Namespace `PyCamcoil`

Sub-modules

- PyCamcoil.camcoil
- PyCamcoil.src

Module `PyCamcoil.camcoil`

Functions

Function `main`

```
def main(
    sequence=None,
    pH=None,
    f_out=None
)
```

This is the main function that is called to initiate the camcoil_engine prediction.

:param sequence: (string) of amino-acids.

:param pH: (float) determines the specific random coil (reference) values that will be used to generate the predictions.

:param f_out: (path) if given, the output will be saved there instead of the screen.

:return: None.

Module `PyCamcoil.src`

Sub-modules

- PyCamcoil.src.camcoil_engine
- PyCamcoil.src.camcoil_properties

Module `PyCamcoil.src.camcoil_engine`

This module provides a "Python implementation" of the camcoil program (originally written in C) to estimate the random coil chemical shift values from a sequence (string) of amino-acids.

The work is described in detail at:

1. Alfonso De Simone, Andrea Cavalli, Shang-Te Danny Hsu, Wim Vranken and Michele Vendruscolo (2009) (https://doi.org/10.1021/ja904937a). "Accurate Random Coil Chemical Shifts from an Analysis of Loop Regions in Native States of Proteins". Journal of the American Chemical Society (JACS), 131 (45), 16332 - 16333.

Note ——= The txt files: 'corr_L1', 'corr_L2', 'corr_R1', 'corr_R2', are required for the estimation of the random coil values. They should be placed in the same directory with the module file. If they do not exist the code will exit with an error.

Classes

Class `CamCoil`

```
class CamCoil(
    pH=7.0
)
```

This class implements the CamCoil code in Python.

Initializes the camcoil object. The pH is given as option during the initialization of the object even though only two actual implementations exist at the moment (i.e., pH=2 and pH=7).

If the user selects another pH value, this will be set automatically to one of these two in the code.

:param pH: (float) the default pH value is set to 7.0.

Instance variables

Variable `df` Return an attribute of instance, which is of type owner.

Variable `pH` Accessor (getter) of the pH parameter.

:return: the pH value.

Methods

Method `predict`

```
def predict(
    self,
    seq=None,
    verbose=False
)
```

Accepts a string amino-acid sequence, and returns a prediction with the random coil chemical shifts.

:param seq: (string) The input amino-acid sequence.

:param verbose: (bool) If the flag is set to True it will print more information on the screen.

:return: a pandas DataFrame, with the results.

Module `PyCamcoil.src.camcoil_properties`

Properties for the CamCoil implementation. These include:

1. `ACCEPTED_RES_ONE`
2. `pH2_prop`
3. `pH7_prop`
4. `weights`
5. `weights_LFP`

Classes

Class `ChemShifts`

```
class ChemShifts(
    N,
    C,
    CA,
    CB,
    H,
    HA
)
```

ChemShifts(N, C, CA, CB, H, HA)

Ancestors (in MRO)

- builtins.tuple

Instance variables

Variable `C`   Random coil chemical shift value for 'C'.

Variable `CA`   Random coil chemical shift value for 'CA'.

Variable `CB`   Random coil chemical shift value for 'CB'.

Variable `H`   Random coil chemical shift value for 'H'.

Variable `HA`   Random coil chemical shift value for 'HA'.

Variable `N`   Random coil chemical shift value for 'N'.

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