methods

**__init__**(*self*, *fin*)

**__read__**(*self*)

Read an Expresso output file; store the data inside this object.

**getPDBcodes**(*self*)

Return PDB code and chain as a tuple for each line.

**writeNonEmpty**(*self*, *fout*)

Writes non-empty PDB IDs to file.

**getNonEmptySequenceNames**(*self*)

Gets non-empty PDB names.

# 9 Module labblouin.homology

## 9.1 Functions

**cleanFastaFile**(*fname*, *targetfolder*=`''`)

Removes gaps from target FASTA file. Allows for BLAST input using this file. Creates new files for every sequence entry. Returns the filename(s) of the new file(s).

**writeModellerPIR**(*pdb_files*, *seq*, *dest_file*)

**writeAlignmentFromFasta**(*fasta_file*, *dest_file*)

Reads a FASTA file and outputs it to a Clustal-like alignment.

**writeSOAPSSAlignment**(*fasta_file*, *pdb1*, *pdb2*, *dest_file*)

Reads a FASTA file and outputs to a SOAPSS alignment file.

**writeFirstFromFasta**(*fasta_file*, *dest_file*)

Extracts first sequence from a FASTA and writes to a new one.

**extractRandomFasta**(*fasta_file*, *numRandom*, *dest_file*)

Extracts a random number of sequences from a FASTA file. Writes to new FASTA.

**completePDB**(*pdbin*, *pdbout*)

Given a PDB, clean/complete the PDB using Modeller's complete_pdb function.

**getRandomPDBFragment**(*pdb*, *k*=`100`)

Given a PDB, get a random fragment of length k.

**getFirstResidueNumber**(*pdb*)

Gets the FASTA residue number of the first ATOM in a PDB file.

**checkForFileCollision**(*path*, *ext*)

Ensures a file is not being overwritten. Will recursively keep adding a '0' to end of base filename until a unique filename is found. Returns the path.

**system**(*instruction*)

Executes a system command line instruction. Returns list of stdout, stderr.

**cleanModellerFolder**(*path*)

Moves intermediate PDBs to another subfolder in the Modeller folder output from Biskit.

**getModellerPDB**(*workflowfolder*, *targetfile*)

Copies the model_00.pdb file from Modeller if present in given workflow directory from homologyWorkflow.

**compareStructures**(*foldername1*, *foldername2*, *outpath*, *verbose*=`False`)

Given 2 folders with PDB files, calculates the RMSDs with all possible pairwise combinations of PDBs; writes to file located at path determined by outpath.

**startPymol**()

Ensures Pymol has been launched.

**radiusOfGyration**(*pdbFile*, *chain*, *pdb*=`None`)

Returns the approximate radius of gyration of a given PDB molecule. Deprecated; now in PDBnet.

**tmscore**(*alignPDB*, *alignFASTA*)

Returns the TMscore and associated P-value. See Xu & Zhang, "How significant is a protein structure similarity with TM-score = 0.5?".

**rrmsd**(*alignPDB*, *alignFASTA*, *rmsd*=`False`, *chains*=`None`)

Returns the rRMSD of an aligned pairwise PDB and FASTA file. See Betancourt & Skolnick, "Universal Similarity Measure for Comparison Protein Structures". Deprecated.

**rmsd**(*pdbFile1*, *pdbFile2*)

Returns the RMSD of two PDB files. Requires: Pymol.

## 9.2 Variables

*continued on next page*

| Name | Description |
|---|---|

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

## 9.3 Class manualModeller

Set up and run Modeller using a given folder of PDB files and a target FASTA sequence.

### 9.3.1 Methods

**__init__**(*self*, *outfolder*, *targetfile*, *templatefldr*)

**__buildList__**(*self*)

Build a string list of all PDB files.

**__prepare__**(*self*)

Prepare input for Modeller.

**run**(*self*)

Run, call Modeller.

**postProcess**(*self*)

Make a copy of all found models and rename.

## 9.4 Class fasta

Open, read, and organize a FASTA file as an object.

### 9.4.1 Methods

**__init__**(*self*, *fname*, *removeGaps*=`True`, *allUpper*=`True`)

**read**(*self*, *rgaps*, *allup*)

# 10 Module labblouin.homstrad

A library to manage interfacing with the Homstrad database raw files.

homstrad Python Library / May 22, 2013 / Alex Safatli

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E-mail: safatli@cs.dal.ca Dependencies: IO (LabBlouinTools)

## 10.1 Functions

**hasNoFolders**(*path*)

## 10.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

## 10.3 Class homstradFolder

Model a single Homstrad folder or set.

### 10.3.1 Methods

**__init__**(*self*, *foldrname*)

**__manifest__**(*self*)

**getNames**(*self*)

**getNumSequences**(*self*)

**getSequences**(*self*)

**getFiles**(*self*)

**getPath**(*self*)

**getFASTA**(*self*)

**writeFASTA**(*self*, *fi*, *names*=`None`)

**getFASTAfor**(*self*, *names*)

**getAlignedPDB**(*self*)

**getPDBs**(*self*)

**getPDBfor**(*self*, *name*)

**getSequenceLength**(*self*)

**getAlignmentLength**(*self*)

## 10.4 Class homstradDatabase

### 10.4.1 Methods

**__init__**(*self*, *dbpath*, *traverse*=`True`)

**__iter__**(*self*)

**traverse**(*self*)

**getPath**(*self*)

**getFolders**(*self*)

**getFailedCount**(*self*)

**getSucceededCount**(*self*)

# 11 Module labblouin.loadingBar

## 11.1 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

## 11.2 Class loadingBar

### 11.2.1 Methods

**__init__**(*self*, *title*, *width*=`300`, *height*=`25`)

**open**(*self*)

**close**(*self*)

**update**(*self*, *ratio*)

**settitle**(*self*, *title*)

# 12 Module labblouin.logfile

## 12.1 Functions

**parseTime**(*time*)

**calculateTime**(*timevector*)

## 12.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

## 12.3 Class XMLfile

### 12.3.1 Methods

**__init__**(*self*, *xmlf*, *root*=`'root'`)

**compile**(*self*)

**read**(*self*)

**write**(*self*)

**add**(*self*, *ele*, *it*, **args*)

## 12.4 Class logfile

### 12.4.1 Methods

**__init__**(*self*, *logf*, *enable*=`True`, *silent*=`False`)

**setTotalNum**(*self*, *tn*)

**incrementTimer**(*self*)

**updateTimer**(*self*, *numat*)

**__fs__**(*self*, *tot*)

**writeTemporary**(*self*, *msg*, *silent*=`None`)

**write**(*self*, *msg*, *silent*=`None`)

**writeElapsedTime**(*self*)

# 13 Module labblouin.mdsa

A library to manage interfacing with the MDSA database raw files (http://dna.cs.byu.edu/mdsas/index.shtm

mdsa Python Library / Oct 8, 2014 / Alex Safatli

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You should have received a copy of the GNU General Public License along with this program. If not, see <http://www.gnu.org/licenses/>.

E-mail: safatli@cs.dal.ca Dependencies: IO, FASTAnet (LabBlouinTools)

## 13.1 Variables

| Name | Description |
|---|---|
| mdsaTypes | **Value:** `['smart', 'balibase', 'oxbench', 'prefab']` |
| __package__ | **Value:** `'labblouin'` |

## 13.2 Class mdsaAlignment

Model a single MDSA alignment.

### 13.2.1 Methods

**__init__**(*self*, *finame*)

**getObject**(*self*)

**getNames**(*self*)

**getNumSequences**(*self*)

**getSequences**(*self*)

**getPath**(*self*)

**writeFASTA**(*self*, *fi*, *names*=`None`)

**getFASTAfor**(*self*, *names*)

**getSequenceLength**(*self*)

**getAlignmentLength**(*self*)

## 13.3 Class mdsaDatabase

### 13.3.1 Methods

**__init__**(*self*, *dbpath*, *traverse*=`True`)

**__iter__**(*self*)

**traverse**(*self*)

**getPath**(*self*)

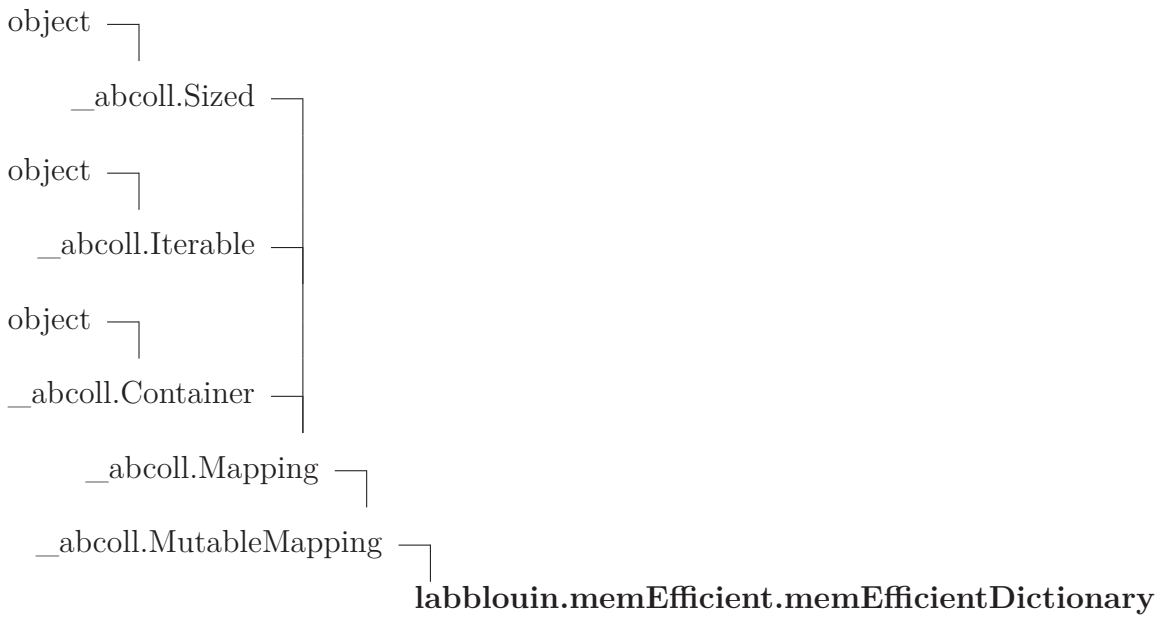
**getFiles**(*self*)

# 14 Module labblouin.memEfficient

## 14.1 Variables

| Name | Description |
|---|---|
| DICT_START_NUM | **Value:** `8` |
| DICT_FREE_SLOT | **Value:** `-1` |
| DICT_DUMMY_SLOT | **Value:** `-2` |
| DICT_SHIFT | **Value:** `5` |
| __package__ | **Value:** `'labblouin'` |

## 14.2 Class memEfficientDictionary




A memory-efficient alternative to the built-in Python dictionary with a trade-off for (insertion) performance. Based on recipe found by Raymond Hettinger (http://code.activestate.com/recipes/578 proof-of-concept-for-a-more-space-efficient -faster/).

### 14.2.1 Methods

**__init__**(*self*, **args*, ***kwds*)

x.__init__(...) initializes x; see help(type(x)) for signature

Overrides: object.__init__ extit(inherited documentation)

**__len__**(*self*)

Overrides: _abcoll.Sized.__len__

**__iter__**(*self*)

Overrides: _abcoll.Iterable.__iter__

**iterkeys**(*self*)

**Return Value**
an iterator over the keys of D

Overrides: _abcoll.Mapping.iterkeys extit(inherited documentation)

**keys**(*self*)

**Return Value**
list of D's keys

Overrides: _abcoll.Mapping.keys extit(inherited documentation)

**itervalues**(*self*)

**Return Value**
an iterator over the values of D

Overrides: _abcoll.Mapping.itervalues extit(inherited documentation)

**values**(*self*)

**Return Value**
list of D's values

Overrides: _abcoll.Mapping.values extit(inherited documentation)

**iteritems**(*self*)

**Return Value**
an iterator over the (key, value) items of D

Overrides: _abcoll.Mapping.iteritems extit(inherited documentation)

**items**(*self*)

**Return Value**
list of D's (key, value) pairs, as 2-tuples

Overrides: _abcoll.Mapping.items extit(inherited documentation)

**__contains__**(*self*, *key*)

Overrides: _abcoll.Container.__contains__

**get**(*self*, *key*, *default*=`None`)

d defaults to None.

**Return Value**
D[k] if k in D, else d

Overrides: _abcoll.Mapping.get extit(inherited documentation)

**popitem**(*self*)

as a 2-tuple; but raise KeyError if D is empty.

**Return Value**
(k, v), remove and return some (key, value) pair

Overrides: _abcoll.MutableMapping.popitem extit(inherited documentation)

**clear**(*self*)

Clear the data structure.

**Return Value**
None

Overrides: _abcoll.MutableMapping.clear

**__getitem__**(*self*, *key*)

Access an item through the [] notation.

Overrides: _abcoll.Mapping.__getitem__

**__setitem__**(*self*, *key*, *value*)

Overrides: _abcoll.MutableMapping.__setitem__

**__delitem__**(*self*, *key*)

Overrides: _abcoll.MutableMapping.__delitem__

***Inherited from __abcoll.MutableMapping***

pop(), setdefault(), update()

***Inherited from __abcoll.Mapping***

__eq__(), __ne__()

***Inherited from __abcoll.Sized***

__subclasshook__()

***Inherited from object***

__delattr__(), __format__(), __getattribute__(), __new__(), __reduce__(), __reduce_ex__(), __repr__(), __setattr__(), __sizeof__(), __str__()

### 14.2.2 Properties

| Name | Description |
|---|---|
| *Inherited from object* | |
| __class__ | |

### 14.2.3 Class Variables

| Name | Description |
|---|---|
| __abstractmethods__ | **Value:** `frozenset([])` |
| *Inherited from __abcoll.Mapping* | |
| __hash__ | |

# 15 Module labblouin.passToqsub

## 15.1 Functions

**returnScript**(*command*, *jobname*=`'default_job'`, *np*=`1`, *npmin*=`1`, *nomail*=`True`, *sync*=`False`)

## 15.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

# 16 Module labblouin.pdbCompare

## 16.1 Functions

**getChecksum**(*pdb_file*)

Given a PDB file, retrieve a unique checksum.

**pdbCrosscheck**(*folder1*, *folder2*)

Given two folder paths, determine what PDBs are unique amongst the two

**outputResults**(*pdbcrosscheck_results*, *fpath*=`None`)

## 16.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |
| __warningregistry__ | **Value:** `{('the md5 module is deprecated; use hashlib instead', <t...` |

# 17 Module labblouin.pfam

## 17.1 Functions

**extractPDBSequences**(*pdb_file*)

Extracts the Amino Acid sequences for a protein structure defined by a PDB file and returns as a dictionary.

**extractPDBChain**(*pdb_file*, *ch*, *dest_file*)

Extracts a PDB file from another that has only information for a single chain.

**writeSequencesToFile**(*seq_list*, *targetfolder*, *fasta*=`True`)

Takes in a dictionary of sequences and writes them to seperate .seq or .fasta files.

**writeSequenceToFasta**(*seq*, *seq_id*, *targetpath*)

Creates FASTA file from given sequence string.

**writeSequencesToFasta**(*seq_list*, *dest_file*)

Creates single FASTA file from given sequence tuple list where first item is sequence ID, second item is the sequence.

**doSequenceSearch**(*seq_file*)

Performs the PFAM search for a sequence file.

**processSequenceSearch**(*search_results*)

Takes in a XML result returned from a sequence search and parses it in order to determine what the most significant results are for related families. Returns a list of the family PFAM IDs.

**downloadFamilySequences**(*pfam_family_id*, *dest_folder*, *atype*=`'seed'`)

Takes in PFAM family ID and acquires the gzipped flat file filled with seed or full sequence allignments.

**decompressGzipFile**(*gzip_file_name*, *destfolder*, *file_ext*=`'ann'`)

Takes in GZIP file from PFAM or PDB and decompresses it to an .ann or specified file extension.

**readPfamFile**(*file_name*)

Takes in PFAM Stockholm file and reads it, returning a pfamFile object.

**grabNCBIAccessionMetadata**(*accession_id*)

Takes in an accession ID and returns NCBI metadata from GenBank.

**grabPDBFile**(*pdb_code*, *dest_folder*)

Takes in a PDB code and acquires the PDB file from the PDB database, placing it in the specified destination folder.

**printListToFile**(*list_in*, *dest*)

Prints a list to a file.

**list2txttable**(*list_in*, *title*)

Converts a list to a string table.

**removeListDuplicates**(*list_in*)

Removes all duplicates in a list.

## 17.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

## 17.3 Class pfamFile

### 17.3.1 Methods

**__init__**(*self*, *filepath*)

**parse**(*self*)

**cluster**(*self*)

# 18 Module labblouin.plotGM

this will plot a gm of a 2D shape

## 18.1 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

# 19 Module labblouin.psub

Run as many of a input set of jobs/commands as there are cores at any given time (i.e. emulate a queue such as qsub present on GRID-powered hardware).

## 19.1 Functions

**call**(*instr*)

## 19.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

# 20 Module labblouin.sabmark

## 20.1 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

## 20.2 Class sabmarkFile

### 20.2.1 Methods

**__init__**(*self*, *path*, *l*, *fp*)

## 20.3 Class sabmarkSummary

### 20.3.1 Methods

**__init__**(*self*, *path*)

**__read__**(*self*)

## 20.4 Class sabmarkFolder

### 20.4.1 Methods

**__init__**(*self*, *foldrname*)

**__manifest__**(*self*)

## 20.5 Class sabmarkDatabase

### 20.5.1 Methods

**__init__**(*self*, *dbpath*)

**traverse**(*self*)

**groups**(*self*, *fkey*)

# 21 Module labblouin.scop

## 21.1 Variables

| Name | Description |
|---|---|
| SCOP_VERSION | **Value:** `'1.75'` |
| SCOP_PARSE_FILE | **Value:** `'http://scop.mrc-lmb.cam.ac.uk/scop/parse/dir.des.scop.tx.` |
| SCOP_PDBDB_FILE | **Value:** `'http://scop.mrc-lmb.cam.ac.uk/scop/parse/dir.cla.scop.tx.` |
| LOCAL_PARSE_FILE | **Value:** `'directory.scop'` |
| LOCAL_PDBDB_FILE | **Value:** `'pdbdb.scop'` |
| LOCAL_FLAT_FILE | **Value:** `'scop.pickl'` |
| __package__ | **Value:** `'labblouin'` |

## 21.2 Class scopHierarchy

### 21.2.1 Methods

**__init__**(*self*, *cacheloc*)

**__downloadparse__**(*self*)

**__downloadpdbdb__**(*self*)

**__parsefile__**(*self*, *fi*)

**__pdbdbfile__**(*self*, *fi*)

**__readpickle__**(*self*, *fi*)

**__writepickle__**(*self*, *fi*)

**populateHierarchy**(*self*)

**getDissimilar**(*self*, *suprfquery*, *num*=`100`)

**query**(*self*, *dicti*, *q*)

**getSimilar**(*self*, *suprfquery*, *num*=100)

**getFamilies**(*self*, *suprfquery*)

### 21.2.2 Class Variables

| Name | Description |
|---|---|
| classes | **Value:** {} |
| folds | **Value:** {} |
| superfamilies | **Value:** {} |
| families | **Value:** {} |
| domains | **Value:** {} |
| species | **Value:** {} |
| entries | **Value:** {} |

## 21.3 Class scopItem

### 21.3.1 Methods

**__init__**(*self*, *sunid*, *sccs*, *shortname*, *desc*)

**addPDB**(*self*, *pdb*)

**getPDBs**(*self*)

# 22 Module labblouin.svm

## 22.1 Class svm_model

### 22.1.1 Methods

**__init__**(*self*, *data*=`[]`, *labels*=`[]`, *kernel*=`svmutil.RBF`, *c*=`10`)

**optimize**(*self*, *low*=`1`, *up*=`50`, *steps*=`5`, *by*=`'proportions'`)

Optimize c-value on the basis of by (default:proportions of correct classifications).

**predict**(*self*, *data*)

**load**(*self*, *fin*)

**save**(*self*, *fin*)

## 22.2 Class cross_validate

### 22.2.1 Methods

**__init__**(*self*, *model*, *test*=`[]`)

**perform**(*self*)

Perform the cross-validation.

# 23 Module labblouin.timer

## 23.1 Functions

**getTime**()

**estimateRemainingTime**(*starttime*, *numAt*, *totalNum*)

## 23.2 Variables

| Name | Description |
|---|---|
| __package__ | **Value:** `'labblouin'` |

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