Dye/DNA Plates Documentation

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CONTENTS:

MODULES

1.1 Wells

src.wells.**column_row_to_well**(*ix: int*, *iy: int*) → str

Convert indices to well

```
>>> column_row_to_well(0, 0)
'A1'
>>> column_row_to_well(0, 7)
'H1'
>>> column_row_to_well(11, 0)
'A12'
>>> column_row_to_well(11, 7)
'H12'
>>> well_to_row(column_row_to_well(11, 7))
7
>>> well_to_column(column_row_to_well(11, 7))
11
```

Parameters

- **ix** (*int*) – a index
- **iy** (*int*) – y index

Returns well

Return type str

src.wells.**number_to_column**(*number: int*) → int

```
>>> number_to_column(1)
1
>>> number_to_column(0)
0
>>> number_to_column(11)
11
>>> number_to_column(95)
11
>>> number_to_column(84)
0
```

src.wells.**number_to_row**(*number: int*) → int

```
>>> number_to_row(0)
0
>>> number_to_row(1)
0
>>> number_to_row(11)
0
>>> number_to_row(12)
1
>>> number_to_row(95)
7
>>> number_to_row(84)
7
```

src.wells.**number_to_well**(*number: int*) → str
> Return number of well

```
>>> number_to_well(0)
'A1'
>>> number_to_well(11)
'A12'
>>> number_to_well(95)
'H12'
>>> number_to_well(84)
'H1'
```

src.wells.**well_to_column**(*well: str*) → int
> Convert well name to column

```
>>> well_to_column('H100')
Traceback (most recent call last):
    ...
ValueError: '100' is not in list
>>> well_to_column('H1')
0
>>> well_to_column('A1')
0
>>> well_to_column('B12')
11
>>> well_to_column('B13')
Traceback (most recent call last):
    ...
ValueError: '13' is not in list
>>> well_to_column('Z1')
0
```

> **Parameters** **well** (*str*) – name of well
>
> **Returns** **ix** – a-index for well
>
> **Return type** int

src.wells.**well_to_number**(*well: str*) → int
> Return number of well

```
>>> well_to_number("A1")
0
>>> well_to_number("A12")
```

```
11
>>> well_to_number("H12")
95
>>> well_to_number("H1")
84
```

src.wells.**well_to_row**(*well: str*) → int
> Well to y index

```
>>> well_to_row('H100')
7
>>> well_to_row('H1')
7
>>> well_to_row('A1')
0
>>> well_to_row('B1')
1
>>> well_to_row('Z1')
Traceback (most recent call last):
    ...
ValueError: 'Z' is not in list
```

> **Parameters well** (*str*) – well name
>
> **Returns iy** – y-index of well
>
> **Return type** int

1.2 Get Data

class src.get_data.**CombinedData**(**replicates*)
> Combined data from several replicate plates. See changes to F and C in *Raw Data and Scaling* portion of *Results and Discussion*.
>
> **Variables**
>
> - **F** (*np.ndarray*) – Fluorescence data, $\mathbf{F}_{\mathbf{D}}^t$ in Equation (16a)
> - **C** (*np.ndarray*) – Dye concentrations, $\mathbf{C}_{\mathbf{D}}^t$ in Equation (16a)
> - **D** (*float*) – DNA concentration, $\mathbf{D}$ in Equation (16a)
> - **t** (*str*) – Type of DNA, t, `"SS"` or `"DS"`
> - **N** (*int*) – number of nucleobases per single strand, N
> - **M_tls** (*np.array*) – $\mathbf{M}^{\text{TLS}}$, set externally, defaults to np.array([])
> - **C_hat** (*np.array*) – $\widehat{\mathbf{C}}$, set externally, defaults to np.array([])
> - **V_M** (*np.array*) – $V(\mathbf{M})$ (see Section S1.2), defaults to np.array([])
> - **V_C** (*np.array*) – $V(\mathbf{C})$ (see Section S1.2), defaults to np.array([])
> - **M_std** (*np.array*) – $\sqrt{V(\mathbf{M})}$ (see Section S1.2), defaults to np.array([])
> - **C_std** (*np.array*) – $\sqrt{V(\mathbf{C})}$ (see Section S1.2), defaults to np.array([])
>
> **__init__**(**replicates*) → None
> > Combine replicate F and C

> Parameters **replicates** (`typing.List[Data]`) – list of plates to gather together as replicates

make_subset(*F_min*)
  Make subset of data as described in *Raw Data and Scaling* portion of manuscript

---

Note: **F** and **C** are overwritten.

---

class `src.get_data.`**RawData**(*fluorescence_file_name*,   *B_d*,   *t*,   *l*,   *N*,
                                        dye_conc_file_name='dye_conc_uM.csv')
  Stores raw data.

  Variables

  - **F** (`np.ndarray`) – Fluorescence data, $F_d^{t\ell}$ (see Equation 14 of main text)
  - **C** (`np.ndarray`) – Dye concentrations, C (see Equation 13 of main text)
  - **B** (`float`) – DNA concentration, B_d in mol/L
  - **t** (`str`) – Type of DNA, t, `"SS"` or `"DS"` or `"None"`.
  - **l** (`str`) – Replicate name, ℓ is A, B, or C
  - **N** (`int`) – number of nucleobases per single strand

  __init__(*fluorescence_file_name*, *B_d*, *t*, *l*, *N*, *dye_conc_file_name='dye_conc_uM.csv'*)
    Scale the data before interpolating/solving optimization problem.

    Parameters

    - **fluorescence_file_name** (`str`) – name of fluorescence file within data folder
    - **B_d** (`float`) – Total concentration of nucleobases in mol/L B_d
    - **dye_conc_file_name** (`str, optional`) – name of dye concentration file name within data folder, defaults to `"dye_conc_uM.csv"`
    - **t** (`str`) – Type of DNA, `"SS"`, `"DS"`, or `"None"`.
    - **l** (`str`) – Replicate name, ℓ is A, B, or C
    - **N** (`int`) – number of nucleobases per single strand

`src.get_data.`**excel_to_data**(*f_name: str*, *channel='GREEN'*)
  Convert "Raw Data" sheet of excel file to pandas dataframe. Uses Equation (12) of manuscript to calculate temperature associated with each cycle.

    Parameters

    - **f_name** (`str`) – name of excel file
    - **channel** (`str, optional`) – name of channel to investigate, defaults to `"GREEN"`

    Returns Formatted data frame, with wells sorted from A1, A2 … H11, H12

    Return type pd.DataFrame

`src.get_data.`**get_C**(*file_name*)
  Get total dye concentration associated with each well.

    Parameters **file_name** (`str`) – CSV file formatted like a 96-well plate. The top left corner looks like

Row	1	2
A	.	.
B	.	.
C	.	.

The values are concentrations of dye in units of mol/L

Returns Mapping of well name ("A1",...) to dye concentration [units of mol/L]

Return type Dictionary

1.3 Noise Removal

src.noise_removal.**compute_M_LS**(*F*, *C*)

Calculate $\mathbf{M}$ by least-squares approximation

Returns $\mathbf{M}^{\mathrm{LS}}$, see Equation (21)

Return type np.array

src.noise_removal.**compute_M_plus**(*F*, *c_plus*)

Get updated guess for M

Parameters

- **F** (*np.ndarray*) – Fluorescence matrix $\mathbf{F}$

- **c_plus** (*np.array*) – Concentration matrix updated $\mathbf{c}_+$

Returns $\mathbf{M}_+$ by Equation (S3b)

Return type np.array

src.noise_removal.**compute_c_plus**(*F*, *C*, *M_minus*, *rho_squared*)

Compute updated guess of concentrations, $\mathbf{c}_+$

Parameters

- **F** (*np.ndarray*) – Fluorescence $\mathbf{F}$

- **C** (*np.array*) – Dye Concentration $\mathbf{C}$

- **M_minus** (*np.array*) – Guess for M, $\mathbf{M}_-$

- **rho_squared** (*float*) – Weight, ρ^2

Returns $\mathbf{c}_+$ by Equation (S3a)

Return type np.ndarray

src.noise_removal.**predictor_corrector**(*F*, *C*, *rho_squared*, *maxiter=100000*, *print_iter=True*)

Solve Equation (22) with predictor–corrector algorithm

Parameters

- **F** (*np.ndarray*) – Fluorescence data $\mathbf{F}$

- **C** (*np.ndarray*) – Dye concentration data $\mathbf{C}$

- **rho_squared** (*float*) – Weighting factor for concentrations, ρ^2 in Equation (22a)

- **maxiter** (*int, optional*) – maximum iterations allowed, by default 100000

- **print_iter**(*bool, optional*) – whether or not to print the total number of iterations performed, by default True

Returns (M, c) – solution, $(\mathbf{M}^{\mathrm{TLS}}, \widehat{\mathbf{C}})$

Return type tuple(np.array, np.array)

1.4 Parameter Extraction

class src.parameter_extraction.**Parameters**(*cls1:   src.get_data.CombinedData,   cls2: src.get_data.CombinedData*)

Stores multiple instances of CombinedData for one DNA type

Variables

- **N** (*int*) – number of nucleobases, N
- **M1** (*np.array*) – $\mathbf{M}^{\mathrm{TLS}}$ associated with $\mathbf{D} = 1$
- **M2** (*np.array*) – $\mathbf{M}^{\mathrm{TLS}}$ associated with $\mathbf{D} = 2$. Several high temperatures are removed to reflect smaller temperature range associated with $\mathbf{D} = 1$
- **C1** (*np.array*) – $\widehat{\mathbf{C}}$ associated with $\mathbf{D} = 1$
- **C2** (*np.array*) – $\widehat{\mathbf{C}}$ associated with $\mathbf{D} = 2$
- **r** (*np.array*) – r, as defined in Equation (S7).
- **V_C1** (*np.array*) – $V(\mathbf{C})$ associated with $\mathbf{D} = 1$
- **V_C2** (*np.array*) – $V(\mathbf{C})$ associated with $\mathbf{D} = 2$
- **V_M1** (*np.array*) – $V(\mathbf{M})$ associated with $\mathbf{D} = 1$
- **V_M2** (*np.array*) – $V(mathbfM)$ associated with $\mathbf{D} = 2$. Several high temperatures are removed to reflect smaller temperature range associated with $\mathbf{D} = 1$
- **dT** (*float*) – Change in temperature from one cycle to next, ΔT

__init__(*cls1: src.get_data.CombinedData, cls2: src.get_data.CombinedData*)

Initialize data

Note: Since different temperature ranges for each, need to make subset of dataset that has more temperatures. Dataset with lower DNA concentration `cls1` always has less temperatures.

Parameters

- **cls1** (`CombinedData`) – Data of DNA type at $\mathbf{D} = 1$
- **cls2** (`CombinedData`) – Data of DNA type at $\mathbf{D} = 2$

get_K() → numpy.array

Get $\mathbf{K}$ from vectorized version of Equation (24)

Returns K

Return type np.array

get_K_std() → numpy.array

Get standard deviation estimate of $\mathbf{K}$

Returns

$$\sqrt{\Delta\mathbf{M}^2\left(4V(\mathbf{M}_1)+2V(\mathbf{M}_2)\right)+\frac{\Delta H^2}{8\Delta\mathbf{M}^4}\left(V(\mathbf{M}_1)+V(\mathbf{M}_2)\right)}$$

where $\Delta H := 2\mathbf{M}_1 - \mathbf{M}_2$, $\Delta\mathbf{M} := \mathbf{M}_2 - \mathbf{M}_1$

Return type np.array

get_dg() $\rightarrow$ numpy.array

Get free energy of dye binding, Δg, vectorized version of Equation (29).

Returns

Return type np.array

get_dg_std() $\rightarrow$ numpy.array

Get estimate of standard deviation in Δg.

Returns

$$\frac{RT_j}{2\Delta\mathbf{M}_j\left(2\mathbf{M}_{j1}-\mathbf{M}_{j2}\right)}\sqrt{\mathbf{M}_{j2}^2 V(\mathbf{M}_{j1})+\mathbf{M}_{j1}^2 V(\mathbf{M}_{j2})}$$

where $\Delta\mathbf{M}_j = \mathbf{M}_{j2} - \mathbf{M}_{j1}$.

Return type np.array

get_dh() $\rightarrow$ numpy.array

Get differential enthalpy of binding, Δh as the vectorized version of Equation (30).

Returns

Return type np.array

get_dh_std() $\rightarrow$ numpy.array

Get estimate of error in Δh_j

Returns

Return type np.array

get_f() $\rightarrow$ numpy.array

Get **f** from vectorized version of Equation (27)

Returns **f**

Return type np.array

get_f_std() $\rightarrow$ numpy.array

Get standard deviation estimate of **f**

Returns

$$\sqrt{V(\mathbf{M}_1)+V(\mathbf{M}_2)+\frac{E_B^2 V_A + E_A^2 V_B}{E_B^4}}$$

where

$$V_A := (V_B + H_+^2)(V(\mathbf{M}_1)+V(\mathbf{M}_2)+\Delta\mathbf{M}^2) - E_A^2$$
$$V_B := 2V(\mathbf{M}_1)+V(\mathbf{M}_2)$$
$$E_A := \Delta\mathbf{M}H_+$$
$$E_B := 2\mathbf{M}_1 - \mathbf{M}_2$$
$$\Delta\mathbf{M} := \mathbf{M}_2 - \mathbf{M}_1$$
$$H_+ := 2\mathbf{M}_1 + \mathbf{M}_2$$

> **Return type** np.array

get_phi_1() → numpy.array
> Get φ_1, vectorized version of Equation (S6a)

> > **Returns**

> > **Return type** np.array

get_phi_2()
> Get φ_2, vectorized version of Equation (S6b)

> > **Returns**

> > **Return type** np.array

get_std_phi_1() → numpy.array
> Get estimate of standard deviation in φ_1

> > **Returns**

$$\frac{2}{\mathbf{M}_{2j}}\sqrt{V(\mathbf{M}_{1j}) + r_j^2 V(\mathbf{M}_{2j})}$$

> > **Return type** np.array

get_std_phi_2()
> Get estimate of standard deviation in φ_2

> > **Returns**

$$\frac{1}{\mathbf{M}_{1j}}\sqrt{V(\mathbf{M}_{2j}) + r_j^{-2} V(\mathbf{M}_{1j})}$$

> > **Return type** np.array

src.parameter_extraction.**calculate_relative_brightness**(*f_SS*, *f_DS*)
> Calculate relative brightness, Equation (28).

> > **Parameters**

> > > - **f_SS** (*np.array*) – Molar fluorescence of single-stranded DNA, $\mathbf{f}^{\mathrm{SS}}$.
> > > - **f_DS** (*np.array*) – Molar fluorescence of double-stranded DNA, $\mathbf{f}^{\mathrm{DS}}$.

> > **Returns** Relative brightness, $\mathbf{f}_j^{\mathrm{DS}}/\mathbf{f}_j^{\mathrm{SS}}$ for each j associated with SS.

> > **Return type** np.array

src.parameter_extraction.**calculate_relative_brightness_err**(*SS_M1*, *SS_M2*, *DS_M1*, *DS_M2*, *SS_V_M1*, *SS_V_M2*, *DS_V_M1*, *DS_V_M2*) → numpy.array
> Estimate error in relative brightness, Equation (28).

> > **Parameters**

> > > - **SS_M1** (*np.array*) – $\mathbf{M}_1^{\mathrm{SS}}$
> > > - **SS_M2** (*np.array*) – $\mathbf{M}_2^{\mathrm{SS}}$
> > > - **DS_M1** (*np.array*) – $\mathbf{M}_1^{\mathrm{DS}}$
> > > - **DS_M2** (*np.array*) – $\mathbf{M}_2^{\mathrm{DS}}$

- **SS_V_M1** (*np.array*) – $V(\mathbf{M}_1^{\mathrm{SS}})$ _description_
- **SS_V_M2** (*np.array*) – $V(\mathbf{M}_2^{\mathrm{SS}})$
- **DS_V_M1** (*np.array*) – $V(\mathbf{M}_1^{\mathrm{DS}})$
- **DS_V_M2** (*np.array*) – $V(\mathbf{M}_2^{\mathrm{DS}})$

Returns Estimate of error in relative brightness

Return type np.array

1.5 Plotting

1.5.1 Raw Data

src.plot_raw_data.**make_figure_2**(*SS_A_1: src.get_data.RawData, SS_B_1: src.get_data.RawData, SS_C_1: src.get_data.RawData, SS_A_2: src.get_data.RawData, SS_B_2: src.get_data.RawData, DS_A_1: src.get_data.RawData, DS_B_1: src.get_data.RawData, DS_A_2: src.get_data.RawData, DS_B_2: src.get_data.RawData, A_1: src.get_data.RawData*)

Makes Figure 2

src.plot_raw_data.**make_figure_S1**()

Makes Figure S1.

src.plot_raw_data.**make_figure_S2**()

Makes Figure SX.

src.plot_raw_data.**plot_linemap**(*cls: src.get_data.RawData, ax, colorbar=False, get_ticks=False, ordered_by_row=True*)

Plot F vs C for various temperatures (colors)

Parameters

- **cls** (*Data*) – Instance of data (i.e., a dataset)
- **ax** (*axis*) – Matplotlib axis to plot on
- **colorbar** (*bool, optional*) – whether or not to plot colorbar, in which case the axis is colorbar axis, by default False
- **get_ticks** (*bool, optional*) – whether or not to return list of ticks, by default False
- **ordered_by_row** (*bool, optional*) – whether or not well concentrations are ordered by row, by default True

Returns Only returns list of get_ticks=True.

Return type None or list

1.5.2 Noise Removal

src.plot_noise_removal.**plot_error_F**(*ax, F_k_tl, F_hat_k_tl, T*)

Plot the predicted fluorescence $\widehat{\mathbf{F}}_{ijk}^{t\ell}$ against $\mathbf{F}_{ijk}^{t\ell}$ for $i = 1, \ldots, n$ and $j = 1, \ldots, n$.

Parameters

- **ax** (*matplotlib.axes*) – axes to plot on

- **F_kl** (*np.ndarray*) – Experimentally measured fluorescence $\mathbf{F}_k^{t\ell}$.

- **F_hat_kl** (*np.ndarray*) – Predicted fluorescence $\widehat{\mathbf{F}}_k^{t\ell}$.

- **T** (*np.array*) – Temperatures in K

Returns image for colorbar

Return type img

1.5.3 Parameters

src.plot_params.**plot_figure_S6**(*T*, *rb*, *d_rb*)
    Plot figure S5, relative brightness

Parameters

- **T** (*np.array*) – array of temperatures

- **rb** (*np.array*) – Relative brightness, $\mathbf{f}_j^{\mathrm{DS}}/\mathbf{f}_j^{\mathrm{SS}}$

- **d_rb** (*np.array*) – standard deviation in relative brightness

1.6 Util

src.util.**figure_name_to_abspath**(*fname: str*) → str
    Figure name to absolute path

Parameters **fname** (*str*) – name of figure

Returns absolute path to name of figure

Return type str

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