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# **cytpower Documentation**

***Release 0.1.1***

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**Oct 17, 2018**



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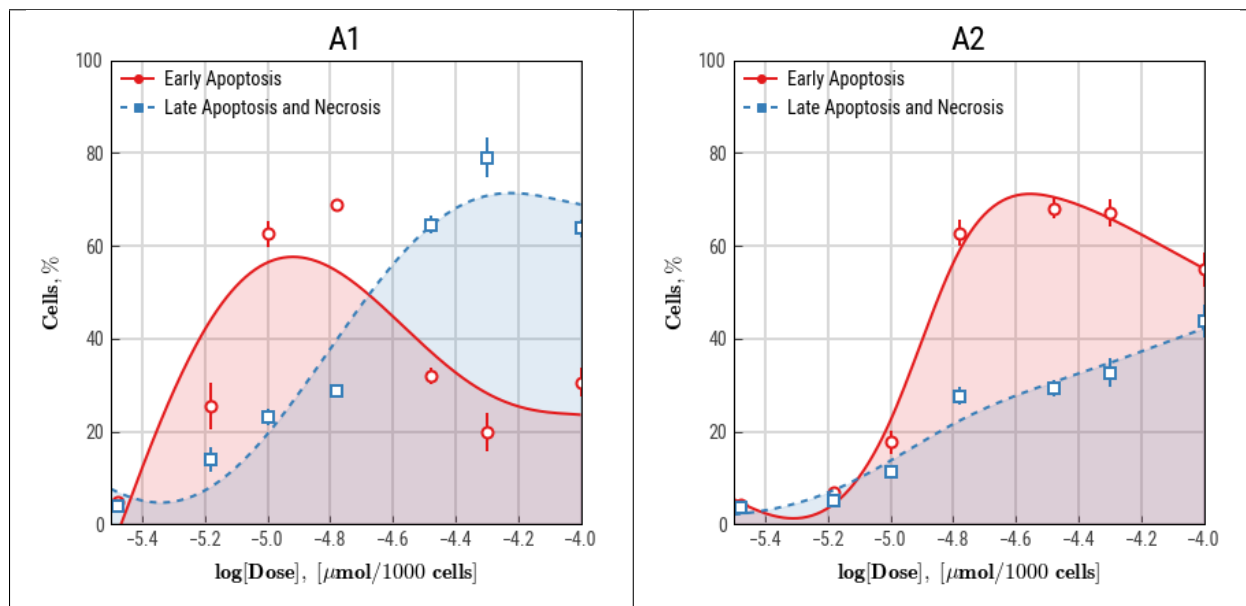
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Cytotoxicity is an ability of chemical compounds to destroy cells either directly or indirectly. Cytotoxicity assays are used in drug discovery to screen potentially toxic compounds. The results are routinely presented as percentages of affected cells vs concentrations used. These data are usually discrete or even disjoint, and do not even rely on the concept of drug dose (concentration per number of cells). Unfortunately, there are no suitable measure indices to estimate cytotoxic potential of a compound within a dose range.



We have recently introduced a concept of cytotoxic power, a parameter that is based on numerical integration and drug doses instead of concentrations (Goncharov et al., 2018). Previously, we endorsed two other indices that may be used to highlight drug specifics (e.g. apoptosis prevalence over necrosis): apoptotic and necrotic difference (AND) and apoptotic and necrotic areas under curves (ANAUCs) (Smetanin et al., 2016, Galenko et al., 2017).

$$CP = \frac{\int_a^b f(x)dx}{\Delta t}$$

where  $x$  is a compound dose,  $f(x)$  is a dose-response function,  $\Delta t$  is incubation duration,  $a$  is minimal dose, and  $b$  is maximum dose.

This Python package is a proof-of-concept implementation of cytotoxic power calculation algorithm to assist researchers in processing cell assay results and presenting data.

The latest version can be installed from PyPi using `pip`:

```
pip install cytpower
```

You can also use `pip` to install the development version from GitHub:

```
pip install git+https://github.com/maximtrp/cytpower.git
```

## 2.1 Dependencies

Package is compatible with both major versions of Python and have the following dependencies:

- `numpy`
- `scipy`
- `statsmodels`
- `pandas`
- `seaborn`
- `matplotlib`

## 2.2 Bugs

Please report any bugs using issues tracker on [GitHub](#).





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<code>calc(cyt_cols, cmp_col, dose_col, data[, ...])</code>	Cytotoxic power calculation.
<code>plot(cyt_cols, cmp_col, dose_col, data[, ...])</code>	Cytotoxic assay data plotting.

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### 3.1 cytpower.calc

`cytpower.calc(cyt_cols, cmp_col, dose_col, data, timedelta=24, iters=16, melted=False, log=False, xlim=None, agg_funcs=None, spline_smth=50, fit_kwds={}, indices_kwds={})`  
 Cytotoxic power calculation. Input data must be converted to a pandas DataFrame object. Also, see reference [\[1\]](#).

#### Parameters

- cyt\_cols** [string or array\_like] Column(s) containing cytotoxic data values.
- cmp\_col** [string] Column containing chemical compounds names.
- dose\_col** [string] Column containing dose values.
- data** [DataFrame object] Long-form dataframe where each row is an observation.
- timedelta** [int or float, optional] Cell incubation duration. Default is 24 hours.
- iters** [int, optional] Bootstrap iterations number to obtain multiple power values (for multiple experiments).
- melted** [bool, optional] Defines if input dataframe is already melted.
- log** [bool, optional] Compute log dose values using basic concentration/dose data in *dose\_col*.
- xlim** [float, optional] Minimum and maximum dose values for calculation.
- agg\_funcs** [array\_like, optional] List of two aggregation functions. Typically, central measure and deviation functions. Passed to Pandas DataFrame *agg* method. Default is `['mean', 'sem']`.

**spline\_smth**: int or float, optional Spline smoothing factor. Passed to *UnivariateSpline* method.

**fit\_kwds** [dict, optional] Dict containing lmfit models as key->val pairs where key is a compound and val is a model created with *lmfit* package (see manual).

**indices\_kwds** [str, dict or array\_like of str, optional] The following options are available: 1) Dict containing the following keys and values: *expr* : array\_like or str Operations to be applied to indices. Available values: -, /, +, \*. Several may be specified.

*cols* : array\_like Columns containing cytotoxic data that must be used to calculate indices.

2) Dict containing *indices* key and values (str or array\_like of str): E.g.: 'E1-E2' or ['E1/E2', 'E1-E2']. Column names must be safe for pandas *eval* func (no spaces or operation symbols in column names).

#### Returns

Pandas DataFrame object containing results.

#### References

[1]

## 3.2 cytpower.plot

`cytpower.plot`(*cyt\_cols*, *cmp\_col*, *dose\_col*, *data*, *agg\_funcs*=None, *colors*={}, *labels*={}, *ls*={}, *markers*={}, *err\_kwds*={}, *fill\_kwds*={'alpha': 0.33}, *fit\_kwds*={}, *grid\_kwds*={}, *legend\_kwds*={}, *leghan\_kwds*={}, *line\_kwds*={}, *log*=False, *markers\_kwds*={}, *melted*=False, *plt\_num*=100, *figname*=None, *savefig\_kwds*={}, *spline\_smth*=50, *subplot\_kwds*={}, *tight\_layout*=True, *title*='{cmp}', *title\_kwds*={}, *xlabel\_kwds*={}, *xlim*=None, *xticks*=None, *xticks\_labels*=None, *xticks\_kwds*={}, *ylabel\_kwds*={}, *ylim*=None, *yticks*=None, *yticks\_labels*=None, *yticks\_kwds*={})

Cytotoxic assay data plotting. Input data must be converted to a pandas DataFrame object.

#### Parameters

**cyt\_cols** [string or array\_like] Column(s) containing cytotoxic data values.

**cmp\_col** [string] Column containing chemical compounds names.

**dose\_col** [string] Column containing dose values.

**data** [DataFrame object] Long-form dataframe where each row is an observation.

**agg\_funcs** [array\_like of str or array\_like of callable, optional] List of two aggregation functions. Typically, central measure and deviation functions. Passed to Pandas DataFrame *agg* method. Default is ['mean', 'sem'].

**colors** [dict, optional] Dictionary with compound names as keys and colors as values.

**labels** [dict, optional] Dictionary with column names (*cyt\_cols*) as keys and plot labels as values.

**ls** [dict, optional] Dictionary with compound names as keys and matplotlib linestyles as values.

**markers** [dict, optional] Dictionary with compound names as keys and matplotlib markers as values.

**err\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.errorbar* method.

**fill\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.fill\_between* method.

**fit\_kwds** [dict, optional] Dict containing lmfit models as key -> value pairs where key is a compound name and value is a model created with *lmfit* package (see manual).

**grid\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.grid* method.

**legend\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.legend* function.

**leghan\_kwds** [dict, optional] Dict of keywords passed to matplotlib *lines.Line2D* method.

**line\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.plot* method.

**log** [bool, optional] Compute log dose values using non-log concentration/dose data in *dose\_col*.

**markers\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.plot* method.

**melted** [bool, optional] Defines if input DataFrame is already melted.

**plt\_num** [int, optional] Number of plot coordinates returned by fitted function.

**figname** [str, optional] Figure filename. *{cmp}* can be used as a variable for compound name.

**savefig\_kwds** [dict, optional] Dict of keywords passed to matplotlib *errorbar* function. File-name is defined by *fname* keyword. *{cmp}* can be used as a variable for compound name.

**spline\_smth** [int, optional] Spline smoothing factor passed to *UnivariateSpline* method.

**subplot\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.subplots* method.

**tight\_layout** [bool, optional] Defines if to use *pyplot.tight\_layout* method to optimize plot.

**title** [str, optional] Plot title. *{cmp}* can be used as a variable for compound name.

**title\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.title* method.

**xlabel\_kwds** [dict, optional] Dict of keywords passed to matplotlib *errorbar* function.

**xlim** [array\_like of ints or floats, optional] Minimum and maximum X values (dose values) for plotting.

**xticks** [array\_like of ints or floats, optional] List of X ticks.

**xticks\_labels** [array\_like, optional] List of X ticks labels.

**xticks\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.xticks* method.

**ylabel\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.ylabel* method.

**ylim** [array\_like of ints or floats, optional] Minimum and maximum Y values for plotting.

**yticks** [array\_like of ints or floats, optional] List of Y ticks.

**yticks\_labels** [array\_like, optional] List of Y ticks labels.

**yticks\_kwds** [dict, optional] Dict of keywords passed to matplotlib *pyplot.yticks* method.

#### Returns

**Pandas DataFrame object containing results.**



## CHAPTER 4

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### Indices and tables

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



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## Bibliography

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- [1] Goncharov, N. V., Terpilowski, M. A., Nadeev, A. D., Kudryavtsev, I. V., Serebriakova, M. K., Zinchenko, V. P., Avdonin, P. V. (2018). Cytotoxic Power of Hydrogen Peroxide Effect on Endothelial Cells in vitro. *Biochemistry (Moscow), Supplement Series A: Membrane and Cell Biology*, 12(2), 180-188.





## C

`calc()` (in module `cytpower`), [5](#)

## P

`plot()` (in module `cytpower`), [6](#)