Thunor Core Documentation

Release 0.1.30+0.g788412e.dirty

Alex Lubbock

Feb 06, 2023

CONTENTS

Thunor Core is a Python package for managing and viewing high throughput screen data. It can calculate and visualize both single-timepoint viability calculations, and the multi-timepoint drug-induced proliferation rate (DIP rate) metric, which is a dynamic measure of drug response.

For further information on Thunor, related projects (including a web interface, Thunor Web), and further help see the Thunor website.

Contents:

CHAPTER

ONE

INSTALLATION

To install Thunor, you can use pip:

```
pip install thunor
```

Please note that Python 3 is required (not compatible with Python 2.7).

CHAPTER

TWO

THUNOR CORE TUTORIAL

Thunor (pronounced THOO-nor) is a free software platform for managing, visualizing, and analyzing high throughput cell proliferation data, which measure the dose-dependent response of cells to one or more drug(s).

This repository, Thunor Core, is a Python package which can be used for standalone analysis or integration into computational pipelines.

A web interface is also available, called Thunor Web. Thunor Web has a comprehensive manual, which goes into further detail about the curve fitting methods, types of plots available and other information you may find relevant.

Please see the Thunor website for additional resources, and a link to our chat room, where you can ask questions about Thunor.

2.1 Start Jupyter Notebook

Run jupyter notebook with the following argument:

```
jupyter notebook --NotebookApp.iopub_data_rate_limit=1.0e10
```

The data rate limit needs to be increased or `init_notebook_mode()` throws an error. This is a plotly requirement.

2.2 Check Thunor Core is available

[1]:
```
# If the import doesn't work, uncomment the following two lines, or "pip install
↪thunor"
import os, sys
sys.path.insert(0, os.path.abspath('../'))

import thunor
```

2.3 Load a file

First, specify a file to load. Here, we use an example dataset from the thunor package itself.

[2]:
```
hts007_file = '../thunor/testdata/hts007.h5'
```

Load the file using `read_hdf` (for HDF5 files), `read_vanderbilt_hts` (for CSV files), or another appropriate reader.

[3]:
```
from thunor.io import read_hdf
hts007 = read_hdf(hts007_file)
```

We'll just use a subset of the drugs, to make the plots manageable.

[4]:
```
hts007r = hts007.filter(drugs=['cediranib', 'everolimus', 'paclitaxel'])
```

[5]:
```
hts007r.drugs
```

[5]:
```
[('cediranib',), ('everolimus',), ('paclitaxel',)]
```

[6]:
```
hts007r.cell_lines
```

[6]:
```
['BT20',
 'HCC1143',
 'MCF10A-HMS',
 'MCF10A-VU',
 'MDAMB231',
 'MDAMB453',
 'MDAMB468',
 'SUM149']
```

2.4 Calculate DIP rates and parameters

These two operations can be done in two lines of code (plus imports). Note that you may see `RuntimeWarning` messages, which indicates that some dose response curves were not able to be fitted. This can happen if the cells do not stop proliferating in response to drug, the response is not closely approximated by a log-logistic curve, or the data are very noisy.

[7]:
```
from thunor.dip import dip_rates
from thunor.curve_fit import fit_params

ctrl_dip_data, expt_dip_data = dip_rates(hts007r)
fp = fit_params(ctrl_dip_data, expt_dip_data)
```

```
/home/docs/checkouts/readthedocs.org/user_builds/thunor/checkouts/stable/thunor/curve_
↪fit.py:157: RuntimeWarning: invalid value encountered in log
  return c + (d - c) / (1 + np.exp(b * (np.log(x) - np.log(e))))
/home/docs/checkouts/readthedocs.org/user_builds/thunor/checkouts/stable/thunor/curve_
↪fit.py:225: RuntimeWarning: invalid value encountered in double_scalars
  1 / self.hill_slope)
```

2.5 Setting up plots

Each of the `plot_X` functions returns a plotly `Figure` object which can be visualised in a number of ways. Here, we use the offline `iplot` function, which generates a plot for use with Jupyter notebook. We could also generate plots using the `plot` function in standalone HTML files. See the plotly documentation for more information on the latter approach.

[8]:
```
from thunor.plots import plot_drc, plot_drc_params, plot_time_course, plot_ctrl_dip_
↪by_plate, plot_plate_map
```

2.6 Plot Types

2.6.1 Plot DIP rate curves

[9]:
```
plot_drc(fp)
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

2.6.2 Plot DIP parameters

[10]:
```
plot_drc_params(fp, 'auc')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

2.6.3 Filtering fit params

The `fp` object is a pandas data frame, so we can filter it before plotting. Some examples:

[11]:
```
fit_params_bt20_pac = fp[fp.index.isin(['BT20'], level='cell_line') & \
                         fp.index.isin(['paclitaxel'], level='drug')]

plot_drc(fit_params_bt20_pac)
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

2.6.4 Plot time course

Time course plot for paclitaxel on BT20 cells:

[12]:
```
plot_time_course(
    hts007.filter(drugs=['paclitaxel'], cell_lines=['BT20'])
)
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

2.6.5 Quality control check: plot DIP rate ranges by cell line and plate (box plot)

[13]:
```
plot_ctrl_dip_by_plate(ctrl_dip_data)
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

2.6.6 Quality control check: plot DIP rate as a plate heat map

[14]:
```
plate_data = hts007.plate('HTS007_149-28A', include_dip_rates=True)
```

[15]:
```
plot_plate_map(plate_data, color_by='dip_rates')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

CHAPTER

THREE

THUNOR CORE MODULES REFERENCE

3.1 I/O, file reading and writing, core formats (`thunor.io`)

class thunor.io.**HtsPandas**(*doses*, *assays*, *controls*)
High throughput screen dataset

Represented internally using pandas dataframes

Parameters

- **doses** (*pd.DataFrame*) – DataFrame of doses
- **assays** (*pd.DataFrame*) – DataFrame of assays
- **controls** (*pd.DataFrame*) – DataFrame of controls

cell_lines
List of cell lines in the dataset

Type list

drugs
List of drugs in the dataset

Type list

assay_names
List of assay names in the dataset

Type list

dip_assay_name
The assay name used for DIP rate calculations, e.g. "Cell count"

Type str

doses_unstacked()
Split multiple drugs/doses into separate columns

filter(*cell_lines=None*, *drugs=None*, *plate=None*)
Filter by cell lines and/or drugs

"None" means "no filter"

Parameters

- **cell_lines** (*Iterable, optional*) – List of cell lines to filter on
- **drugs** (*Iterable, optional*) – List of drugs to filter on
- **plate** (*Iterable, optional*) –

Returns A new dataset filtered using the supplied arguments

Return type *HtsPandas*

plate(*plate_name*, *plate_size=384*, *include_dip_rates=False*)
Return a single plate in PlateData format

Parameters

- **plate_name** (*str*) – The name of a plate in the dataset
- **plate_size** (*int*) – The number of wells on the plate (default: 384)
- **include_dip_rates** (*bool*) – Calculate and include DIP rates for each well if True

Returns The plate data for the requested plate name

Return type *PlateData*

class thunor.io.**PlateData**(*width=24*, *height=16*, *dataset_name=None*, *plate_name=None*, *cell_lines=[]*, *drugs=[]*, *doses=[]*, *dip_rates=[]*)
A High Throughput Screening Plate with Data

exception thunor.io.**PlateFileParseException**

class thunor.io.**PlateMap**(***kwargs*)
Representation of a High Throughput Screening plate

Parameters **kwargs** (*dict, optional*) – Optionally supply "width" and "height" values for the plate

col_iterator()
Iterate over the column numbers in the plate

Returns Iterator over the column numbers (1, 2, 3, etc.)

Return type Iterator of int

property num_wells
Number of wells in the plate

classmethod plate_size_from_num_wells(*num_wells*)
Calculate plate size from number of wells, assuming 3x2 ratio

Parameters **num_wells** (*int*) – Number of wells in a plate

Returns Width and height of plate (numbers of wells)

Return type tuple

row_iterator()
Iterate over the row letters in the plate

Returns Iterator over the row letters (A, B, C, etc.)

Return type Iterator of str

well_id_to_name(*well_id*)
Convert a Well ID into a well name

Well IDs use a numerical counter from left to right, top to bottom, and are zero based.

Parameters **well_id** (*int*) – Well ID on this plate

Returns Name for this well, e.g. A1

Return type str

well_iterator()
Iterator over the plate's wells

Returns Iterator over the wells in the plate. Each well is given as a dict of 'well' (well ID), 'row' (row character) and 'col' (column number)

Return type Iterator of dict

well_list()
List of the plate's wells

Returns The return value of *well_iterator()* as a list

Return type list

well_name_to_id(*well_name*, *raise_error=True*)
Convert a well name to a Well ID

Parameters

- **well_name** (*str*) – A well name, e.g. A1
- **raise_error** (*bool*) – Raise an error if the well name is invalid if True (default), otherwise return -1 for invalid well names

Returns Well ID for this well. See also *well_id_to_name()*

Return type int

thunor.io.**read_hdf**(*filename_or_buffer*)
Read a HtsPandas dataset from Thunor HDF5 format file

Parameters **filename_or_buffer** (*str or object*) – Filename or buffer from which to read the data

Returns Thunor HTS dataset

Return type *HtsPandas*

thunor.io.**read_vanderbilt_hts**(*file_or_source*, *plate_width=24*, *plate_height=16*, *sep=None*, *_unstacked=False*)
Read a Vanderbilt HTS format file

See the wiki for a file format description

Parameters

- **file_or_source** (*str or object*) – Source for CSV data
- **plate_width** (*int*) – Width of the microtiter plates (default: 24, for 384 well plate)
- **plate_height** (*int*) – Width of the microtiter plates (default: 16, for 384 well plate)
- **sep** (*str*) – Source file delimiter (default: detect from file extension)

Returns HTS Dataset containing the data read from the CSV

Return type *HtsPandas*

thunor.io.**write_hdf**(*df_data*, *filename*, *dataset_format='fixed'*)
Save a dataset to Thunor HDF5 format

Parameters

- **df_data** (HtsPandas) – HTS dataset
- **filename** (*str*) – Output filename

- **dataset_format** (*str*) – One of 'fixed' or 'table'. See pandas HDFStore docs for details

thunor.io.**write_vanderbilt_hts**(*df_data*, *filename*, *plate_width=24*, *plate_height=16*, *sep=None*)

Read a Vanderbilt HTS format file

See the wiki for a file format description

Parameters

- **df_data** (HtsPandas) – HtsPandas - HTS dataset
- **filename** (*str or object*) – filename or buffer to write into
- **plate_width** (*int*) – plate width (number of wells)
- **plate_height** (*int*) – plate height (number of wells)
- **sep** (*str*) – Source file delimiter (default: detect from file extension)

3.2 DIP calculations and statistics (thunor.dip)

thunor.dip.**adjusted_r_squared**(*r*, *n*, *p*)

Calculate adjusted r-squared value from r value

Parameters

- **r** (*float*) – r value (between 0 and 1)
- **n** (*int*) – number of sample data points
- **p** (*int*) – number of free parameters used in fit

Returns Adjusted r-squared value

Return type float

thunor.dip.**ctrl_dip_rates**(*df_controls*)

Calculate control DIP rates

Parameters **df_controls** (*pd.DataFrame*) – Pandas DataFrame of control cell counts from a *thunor.io.HtsPandas* object

Returns Fitted control DIP rate values

Return type pd.DataFrame

thunor.dip.**dip_rates**(*df_data*, *selector_fn=<function tyson1>*)

Calculate DIP rates on a dataset

Parameters

- **df_data** (thunor.io.HtsPandas) – Thunor HTS dataset
- **selector_fn** (*function*) – Selection function for choosing optimal DIP rate fit (default: *tyson1()*

Returns Two entry list, giving control DIP rates and experiment (non-control) DIP rates (both as Pandas DataFrames)

Return type list

thunor.dip.**expt_dip_rates**(*df_doses*, *df_vals*, *selector_fn=<function tyson1>*)

Calculate experiment (non-control) DIP rates

Parameters

- **df_doses** (*pd.DataFrame*) – Pandas DataFrame of dose values from a *thunor.io.HtsPandas* object
- **df_vals** (*pd.DataFrame*) – Pandas DataFrame of cell counts from a *thunor.io.HtsPandas* object
- **selector_fn** (*function*) – Selection function for choosing optimal DIP rate fit (default: *tyson1()*

Returns Fitted DIP rate values

Return type pd.DataFrame

thunor.dip.**tyson1**(*adj_r_sq*, *rmse*, *n*)

Tyson1 algorithm for selecting optimal DIP rate fit

Parameters

- **adj_r_sq** (*float*) – Adjusted r-squared value
- **rmse** (*float*) – Root mean squared error of fit
- **n** (*int*) – Number of data points used in fit

Returns Fit value (higher is better)

Return type float

3.3 Viability calculations and statistics (thunor.viability)

thunor.viability.**viability**(*df_data*, *time_hrs=72*, *assay_name=None*, *include_controls=True*)

Calculate viability at the specified time point

Viability is calculated as the assay value over the mean of controls from the same plate, cell line, and time point

Parameters

- **df_data** (HtsPandas) – HTS dataset
- **time_hrs** (*float*) – Time in hours to use for viability. The closest time point in each well to the one specified is used.
- **assay_name** (*str, optional*) – The assay name to use for viability calculation, or None to use the default proliferation assay
- **include_controls** (*bool*) – Return the control values for reference as a the second entry in a two-tuple, if True

Returns A DataFrame containing the viability results and a Series containing the control values, if requested (None is returned as the second return value otherwise)

Return type pd.DataFrame, pd.Series or None

3.4 Dose Response Curve Fitting (thunor.curve_fit)

exception thunor.curve_fit.**AAFitWarning**

exception thunor.curve_fit.**AUCFitWarning**

exception thunor.curve_fit.**DrugCombosNotImplementedError**
This function does not support drug combinations yet

class thunor.curve_fit.**HillCurve**(*popt*)
Base class defining Hill/log-logistic curve functionality

null_response_fn(*axis=None*, *dtype=None*, *out=None*, *keepdims=<no value>*)
Compute the arithmetic mean along the specified axis.

Returns the average of the array elements. The average is taken over the flattened array by default, otherwise over the specified axis. *float64* intermediate and return values are used for integer inputs.

Parameters

- **a** (*array_like*) – Array containing numbers whose mean is desired. If *a* is not an array, a conversion is attempted.
- **axis** (*None or int or tuple of ints, optional*) – Axis or axes along which the means are computed. The default is to compute the mean of the flattened array.

  New in version 1.7.0.

  If this is a tuple of ints, a mean is performed over multiple axes, instead of a single axis or all the axes as before.
- **dtype** (*data-type, optional*) – Type to use in computing the mean. For integer inputs, the default is *float64*; for floating point inputs, it is the same as the input dtype.
- **out** (*ndarray, optional*) – Alternate output array in which to place the result. The default is None; if provided, it must have the same shape as the expected output, but the type will be cast if necessary. See *ufuncs-output-type* for more details.
- **keepdims** (*bool, optional*) – If this is set to True, the axes which are reduced are left in the result as dimensions with size one. With this option, the result will broadcast correctly against the input array.

  If the default value is passed, then *keepdims* will not be passed through to the *mean* method of sub-classes of *ndarray*, however any non-default value will be. If the sub-class' method does not implement *keepdims* any exceptions will be raised.

Returns **m** – If *out=None*, returns a new array containing the mean values, otherwise a reference to the output array is returned.

Return type ndarray, see dtype parameter above

See also:

average Weighted average

std, var, nanmean, nanstd, nanvar

Notes

The arithmetic mean is the sum of the elements along the axis divided by the number of elements.

Note that for floating-point input, the mean is computed using the same precision the input has. Depending on the input data, this can cause the results to be inaccurate, especially for *float32* (see example below). Specifying a higher-precision accumulator using the *dtype* keyword can alleviate this issue.

By default, *float16* results are computed using *float32* intermediates for extra precision.

Examples

```
>>> a = np.array([[1, 2], [3, 4]])
>>> np.mean(a)
2.5
>>> np.mean(a, axis=0)
array([2., 3.])
>>> np.mean(a, axis=1)
array([1.5, 3.5])
```

In single precision, *mean* can be inaccurate:

```
>>> a = np.zeros((2, 512*512), dtype=np.float32)
>>> a[0, :] = 1.0
>>> a[1, :] = 0.1
>>> np.mean(a)
0.54999924
```

Computing the mean in float64 is more accurate:

```
>>> np.mean(a, dtype=np.float64)
0.55000000074505806 # may vary
```

class thunor.curve_fit.**HillCurveLL2**(*popt*)

classmethod fit_fn(*x*, *b*, *e*)
Two parameter log-logistic function ("Hill curve")

Parameters

- **x** (*np.ndarray*) – One-dimensional array of "x" values
- **b** (*float*) – Hill slope
- **e** (*float*) – EC50 value

Returns Array of "y" values using the supplied curve fit parameters on "x"

Return type np.ndarray

classmethod initial_guess(*x*, *y*)
Heuristic function for initial fit values

Uses the approach followed by R's drc library: https://cran.r-project.org/web/packages/drc/index.html

Parameters

- **x** (*np.ndarray*) – Array of "x" (dose) values
- **y** (*np.ndarray*) – Array of "y" (response) values

Returns Four-valued list corresponding to initial estimates of the parameters defined in the `ll4()` function.

Return type list

class thunor.curve_fit.**HillCurveLL3u**(*popt*)

Three parameter log logistic curve, for viability data

classmethod fit_fn(*x*, *b*, *c*, *e*)

Three parameter log-logistic function ("Hill curve")

Parameters

- **x** (*np.ndarray*) – One-dimensional array of "x" values
- **b** (*float*) – Hill slope
- **c** (*float*) – Maximum response (lower plateau)
- **e** (*float*) – EC50 value

Returns Array of "y" values using the supplied curve fit parameters on "x"

Return type np.ndarray

classmethod initial_guess(*x*, *y*)

Heuristic function for initial fit values

Uses the approach followed by R's drc library: https://cran.r-project.org/web/packages/drc/index.html

Parameters

- **x** (*np.ndarray*) – Array of "x" (dose) values
- **y** (*np.ndarray*) – Array of "y" (response) values

Returns Four-valued list corresponding to initial estimates of the parameters defined in the `ll4()` function.

Return type list

static null_response_fn(*_*)

Compute the arithmetic mean along the specified axis.

Returns the average of the array elements. The average is taken over the flattened array by default, otherwise over the specified axis. *float64* intermediate and return values are used for integer inputs.

Parameters

- **a** (*array_like*) – Array containing numbers whose mean is desired. If *a* is not an array, a conversion is attempted.
- **axis** (*None or int or tuple of ints, optional*) – Axis or axes along which the means are computed. The default is to compute the mean of the flattened array.

  New in version 1.7.0.

  If this is a tuple of ints, a mean is performed over multiple axes, instead of a single axis or all the axes as before.
- **dtype** (*data-type, optional*) – Type to use in computing the mean. For integer inputs, the default is *float64*; for floating point inputs, it is the same as the input dtype.
- **out** (*ndarray, optional*) – Alternate output array in which to place the result. The default is `None`; if provided, it must have the same shape as the expected output, but the type will be cast if necessary. See *ufuncs-output-type* for more details.

- **keepdims** (*bool, optional*) – If this is set to True, the axes which are reduced are left in the result as dimensions with size one. With this option, the result will broadcast correctly against the input array.

  If the default value is passed, then *keepdims* will not be passed through to the *mean* method of sub-classes of *ndarray*, however any non-default value will be. If the sub-class' method does not implement *keepdims* any exceptions will be raised.

Returns **m** – If *out=None*, returns a new array containing the mean values, otherwise a reference to the output array is returned.

Return type ndarray, see dtype parameter above

See also:

average Weighted average

`std`, `var`, `nanmean`, `nanstd`, `nanvar`

Notes

The arithmetic mean is the sum of the elements along the axis divided by the number of elements.

Note that for floating-point input, the mean is computed using the same precision the input has. Depending on the input data, this can cause the results to be inaccurate, especially for *float32* (see example below). Specifying a higher-precision accumulator using the *dtype* keyword can alleviate this issue.

By default, *float16* results are computed using *float32* intermediates for extra precision.

Examples

```
>>> a = np.array([[1, 2], [3, 4]])
>>> np.mean(a)
2.5
>>> np.mean(a, axis=0)
array([2., 3.])
>>> np.mean(a, axis=1)
array([1.5, 3.5])
```

In single precision, *mean* can be inaccurate:

```
>>> a = np.zeros((2, 512*512), dtype=np.float32)
>>> a[0, :] = 1.0
>>> a[1, :] = 0.1
>>> np.mean(a)
0.54999924
```

Computing the mean in float64 is more accurate:

```
>>> np.mean(a, dtype=np.float64)
0.55000000074505806 # may vary
```

class thunor.curve_fit.**HillCurveLL4**(*popt*)

aa(*min_conc*, *max_conc*)
Find the activity area (area over the curve)

Parameters

- **min_conc** (*float*) – Minimum concentration to consider for fitting the curve
- **max_conc** (*float*) – Maximum concentration to consider for fitting the curve

Returns Activity area value

Return type float

auc(*min_conc*)
Find the area under the curve

Parameters **min_conc** (*float*) – Minimum concentration to consider for fitting the curve

Returns Area under the curve (AUC) value

Return type float

ec(*ec_num=50*)
Find the effective concentration value (e.g. IC50)

Parameters **ec_num** (*int*) – EC number between 0 and 100 (response level)

Returns Effective concentration value for requested response value

Return type float

classmethod fit_fn(*x*, *b*, *c*, *d*, *e*)
Four parameter log-logistic function ("Hill curve")

Parameters

- **x** (*np.ndarray*) – One-dimensional array of "x" values
- **b** (*float*) – Hill slope
- **c** (*float*) – Maximum response (lower plateau)
- **d** (*float*) – Minimum response (upper plateau)
- **e** (*float*) – EC50 value

Returns Array of "y" values using the supplied curve fit parameters on "x"

Return type np.ndarray

ic(*ic_num=50*)
Find the inhibitory concentration value (e.g. IC50)

Parameters **ic_num** (*int*) – IC number between 0 and 100 (response level)

Returns Inhibitory concentration value for requested response value

Return type float

classmethod initial_guess(*x*, *y*)
Heuristic function for initial fit values

Uses the approach followed by R's drc library: https://cran.r-project.org/web/packages/drc/index.html

Parameters

- **x** (*np.ndarray*) – Array of "x" (dose) values
- **y** (*np.ndarray*) – Array of "y" (response) values

Returns Four-valued list corresponding to initial estimates of the parameters defined in the `ll4()` function.

Return type list

class thunor.curve_fit.**HillCurveNull**(*popt*)

exception thunor.curve_fit.**ValueWarning**

thunor.curve_fit.**aa_obs**(*responses*, *doses=None*)
Activity Area (observed)

Parameters

- **responses** (*np.array or pd.Series*) – Response values, with dose values in the Index if a Series is supplied
- **doses** (*np.array or None*) – Dose values - only required if responses is not a pd.Series

Returns Activity area (observed)

Return type float

thunor.curve_fit.**fit_drc**(*doses*, *responses*, *response_std_errs=None*, *fit_cls=<class 'thunor.curve_fit.HillCurveLL4'>*, *null_rejection_threshold=0.05*, *ctrl_dose_test=False*)
Fit a dose response curve

Parameters

- **doses** (*np.ndarray*) – Array of dose values
- **responses** (*np.ndarray*) – Array of response values, e.g. viability, DIP rates
- **response_std_errs** (*np.ndarray, optional*) – Array of fit standard errors for the response values
- **fit_cls** (*Class*) – Class to use for fitting (default: 4 parameter log logistic "Hill" curve)
- **null_rejection_threshold** (*float, optional*) – p-value for rejecting curve fit against no effect "flat" response model by F-test (default: 0.05). Set to None to skip test.
- **ctrl_dose_test** (*boolean*) – If True, the minimum dose is assumed to represent control values (in DIP rate curves), and will reject fits where E0 is greater than a standard deviation higher than the mean of the control response values. Leave as False to skip the test.

Returns A HillCurve object containing the fit parameters

Return type *HillCurve*

thunor.curve_fit.**fit_params**(*ctrl_data*, *expt_data*, *fit_cls=<class 'thunor.curve_fit.HillCurveLL4'>*, *ctrl_dose_fn=<function <lambda>>*)
Fit dose response curves to DIP rates or viability data

This method computes parameters including IC50, EC50, AUC, AA, Hill coefficient, and Emax. For a faster version, see *fit_params_minimal()*.

Parameters

- **ctrl_data** (*pd.DataFrame or None*) – Control DIP rates from `dip_rates()` or `ctrl_dip_rates()`. Set to None to not use control data.
- **expt_data** (*pd.DataFrame*) – Experiment (non-control) DIP rates from `dip_rates()` or `expt_dip_rates()`, or viability data from `viability()`
- **fit_cls** (*Class*) – Class to use for curve fitting (default: *HillCurveLL4()*)

- **ctrl_dose_fn** (*function*) – Function to use to set an effective "dose" (non-zero) for controls. Takes the list of experiment doses as an argument.

Returns DataFrame containing DIP rate curve fits and parameters

Return type pd.DataFrame

thunor.curve_fit.**fit_params_from_base**(*base_params*, *ctrl_resp_data=None*, *expt_resp_data=None*, *ctrl_dose_fn=<function <lambda>>*, *custom_ic_concentrations=frozenset({})*, *custom_ec_concentrations=frozenset({})*, *custom_e_values=frozenset({})*, *custom_e_rel_values=frozenset({})*, *include_aa=False*, *include_auc=False*, *include_hill=False*, *include_emax=False*, *include_einf=False*, *include_response_values=True*)

Attach additional parameters to basic set of fit parameters

thunor.curve_fit.**fit_params_minimal**(*ctrl_data*, *expt_data*, *fit_cls=<class 'thunor.curve_fit.HillCurveLL4'>*, *ctrl_dose_fn=<function <lambda>>*)

Fit dose response curves to DIP or viability, and calculate statistics

This function only fits curves and stores basic fit parameters. Use *fit_params()* for more statistics and parameters.

Parameters

- **ctrl_data** (*pd.DataFrame or None*) – Control DIP rates from `dip_rates()` or `ctrl_dip_rates()`. Set to None to not use control data.
- **expt_data** (*pd.DataFrame*) – Experiment (non-control) DIP rates from `dip_rates()` or `expt_dip_rates()`
- **fit_cls** (*Class*) – Class to use for curve fitting (default: *HillCurveLL4()*)
- **ctrl_dose_fn** (*function*) – Function to use to set an effective "dose" (non-zero) for controls. Takes the list of experiment doses as an argument.

Returns DataFrame containing DIP rate curve fits and parameters

Return type pd.DataFrame

thunor.curve_fit.**is_param_truncated**(*df_params*, *param_name*)

Checks if parameter values are truncated at boundaries of measured range

Parameters

- **df_params** (*pd.DataFrame*) – DataFrame of DIP curve fits with parameters from *fit_params()*
- **param_name** (*str*) – Name of a parameter, e.g. 'ic50'

Returns Array of booleans showing whether each entry in the DataFrame is truncated

Return type np.ndarray

3.5 Plots and visualization (thunor.plots)

exception thunor.plots.**CannotPlotError**

thunor.plots.**plot_ctrl_cell_counts_by_plate**(*df_controls*, *title=None*, *subtitle=None*, *template='none'*)

Parameters

- **df_controls** (*pd.DataFrame*) – Control well cell counts
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_ctrl_dip_by_plate**(*df_controls*, *title=None*, *subtitle=None*, *template='none'*)

Parameters

- **df_controls** (*pd.DataFrame*) – Control well DIP values
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_drc**(*fit_params*, *is_absolute=False*, *color_by=None*, *color_groups=None*, *title=None*, *subtitle=None*, *template='none'*)

Plot dose response curve fits

Parameters

- **fit_params** (*pd.DataFrame*) – Fit parameters from *thunor.curve_fit.fit_params()*
- **is_absolute** (*bool*) – For DIP rate plots, use absolute (True) or relative (False) y-axis scale. **Ignored for viability plots.**
- **color_by** (*str or None*) – Color the traces by cell lines if 'cl', drugs if 'dr', or arbitrarily if None (default)
- **color_groups** (*dict or None*) – If using color_by, provide a dictionary containing the color groups, where the values are cell line or drug names
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_drc_params**(*df_params*, *fit_param*, *fit_param_compare=None*, *fit_param_sort=None*, *title=None*, *subtitle=None*, *aggregate_cell_lines=False*, *aggregate_drugs=False*, *multi_dataset=False*, *color_by=None*, *color_groups=None*, *template='none'*, ***kwargs*)

Box, bar, or scatter plots of DIP rate fit parameters

Parameters

- **df_params** (*pd.DataFrame*) – DIP fit parameters from `thunor.dip.dip_params()`
- **fit_param** (*str*) – Fit parameter name, e.g. 'ic50'
- **fit_param_compare** (*str, optional*) – Second fit parameter name for comparative plots, e.g. 'ec50'
- **fit_param_sort** (*str, optional*) – Fit parameter name to use for sorting the x-axis, if different from fit_param
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **aggregate_cell_lines** (*bool or dict, optional*) – Aggregate all cell lines (if True), or aggregate by the specified groups (dict of cell line names as values, with group labels as keys)
- **aggregate_drugs** (*bool or dict, optional*) – Aggregate all drugs (if True), or aggregate by the specified groups (dict of drug names as values, with group labels as keys)
- **multi_dataset** (*bool*) – Set to true to compare two datasets contained in fit_params
- **color_by** (*str or None*) – Color by cell lines if "cl", drugs if "dr", or arbitrarily if None (default)
- **color_groups** (*dict or None*) – Groups of cell lines of drugs to color by
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)
- **kwargs** (*dict, optional*) – Additional keyword arguments

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_drug_combination_heatmap**(*ctrl_resp_data*, *expt_resp_data*, *title=None*, *subtitle=None*, *template='none'*)

Plot heatmap of drug combination response by DIP rate

Two dimensional plot (each dimension is a drug concentration) where squares are coloured by DIP rate value.

Parameters

- **ctrl_resp_data** (*pd.DataFrame*) – Control DIP rates from *thunor.dip.dip_rates()*
- **expt_resp_data** (*pd.DataFrame*) – Experiment (non-control) DIP rates from *thunor.dip.dip_rates()*
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_plate_map**(*plate_data*, *color_by='dip_rates'*, *missing_color='lightgray'*, *subtitle=None*, *template='none'*)

Parameters

- **plate_data** (*thunor.io.PlateData*) – Plate map layout data
- **color_by** (*str*) – Attribute to color wells by, must be numerical (default: dip_rates)
- **missing_color** (*str*) – Color to use for missing values (default: lightgray)
- **subtitle** (*str or None*) – Subtitle, or None to auto-generate
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_time_course**(*hts_pandas*, *log_yaxis=False*, *assay_name='Assay'*, *title=None*, *subtitle=None*, *show_dip_fit=False*, *template='none'*)

Plot a dose response time course

Parameters

- **hts_pandas** (*HtsPandas*) – Dataset containing a single cell line/drug combination
- **log_yaxis** (*bool*) – Use log scale on y-axis
- **assay_name** (*str*) – The name of the assay to use for the time course (only used for multi-assay datasets)
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **show_dip_fit** (*bool*) – Overlay the DIP rate fit on the time course
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

thunor.plots.**plot_two_dataset_param_scatter**(*df_params*, *fit_param*, *title*, *subtitle*, *color_by*, *color_groups*, *template='none'*, ***kwargs*)

Plot a parameter comparison across two datasets

Parameters

- **df_params** (*pd.DataFrame*) – DIP fit parameters from `thunor.dip.dip_params()`
- **fit_param** (*str*) – The name of the parameter to compare across datasets, e.g. ic50
- **title** (*str, optional*) – Title (or None to auto-generate)
- **subtitle** (*str, optional*) – Subtitle (or None to auto-generate)
- **template** (*str*) – Name of plotly template (https://plot.ly/python/templates/)
- **kwargs** (*dict, optional*) – Additional keyword arguments

Returns A plotly figure object containing the graph

Return type plotly.graph_objs.Figure

3.6 Miscellaneous "helper" functions (thunor.helpers)

thunor.helpers.**format_dose**(*num*, *sig_digits=12*, *array_as_string=None*)
Format a numeric dose like 1.2e-9 into 1.2 nM

Parameters

- **num** (*float or np.ndarray*) – Dose value, or array of such
- **sig_digits** (*int*) – Number of significant digits to include
- **array_as_string** (*str, optional*) – Combine array into a single string using the supplied join string. If not supplied, a list of strings is returned.

Returns Formatted dose values

Return type str or list of str

thunor.helpers.**plotly_to_dataframe**(*plot_fig*)
Extract data from a plotly figure into a pandas DataFrame

Parameters **plot_fig** (*plotly.graph_objs.Figure*) – A plotly figure object

Returns A pandas DataFrame containing the extracted traces from the figure

Return type pd.DataFrame

3.7 Conversion tools for external formats and databases (thunor.converters)

thunor.converters.**convert_ctrp**(*directory='.'*, *output_file='ctrp_v2.h5'*)
Convert CTRP v2.0 data to Thunor format

CTRP is the Cancer Therapeutics Response Portal, a project which has generated a large quantity of viability data.

The data are freely available from the CTD2 Data Portal:

https://ocg.cancer.gov/programs/ctd2/data-portal

The required files can be downloaded from their FTP server:

ftp://caftpd.nci.nih.gov/pub/OCG-DCC/CTD2/Broad/CTRPv2.0_2015_ctd2_ExpandedDataset/

You'll need to download and extract the following file:

- "CTRPv2.0_2015_ctd2_ExpandedDataset.zip"

Please note that the layout of wells in each plate after conversion is arbitrary, since this information is not in the original files.

Please make sure you have the "tables" python package installed, in addition to the standard Thunor Core requirements.

You can run this function at the command line to convert the files; assuming the two files are in the current directory, simply run:

```
python -c "from thunor.converters import convert_ctrp; convert_ctrp()"
```

This script will take several minutes to run, please be patient. It is also resource-intensive, due to the size of the dataset. We recommend you utilize the highest-spec machine that you have available.

This will output a file called (by default) `ctrp_v2.h5`, which can be opened with *thunor.io.read_hdf()*, or used with Thunor Web.

Parameters

- **directory** (*str*) – Directory containing the extracted CTRP v2.0 dataset
- **output_file** (*str*) – Filename of output file (Thunor HDF5 format)

thunor.converters.**convert_gdsc**(*drug_list_file='Screened_Compounds.xlsx'*, *screen_data_file='v17a_public_raw_data.xlsx'*, *output_file='gdsc-v17a.h5'*)

Convert GDSC data to Thunor format

GDSC is the Genomics of Drug Sensitivity in Cancer, a project which has generated a large quantity of viability data.

The data are freely available under the license agreement described on their website:

https://www.cancerrxgene.org/downloads

The required files can be downloaded from here:

ftp://ftp.sanger.ac.uk/pub/project/cancerrxgene/releases/release-6.0/

You'll need to download two files to convert to Thunor format:

- The list of drugs, "Screened_Compounds.xlsx"
- Sensitivity data, "v17a_public_raw_data.xlsx"

Please note that the layout of wells in each plate after conversion is arbitrary, since this information is not in the original files.

Please make sure you have the "tables" and "xlrd" python packages installed, in addition to the standard Thunor Core requirements.

You can run this function at the command line to convert the files; assuming the two files are in the current directory, simply run:

```
python -c "from thunor.converters import convert_gdsc; convert_gdsc()"
```

This script will take several minutes to run, please be patient. It is also resource-intensive, due to the size of the dataset. We recommend you utilize the highest-spec machine that you have available.

This will output a file called (by default) `gdsc-v17a.h5`, which can be opened with *thunor.io.read_hdf()*, or used with Thunor Web.

Parameters

- **drug_list_file** (*str*) – Filename of GDSC list of drugs, to convert drug IDs to names
- **screen_data_file** (*str*) – Filename of GDSC sensitivity data
- **output_file** (*str*) – Filename of output file (Thunor HDF5 format)

thunor.converters.**convert_gdsc_tags**(*cell_line_file='Cell_Lines_Details.xlsx'*, *output_file='gdsc_cell_line_primary_site_tags.txt'*)

Convert GDSC cell line tissue descriptors to Thunor tags

GDSC is the Genomics of Drug Sensitivity in Cancer, a project which has generated a large quantity of viability data.

The data are freely available under the license agreement described on their website:

https://www.cancerrxgene.org/downloads

The required files can be downloaded from here:

ftp://ftp.sanger.ac.uk/pub/project/cancerrxgene/releases/release-6.0/

You'll need to download one file:

- Cell line details, "Cell_Lines_Details.xlsx"

You can run this function at the command line to convert the files; assuming the downloaded file is in the current directory, simply run:

```
python -c "from thunor.converters import convert_gdsc_tags; convert_gdsc_tags()"
```

This will output a file called (by default) `gdsc_cell_line_primary_site_tags.txt`, which can be loaded into Thunor Web using the "Upload cell line tags" function.

Parameters

- **cell_line_file** (*str*) – Filename of GDSC cell line details (Excel .xlsx format)
- **output_file** (*str*) – Filename of output file (tab separated values format)

thunor.converters.**convert_teicher**(*directory='.'*, *output_file='teicher.h5'*)

Convert Teicher data to Thunor format

The "Teicher" data is a dataset of dose-response data on a panel of small cell lung cancer (SCLC) cell lines. The data can be downloaded from the following link (select the Compound Concentration/Response Data link):

https://sclccelllines.cancer.gov/sclc/downloads.xhtml

Unzip the downloaded file. The dataset can then be converted on the command line:

```
python -c "from thunor.converters import convert_teicher; convert_teicher()"
```

Please note that the layout of wells in each plate after conversion is arbitrary, since this information is not in the original files.

This will output a file called (by default) `teicher.h5`, which can be opened with *thunor.io.read_hdf()*, or used with Thunor Web.

Parameters

- **directory** (*str*) – Directory containing the Teicher dataset
- **output_file** (*str*) – Filename of output file (Thunor HDF5 format)

CHAPTER

FOUR

INDICES AND TABLES

- genindex
- modindex

PYTHON MODULE INDEX

t

INDEX