pytc Documentation

Release 1.1.5

Michael J. Harms

Mar 25, 2019

Contents:

1 Download 3

2 Philosophy 5

3 Features 7

4 Documentation 9

5 GUI Demo 11

6 API Demo 13

7 Implementation 15
7.1 pytc package 15

8 Indices and tables 17

Open source python software for extracting thermodynamic information from Isothermal Titration Calorimetry experiments.

- We welcome bug reports, patches, and new thermodynamic models. See the contributing page for how to get involved.
- If you find pytc useful, please star and/or fork the project on github.
- *Citation*: Duvvuri H, Wheeler LC, Harms MJ. (2018) "pytc: Open-Source Python Software for Global Analyses of Isothermal Titration Calorimetry Data" *Biochemistry*. doi://10.1021/acs.biochem.7b01264

CHAPTER 1

Download

Windows GUI | Mac GUI | Linux GUI | API | Source code

CHAPTER 2

Philosophy

- **Open source and cross platform**. The full source code should be available. The program should not require proprietary software to run.
- **Rigorous**. Program should use best practices and current algorithms for performing fits and assessing fit quality.
- **Ease of use**. Fitting basic models should be easy. Implementing completely new thermodynamic models should be straightforward.
- **Accessible for users and programmers**. It should have both a graphical user interface and a well-designed API.

CHAPTER 3

Features

- Simple, cross-platform graphical user interface.
- Clean, pythonic API
- New models can be defined using a few lines of python code
- Easy integration with jupyter notebooks for writing custom fitting scripts

CHAPTER 4

Documentation

- Installation
- Fitting models using the GUI
- Fitting models using the API
- **Reference:**
  - Thermodynamic models for individual experiments
  - Global fits
  - Fit strategies
  - Fit statistics
  - Defining new models
  - Contributing to the project

Warning: **pytc** will fit all sorts of complicated models to your data. It is up to you to make sure the fit is justified by the data. See the Fitting and statistics section to see what **pytc** reports to help in this decision making.

CHAPTER 5

GUI Demo

An animated gif showing the GUI in action.

CHAPTER 6

API Demo

Fit a single-site binding model to a $Ca^{2+}/EDTA$ binding experiment.

```
import pytc

# Load in integrated heats from an ITC experiment
e = pytc.ITCExperiment("demos/ca-edta/tris-01.DH",
                       pytc.indiv_models.SingleSite)

# Create the global fitter, add the experiment
g = pytc.GlobalFit()
g.add_experiment(e)

# Do the fit
g.fit()

# Print the results out
g.plot()
print(g.fit_as_csv)
```

CHAPTER 7

Implementation

Our implementation is built on python3 extended with numpy, scipy, matplotlib and emcee. The GUI is built on pytq5.

7.1 pytc package

7.1.1 Subpackages

pytc.experiments package

Submodules

pytc.experiments.base module

Module contents

pytc.global_connectors package

Submodules

pytc.global_connectors.base module

pytc.global_connectors.num_protons module

pytc.global_connectors.vant_hoff module

pytc.global_connectors.vant_hoff_extended module

Module contents

pytc.indiv_models package

Submodules

pytc.indiv_models.base module

pytc.indiv_models.binding_polynomial module

pytc.indiv_models.blank module

pytc.indiv_models.single_site module

pytc.indiv_models.single_site_competitor module

Module contents

pytc.util package

Submodules

pytc.util.util module

Module contents

7.1.2 Submodules

7.1.3 pytc.fit_param module

7.1.4 pytc.global_fit module

7.1.5 Module contents

CHAPTER 8

Indices and tables

- genindex
- modindex
- search