
pytc-gui Documentation

Release 1.0.1

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Aug 25, 2018

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pytc-gui is a graphical interface for [pytc](#), a flexible package for fitting Isothermal Titration Calorimetry data.

- [Installation](#)
- [Basic fits](#)
- [Video examples](#)
- [Full pytc docs](#)

CHAPTER 1

Start-up

either: + double-click the icon for the installed program + run `pytc-gui` on command line

- load experiments
- link individual fit parameters to global parameters
- set fit parameter guesses
- fit the model to the data
- export the results, which will save a csv file with the fit parameters and a pdf showing the fit

2.1 Installation

Note: If you would like to use the [pytc API](#) in addition to the GUI, we recommend installing the python scientific computing stack and then installing pytc-gui via the *pip* method.

Demo heat files for testing the GUI are [here](#).

2.1.1 Windows or Mac installation

For users who only want to use the GUI

- **Windows:** download the [installation file](#) and follow the prompts for the installer.
- **Mac:** download the [dmg](#), unpack it, and then drag the pytc icon into the Applications folder.

It will install its own mini python scientific computing stack, independent of other python distributions installed on the system.

2.1.2 pip installation (windows, mac, or linux)

For users who want to use the GUI and API or for users who want to use an existing python installation

Make sure that python3 and pip3 are already installed (see below).

Option 1: pip. In a terminal, type:

```
pip3 install pytc-gui
```

Option 2: git. In a terminal, type:

```
git clone https://github.com/harmslab/pytc-gui.git
cd pytc-gui
pip3 install .
```

2.1.3 Installing python3

You can obtain python3 from the following sources:

- [Anaconda](#). A single large installation with binaries for windows, mac, and linux.
- [WinPython](#). A single large installation for windows.
- Package managers (linux and mac). For example, the Ubuntu command would be: `sudo apt-get install python3 python3-pip`
- [python.org](#). The main python binary for windows, mac, and linux.

2.1.4 Indices and tables

- [genindex](#)
- [modindex](#)
- [search](#)

2.2 How-To: Basic Fits with GUI

2.2.1 Setting Up

Single-Site Model

For performing a single-site model fit to a single experiment.

This can be repeated for more experiments. Any new experiments you load will be added to the GUI.

2.2.2 Sliders

Each loaded experiment has a model with associated fit parameters. These parameters can be manipulated using a set of “sliders”. These have the same general layout. Each time a value is changed on a slider, the graph is updated with the new guesses. The graph will update to show the fit results once the fit is performed.

2.2.3 Global Variables

Simple Global

For using a global variable that is shared across multiple experiments.

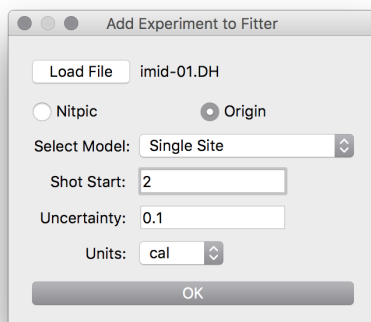


Fig. 1: First, go to File -> Add Experiment. Select the model, load in the file, and select the shot start.

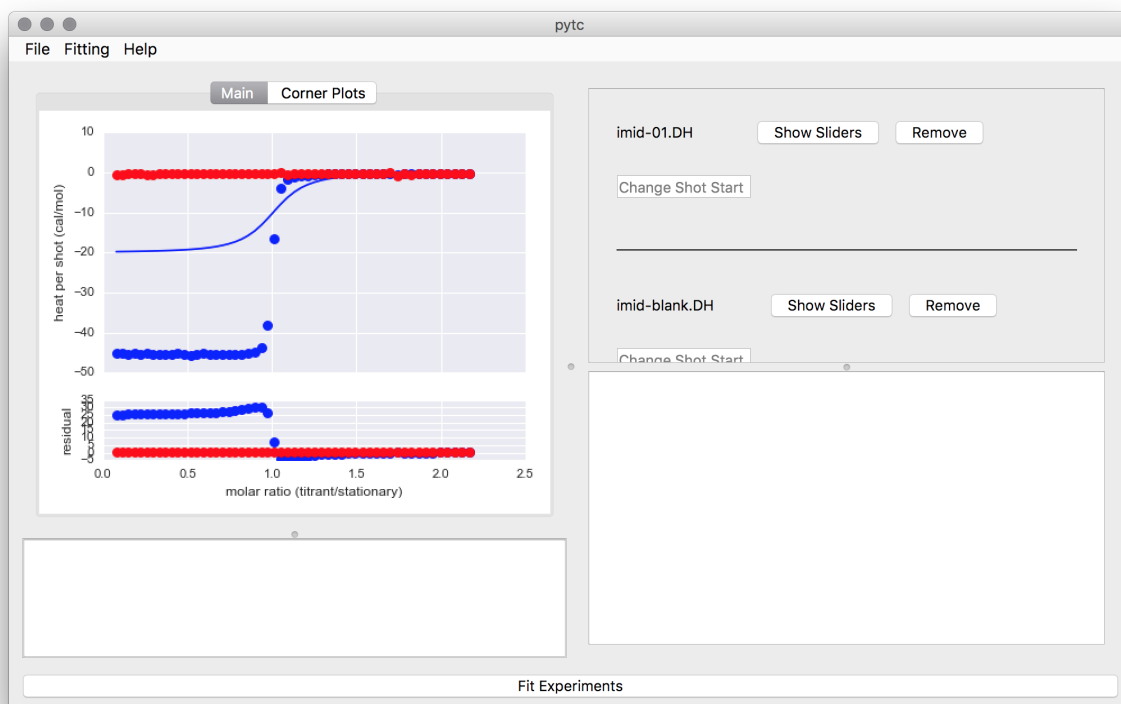


Fig. 2: Before fitting, the graph shows the model calculated using the parameter guesses.

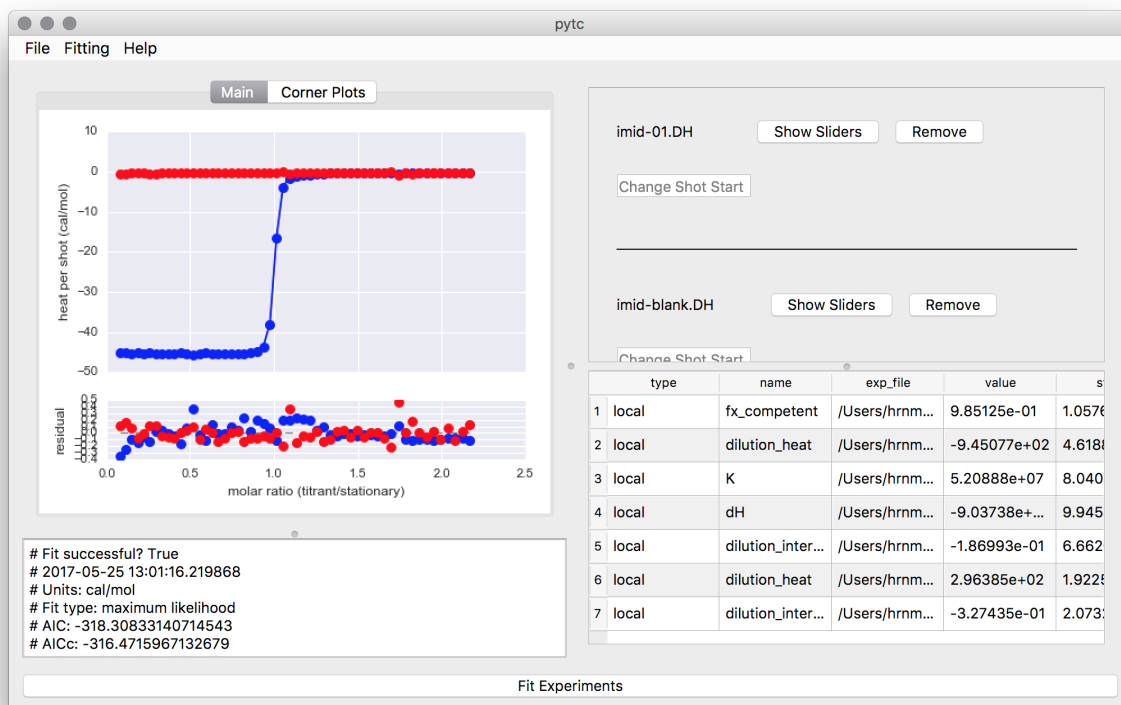


Fig. 3: To fit the model, go to Fitting -> Fit Experiments.

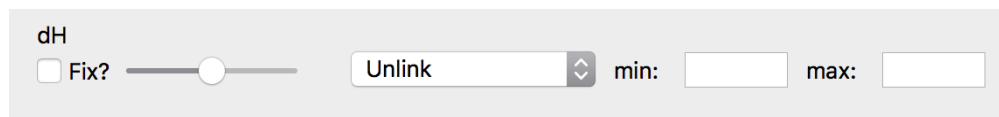


Fig. 4: The general layout for each slider. Global parameters are similar except they exclude the dropdown menu.

	Use
Fix	When checked, allows you to enter a fixed parameter value
Slider	Changes the parameter guess value.
Dropdown	Allows you to link and unlink parameters from global parameters as well as creation of new global parameters or connectors.
Min/Max	Allows you to change the bounds of allowed values for a parameter.

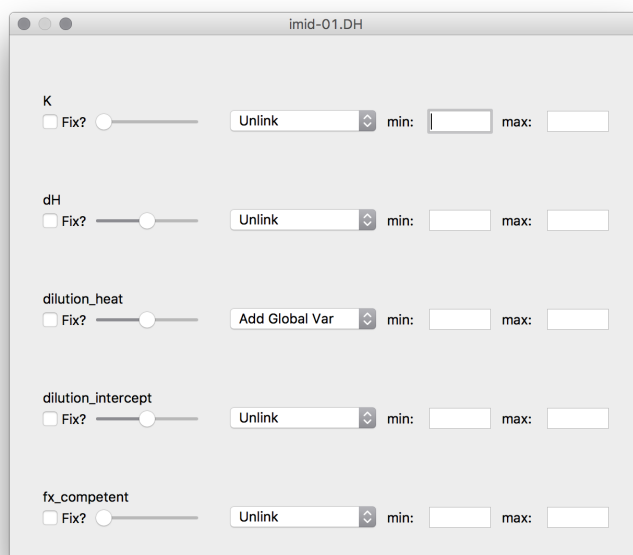


Fig. 5: `pytc-gui` uses sliders to select guesses for each fit parameter. To get to the sliders for an experiment, click on the **Show Sliders** button next to the experiment name. Each pop-up has the same basic layout.

To add a new global variable, select **Add Global Var** from the dropdown menu.

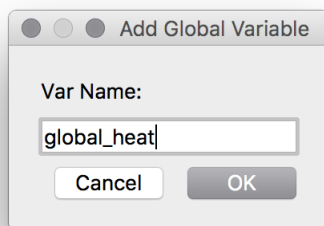


Fig. 6: The pop-up allows you to create a new global variable.

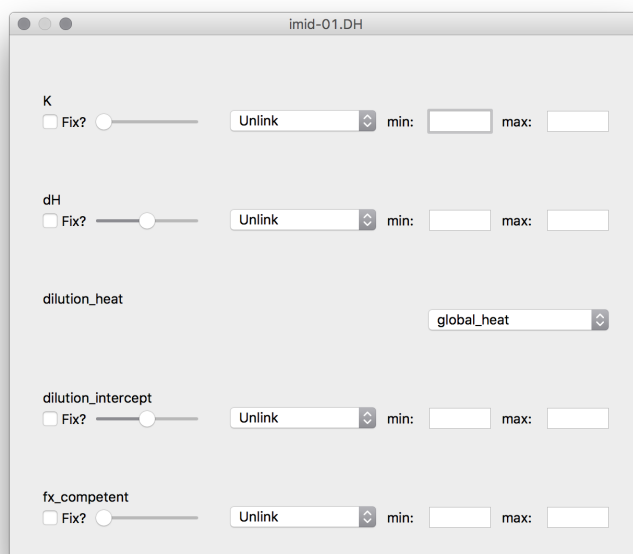


Fig. 7: Once a global variable is made, it can be linked to any parameter by selecting it from the dropdown menu for that parameter.

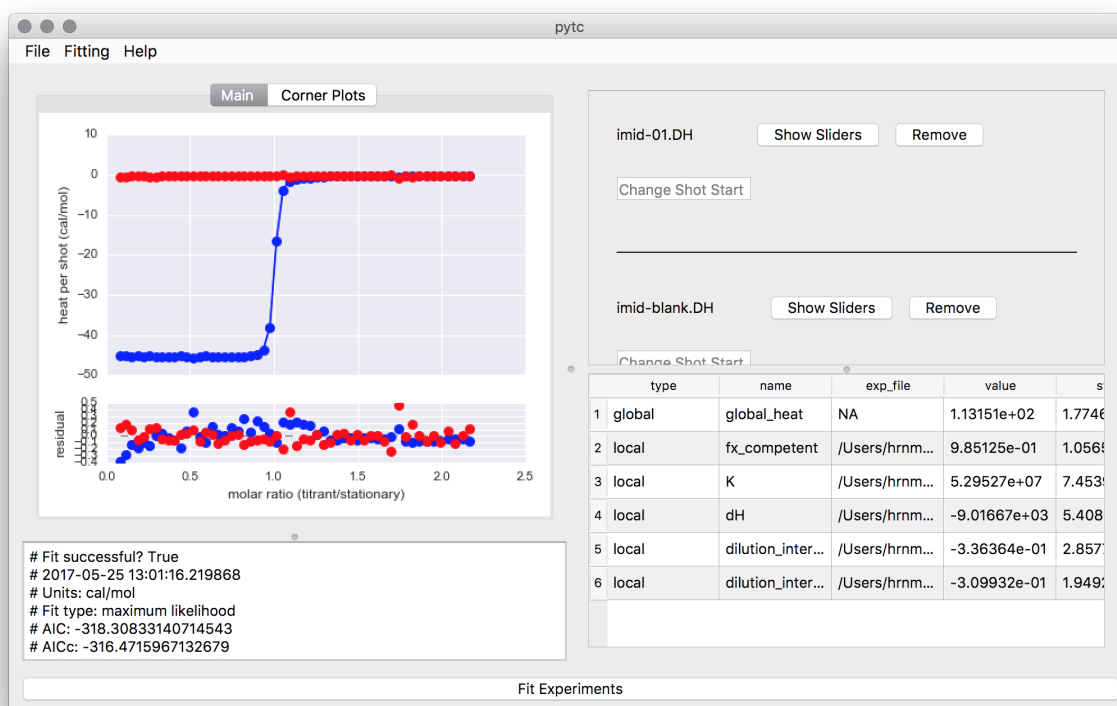


Fig. 8: A new entry is made for the global variable. After this select `Fitting -> Fit Experiments`. This will fit the new global model to the data and update the graph and parameter list.

Connectors

For defining more complex linkages between experiments (such as a van't Hoff relationship).

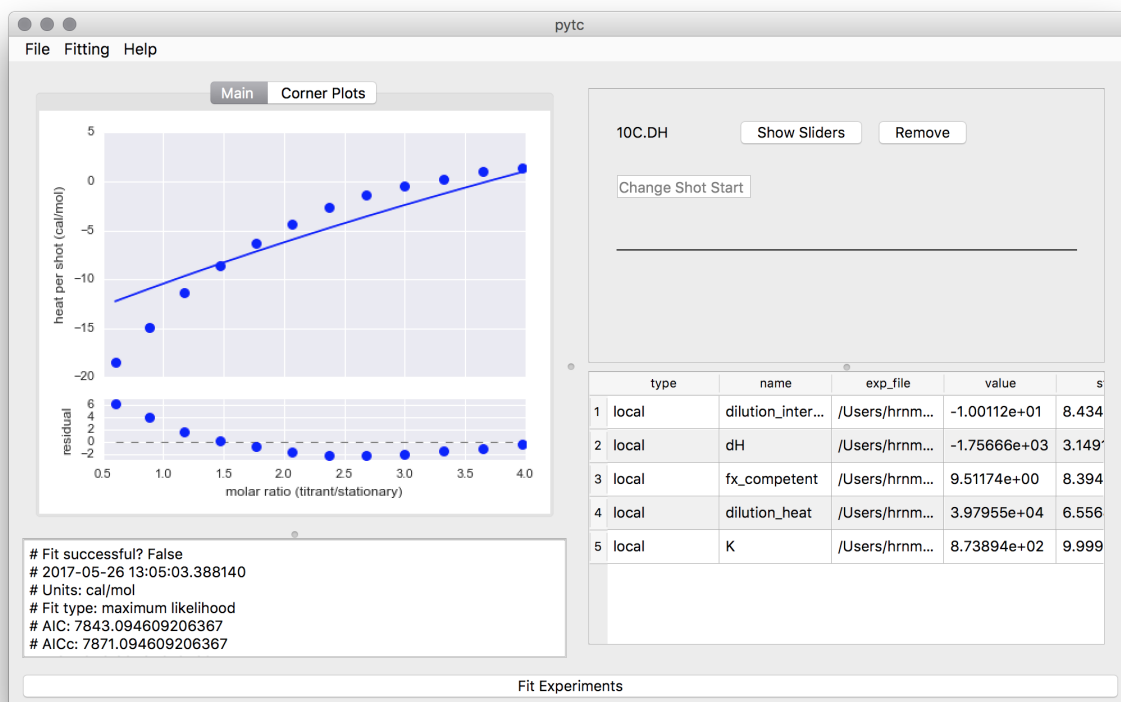


Fig. 9: Fit using a temperature dependant experiment.

2.2.4 Indices and tables

- genindex
- modindex
- search

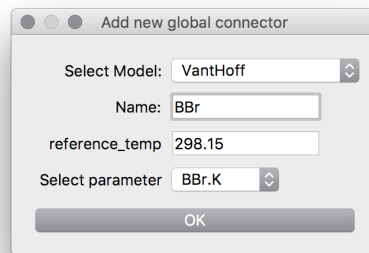


Fig. 10: Connectors are linked in a similar way to global variables, except select **Add Connector** from the dropdown menu rather than **Add Global Var**. A new pop-up will come up allowing you to select the type of connector you'd like to make, the name of the connector, and nay variables linked to that connector.

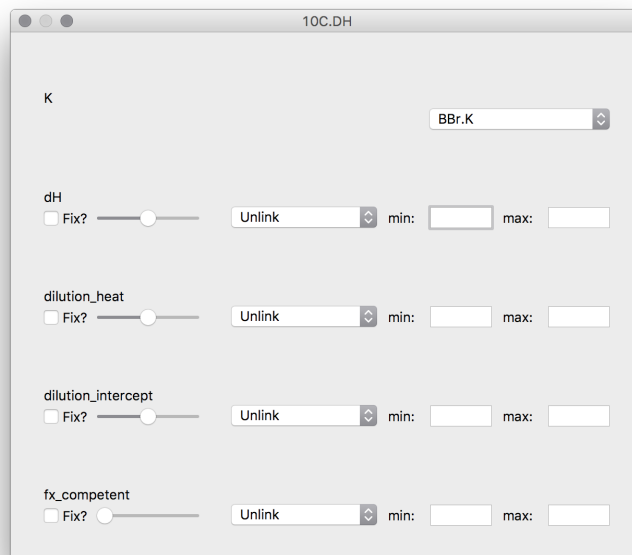


Fig. 11: As with global variables, link parameters to a connector parameter by selecting the connector from the dropdown menu.

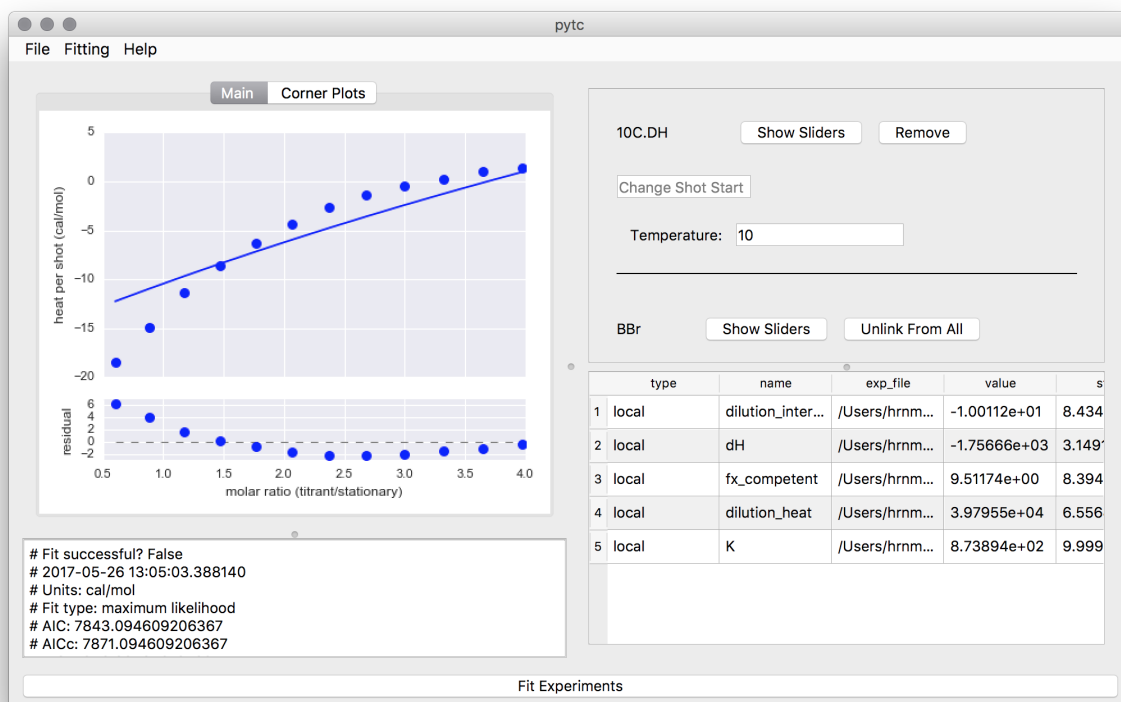


Fig. 12: Some connectors might require experimental metadata (temperature, ionization enthalpy, etc.). These need to be defined before performing the new fit.

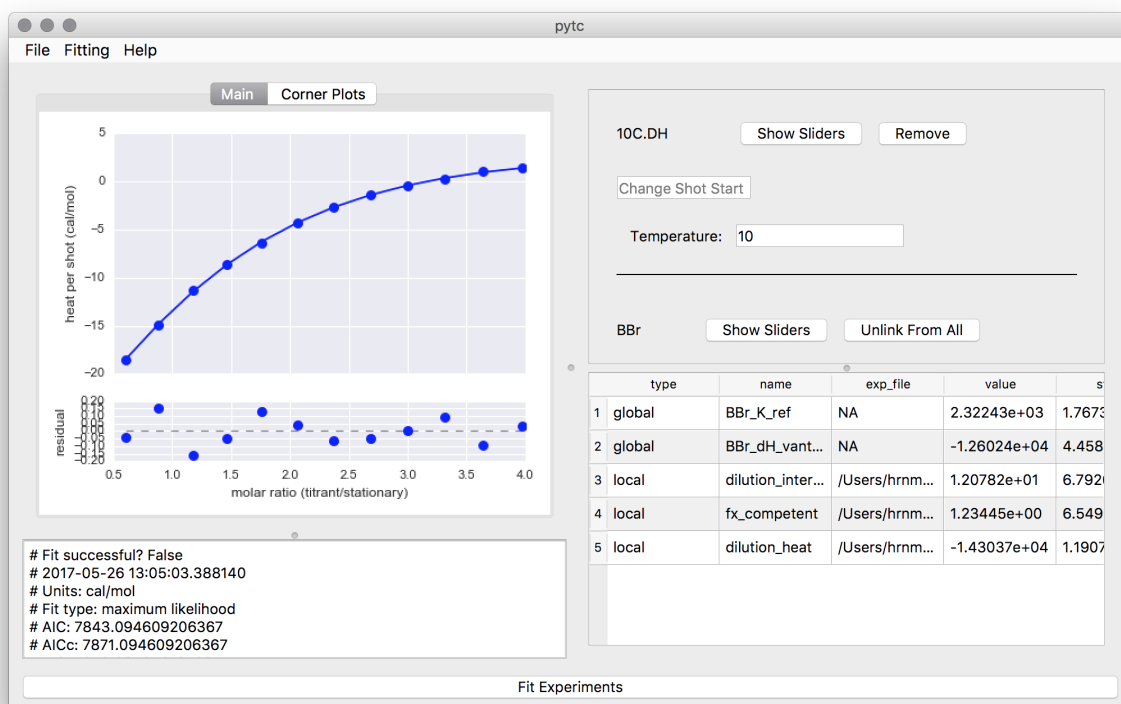


Fig. 13: Once everything is set, perform the new fit.

2.3 Video Examples of Fits

2.3.1 Single Site - Single w/ Blank

2.3.2 Connectors - Num Proton

2.3.3 Connectors - Van't Hoff

2.3.4 Single Site - Replicate + Blank

2.4 GUI Module

2.4.1 Main Interface

Main Window

Fit Update

Set-up

2.4.2 Experiments

Local

Global

Connectors

2.4.3 Sliders

Main Sliders

Local

Global/Connectors

Pop-ups

CHAPTER 3

Indices and tables

- `genindex`
- `modindex`
- `search`