pytc Documentation

Release 1.1

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Aug 25, 2018

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A python software package for analyzing Isothermal Titration Calorimetry data. The name is a portmanteau of Python and ITC.

CHAPTER 1

Introduction

pytc is python software used to extract thermodynamic information from isothermal titration calorimetry (ITC) experiments. It fits arbitrarily complex thermodynamic models to multiple ITC experiments simultaneously. We built it with three design principles:

- **Open source and cross platform**. The full source code should be available. The program should not require proprietary software to run.
- **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 GUI and a well-documented API.

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

CHAPTER 2

Features

- Clean, pythonic API
- Simple, cross-platform GUI based on PyQt5.
- New models can be defined using a few lines of python code.
- Easy integration with jupyter notebooks for writing custom fitting scripts.

CHAPTER 3

Documentation

- Installation
- Fitting models using the API.
- Fitting models using the GUI.
- Fitting and statistics.
- Description of individual experiment models included in package.
- Description of global fits included in package.
- Defining new models.

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 4

API Quick Start

If you already have a python3-based scientific computing environment installed, you can start using the API by:

```
# Install pytc
pip3 install pytc-fitter

# Clone the demos repo
git clone https://github.com/harmslab/pytc-demos

# Fire up jupyter
cd pytc-demos
jupyter notebook
```

CHAPTER 5

Example code using the API

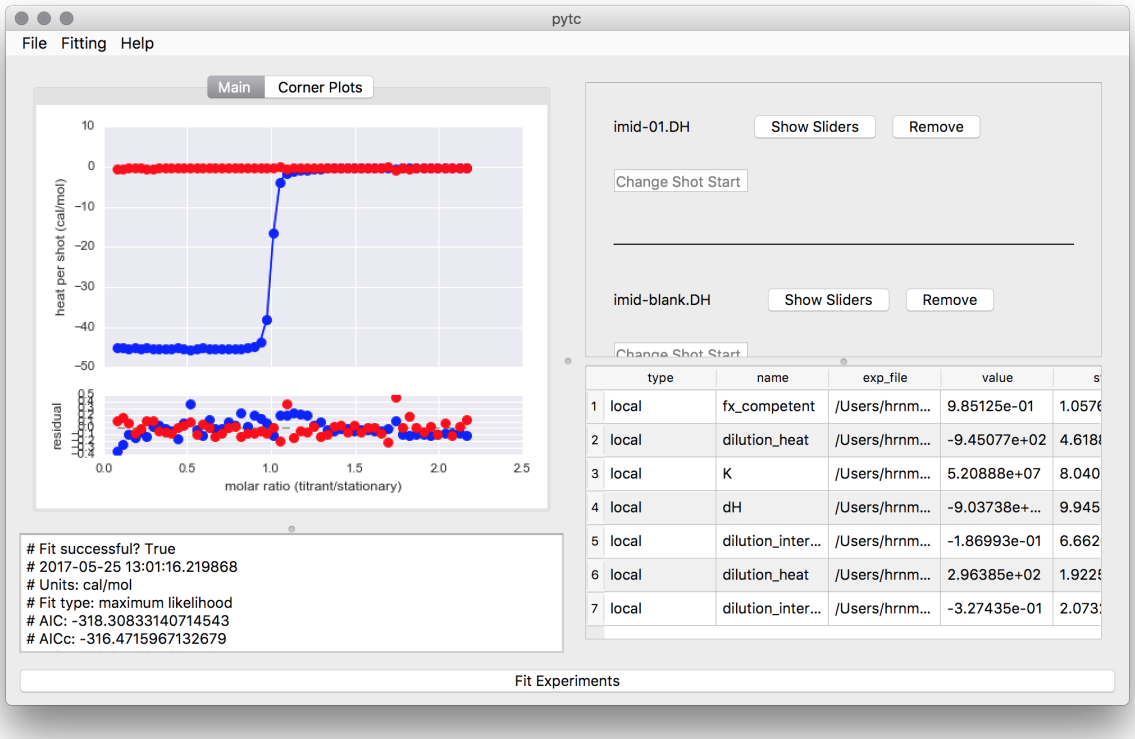
Fit a $Ca^{2+}/EDTA$ binding experiment to a single-site binding model.

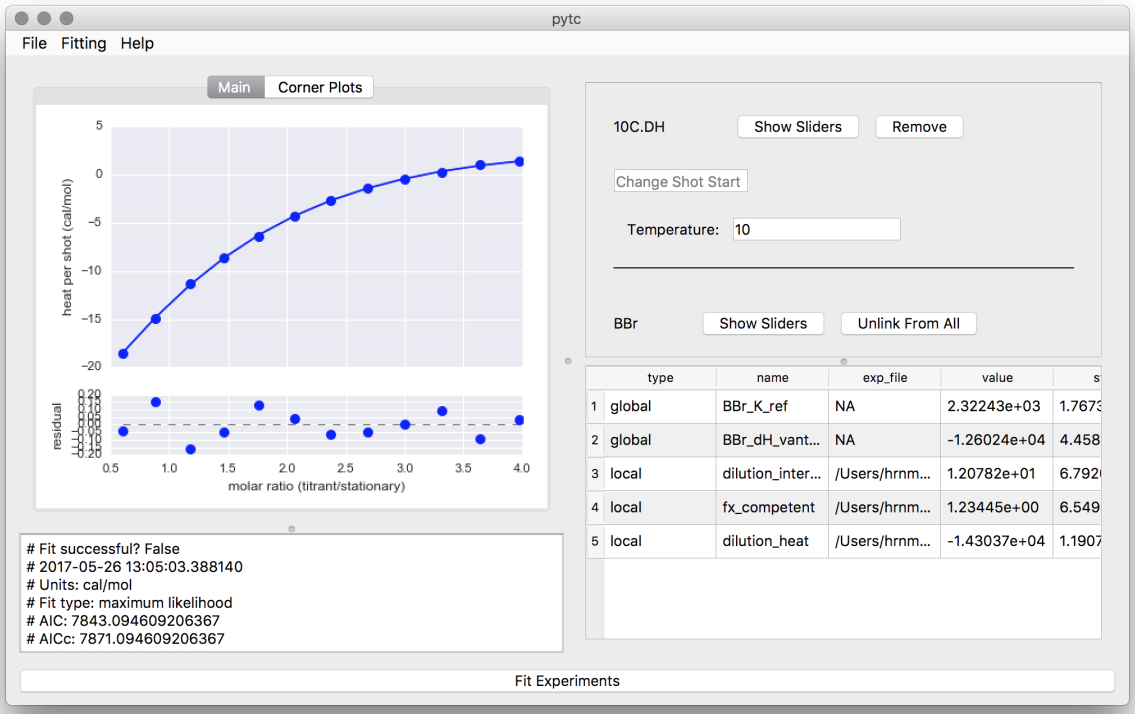
```
import pytc

# 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, and fit
g = pytc.GlobalFit()
g.add_experiment(e)
g.fit()

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

CHAPTER 6

GUI

The GUI is installed separately from the API. Instructions are here. The GUI docs are here. A few screenshots showing the GUI in action are below.




pytc
File Fitting Help
Main
Corner Plots
heat per shot (cal/mol)
residual
molar ratio (titrant/stationary)
10C.DH
Show Sliders
Remove
Change Shot Start
Temperature: 10
BBr
Show Sliders
Unlink From All
type name exp_file value
1 global BBr_K_ref NA 2.32243e+03
2 global BBr_dH_vant... NA -1.26024e+04
3 local dilution_inter... /Users/hrnm... 1.20782e+01
4 local fx_competent /Users/hrnm... 1.23445e+00
5 local dilution_heat /Users/hrnm... -1.43037e+04
Fit successful? False
2017-05-26 13:05:03.388140
Units: cal/mol
Fit type: maximum likelihood
AIC: 7843.094609206367
AICc: 7871.094609206367
Fit Experiments

6.1 pytc package

6.1.1 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

6.1.2 Submodules

CHAPTER 7

Indices and tables

- genindex
- modindex
- search