

Package: tidymst (via r-universe)

October 24, 2026

Title Read and Analyse NanoTemper Microscale Thermophoresis Exports

Version 0.1.0

Description Read the Excel exports written by NanoTemper's MO.Affinity Analysis software (MST traces, capillary scans, dose-response and fit results) into tidy data frames, and analyse them: recompute normalised fluorescence (Fnorm) from traces, fit Kd and Hill binding models, and convert responses to delta Fnorm or fraction bound.

License MIT + file LICENSE

URL <https://github.com/BradyAJohnston/tidymst>,
<https://bradyajohnston.github.io/tidymst/>

BugReports <https://github.com/BradyAJohnston/tidymst/issues>

Depends R (>= 4.1.0)

Imports cli, DBI, dplyr (>= 1.1.0), readxl, rlang (>= 1.1.0), RSQLite, stats, tibble, tidyselect, utils, vctrs

Suggests ggplot2, knitr, quarto, testthat (>= 3.0.0), withr

VignetteBuilder quarto

Config/roxygen2/version 8.1.1

Config/testthat/edition 3

Encoding UTF-8

Language en-GB

Roxygen list(markdown = TRUE)

Repository <https://bradyajohnston.r-universe.dev>

Date/Publication 2026-10-24 11:22:03 UTC

RemoteUrl <https://github.com/bradyajohnston/tidymst>

RemoteRef HEAD

RemoteSha 1713a909590d69a89fde0b6b40cfec2ed8ca1345

Contents

mst_coefs	2
mst_curve	3
mst_export_type	4
mst_fit	5
mst_fnorm	6
mst_normalise	7
mst_plot_dose_response	8
mst_plot_traces	9
read_mst	9
read_mst_capillary_scan	11
read_mst_dose_response	11
read_mst_fit	13
read_mst_fit_curve	14
read_mst_metadata	14
read_mst_traces	15
tidymst_example	16
Index	17

mst_coefs	<i>Get fitted model coefficients</i>
-----------	--------------------------------------

Description

Get fitted model coefficients

Usage

```
mst_coefs(fits, conf_level = 0.95)
```

Arguments

- | | |
|------------|--|
| fits | A tibble of fits from <code>mst_fit()</code> . |
| conf_level | Confidence level of the intervals. |

Value

- A tibble with one row per parameter per fit, with the grouping columns of fits and:
- model: the model fitted.
 - term: the parameter: unbound, bound, and kd and target_concentration for the Kd model or ec50 and hill for the Hill model. A fixed target_concentration is not included.
 - estimate and std_error: the estimate and its standard error. Concentrations are molar.
 - conf_low and conf_high: the confidence interval, from the t-distribution. Concentrations are fitted on a log scale, so their intervals are calculated on that scale and are asymmetric, and their standard errors are approximate.

Examples

```
doses <- read_mst_dose_response(  
  tidymst_example("dppr10-cy5_dose-response-flat.xlsx")  
)  
fits <- mst_fit(doses, .by = target)  
mst_coefs(fits)
```

mst_curve

Predict fitted binding curves

Description

Predict fitted binding curves

Usage

```
mst_curve(fits, n = 100)
```

Arguments

fits	A tibble of fits from <code>mst_fit()</code> .
n	Number of points on each curve, spaced evenly on a log scale over the range of concentrations fitted.

Value

A tibble with n rows per fit, with the grouping columns of fits and:

- The concentration, named as in `mst_fit()` (ligand_concentration by default).
- response: the fitted response.
- delta_fnorm: the response relative to the unbound state.
- fraction_bound: the fraction of target bound.

Examples

```
doses <- read_mst_dose_response(  
  tidymst_example("dppr10-cy5_dose-response-flat.xlsx")  
)  
fits <- mst_fit(doses, .by = target)  
mst_curve(fits)
```

mst_export_type	<i>Detect the type of a MO.Affinity Analysis export</i>
-----------------	---

Description

MO.Affinity Analysis records which view an Excel export was made from in its Exported from: field. `mst_export_type()` reads that field and returns a short identifier, which `read_mst()` uses to pick a reader. It also recognises the project files written by MO.Control (.moc) and MO.Affinity Analysis (.nta), which are SQLite databases.

Usage

```
mst_export_type(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Value

A string, one of:

- "traces": MST Traces, including the Raw Data Inspection variant.
- "capillary_scan": Capillary Scan.
- "compare_chart": Compare Results (Chart).
- "compare_grid": Compare Results (Grid).
- "dose_response_grouped": Dose-Response (Grouped).
- "dose_response_flat": Dose-Response (Flat).
- "affinity_project": an MO.Affinity Analysis project (.nta), with both the measurements and their analysis.
- "control_project": an MO.Control project (.moc), with the measurements only.

Examples

```
mst_export_type(tidymst_example("dppr10-cy5_traces.xlsx"))
mst_export_type(tidymst_example("dppr10-cy5_compare-fnorm.xlsx"))
mst_export_type(tidymst_example("dppr10-cy5.nta"))
```

mst_fit

Fit binding models to dose-response data

Description

Fits the binding models used by MO.Affinity Analysis by non-linear least squares, with `stats::nls()`.

Usage

```
mst_fit(
  data,
  model = c("kd", "hill"),
  concentration = ligand_concentration,
  response = response,
  target_concentration = NULL,
  .by = NULL
)
```

Arguments

data	A data frame with a row for each concentration, such as from <code>read_mst_dose_response()</code> or <code>mst_fnorm()</code> . If data is grouped with <code>dplyr::group_by()</code> , each group is fitted separately.
model	The model to fit, "kd" or "hill". See the Models section.
concentration, response	<code><data-masking></code> The columns of ligand concentration (molar) and response.
target_concentration	For the Kd model, the target concentration in molar. If NULL, the default, it is estimated along with the other parameters, as MO.Affinity Analysis can do. If it is known, fixing it gives a more stable fit.
.by	<code><tidy-select></code> Columns to group by, fitting each group separately. An alternative to grouping data.

Value

A tibble with one row per group, with the grouping columns and:

- model: the model fitted.
- n: the number of points fitted.
- sigma: the residual standard deviation.
- fit: the fitted model, used by `mst_coefs()`, `mst_curve()` and `mst_normalise()`. NULL if the fit failed.

Models

The **Kd** model describes 1:1 binding of a ligand to a target, accounting for depletion of free ligand:

$$f = \frac{c + c_T + K_d - \sqrt{(c + c_T + K_d)^2 - 4cc_T}}{2c_T}$$

$$y = U + (B - U)f$$

where c is the ligand concentration, c_T the target concentration, f the fraction of target bound, and U and B the responses of the unbound and bound states.

The **Hill** model describes cooperative binding:

$$y = U + \frac{B - U}{1 + (EC_{50}/c)^n}$$

Examples

```
doses <- read_mst_dose_response(
  tidymst_example("dppr10-cy5_dose-response-flat.xlsx")
)
fits <- mst_fit(doses, .by = target)
fits

mst_coefs(fits)

# Fix the target concentration at its nominal value
mst_fit(doses, target_concentration = 50e-9, .by = target)
```

mst_fnorm

Calculate normalised fluorescence from MST traces

Description

Fnorm is the ratio of the mean fluorescence in a "hot" window, while the IR laser is on, to the mean fluorescence in a "cold" window just before it, expressed in per mille. Recalculating Fnorm from [read_mst_traces\(\)](#) lets you choose the windows without going back to MO.Affinity Analysis.

Usage

```
mst_fnorm(data, hot, cold = c(-1, 0))
```

Arguments

data	A data frame of traces, as returned by read_mst_traces() , with columns time and fluorescence.
hot, cold	Start and end times of the hot and cold windows, in seconds, as numeric vectors of length 2. The hot window depends on how long the laser was on; look up the one used in MO.Affinity Analysis with read_mst_metadata() .

Details

Windows include their start and exclude their end, as MO.Affinity Analysis does, so the results match its Fnorm for the same windows.

Value

A tibble with one row per capillary, with the columns of data other than time, fluorescence and fluorescence_raw, plus response_type (always "fnorm") and response, the Fnorm in per mille. This is the same form as `read_mst_dose_response()`, ready for `mst_fit()`.

Examples

```
traces <- read_mst_traces(tidymst_example("dppr10-cy5_traces.xlsx"))
mst_fnorm(traces, hot = c(19, 20))

# Use a shorter hot window, excluding outliers
traces |>
  dplyr::filter(included) |>
  mst_fnorm(hot = c(1.5, 2.5))
```

mst_normalise	<i>Normalise responses to delta Fnorm and fraction bound</i>
---------------	--

Description

Uses the unbound and bound states of fitted models to express responses relative to the unbound state (delta Fnorm), and as the fraction of target bound. This puts merge sets with different baselines on the same scale.

Usage

```
mst_normalise(data, fits, response = response)
```

Arguments

data	A data frame of dose-response data, as passed to <code>mst_fit()</code> .
fits	A tibble of fits from <code>mst_fit()</code> . Its grouping columns must also be in data.
response	<code><data-masking></code> The column of response, in the same units as the fits.

Value

data with two new columns:

- `delta_fnorm`: the response minus the unbound response.
- `fraction_bound`: `delta_fnorm` divided by the difference between the bound and unbound responses.

Examples

```
doses <- read_mst_dose_response(
  tidymst_example("dppr10-cy5_dose-response-flat.xlsx")
)
fits <- mst_fit(doses, .by = target)
mst_normalise(doses, fits)
```

mst_plot_dose_response

Plot dose-response curves

Description

Draws the response at each concentration, with error bars if data has an error column, and optionally the fitted curves. Requires ggplot2.

Usage

```
mst_plot_dose_response(
  data,
  fits = NULL,
  concentration = ligand_concentration,
  response = response,
  colour = NULL
)
```

Arguments

data	A data frame of dose-response data, such as from read_mst_dose_response() or mst_fnorm() .
fits	Optionally, a tibble of fits from mst_fit() to draw.
concentration, response, colour	<data-masking> The columns of ligand concentration, response, and colour of the points.

Value

A ggplot.

Examples

```
doses <- read_mst_dose_response(
  tidymst_example("dppr10-cy5_dose-response-flat.xlsx")
)
fits <- mst_fit(doses, .by = target)
mst_plot_dose_response(doses, fits, colour = target)
```

mst_plot_traces	<i>Plot MST traces</i>
-----------------	------------------------

Description

Draws one line per capillary. Requires ggplot2.

Usage

```
mst_plot_traces(data, colour = ligand_concentration)
```

Arguments

data	A data frame of traces, as returned by <code>read_mst_traces()</code> .
colour	<code><data-masking></code> The column to colour lines by. Numeric columns are coloured on a log scale.

Value

A ggplot.

Examples

```
traces <- read_mst_traces(tidymst_example("dppr10-cy5_traces.xlsx"))
mst_plot_traces(traces)
```

read_mst	<i>Read a MO.Affinity Analysis export</i>
----------	---

Description

`read_mst()` detects the type of export with `mst_export_type()` and reads its main table:

Usage

```
read_mst(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Details

- MST Traces: `read_mst_traces()`.
- Capillary Scan: `read_mst_capillary_scan()`.
- Compare Results (Chart) and Dose-Response (Grouped and Flat): `read_mst_dose_response()`.
- Compare Results (Grid): `read_mst_fit()`.
- MO.Control (.moc) and MO.Affinity Analysis (.nta) project files: `read_mst_traces()`.

Value

A tibble.

Project files

MO.Control (.moc) and MO.Affinity Analysis (.nta) save projects as SQLite databases, which hold everything the Excel exports are made from. `read_mst_traces()`, `read_mst_capillary_scan()` and `read_mst_metadata()` read both kinds of project; `read_mst_dose_response()` and `read_mst_fit()` read MO.Affinity Analysis projects, which include the analysis. They return the same columns as for the Excel exports, with these differences:

- An `analysis_set` column names the analysis set, as a project can hold several. A trace in more than one analysis set appears once for each. MO.Control projects have no analysis, so `analysis_set`, `merge_set` and `included` are missing, and `run` is named as MO.Affinity Analysis would name it.
- Traces also have `fluorescence_raw`, the fluorescence in raw counts. `fluorescence` is normalised to the mean before the laser switches on, which is within about 0.2% of MO.Affinity Analysis's normalisation.
- Measurement times are in UTC (the Excel exports use local time), and `temperature` is the measured temperature in degrees Celsius.
- `mst_power` is a percentage, such as "40%", rather than a label such as "Medium", and `excitation_type` is not available.
- The fits from `read_mst_fit()` are those saved in the project, which may differ from an export made at another time. They include each parameter's standard error as reported by MO.Affinity Analysis (`*_std_error`), and `fixed` lists any parameters that were fixed.

Fit curves (`read_mst_fit_curve()`) are not read from projects; calculate them with `mst_fit()` and `mst_curve()`.

See Also

`read_mst_metadata()` for the file-level header, and `read_mst_fit()` and `read_mst_fit_curve()` for the fits included in Compare Results and Dose-Response (Grouped) exports.

Examples

```
read_mst(tidymst_example("dppr10-cy5_dose-response-flat.xlsx"))

# A project file from MO.Affinity Analysis
read_mst(tidymst_example("dppr10-cy5.nta"))
```

`read_mst_capillary_scan`*Read capillary scans*

Description

Reads a Capillary Scan export: the raw fluorescence across the tray before each measurement, which is used to check for sticking, aggregation and pipetting errors.

Usage

```
read_mst_capillary_scan(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Value

A tibble with one row per scan position per capillary. Alongside the sample and measurement settings of each capillary, it has columns:

- included: FALSE if the capillary was marked as an outlier.
- position: position along the tray, in capillary index units.
- fluorescence: raw fluorescence counts.

Project files give some extra columns; see the Project files section of [read_mst\(\)](#).

Examples

```
read_mst_capillary_scan(tidymst_example("dppr10c2_capillary-scan.xlsx"))  
read_mst_capillary_scan(tidymst_example("dppr10-cy5.nta"))
```

`read_mst_dose_response`*Read dose-response data*

Description

Reads the response of each ligand concentration from a dose-response export.

Usage

```
read_mst_dose_response(path)
```

Arguments

path Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.

Details

- Compare Results (Chart) and Dose-Response (Grouped) exports give the mean response of each concentration in each merge set, with its error. Capillaries marked as outliers are excluded.
- Dose-Response (Flat) exports give the Fnorm of every capillary. They do not record which capillaries were marked as outliers, so all are included; join to `read_mst_traces()` by run and capillary to find them.
- MO.Affinity Analysis project files (.nta) give the Fnorm of every capillary, calculated with `mst_fnorm()` using the cold and hot regions of its analysis set, and whether it was included. See the Project files section of `read_mst()`.

Note that dates of measurement in Dose-Response (Flat) exports appear to be in UTC, while other exports use the local time of the instrument computer. Both are returned as recorded, labelled as UTC.

Value

A tibble with one row per concentration per series. It always has columns `merge_set`, `target`, `target_concentration`, `ligand`, `ligand_concentration`, `response_type` and `response`, followed by the other settings in the export.

- `response_type` is one of "fnorm", "delta_fnorm" or "fraction_bound", depending on how the data was exported. Fnorm and delta Fnorm are in per mille.
- `series` numbers the merge sets in the order they appear in the export, to tell apart series that share a name. It matches series in `read_mst_fit()` and `read_mst_fit_curve()`.
- `error` is the error of the mean response.

Concentrations are molar.

Examples

```
read_mst_dose_response(tidymst_example("dppr10-cy5_compare-fnorm.xlsx"))

read_mst_dose_response(
  tidymst_example("dppr10-cy5_dose-response-flat.xlsx")
)

read_mst_dose_response(tidymst_example("dppr10-cy5.nta"))
```

read_mst_fit	<i>Read binding fits</i>
--------------	--------------------------

Description

Reads the fits that MO.Affinity Analysis made to each merge set. These are included in Compare Results (Chart and Grid) and Dose-Response (Grouped) exports.

Usage

```
read_mst_fit(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Value

A tibble with one row per merge set, with columns:

- series, merge_set, target, target_concentration and ligand identify the merge set. series is missing for Grid exports.
- model: the fit model, "kd" or "hill".
- unbound and bound: the response of the unbound and bound states.
- kd and kd_confidence (Kd model): the dissociation constant and its confidence, in molar.
- target_concentration_fit (Kd model): the target concentration used in the fit, which may differ from the nominal target_concentration if it was a free parameter.
- ec50, ec50_confidence and hill (Hill model): the half-maximal concentration, its confidence, and the Hill coefficient.
- std_dev: the standard deviation of the residuals.

Grid exports also include fit statistics such as std_error, reduced_chi_sq and signal_to_noise. MO.Affinity Analysis project files (.nta) give one row per merge set per model fitted, with standard errors instead of confidences; see the Project files section of [read_mst\(\)](#).

Examples

```
read_mst_fit(tidymst_example("dppr10-cy5_compare-fnorm.xlsx"))  
read_mst_fit(tidymst_example("dsnppr10_compare-delta-fnorm.xlsx"))
```

read_mst_fit_curve	<i>Read fitted binding curves</i>
--------------------	-----------------------------------

Description

Reads the curves MO.Affinity Analysis fitted to each merge set, from the Fit-Values sheet of Compare Results (Chart) and Dose-Response (Grouped) exports.

Usage

```
read_mst_fit_curve(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Value

A tibble with one row per point on each curve, with columns series, merge_set, target, ligand_concentration, fnorm, response_type and response. response is the curve in the units the data was exported in (see response_type); fnorm is the same curve as Fnorm. Some exports leave the curves empty, giving a tibble with no rows.

Examples

```
read_mst_fit_curve(tidymst_example("dsnppr10_compare-delta-fnorm.xlsx"))
```

read_mst_metadata	<i>Read export metadata</i>
-------------------	-----------------------------

Description

Reads the header that MO.Affinity Analysis writes at the top of every export: where the data came from, when it was exported, and (for most exports) the analysis settings.

Usage

```
read_mst_metadata(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Value

A tibble with one row. Columns include software, project, analysis_set, exported_from and exported_on, and, when the export has a single set of analysis settings, analysis_type, evaluation_strategy and the cold and hot regions in seconds (cold_start, cold_end, hot_start, hot_end).

For project files, it gives the software that wrote the file, the project name, when it was created and updated, and the instrument's device_type and optics_type. MO.Affinity Analysis projects have one row for each analysis set, with its settings.

Examples

```
read_mst_metadata(tidymst_example("dppr10-cy5_traces.xlsx"))
read_mst_metadata(tidymst_example("dppr10-cy5.nta"))
```

read_mst_traces	<i>Read MST traces</i>
-----------------	------------------------

Description

Reads an MST Traces export: the fluorescence of each capillary over time, before and while the IR laser heats it. Normalised fluorescence (Fnorm) can be recalculated from the traces with [mst_fnorm\(\)](#).

Usage

```
read_mst_traces(path)
```

Arguments

path	Path to an .xlsx file exported from MO.Affinity Analysis, or a .moc or .nta project file.
------	---

Value

A tibble with one row per time point per capillary. Alongside the sample and measurement settings of each capillary, it has columns:

- included: FALSE if the capillary was marked as an outlier.
- time: time in seconds relative to the laser switching on.
- fluorescence: fluorescence, normalised by MO.Affinity Analysis.

Concentrations are molar. Project files give some extra columns; see the Project files section of [read_mst\(\)](#).

Examples

```
read_mst_traces(tidymst_example("dppr10-cy5_traces.xlsx"))
read_mst_traces(tidymst_example("dppr10-cy5.nta"))
```

tidymst_example	<i>Get paths to example exports</i>
-----------------	-------------------------------------

Description

tidymst comes bundled with example MO.Affinity Analysis exports in its `inst/extdata` directory. This function makes them easy to access.

Usage

```
tidymst_example(file = NULL)
```

Arguments

file	Name of a file. If NULL, the example files will be listed.
------	--

Details

Most of the files are from one experiment: the binding of a Cy5-labelled PPR protein, dPPR10-Cy5, to two RNA targets (atpH-fl and NEAT1-fl), exported in several formats.

Value

A path, or a character vector of file names.

Examples

```
tidymst_example()  
tidymst_example("dppr10-cy5_traces.xlsx")
```

Index

`dplyr::group_by()`, 5

`mst_coefs`, 2
`mst_coefs()`, 5
`mst_curve`, 3
`mst_curve()`, 5, 10
`mst_export_type`, 4
`mst_export_type()`, 9
`mst_fit`, 5
`mst_fit()`, 2, 3, 7, 8, 10
`mst_fnorm`, 6
`mst_fnorm()`, 5, 8, 12, 15
`mst_normalise`, 7
`mst_normalise()`, 5
`mst_plot_dose_response`, 8
`mst_plot_traces`, 9

`read_mst`, 9
`read_mst()`, 4, 11–13, 15
`read_mst_capillary_scan`, 11
`read_mst_capillary_scan()`, 10
`read_mst_dose_response`, 11
`read_mst_dose_response()`, 5, 7, 8, 10
`read_mst_fit`, 13
`read_mst_fit()`, 10, 12
`read_mst_fit_curve`, 14
`read_mst_fit_curve()`, 10, 12
`read_mst_metadata`, 14
`read_mst_metadata()`, 6, 10
`read_mst_traces`, 15
`read_mst_traces()`, 6, 9, 10, 12

`stats::nls()`, 5

`tidymst_example`, 16