FT-ITC Analysis
User manual

Processing, fitting, and interpreting isothermal titration calorimetry experiments.

VERSION 1.5.0 · FOR MACOS, WINDOWS, AND LINUX

Contents

CHAPTER 01

FT-ITC Analysis user manual

Start here for a tour of FT-ITC Analysis and the conventions used throughout this manual.

Last verified: 2026-08-28

FT-ITC Analysis is a desktop application for processing, fitting, comparing, and presenting isothermal titration calorimetry (ITC) experiments.

This manual is for ITC practitioners who are new to FT-ITC Analysis. It explains user workflows and provides scientific interpretation guidance; no programming knowledge is required.

These instructions apply on macOS, Windows, and Linux. The manual treats the supported desktop applications as one product. A **Platform note** appears only when an operating-system or interface difference changes how you complete a task.

> **VERIFIED:**
> This edition reflects FT-ITC Analysis 1.5.0 and was verified on the date shown for each page.

What the application does

FT-ITC Analysis supports the complete path from compatible instrument data to an analysis project and publication-oriented output:

1. Import of a raw thermogram, integrated heats, or an existing project.
2. Experiment details, concentrations, comments, and attributes.

3. Thermogram processing with model-based baselines, detailed spline editing, and rapid or automatic injection-region adjustment.
4. Single- or multiple-experiment fitting with a supported model.
5. Solution, uncertainty, residual, and result-validity views.
6. Portable project storage in the `.ftxtc` format.
7. Final figures, numerical data, and result-table exports.

Raw input files are read, not rewritten. Desktop analysis is local: experiment data are not uploaded during ordinary analysis. An optional launch-time online check retrieves version and citation information.

Product tour

The data list contains loaded experiments and completed Analysis Results. Selecting an experiment exposes four shared task views:

- **Overview** summarizes the experiment and provides access to its details.
- **Process Data** builds and refines baselines, adjusts injection regions, and converts a raw thermogram into integrated heats with estimated uncertainties.
- **Analyze Data** fits a single experiment or multiple experiments.
- **Final Figure** presents the thermogram, heats, fitted curve, residuals, and annotations.

Selecting an Analysis Result opens its result workspace, with a parameter summary, member fits, parameter correlation, uncertainty display, and any compatible advanced analyses. The menus provide project operations, experiment management, export commands, preferences, additional tools, citation information, and support links. The FT-ITC Analysis website, latest release, source repository, and software DOI provide project, installation, and citation context.

Manual conventions

The shortest route to a first result is Quick start, which uses the reader's own compatible data instead of a bundled tutorial dataset. The relevant task chapter provides setting details and diagnostic guidance when a workflow needs closer inspection.

Manual directory

The manual uses these callouts:

> **NOTE:**
> A detail that affects how the application behaves.

> **CAUTION:**
> A condition that can produce a failed task, invalid result, or misleading output.

> **INTERPRETATION:**
> Scientific context for judging output; it is not an automated conclusion made by the application.

> **RECOMMENDATION:**
> A defensible working practice rather than a software requirement.

PLATFORM NOTE:

A genuine operating-system or interface difference that changes how a task is completed.

CALCULATION:

A compact relationship used by FT-ITC Analysis or needed to interpret its output.

Interface labels appear in **bold**. A path such as **File > Save As…** means choose the menu and then the command. The names of views and controls are used instead of position-dependent phrases, so the instruction remains usable when the window size or platform changes.

Help and support

Citation presents the current paper and versioned software citations and supports copying or exporting BibTeX. **Contact Support…** prepares access to email support and a diagnostic report containing the application version, operating system, recent activity, and full application log. **Copy Support Report** places that report on the clipboard. Official links include the FT-ITC Analysis website, latest release, project viewer, source repository, issue tracker, and software DOI 10.5281/zenodo.14832177.

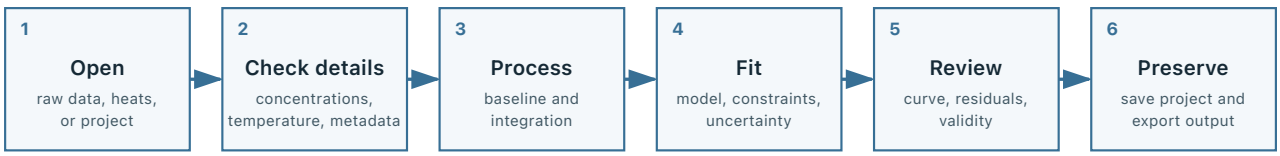
CHAPTER 02

Quick start

Open your own ITC dataset, process it, fit a one-set-of-sites model, review the result, save the project, and export a figure.

Last verified: 2026-08-28

This procedure takes a compatible file through an ordinary one-set-of-sites analysis. Use a dataset for which that model is scientifically plausible. The goal is to learn the application workflow, not to prescribe the correct model for every interaction.



The overall analysis workflow. Integrated-heat imports enter after thermogram processing.

Before you begin

Have one of these inputs available:

- a raw thermogram from a MicroCal-style file (`.itc`), native TA Instruments NanoITC file (`.nitc`), NanoAnalyze export (`.ta`), or PEAQ-ITC project (`.apj`).
- an Origin project file (`.opj`). When a recognized ITC worksheet contains the original time/power trace, FT-ITC Analysis restores it for processing; otherwise, it uses the worksheet heat values as integrated input.
- injection-level integrated heats (`.dat` , `.aff` , or `.dh`).
- an FT-ITC project (`.ftxtc`).

Supported formats and project behavior are described in Installation, files, and projects.

> **NOTE:**
> Integrated-heat files and Origin projects without an original time/power trace skip baseline correction and peak integration; begin with experiment details and fitting.

1. Open your data

Launch FT-ITC Analysis and choose **Open File...** on the welcome screen, choose **File > Open...**, or drag compatible files into the application window. Select your file and confirm the open operation.

The experiment appears in the data list. Select it and open **Overview** to orient yourself in the imported experiment. Drag any non-button area of a data or result row to change its position. This order is used throughout the application and is retained when the project is saved as `.ftxtc`.

2. Edit experiment details

Open **Details...** for the selected experiment. Concentration entries and the experiment date/time can be changed here when needed. Comments and attributes relevant to later analysis can also be added or edited. A changed date is marked as user-modified in the experiment overview.

Apply corrections only when you have an independent experimental basis. Concentration entries influence the calculated concentration ratio and fitted parameters.

3. Process a raw thermogram

If the import contains a thermogram, open **Process Data**.

1. If the trace shows a smooth global drift, try **Polynomial** baseline. For more complicated baseline shapes, choose **Spline**; for local baseline behavior, choose **Segmented**. Keep the default integration settings initially.

2. Inspect whether the baseline represents the signal between injections rather than the peaks.
3. Inspect the start and end of every integration region. A region should include the injection response without extending unnecessarily into baseline noise. Zoom to a peak and adjust the integration end point. Use **Space** to copy the integration length to the next injection; the start is also copied when **Copy start time to next** is enabled.

These baseline alternatives are explained in Processing.

> **INTERPRETATION:**
> A visually smooth baseline is generally desired. As a rough rule of thumb, aim for about 20% of the data points to be baseline data; this is guidance, not a hard threshold. Apparent jumps in the baseline may indicate insufficient equilibration time between injections. Major spikes may require advanced baseline editing; the **Spline** baseline type provides more flexibility.

4. Fit one set of sites

Open **Analyze Data**, choose **Single experiment**, and select **One-Set-Of-Sites**.

1. Review the initial parameter values. Use physically plausible orders of magnitude for affinity, enthalpy, and stoichiometry.
2. Choose an optimizer. **Levenberg-Marquardt** is efficient near a suitable solution; **Nelder-Mead** can be useful when the starting surface is less cooperative.
3. Optionally enable **Weight by injection error** when the integration uncertainties are meaningful for the dataset.
4. Choose **None**, **Bootstrap residuals**, **Leave-one-out**, or **Profile likelihood** for error estimation.
5. Choose **Run Fit**.

Create analysis result determines whether a usable fit also creates a separate Analysis Result. Enable it to continue through the result workspace in the next step; otherwise, the fitted solution remains attached to the Experiment Data.

If the fit fails or reaches a limit, the possible causes are described under Fit availability and non-convergence.

5. Review the result

Inspect the fitted curve together with the residuals. When **Create analysis result** is enabled, select the resulting **Analysis Result** and check:

- the included experiment and injections;
- fitted parameter values and units;
- convergence and fit loss;
- whether weighting and uncertainty estimation match your intention;
- parameter uncertainty or confidence intervals, when calculated;
- result validity.

When **Create analysis result** is disabled, the fitted solution remains available in **Analyze Data** rather than as a stored Analysis Result.

> **INTERPRETATION:**
> Parameter precision does not establish model adequacy. Look for structured residuals, sensitivity to initial values, values at limits, excessive parameter correlation, or disagreement with known stoichiometry and experimental conditions.

6. Save a portable project

Choose **File > Save As...** and save the project as `.ftxtc`. The project contains imported data, experiment details, processing state, fits, results, and available advanced-analysis output. Keep the original instrument files as source records even though the project is portable.

If autosave is enabled, it supplements normal saving; it is not a replacement for a named project file.

7. Export a figure

Return to the experiment and open **Final Figure**. Choose the elements you need, such as the thermogram, integrated heats, fitted curve, residuals, confidence band, or parameter information. Review axis ranges and labels, then use the figure export or print command provided by the view.

Use **Analysis Result Exporter...** when you need numerical result tables rather than a graphic. For injection-level heats, choose **File > Export Integrated Peaks...**. The same output is available through **File > Export Data...** by choosing **Integrated Peaks**.

The figure and table workflows continue in Figures and export.

CHAPTER 03

Installation, files, and projects

Install FT-ITC Analysis, open supported data, save portable projects, and use autosave or recovery safely.

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Install the application

Use the latest FT-ITC Analysis release for current packages and release notes. Verify that the file came from the project release channel before accepting an operating-system security prompt. The examples below describe package types available at this manual's verification date and may change between releases. Installation problems can be reported through the GitHub issue tracker.

macOS

Open the DMG, drag **FT-ITC Analysis** to **Applications**, and eject the disk image. If macOS blocks a verified download, review it in **System Settings > Privacy & Security** and use **Open Anyway** only after confirming its source.

Windows

Run the supplied Windows x64 `.exe` installer and follow the setup prompts. The installer registers `.ftxtc` project associations. If Windows displays an **Unknown publisher** or Microsoft Defender SmartScreen warning, continue only after confirming that the installer came from the project repository.

Linux

Install the supplied `.deb` package matching the system architecture (AMD64 or ARM64, when available) on a compatible Debian-based distribution. Package trust and dependency behavior depend on the channel through which the package was obtained. Review the current release notes for known platform limitations.

> **PLATFORM NOTE:**
> Package installation and file-association prompts are controlled by the operating system. The analysis workflow is otherwise shared; the manual notes the few interface labels that differ between desktop editions.

Supported input formats

EXTENSION	SOURCE	IMPORTED CONTENT
`.itc`	MicroCal-style raw data	Raw thermogram and injections
`.nitc`	TA Instruments NanoITC native data	Raw thermogram and injections
`.ta`	TA Instruments/NanoAnalyze export	Raw thermogram and injections
`.apj`	PEAQ-ITC project	Raw thermogram and injections from the first experiment
`.opj`	Origin project file	Raw thermogram or integrated heats, according to the recognized worksheet
`.dat`	Integrated-heats table	Integrated heats and injections
`.aff`	Integrated-heats table	Integrated heats and injections
`.dh`	Fixed-layout integrated-heats file	Integrated heats, injections, and experiment metadata
`.ftxtc`	Current FT-ITC project	Stored project state

NanoAnalyze `.ta` files are raw thermogram exports. FT-ITC Analysis restores their time/power data and injection information as unprocessed Experiment Data.

PEAQ-ITC `.apj` projects contain a raw thermogram as well as injection and analysis information. FT-ITC Analysis imports the raw thermogram and injection information from the first experiment in the project. Integrated heats, processing choices, and fitted results produced by PEAQ are not imported; process and fit the restored raw data in FT-ITC Analysis.

Native NanoITC `.nitc` imports restore the raw thermogram, injection schedule, concentrations, cell volume, temperature and stirring information, and available source provenance. They open as unprocessed Experiment Data and follow the normal thermogram-processing workflow.

Origin `.opj` files are general project containers. FT-ITC Analysis searches them for the first recognized ITC worksheet and can restore either its original time/power trace or its integrated heats. When a raw trace is available, it is imported as an unprocessed thermogram and is authoritative even if the worksheet also contains integrated heats. If no usable trace is present, the worksheet heat values are used as integrated input and **Process Data** is skipped. ResultsLog text is retained in the experiment comments as provenance. Origin baseline processing, fitted models, and Fit/DY columns are not imported or converted into native FT-ITC fits. Newer `.opju` files are not supported.

Delimited `.dat` and `.aff` inputs must provide positive `INJV` injection volumes and at least one usable heat column. FT-ITC Analysis prefers a complete `DH` column as absolute injection heat. If `DH` is absent or incomplete, it accepts a complete `NDH` column as normalized heat per mole; `NDH` may be absent for the automatically excluded first injection. The separate `.dh` format uses a fixed metadata-and-injection layout rather than the delimited `.dat` / `.aff` column contract.

These files do not encode an unambiguous heat unit. For `DH`, select the absolute-energy unit used by that column. For an `NDH`-based import, select the energy numerator used by the per-mole values (for example, select **calorie** for cal/mol). The reader converts normalized heat to absolute injection heat using the syringe concentration and injection volume. If the syringe concentration cannot be inferred from `Xt` / `Mt`, it must be supplied before an NDH-based import can continue; canceling that prompt skips only the current file. Reuse the selected unit for the remaining files only when every file in that import operation uses the same heat unit and heat-column convention.

When available, the reader infers cell volume and syringe concentration from the energy-independent `Mt` / `Xt` concentration trajectory using the selected dilution model. Each injection row stores the concentrations before that injection; an optional state-only final row stores the concentrations after the last injection. `Mt` and `Xt` are interpreted as mM in normal application

imports. If the trajectory is absent, malformed, or internally inconsistent, `DH` heat and injection-volume rows remain importable; an `NDH`-based import first requires a syringe concentration, and validation asks for any other unresolved metadata instead of silently guessing it. These formats contain no thermogram, so importing them cannot reconstruct a baseline or processing-derived injection uncertainties.

Open files

Choose **File > Open...**, use the welcome-screen action, or drag files into the application. Multiple supported files can be opened together. Files opened into a populated document are added to its existing Data / Results list; this includes current `.ftxtc` projects. Clear the current document first when a current project should be opened by itself.

> **CAUTION:**
> After a current `.ftxtc` project is added to an existing document, that opened project becomes the document's current save destination. Use **Save As...** before saving if you do not intend to replace it with the combined document.

> **CAUTION:**
> Appending can create similarly named experiments or results. Confirm the data list and details before fitting or exporting.

Save projects

Choose **File > Save** to update a named current project, or **File > Save As...** to choose a new name or location. Use the current `.ftxtc` format for ongoing work.

An `.ftxtc` project preserves the data and metadata needed to continue analysis, including thermograms where imported, concentrations and uncertainties, attributes and comments, injection inclusion, processing state, fit solutions, Analysis Results, and completed derived analyses. The package is portable and does not depend on the original raw-file path for ordinary reopening.

Save Selected... writes selected project content when you need a smaller handoff. Confirm the selection before saving and reopen the result if the subset is critical. Saving the selected experiments saves only the experiment with any solution. Saving the selected Analysis Results saves the result along with the involved experiments.

> **RECOMMENDATION:**
> Save a processed version of the project before fitting if you want a reusable starting point. After fitting, save the project again—under a new name if you want to preserve the processed-only version—to retain the fitted solutions and Analysis Results.

Autosave and recovery

Autosave behavior is configured in **Preferences...**. When recovery data is available after an interrupted session, the application offers a recovery path. Open the recovered document, inspect the data list and recent changes, then save it under a deliberate `.ftxtc` name.

Recovery mode is designed to salvage valid project components when possible. If an experiment is unavailable, its saved fit is omitted; Analysis Results that depend on that fit are also omitted rather than being restored with a scientifically different set of members. Unaffected experiments, fits, and results can still be recovered. When recovery was required, the application displays a warning and records the individual recovery issues in the application log. A recovered project can be detached from its former save location and marked as changed. Use **Save As...** rather than assuming the damaged or interrupted file was repaired in place.

> **CAUTION:**
> Recovery cannot guarantee that every optional result or cached component survived. Confirm experiment counts, processing, fits, and result validity before continuing.

Remove and clear content

Removing an experiment or Analysis Result changes only the open document; it does not delete the original raw file. **Remove All Data/Results** clears the current document after confirmation. **Clear Processing/Results** removes all Analysis Results from the open document.

Saving after removal makes the removal part of the saved project. Use **Save As…** first if you want to preserve the original project version.

Privacy and online checks

Analysis and the surrounding workflow—including saving, recovery, export, and printing—run locally. The application has no online analysis features. If **Check for updates and online resources on launch** is enabled, it retrieves GitHub release metadata and the repository's citation metadata file; it does not upload experiment data. Disable the setting when launch-time network access is undesirable. A failed or disabled check does not prevent local processing, fitting, or saving.

Update safely

Before installing a new application version, save important projects and retain the current installer when reproducibility policy requires it. After updating, open a copy of a representative project, confirm processing and results, and save only when you intend the project to be written by the new version.

CHAPTER 04

Workspace

The application window, Experiment Data capabilities, and Analysis Result capabilities.

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Application window

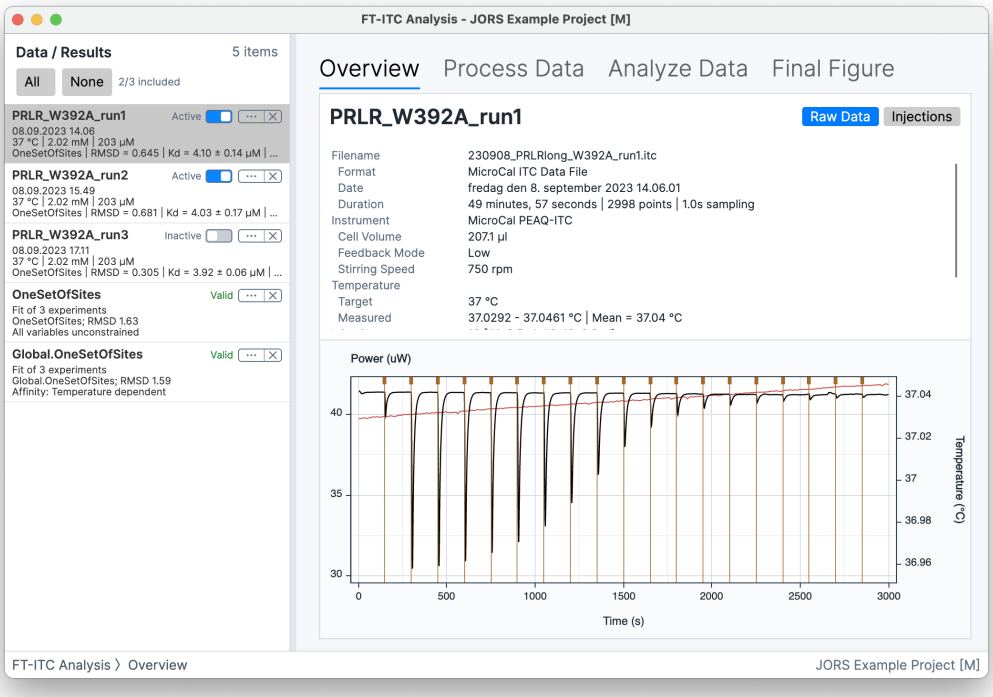
The **Data / Results** list is the project navigator. It contains two types of project item: Experiment Data and completed Analysis Results. Selecting an item shows it in the workspace; selection does not change whether an experiment is Active.

Only Experiment Data has an **Active** toggle. Active experiments participate in operations that use a group of datasets, such as multiple-experiment fitting, processing propagation, and coordinated export. The toggle becomes available after the experiment has been processed. **Enable All**, **Disable All**, and **Invert Active** change several experiments, while the sorting commands change the list order. Multiple-experiment fitting is described in Multiple-experiment fitting, and the processing prerequisite is covered in Processing.

The rest of the window follows the selected item and task:

- The workflow navigator switches between the available stages of an experiment.
- The workspace contains the graphs, tables, and controls for the current task.
- Workflow controls provide options for the view or analysis currently open.
- Item actions apply to the selected Experiment Data or Analysis Result.
- The application menu contains project commands, tools, preferences, and help.

Experiment Data



Selecting Experiment Data opens its experiment workflow in the shared workspace.

Experiment Data represents an imported or application-created dataset. Its list entry provides identifying information and a summary of its processing or fitted state.

Experiment workflow

Four task views are available for Experiment Data:

- **Overview** presents the imported data and available experiment information.
- **Process Data** turns a raw thermogram into integrated heats through baseline modeling and injection-region control.
- **Analyze Data** configures and runs single- or multiple-experiment fitting.
- **Final Figure** prepares the thermogram, integrated heats, fit, residuals, and annotations for presentation.

Details and attributes

The **Details…** view contains editable concentrations, comments, and experiment attributes. The macOS sheet has separate **Details** and **Attributes** tabs: Details contains the experiment name, date/time, conditions, concentrations, and comments; Attributes contains optional metadata. Attributes describe conditions and analysis inputs such as buffer, salt, ionic strength, competitor, or prebound species.

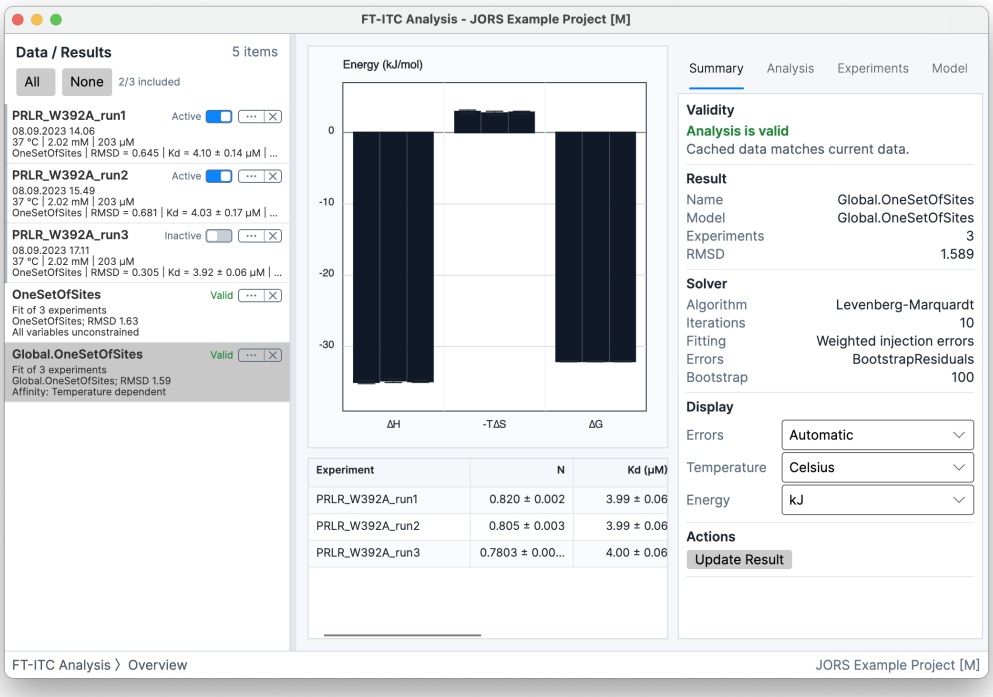
> **PLATFORM NOTE (MACOS):**
> Edit the date and time using separate native controls, including seconds. Use **Add Attribute** on the Attributes tab to add a row. Each tab scrolls independently while **Cancel** and **Apply** remain visible at the bottom. Cancel discards edits; Apply saves them.

Attribute Operations… copies either one attribute or all attributes from the selected Experiment Data to **All other experiments**, **Active experiments**, a **Specific experiment**, or **Experiment names containing…**. The name option targets every other experiment whose name contains the entered text, without regard to capitalization.

Experiment Data actions

- **Details…** opens the editable experiment information and attributes.
- **Duplicate Data** creates another project item from the selected Experiment Data.
- **Export Selected Data…** exports the selected dataset.
- **Clear Solution** removes the fitted solution currently attached to the Experiment Data.
- **Remove Data** removes the item from the open project without deleting its source file.

Analysis Result



An Analysis Result opens its dedicated result workspace when selected.

An Analysis Result stores a fit for one or more experiments together with its model, constraints, fitting settings, uncertainty output, and member solutions. Its list entry summarizes the stored fit.

Result workspace

The result workspace provides these views:

- **Summary** compares fitted and derived parameters across the result and provides its member table.
- **Fit** shows the stored fitted curve and residuals for a selected member experiment.
- **Correlation** shows parameter correlations calculated from residual-bootstrap refits when sufficient bootstrap information is available.
- **Temperature**, **Salt**, and **Protonation** appear when the result and its experiment information support those analyses.

The inspector organizes result information under **Summary**, **Analysis**, **Experiments**, and **Model**. See Results and advanced analyses for interpretation and prerequisites.

Analysis Result actions

Changes to the fit-relevant state of Experiment Data stored in an Analysis Result can invalidate the result. The validity indicator shows whether the stored result still matches the current data.

- **Details…** edits the result name and comments.
- **Copy Result Table** copies the current result table; **Analysis Result Exporter…** provides controlled table export.
- **Update Result** reruns the stored model and fitting settings using the current member experiments and replaces the result only after a successful fit. For a residual-bootstrap result, the update dialog keeps the stored bootstrap count by default and offers larger supported iteration presets. Changing that count affects only this rerun; the stored parameter limits and other fitting settings remain unchanged.
- **Set Active Experiments** makes the result's member experiments Active.
- **Load Solutions to Experiments** attaches the stored member solutions to their corresponding Experiment Data.
- **Export Associated Final Figures…** exports figures for the member experiments.
- **Remove Result** removes the Analysis Result from the open project.

Separate tools

The **Tools** menu opens separate windows for tasks outside the main experiment and result workflows. These include **Experiment Designer…**, **Buffer Subtraction…**, and **Experiment Merger…**. Their features are described in Tools.

CHAPTER 05

Processing

Baseline models, integration regions, injection uncertainty, and processing propagation and locking.

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The **Process Data** workspace estimates and subtracts a baseline from the differential-power trace, integrates the corrected response for each injection, and estimates an uncertainty for the resulting heat. Polynomial and Segmented baselines provide repeatable, model-based treatment with less manual shaping when their assumptions suit the trace. Spline-point editing provides precise local control for difficult cases, while graphical boundary editing, **Fit Peaks**, and copying between injections accelerate integration-region adjustment.

These controls make processing efficient without deciding the scientific interpretation for you. Confirm that the chosen baseline represents the signal between injections and that each integration region captures the observed response.

Raw `.itc`, `.nitc`, `.ta`, and `.apj` imports use this workflow, as do Origin `.opj` imports that contain a usable time/power trace. Integrated-heat imports and Origin projects without a usable trace skip **Process Data**.

CALCULATION:

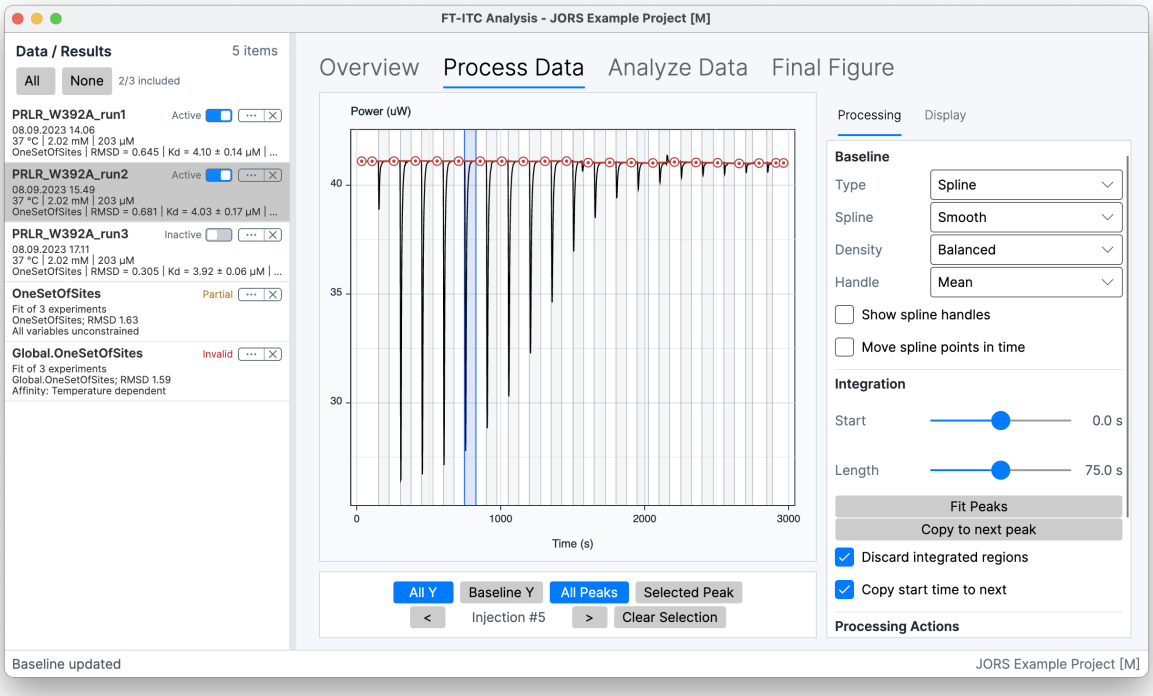
$$q_{i,\mathrm{raw}} = \int [P(t) - b(t)]\,\mathrm{d}t$$

$$\Delta H_i = \frac{q_i}{n_i}$$

$$n_i = c_{\mathrm{syr}} V_i$$

The integral is evaluated between the injection's integration boundaries. Each recorded power value represents the trailing-period average ending at its timestamp, so fractional intervals at either selected boundary are included using the appropriate right-endpoint sample. $P(t)$ is differential power, $b(t)$ is the estimated baseline, and $q_{i,\mathrm{raw}}$ is the raw integrated heat. The heat q_i equals that raw value unless optional buffer subtraction changes it. c_{syr} is the syringe concentration, V_i is the injection volume, n_i is the injected amount, and ΔH_i is the molar heat.

Processing workspace



Process Data combines the thermogram with baseline, integration, display, and navigation controls.

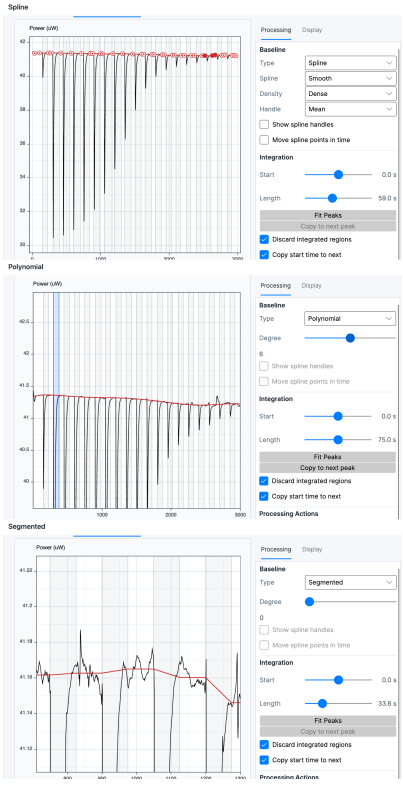
The **Processing** controls configure the baseline and integration regions. The **Display** controls show or hide the baseline, integration regions, corrected data, and cursor information.

With **All injections** selected, **Start** and **Length** apply to every injection. A selected graph region targets one injection, and double-clicking it focuses the graph on that peak. The previous and next controls move through the injections; **Clear Selection** returns to all injections.

The view controls separate horizontal and vertical scaling:

- **All Y** shows the complete power range, while **Baseline Y** emphasizes the baseline region.
- **All Peaks** shows the full injection series, while **Selected Peak** focuses on the current injection.
- Dragging an empty part of the graph zooms into the selected region.

Baseline models and editing



Spline, Polynomial, and Segmented provide different baseline representations for thermogram processing.

Spline

Spline places points in usable baseline regions and interpolates between them. It provides the most direct graphical control.

- **Linear** connects the spline points with straight sections. **Smooth** produces a continuously varying baseline and supports editable slope handles.
- **Sparse**, **Balanced**, and **Dense** change the number of automatically generated points.
- **Mean**, **Median**, and **Min volatility** determine the representative power used for an automatically generated point.
- **Show spline handles** displays the slope handles for a Smooth spline. **Move spline points in time** allows a point to be dragged horizontally as well as vertically.

Dragging a point corrects its position. A secondary-click on the graph adds a point **At Data** or **At Baseline**. A secondary-click on an existing point exposes **Lock** or **Unlock**, **Mark Linear** or **Unmark Linear**, and **Remove**. Marking neighboring points as linear makes the interval between them straight. Locked points are retained when automatic spline points are regenerated.

Balanced provides the middle spline-point density. Greater density increases local flexibility but can also follow noise or absorb part of an injection response.

Polynomial

Polynomial fits one polynomial across the complete thermogram and is suited to smooth global drift. **Degree** controls flexibility.

Polynomial behavior is least constrained at the beginning and end of the run, where a high degree can produce strong edge behavior. Additional degree increases flexibility whether it represents baseline drift or follows more of the trace.

Segmented

Segmented fits local constant, linear, or quadratic baseline behavior between integration regions and blends the local estimates across the run. It is suited to locally changing drift for which one global polynomial is too rigid. **Degree** selects the local behavior.

Local flexibility can follow genuine drift, but it also makes the result more dependent on the integration boundaries and on the baseline immediately around each peak.

Exclude integration regions from the baseline

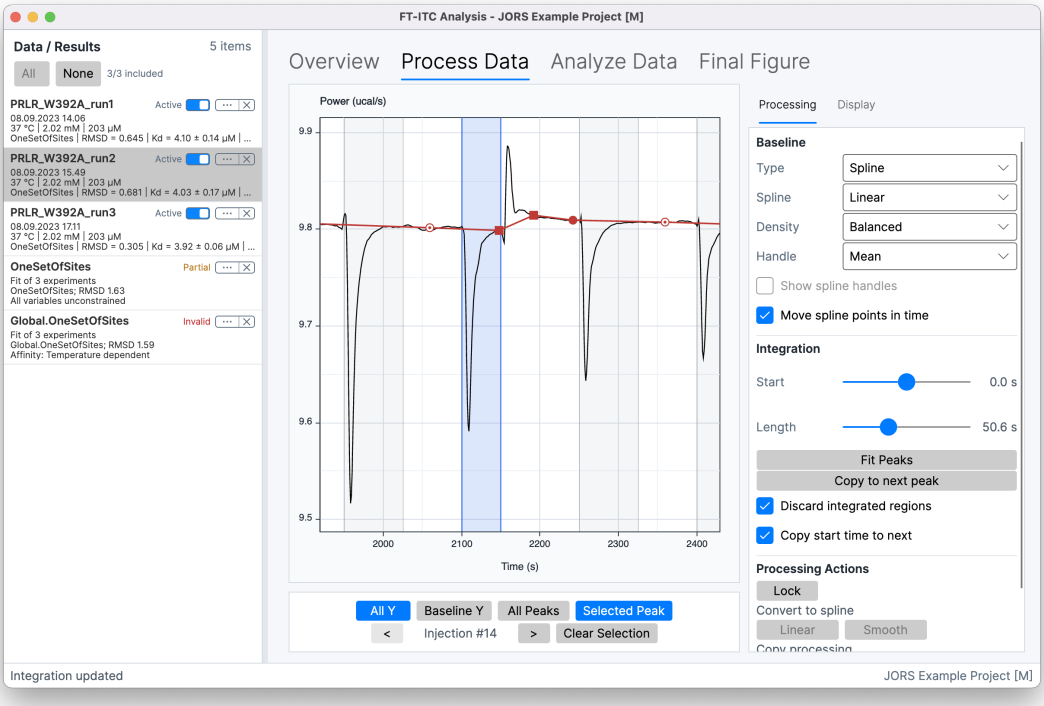
When **Discard integrated regions** is enabled, data inside the current integration regions are excluded when the baseline is recalculated. Moving a boundary can therefore change both the integrated area and the estimated baseline.

> **CAUTION:**
> Boundaries should follow the observed response and a consistent processing rule, not the heat expected from a model.

Convert to a spline

A Polynomial or Segmented baseline can be converted to a **Smooth** or **Linear** Spline when the automatic baseline is a useful starting point for graphical editing. Conversion changes the baseline representation and creates editable spline points.

Integration regions



Selecting an injection exposes its individual boundaries and navigation controls.

Each injection region has a start and an end boundary. **Start** sets the offset of the start boundary relative to the injection. The value displayed as **Length** positions the end boundary that many seconds after the injection begins; it is not a separate processing mode.

Either boundary can be dragged in the graph or adjusted with the controls. The application constrains the start and end to a valid interval within the injection scope and preserves a minimum separation between them.

Estimate end points with Fit Peaks

Fit Peaks estimates the end point of each injection from the decay of the baseline-corrected response. It changes the end boundaries and then integrates the resulting regions; it does not fit the integrated heats or select a persistent integration mode.

When peak fitting converges, the estimated boundaries replace the previous end points. If fitting fails or does not converge, the previous regions remain unchanged. Peak kinetics can vary across the titration, and the first injection can behave differently from the remaining series.

Copy a region to the next injection

Selecting an injection and choosing **Copy to next peak**, or pressing **Space**, copies its end boundary and advances to the next injection. **Copy start time to next** includes the start boundary in that operation.

Injection uncertainty

Each injection error bar represents an estimated ±1 standard deviation for that injection's molar heat. The estimate describes how local noise in the baseline-corrected thermogram propagates through the selected integration region. It is calculated independently for every injection, so the bars can vary across a titration.

The calculation uses baseline-corrected samples around the injection. It combines an estimate of local power noise with the temporal correlation between neighboring samples, the integration-region length, and uncertainty in the baseline level. A longer or noisier region will therefore often have a larger estimated uncertainty. When Buffer Subtraction is applied, the independent target and reference heat uncertainties are combined.

> **CAUTION:**
> At least two surrounding baseline samples and two samples inside the integration region are required. When the estimate cannot be calculated, the application stores zero. Integrated-heat imports also lack a thermogram from which to estimate this uncertainty. A zero or absent error bar can therefore mean that no processing-derived estimate is available; it does not establish that the injection has no uncertainty.

The bars do not include uncertainty in cell or syringe concentration, fitted parameters, or model-derived confidence bands. They also do not quantify baseline-model choice, integration-boundary choice, calibration error, other instrumental effects, or other systematic uncertainty. Consequently, they do not validate the selected processing or constitute confidence intervals for the true heat.

Weight by injection error can use these estimates in the fitting objective. Concentration uncertainty is handled separately in supported resampling calculations. Both behaviors are described under Fitting calculation.

Propagate and lock processing

Active under **Copy processing** copies the selected experiment's processing to the other Active experiments. This can replace existing processing when a destination is unlocked. **New** targets experiments that do not yet have processing.

Processing can be propagated while the source is unlocked. Locked destinations are not overwritten. After propagation, each processor that should be protected can be selected and set to **Lock**. Locking disables baseline, spline-point, integration-region, and peak-fitting edits; **Unlock** makes changes available again.

CHAPTER 06

Single-experiment fitting

Fit one experiment, configure model and uncertainty options, control injection inclusion, and interpret fit diagnostics.

Last verified: 2026-08-26

Analyze Data in **Single experiment** mode fits the integrated heats of the selected Experiment Data. The fit uses the included injections together with the experiment concentrations, injection volumes, cell volume, temperature, and any model-specific information.

The inspector has four tabs:

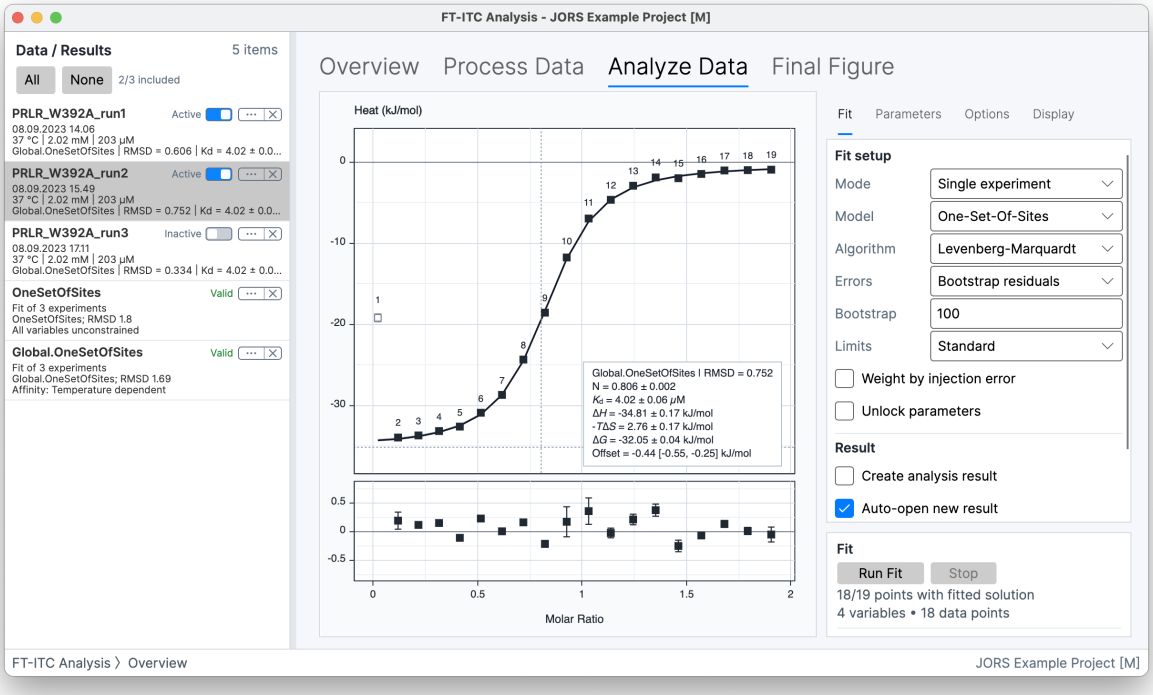
- **Fit** selects the model, optimizer, error-estimation method, limits, weighting, and result output.
- **Parameters** shows the model parameters and their starting or fixed values.
- **Options** contains settings specific to the selected model.
- **Display** controls the fitted curve and diagnostic information shown in the graph.

Profile-likelihood uncertainty

Profile likelihood is a fixed-95% uncertainty method. After a successful primary fit, one fitted coordinate at a time is fixed while nuisance coordinates are refit. Unweighted fits use an F-calibrated RSS interval assuming independent Gaussian residuals; weighted fits use a one-degree-of-freedom chi-square increment conditional on the supplied peak-area SDs. The primary fit remains the reported value.

Integration graphs can display the envelope from available leave-one-out refits (typically a small ensemble); profile likelihood creates no refit ensemble or confidence band.

An endpoint is reported only when both sides cross the threshold. Reaching a parameter limit is computational censoring, not a confidence endpoint, so that side remains unavailable. The displayed `value ± SD` uses an explicitly equivalent symmetric scale computed from the asymmetric profile interval; it is not a Gaussian sample standard deviation. Save profile results as FTXTC to preserve the profile run diagnostics.

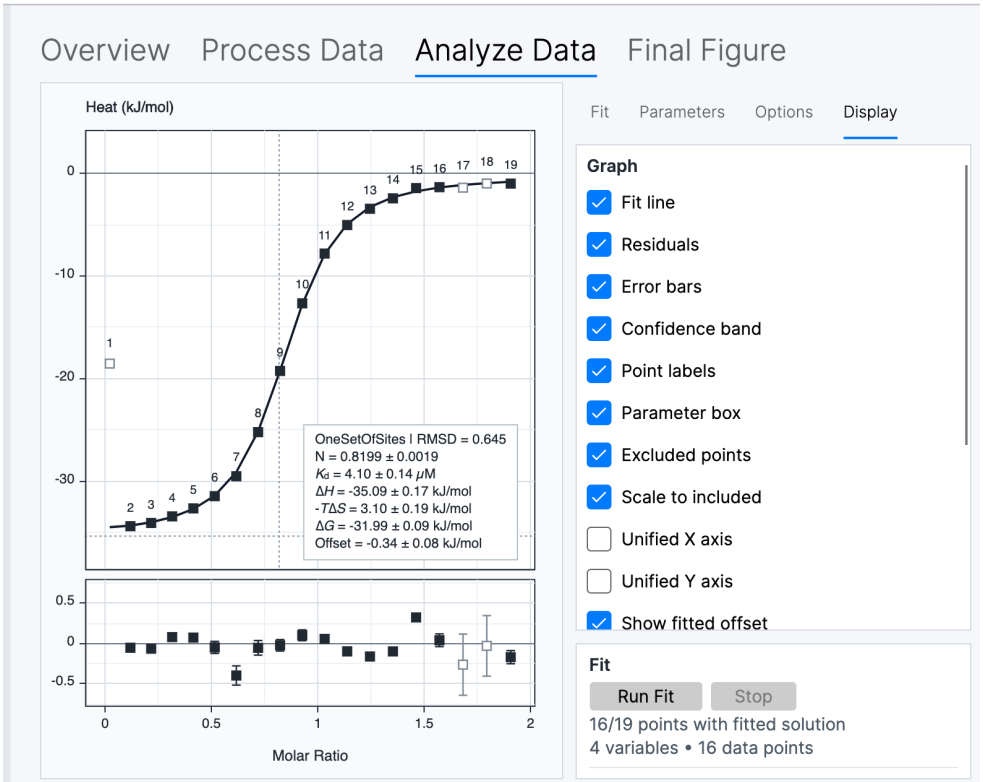


Analyze Data combines the fitted-heats graph and residuals with the controls for configuring and running the fit.

Multiple-experiment fitting uses additional experiment selection and parameter constraints; see Multiple-experiment fitting.

Injection inclusion

Selecting an injection point in the integrated-heats graph changes whether it is included in the fit. Excluded injections do not contribute to the objective function. The **Excluded points** option in **Display** keeps excluded injections visible and available for selection.



Excluded injections remain visible when Excluded points is enabled and can be selected for inclusion again.

Changing injection inclusion does not rerun the fit. The fitted curve and parameters continue to represent the previous fit until **Run Fit** is used again. An inclusion change can also invalidate an Analysis Result that contains the experiment.

Models

One-Set-Of-Sites

One-Set-Of-Sites represents one class of equivalent, independent binding sites. It fits stoichiometry, dissociation constant, binding enthalpy, and an injection-heat offset. The solution also reports thermodynamic quantities derived from the fitted affinity and enthalpy.

The **Options** tab provides **Use Syringe Correction** and **Stoichiometry**. Without syringe correction, the fitted N-value represents the apparent site stoichiometry. With syringe correction enabled, **Stoichiometry** fixes the number of cell-side sites and the fitted N parameter becomes the active syringe-concentration factor `alpha`.

The model cannot by itself distinguish a concentration error from other effects that change an apparent stoichiometry.

Two-Sets-Of-Sites

Two-Sets-Of-Sites represents two independent classes of sites. It fits separate stoichiometries, dissociation constants, and enthalpies for the two classes, together with a shared injection-heat offset.

Shared N-Values makes the two site classes use the same fitted stoichiometry. **Use Syringe Correction** instead fixes the first and second **Stoichiometry** values and fits one active syringe-concentration factor, `alpha`.

The two site labels are interchangeable: exchanging all parameters assigned to site 1 and site 2 describes the same physical model. A lower fitting loss alone does not establish that two distinguishable binding processes are supported by the experiment.

Sequential Binding Sites

Sequential Binding Sites represents two, three, or four ordered binding steps on a macromolecule in the cell. **Sequential binding steps** in the **Options** tab selects the fixed integral step count. The model fits one macroscopic stepwise association constant and one molar step enthalpy for each transition, together with the ordinary molar injection-heat offset. It does not fit an N-value or syringe activity.

For step count n, let $\beta_0 = 1$, $\beta_i = \prod_{j=1\ldots i} K_j$, and let x be free ligand. The state weights and fractions are

CALCULATION:

$$w_i = \beta_i x^i$$

$$F_i = \frac{w_i}{\sum_{j=0}^{n} w_j}$$

$$\overline{\nu} = \sum_{i=0}^{n} i F_i$$

$$X_t = x + M_t \overline{\nu}$$

Here M_t and X_t are total macromolecule and ligand concentrations in the cell. The model solves the ligand balance internally and calculates the cell heat content from the population of every sequential state:

CALCULATION:

$$Q = VM_t \sum_{i=1}^{n} F_i \left(\sum_{j=1}^{i} \Delta H_j \right)$$

The reported K_i values are phenomenological, macroscopic step constants for the ordered transitions $M \rightarrow MX \rightarrow MX_2$ and so on. They are not microscopic intrinsic site constants. Step numbers therefore have physical order and fitted steps are never sorted or treated as exchangeable.

The macromolecule must be in the cell and ligand in the syringe. Reverse titrations with macromolecule in the syringe are outside this model. Multi-step fits can be weakly identifiable, especially when the concentration window does not populate every transition. Inspect parameter bounds, residuals, bootstrap uncertainty, and parameter correlations; an improved RMSD does not by itself establish the selected number of sequential steps.

Competitive Binding

Competitive Binding represents titration of a target ligand into a macromolecule that is initially in equilibrium with a prebound ligand in the cell. It fits the target ligand's stoichiometry, dissociation constant, binding enthalpy, and injection-heat offset.

The **Options** tab requires the prebound ligand **[Ligand]**, **Ligand Affinity**, and **Ligand Enthalpy**. **From attributes** makes **[Ligand]** use the corresponding value stored in the Experiment Data attributes instead of the value entered in the model options. The model also provides **Use Syringe Correction** and **Stoichiometry** with the same concentration-factor interpretation as One-Set-Of-Sites.

The fitted target affinity and enthalpy depend on the supplied prebound-ligand properties. Those values are model inputs rather than quantities independently determined by the competitive fit.

Dissociation

Dissociation represents dilution-driven monomer-dimer self-association. The syringe contains the macromolecule and the cell initially contains buffer. Dilution and mixing change the dimer population, and the model fits the association equilibrium through its reported dissociation constant, the association enthalpy per mole of dimer formed, and an injection-heat offset.

CALCULATION:

$$2M \rightleftharpoons D$$

$$K_a = \frac{[D]}{[M]^2}$$

Here, [*M*] and [*D*] are the monomer and dimer concentrations, and K_a is the association constant.

This is not a general model for dissociation of an arbitrary preformed complex or for other oligomerization schemes. It has no stoichiometry or syringe-correction options.

Thermodynamic relationships

The application derives thermodynamic quantities from the fitted affinity and enthalpy. Temperature *T* is expressed in kelvin.

CALCULATION:

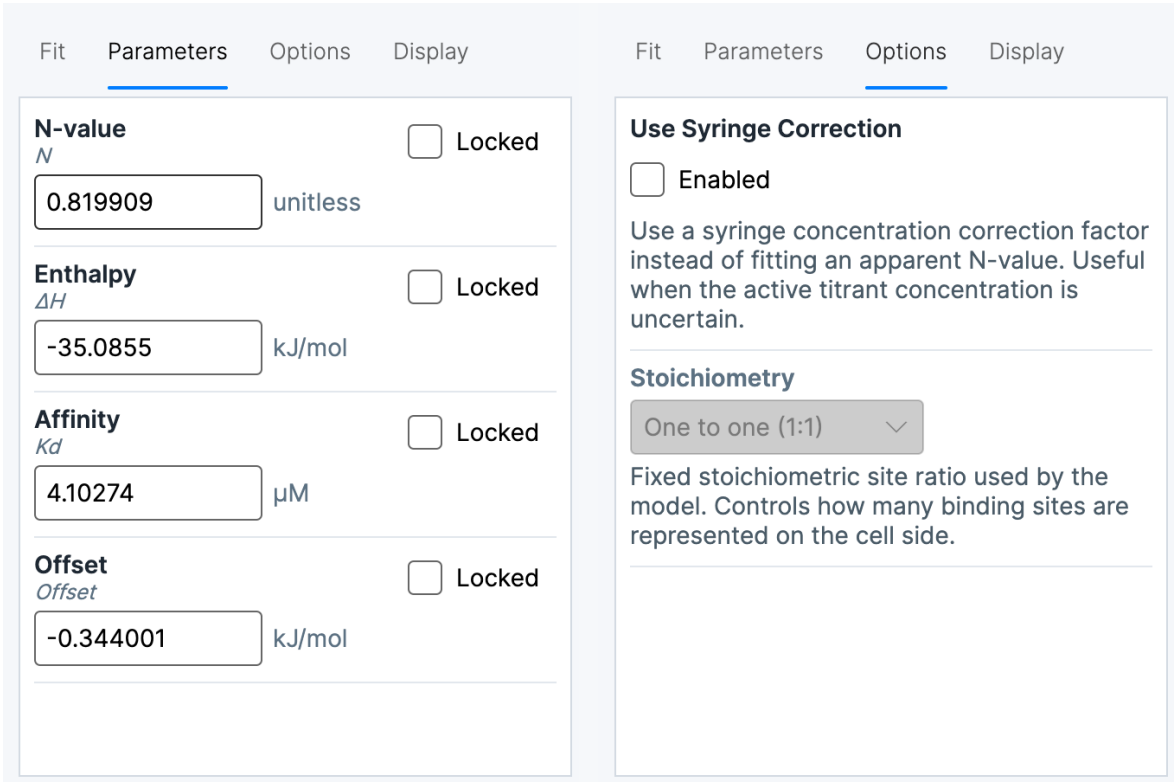
$$K_d = 1/K_a$$

$$\Delta G = RT\ln(K_d) = -RT\ln(K_a)$$

$$-T\Delta S = \Delta G - \Delta H$$

Here, *R* is the gas constant, and the final relationship matches the **–TΔS** quantity reported by the application.

Parameters and model options



Parameters exposes parameter values and locks; Options contains settings specific to the selected model.

The application generates initial parameter values from the experiment and can reuse an attached fitted solution where applicable. Entering a value replaces the generated starting value for that parameter. Values are displayed in the current application units. Clearing a value returns the parameter to automatic initialization.

Locked holds a parameter at its displayed value during the primary fit. An unlocked parameter is adjusted by the optimizer. Locked values remain part of the model and affect every other fitted parameter even though they are not estimated by that fit.

Analysis choices are retained separately for the available fitting modes and models. **Restore defaults** clears the stored analysis inputs and reloads the live inspector fitting controls from the current Preferences. It also resets inspector-only parameter unlocking. The action does not change Preferences or preference-backed limits, result-output, and display settings.

The **Limits** control selects a common parameter-bound policy:

- **Standard** uses the normal parameter bounds.
- **Expanded** permits a wider parameter range.

- **No limits** removes the configured parameter bounds.

A fitted value at a bound is not an interior estimate. It indicates that the reported value depends on the selected bound as well as on the data and model.

Before a fit starts, the application checks every free starting parameter against the currently selected limits. This includes values entered manually, values reused from an attached solution, and automatic values that become stale after the **Limits** policy changes. Bounds are inclusive, so a value exactly at a bound is allowed. Locked and globally determined parameters are not checked because they are not optimizer coordinates. An out-of-range value is marked in the **Parameters** inspector and **Run Fit** remains available so it can be corrected. The fit is blocked with a list of affected parameters; edit the value, clear it to restore the automatic default, or widen **Limits**. In a global fit, a local parameter that has no exposed global editor is identified by its experiment name in the fit status area; edit that experiment in single-experiment mode if needed.

Fitting calculation

Algorithm

Levenberg-Marquardt uses local derivative information and can be efficient when the starting values describe a suitable region of the fitting surface.

Nelder-Mead is a derivative-free simplex optimizer. It provides an alternative calculation for surfaces or starting conditions that are less cooperative for the local derivative-based method. Agreement between optimizers does not by itself establish that the selected model is scientifically adequate.

Weight by injection error

Weight by injection error uses the integration uncertainty estimated during thermogram processing when calculating the fitting objective. Injections with larger estimated uncertainty consequently have less influence than injections with smaller estimated uncertainty.

CALCULATION:

$$r_i = q_{i,\,\mathrm{obs}} - q_{i,\,\mathrm{model}}$$

$$\mathrm{RMSD} = \sqrt{\left[\frac{\Sigma\, r_i^{\,2}}{N}\right]}$$

$$\text{weighted objective} = \Sigma\left(r_i/\sigma_i\right)^2$$

Only included injections enter these sums. The value σ_i is the processing-derived uncertainty for injection *i*; weighting changes the fitting objective but does not remove systematic uncertainty.

The displayed RMSD is always calculated from the unweighted residuals, including after a weighted fit. It therefore remains distinct from the weighted objective minimized by the optimizer.

For a multiple-experiment result, the displayed global RMSD is pooled across every included injection in every member experiment. Each member row retains its own local RMSD, so the global value remains comparable when members contain different numbers of included injections.

If an included injection does not have a finite positive peak-area SD, the application uses the mean of the finite positive SD values from the other included injections. If none is available, it uses a small numerical fallback so the calculation remains defined. A substituted value prevents division by zero; it does not turn a missing processing estimate into a measured uncertainty.

The weighting describes the application's processing-derived uncertainty model. It does not account for every systematic source of experimental or processing uncertainty.

Parameter uncertainty

The **Errors** control determines whether the primary best fit is followed by repeated refitting:

- **None** retains the primary fit without resampling-based parameter uncertainty.
- **Bootstrap residuals** standardizes each included injection's primary-fit residual by the same effective peak-area SD described above, centers that standardized pool, samples independently with replacement, rescales each draw by the target injection's effective SD,

and adds it to the best-fit prediction. The synthetic injection retains the target injection's stored peak-area SD; when error weighting is enabled, the refit therefore uses the same per-injection weighting inputs and fallback rule.

- **Leave-one-out** performs one deterministic refit for each deletion: one refit per included injection in a single-experiment analysis, or one refit per omitted experiment in a globally fitted multiple-experiment analysis. Concentrations, uncertain model options, and parameter locks are held at their primary-fit values so the resulting spread isolates deletion sensitivity.
- **Profile likelihood** fixes each fitted coordinate in turn and refits nuisance coordinates against the conditional likelihood. It uses the local objective for independent members and the complete objective for shared global coordinates; complete asymmetric crossings are retained as endpoints, while a bound reached before crossing is reported as censoring.

Bootstrap sets the requested number of residual-bootstrap iterations. It is enabled and used only for residual bootstrap; leave-one-out and profile likelihood have deterministic schedules and do not use this count. Only included injections supply residuals, and only retained usable refits enter the parameter distributions. Because residual-bootstrap sampling is with replacement, one residual can occur more than once in a synthetic dataset while another may not occur at all. The fit status distinguishes successful and failed refits.

Correlation diagnostics distinguish attempted refits, optimizer-usable refits, and the listwise-complete refits whose displayed coordinates are all finite. A high failed-refit fraction can make the retained ensemble selective; increasing the requested count improves Monte Carlo resolution but does not correct a systematically failing refit process.

Each replicate uses a fresh independent random stream; seeds are not stored, so rerunning a bootstrap does not reproduce the same random sequence.

When **Update Result** is used on a stored residual-bootstrap Analysis Result, its dialog shows the retained usable-refit count and offers the stored behavior plus larger supported presets up to 10,000 requested iterations. The update performs a fresh complete fit and bootstrap; it does not append samples to the saved distribution. Cancelling the calculation or completing it without any usable bootstrap refits preserves the previous Analysis Result.

The primary best-fit parameter remains the reported value. For a parameter with best-fit value $\hat{\theta}$ and values θ_b from B retained refits, the application summarizes the bootstrap distribution as follows:

CALCULATION:

$$\mathrm{SD} = \sqrt{\frac{\sum_b \left(\theta_b - \widehat{\theta}\right)^2}{B}}$$

$$95\%\ \mathrm{CI} = \left[P_{2.5}(\{\theta_b\}), P_{97.5}(\{\theta_b\})\right]$$

SD is the root-mean-square deviation of the retained refits from the primary best fit. The confidence limits are the 2.5th and 97.5th percentiles of the retained refit distribution itself, so they need not be equally spaced around the best fit. Neither calculation replaces the best-fit value with the bootstrap mean or median.

The uncertainty display can show SD, the 95% confidence interval, both, or select between them automatically. This presentation rule is described under Uncertainty and evaluation temperature.

Concentration uncertainty

With **Concentration uncertainty** enabled in the **Fit** tab, the concentration SDs entered in **Details…** are propagated through residual-bootstrap calculations. The control is initialized from the corresponding preference and is active only for residual bootstrap; leave-one-out and profile likelihood keep primary concentrations fixed. Each nonzero fractional SD is the arithmetic standard deviation relative to the entered concentration. Synthetic clones draw a positive, mean-preserving lognormal multiplier: if the fractional SD is c, then $\sigma^2_{\log} = \ln(1 + c^2)$, $\mu_{\log} = -\sigma^2_{\log}/2$, and the multiplier is $\exp(\mu_{\log} + \sigma_{\log} Z)$ for a standard-normal Z. Thus the multiplier has mean 1 and SD c, so cloned concentrations remain positive while preserving the entered arithmetic mean and SD. Explicit cell or syringe SDs take precedence over the automatic value configured in Preferences. These uncertainties affect the synthetic experiment concentrations used for bootstrap refits, not the concentrations used for the primary best fit.

Displayed parameter uncertainty

The bootstrap summary is first calculated for each fitted parameter coordinate. The application then converts that summary into the quantity shown to the user. For example, affinity is fitted as $\log_{10}(K_a)$ but is normally displayed as K_d. The displayed central value comes from the primary best fit, SD is propagated through the transformation, and the percentile limits are transformed and reordered as required.

Quantities calculated from more than one reported parameter, such as $-T\Delta S$, use the application's uncertainty-propagation rules for that calculation. Their displayed limits are therefore not necessarily the percentiles that would be obtained by recalculating the complete derived quantity independently for every bootstrap refit. The **Automatic** SD-or-CI decision is applied after transformation or propagation, separately for each displayed quantity.

Unlock parameters during error estimation

Locked parameters remain fixed during the primary fit. With **Unlock parameters** enabled, copies of those parameters are unlocked only for residual-bootstrap refits and can vary in the resampled solutions. Leave-one-out and profile likelihood always preserve the primary-fit locks.

This setting does not change or rerun the primary best fit. It changes only the parameter state used by the repeated error-estimation fits, and it has no effect when no fitted parameter is locked.

Fit execution and diagnostics

Run Fit starts the primary optimization and the selected error-estimation calculation. **Stop** requests cancellation of the active calculation. When fitting ends, the status reports the termination state, RMSD, iteration count, and elapsed time. A resampling calculation also reports its outcome and the number of successful and failed refits.

The **Display** tab exposes complementary diagnostics:

- **Fit line** shows the curve calculated from the current fitted solution.
- **Residuals** show the difference between each included observation and the fitted curve.
- **Error bars** show the processing-derived integration uncertainty.
- **Confidence band** shows uncertainty around the fitted curve when the solution contains suitable resampling results.
- **Excluded points** shows injections that do not contribute to the current fit.

These displays describe different aspects of the fitted solution. A small RMSD does not rule out systematic residual structure, poorly identified parameters, or dependence on model assumptions.

Store the fitted solution

With **Create analysis result** disabled, a successful single-experiment solution remains attached to its Experiment Data and is available in that experiment's analysis and figure workflows.

With **Create analysis result** enabled, a usable completed fit also creates a separate Analysis Result containing the experiment, model, fit settings, and solution. **Auto-open new result** determines whether the new result workspace opens immediately. A stopped or unusable fit does not create or replace an Analysis Result.

Fit availability and non-convergence

A single-experiment analysis requires processed or imported heats and at least three included injections with usable numerical values. The binding models also require nonzero cell and syringe concentrations. **Dissociation** uses the syringe concentration and does not require a macromolecule concentration in the initially buffered cell.

An unavailable model, failed termination, bound-limited solution, or failed resampling population can reflect missing or degenerate heat and concentration information, the supplied starting values, the selected limit policy, the optimizer's interaction with the fitting surface, model complexity, or weak parameter identifiability. Resampling can fail even when the primary fit succeeds because each refit presents a different or reduced dataset to the same model.

CHAPTER 07

Multiple-experiment fitting

Multi-dataset fitting across processed Active experiments, including constraints, shared options, diagnostics, and combined results.

Last verified: 2026-08-26

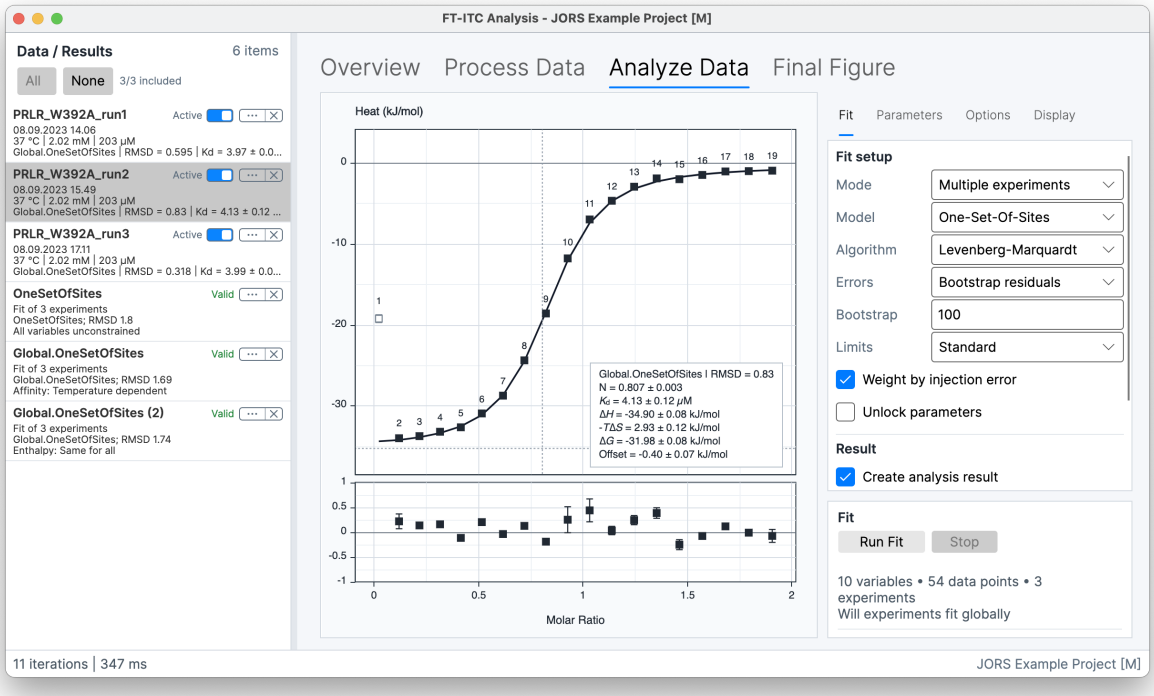
Multiple experiments is the multi-dataset mode in **Analyze Data**. It represents at least two processed **Active** experiments with one shared model context and one combined **Analysis Result**. When every constraint is **None**, the members are fitted independently. When one or more supported constraints are active, the solver performs one connected global optimization. Each experiment remains a member of the result, with member-specific parameters where the constraint state is **None**.

The model and model options apply across the active set. The resulting **Analysis Result** retains the member fits, any shared or temperature-dependent parameters, constraints, solver settings, diagnostics, and uncertainty output. Shared fitting controls are described in Single-experiment fitting.

Fit

The **Fit** tab identifies the **Mode** as **Multiple experiments** and exposes the shared **Model** selection. The solver controls include **Algorithm**, **Errors**, **Bootstrap**, **Limits**, **Weight by injection error**, **Concentration uncertainty**, and **Unlock parameters**. The available **Algorithm** values are **Nelder-Mead** and **Levenberg-Marquardt**; the error-estimation values are **None**, **Bootstrap residuals**, **Leave-one-out**, and **Profile likelihood**. For a globally fitted model, leave-one-out performs one deterministic refit per omitted experiment; profile likelihood uses the complete global objective and total observation/coordinate counts, while independent members use each member's local counts. Bootstrap count, concentration uncertainty, and parameter unlocking are disabled because they do not participate in deletion or profile schedules.

The **Result** controls describe whether a completed fit is stored as an **Analysis Result** and whether that result opens automatically. **Run Fit** and **Stop** are the fit controls. The status area records termination state, RMSD, iteration count, elapsed time, and error-estimation outcome when applicable. A multiple-experiment analysis is ready only when every member has usable processed data and the set contains at least two members.



A shared enthalpy constraint connects the three Active experiments in one global fit.

Parameters

The **Parameters** tab contains the exposed fit parameters and, in multiple-experiment mode, the **Global constraints** section. Parameter rows show the current value, units, uncertainty information when available, and the parameter lock state. A parameter value or lock state is a parameter setting; it is separate from the relationship between members.

The constraint states have these meanings:

STATE	MEANING
None	The parameter remains member-specific. Each experiment has its own fitted value.
Same for all	One common value is fitted for every member in the set.
Temperature dependent	A supported parameter is represented across the temperature series by the relationship exposed by the model.

The **Locked** state fixes an exposed parameter at its displayed value during fitting. **Locked** is not a constraint state and does not make a parameter common to the member experiments. A locked global value and a member-specific locked value therefore have different scopes.

For the core binding parameters, the available relationship states are model- and data-dependent:

PARAMETER	AVAILABLE STATES
Affinity	**None**, **Same for all**, or **Temperature dependent**
Enthalpy	**None** or **Same for all**; **Temperature dependent** is also available when the selected set exposes temperature dependence
N-value	**None** or **Same for all**
Offset	**None** or **Same for all**

The interface omits unsupported states for the current model. The corresponding labels can appear as **Temp. dependent**, **Independent**, or **Shared**; they describe the same temperature-dependent, member-specific, and common relationships.

For **Sequential Binding Sites**, the step count is one shared model option for the complete experiment set. The interface shows one **Affinity** constraint selector and one **Enthalpy** constraint selector, regardless of whether two, three, or four steps are active. A selected family style is applied to every active step while retaining a separate coordinate for each step: **Same**

for all shares K_1 across members, separately shares K_2, and so on; it does not force the different steps to equal one another. **Temperature dependent** likewise uses one ΔG_i per affinity step and one reference $\Delta H_i/\Delta C_{p,i}$ pair per enthalpy step. Reducing the step count discards inactive step values and constraints; increasing it later creates new defaults for those steps.

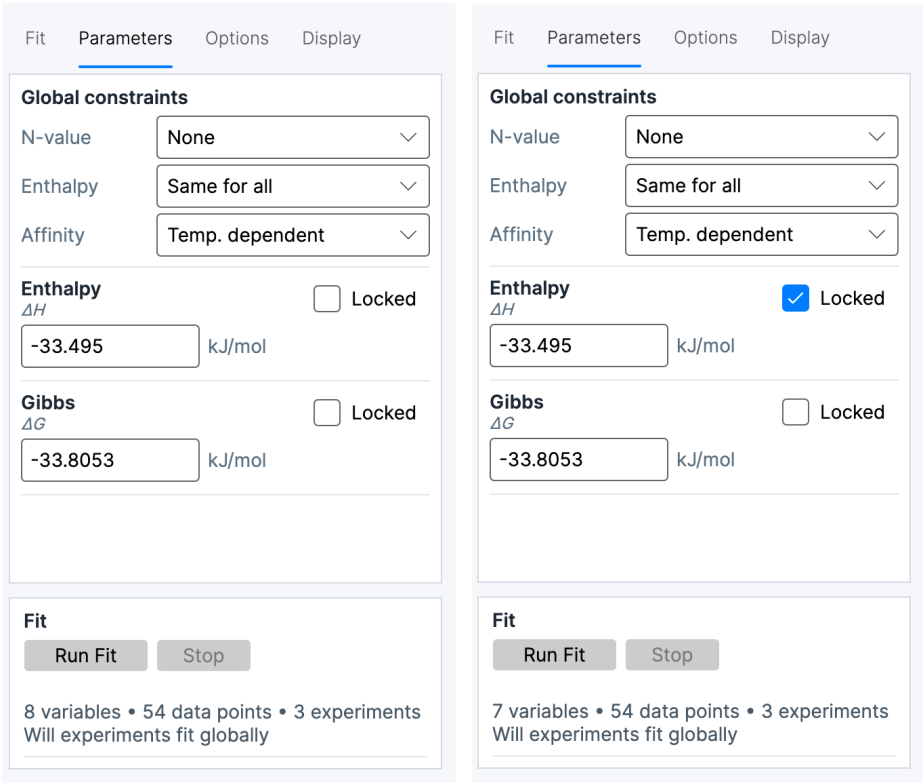
Offset is an energy-per-mole-of-injectant correction. For each injection, its absolute heat contribution scales with the injected amount—the injection volume multiplied by the syringe concentration. With **Offset: None**, each experiment has its own fitted molar offset. With **Offset: Same for all**, the **Parameters** tab exposes one common molar offset for the complete set. That shared value has its own **Locked** control; locking it fixes the common value for every member.

CALCULATION:

$$\Delta H(T) = \Delta H_{\mathrm{ref}} + \Delta C_p(T - T_{\mathrm{ref}})$$

$$K_a(T) = \exp\left[-\frac{\Delta G}{RT}\right]$$

ΔH_{ref} is the enthalpy at the reference temperature, and ΔC_p is the common heat-capacity term. Temperature-dependent affinity is represented through a common free-energy term. T and T_{ref} are absolute temperatures.



Global constraints define relationships between member parameters; Locked separately fixes an exposed value.

Options

The **Options** tab contains the options exposed by the selected model. In multiple-experiment mode, an option is a property of the shared model context and applies to every member. This includes model-specific concentration, stoichiometry, syringe-correction, or prebound-species settings when those options are exposed. The option values are preserved with the combined Analysis Result.

An option that changes which parameters are exposed can also change the available parameter rows and constraint states. For example, model options that share or replace stoichiometry alter which N-values are independently represented. The available rows always describe the active model and option combination.

Display

The **Display** tab controls the graph presentation for the active member set. Its controls cover the fitted line, residuals, error bars, confidence band, point labels, parameter box, excluded points, automatic scaling, unified axes, fitted offset, and fit-line interpolation. The parameter box can separately show model, fitted, and derived parameters.

Display settings affect the graph presentation, not the model, the member data, or the fitted values. The graph can therefore show the current member fits or connected global fit alongside member observations while the Parameters tab remains the source of the stored parameter and constraint state.

Combined Analysis Result

The combined **Analysis Result** contains the exact member experiments, the shared model and options, member parameters, any shared or temperature-dependent parameters, active constraints, solver and weighting settings, convergence diagnostics, and uncertainty results. Its result table can represent both global values and member-specific values. A selected member retains its own fitted curve and residual information even when a parameter is common across the set.

The status and diagnostics distinguish a successful solver termination from the quality and uncertainty of the fit. RMSD, iteration count, weighting, error-estimation method, and the number of successful uncertainty refits describe how the combined result was obtained. Wide or asymmetric uncertainty, a member with a markedly different residual pattern, or a member solution with an invalid status remains visible as member-level information rather than being hidden by a combined value. Result interpretation and validity are covered in Results and advanced analyses.

CHAPTER 08

Results and advanced analyses

Analysis Result views, validity, uncertainty presentation, evaluation temperature, and conditional advanced analyses.

Last verified: 2026-08-26

An **Analysis Result** is a stored fit for one or more experiments. It contains the model and options, constraints, solver state, weighting and uncertainty settings, member solutions, and a validity snapshot. The result workspace presents those stored values together with graph and analysis views. The fitting controls are described in Single-experiment fitting, and multi-dataset constraints are described in Multiple-experiment fitting.

Result views

The result view selector contains **Fit**, **Correlation**, and **Summary** for every Analysis Result. Ordinary thermodynamic temperature plots and parameter evaluation can contain every active sequential step. **Temperature** advanced analysis (Spolar Record method), **Salt**, and **Protonation** appear only when the selected model defines those analyses and the member metadata satisfy their additional requirements.

Summary presents the combined parameter graph and result table. The table can show fitted values, derived values, and the selected uncertainty representation for each stored solution. Columns initially size to their headers and displayed values within compact limits; drag a header boundary to adjust an individual width. Wider tables retain their column widths and scroll horizontally, while spare space is assigned to the Experiment column. Molar-energy columns share one automatically resolved unit (or the fixed unit selected for result export), while ΔCp columns resolve independently. Selecting a row makes that member the current result solution;

the selection is retained by the result workspace and drives **Fit** and the local portion of **Correlation**. When switching directly between analysis results, the selected experiment is retained when the destination contains a member with the same experiment ID. The result workspace no longer has a separate four-choice energy-prefix menu; use **Preferences > General > Energy units** for the Joules/Calories family.

Profile-likelihood results retain ordinary `FloatWithError` values and may still be sampled by existing advanced analyses; profile intervals do not create a bootstrap refit ensemble or a new covariance model. Leave-one-out refits remain available for the integration-graph envelope when saved refits exist.

Fit presents the saved fitted curve, residuals, error bars, confidence band, and excluded points for the selected member. The graph is read-only: it represents the stored solution and does not expose fit controls or alter the underlying experiment.

Correlation presents a matrix calculated from residual-bootstrap refits. Its availability, scope, and interpretation are described under Parameter correlation.

Inspector tabs

The result inspector has four tabs with shared labels across the supported desktop versions: **Summary**, **Analysis**, **Experiments**, and **Model**.

The **Summary** tab contains the result identity, model, member count, RMSD, information criteria, and solver diagnostics. The validity section reports **Analysis is valid**, **Partially invalid**, **Invalid**, or **Unknown status**, with reasons when the stored validity snapshot differs from current member inputs. In the browser viewer, a valid result can also show **Saved result has analysis warnings** when a saved best fit or uncertainty refit reached a parameter boundary, or uncertainty refits reached an optimizer limit; these warnings remain visible alongside validity reasons. Solver information includes algorithm, iterations, weighted or unweighted injection errors, error-estimation method, and bootstrap count.

In the browser viewer, RMSD is shown as a saved unweighted display diagnostic in µJ, separate from the weighted fitting objective. When the saved convergence record contains it, **Molar RMSD (kJ/mol)** is shown separately: the result summary uses the saved global metric, while an individual fit uses that fit's saved metric. Missing or non-finite saved values remain unavailable; member values are not averaged to reconstruct the result metric.

Information criteria

The **Information criteria** section reports the analysis-level AICc when it is available, otherwise AIC, together with the included observation count n and likelihood parameter count K. Both weighted and unweighted criteria estimate one residual-variance parameter, so $K = p + 1$, where p is the number of free fitted parameters. Weighted criteria use the injection integration errors as relative uncertainties and estimate one common variance multiplier from the standardized residuals. AICc is unavailable when $n \leq K + 1$, in which case AIC is shown instead. If the likelihood cannot be evaluated, the displayed criterion shows its diagnostic reason.

When members were fitted independently, the result table also includes an **AICc / AIC** column. It reports each member's own criterion and is intended for comparing alternative models fitted to the same experiment, observations, response definition, and weighting mode. Values in different experiment rows are not comparable because they use different observations. AICc is shown when available, with AIC as the fallback when the small-sample correction is undefined; **Unavailable** means that the member likelihood could not be evaluated. Shared-parameter global fits expose only the analysis-level criterion and omit this member column. Neither AIC nor AICc establishes model adequacy.

The criteria use the saved result's included injections and response definition. At analysis level, residual statistics are pooled before estimating the variance, including when members were fitted independently. Unweighted criteria estimate one common variance across all members; weighted criteria estimate one common multiplier of the injection-error variances. Each independent member's own criterion estimates its variance separately. Consequently, neither pooled AIC nor pooled AICc is a sum of the member values.

With residuals r_i, raw residual sum of squares $RSS = \Sigma r_i^2$, integration-error SDs σ_i, and standardized residual sum of squares $Q = \Sigma (r_i/\sigma_i)^2$, the maximized likelihood terms are:

CALCULATION:

$$\text{Unweighted, estimated common variance:} \quad -2\log L = n\left[\log\left(\frac{2\pi \mathrm{RSS}}{n}\right) + 1\right]$$

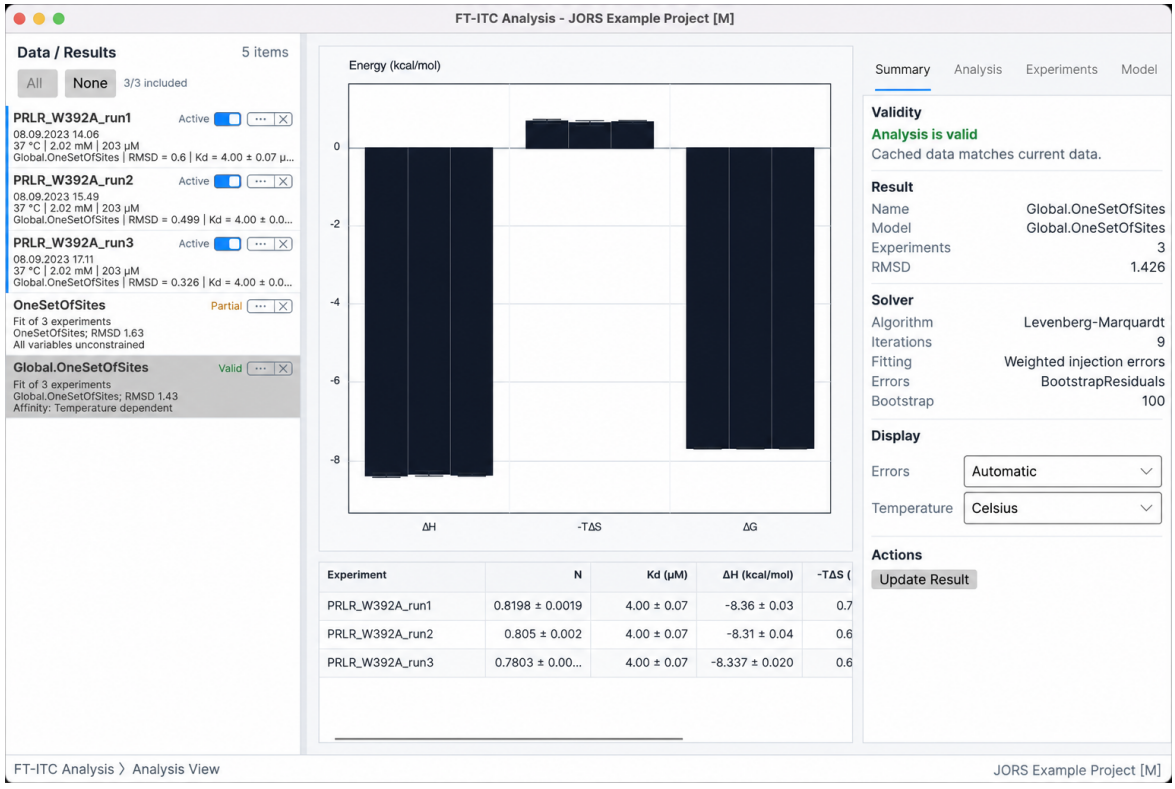
$$\text{Weighted, estimated variance multiplier:} \quad -2\log L = n\left[\log\left(\frac{2\pi Q}{n}\right) + 1\right] + \Sigma \log \sigma_i^2$$

The weighted variance multiplier is Q/n, calculated analytically without adding an optimizer variable or changing the stored integration errors or fitted parameters. Sigma selection uses the same per-injection values and per-member fallback as weighted fitting. Zero residual variance makes the estimated-variance likelihood unavailable. Weighted profile-likelihood intervals retain their fixed observation-sigma convention, which is separate from the AIC/AICc convention.

The fitted parameter count p includes only parameters free in the saved global model. Shared coordinates count once; member-specific coordinates count once per member. For a member criterion, p includes only that member model's free fitted parameters. In both weighting modes, the reported values use $K = p + 1$, $\mathrm{AIC} = -2 \log L + 2K$, and $\mathrm{AICc} = \mathrm{AIC} + 2K(K + 1)/(n - K - 1)$. This standard small-sample correction is an approximation for nonlinear ITC models.

Smaller values are preferred only when comparing models that use the same observations, response definition, and weighting mode. AIC and AICc do not establish model adequacy or replace residual and scientific checks. Prefer AICc when it is available.

Information criteria are recalculated when a saved project is opened. Weighted values from the former fixed-sigma calculation can therefore change; compare results calculated under the same likelihood convention.



Summary combines result validity, stored solver information, display controls, and the member parameter overview.

The **Analysis** tab contains the result view selector, parameter evaluation, and the analysis-specific controls and outputs. It is also the location of the uncertainty display, correlation information, and evaluation-temperature presentation associated with the selected view. Energy labels and values use the family resolver for the visible central-value group, including graph axes, errors, fitted bands, tooltips, and parameter lists.

The **Experiments** tab lists the result members and their stored status and condition information, including member temperature. The member represented as selected in the result table drives **Fit**, while this tab provides the corresponding member context.

The **Model** tab shows the stored model options, locked parameters and their fixed values, and the active constraints. A constraint with state **None** is not listed as an active global constraint; **Same for all** and **Temperature dependent** entries identify the relationships retained by the Analysis Result. The corresponding labels **Independent** and **Shared** describe the same member-specific and common relationships.

Uncertainty and evaluation temperature

The **Errors** display control provides **Automatic**, **Standard deviation**, **95% confidence interval**, and **SD + 95% CI**. **Standard deviation** presents the primary best-fit value with a symmetric ± SD; **95% confidence interval** presents that same best-fit value with the lower and upper percentile limits; and **SD + 95% CI** presents both. The central value is always the primary best fit, not the mean or median of the resampled values.

Automatic makes this choice separately for each reported quantity. Let L and U be its stored 95% confidence limits and $\hat{\theta}$ its primary best-fit value:

CALCULATION:

$$w_{\text{lower}} = \widehat{\theta} - L; \quad w_{\text{upper}} = U - \widehat{\theta}$$

$$\text{asymmetry} = \frac{|w_{\text{upper}} - w_{\text{lower}}|}{w_{\text{upper}} + w_{\text{lower}}}$$

Automatic shows the 95% confidence interval when both widths are positive and the asymmetry is at least 0.18; otherwise it shows SD. This is a display rule based on interval imbalance around the best fit, not a formal statistical test of distribution skewness.

The decision is made after a fitted coordinate has been transformed into the displayed quantity. A nonlinear transformation—such as fitting $\log_{10}(K_a)$ and displaying K_d—can therefore make the displayed interval asymmetric and cause **Automatic** to select CI for that quantity.

Changing **Errors** changes only how stored uncertainty is presented in tables, parameter evaluation, and graphs. It does not rerun the fit, change the best-fit parameters, or turn one error-estimation method into another. Bootstrap construction, parameter transformation, and the SD and percentile calculations are described under Parameter uncertainty.

The **Parameter Evaluation** section contains an evaluation **Temperature** field and the displayed thermodynamic quantities at that temperature. Temperature display can be **Celsius** or **Kelvin**. Changing the evaluation temperature changes derived presentation from the stored model; it does not change injection heats or refit the result. Temperature-dependent values are meaningful together with their model, units, uncertainty representation, and evaluation temperature.

Parameter correlation

Correlation shows Pearson correlations between fitted parameter coordinates across residual-bootstrap refits. It requires **Bootstrap residuals**, at least 30 complete refits, and at least two parameters that vary across those refits. Parameters with no variation are omitted. Parameters fixed in the primary fit are also omitted unless **Unlock parameters** allowed them to vary during bootstrap error estimation; such parameters are marked with an asterisk and a warning that bootstrap parameter unlocking was enabled.

CALCULATION:

$$r_{jk} = \frac{\Sigma_b\left[\left(\theta_{bj} - \overline{\theta}_j\right)\left(\theta_{bk} - \overline{\theta}_k\right)\right]}{\sqrt{\left[\Sigma_b\left(\theta_{bj} - \overline{\theta}_j\right)^2 \Sigma_b\left(\theta_{bk} - \overline{\theta}_k\right)^2\right]}}$$

r_{jk} is the Pearson correlation between fitted coordinates j and k. The index b runs over complete residual-bootstrap refits, and $\bar{\theta}$ is the corresponding mean coordinate.

For each off-diagonal cell, the application also reports an approximate 95% Monte Carlo precision interval using Fisher's transformation. Matrix values range from –1 to +1; an interval spanning zero marks the sign as unresolved at the current simulation precision. The result panel

separately reports attempted, usable, failed, and complete refits. It warns when fewer than 100 complete refits make precision coarse, at least 20% of attempted refits failed, a usable refit lacked a finite displayed coordinate, a sign is unresolved, or the matrix is structurally rank limited. The correlation matrix remains unavailable below 30 complete refits. For a single-experiment result, the scope is **Single experiment**. A multiple-experiment result can show **Shared** coordinates alone or **Shared + selected local** coordinates when a member is selected. Shared and local labels identify the scope of each parameter.

Sequential correlations use the actual fitted coordinates. Affinity coordinates are labeled **log10 Ka1** through **log10 Ka4**, active enthalpy coordinates are included, and no N-value coordinate is added. A global result shows the shared per-step coordinates and, when requested, unconstrained coordinates for the selected member without duplicating constrained member values.

INTERPRETATION:

Correlation shows how fitted coordinates varied together under the residual bootstrap. The Fisher interval describes the finite-bootstrap Monte Carlo precision of the correlation coefficient *r* itself; it is not a confidence interval for either fitted parameter and does not replace the parameter uncertainty display. It does not establish identifiability, causality, model adequacy, or model validity. An interval spanning zero means only that the sign is unresolved at this Monte Carlo precision. Frequent refit failures can make the retained ensemble selective, and the Fisher interval does not account for those failures. Affinity is evaluated in the fitted coordinate system—$\log_{10}(K_a)$—rather than as the displayed K_d. A rank warning states the structural limit $rank \le B - 1$ for the displayed parameter count; it is distinct from numerical rank and scientific model validity.

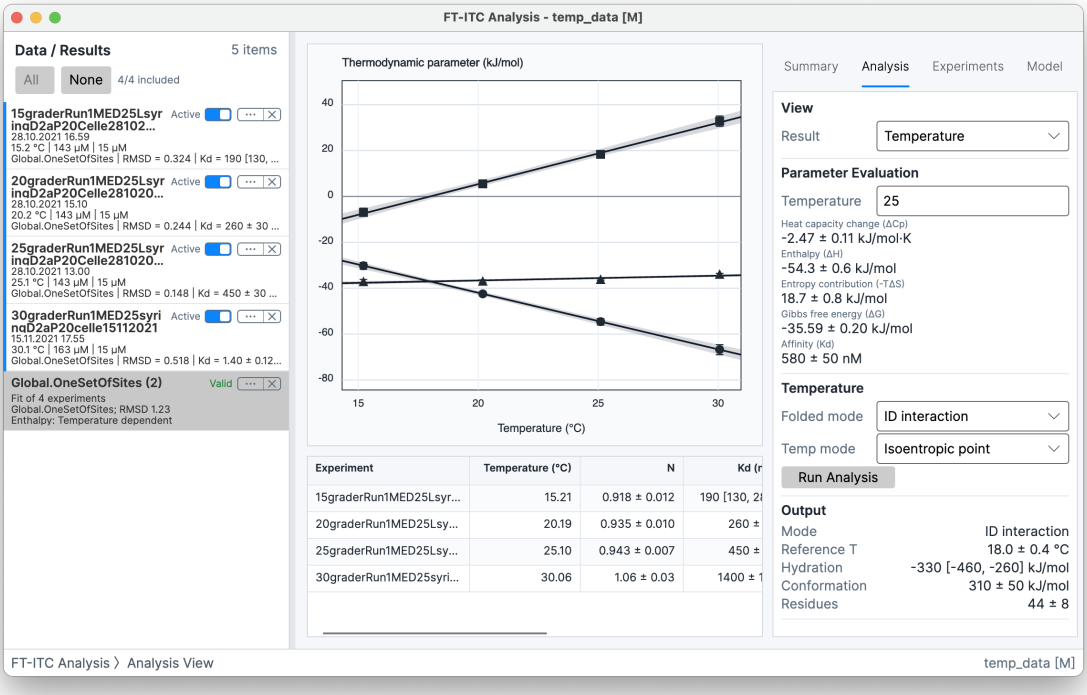
Advanced analysis views

All advanced analyses require a **One-Set-Of-Sites** Analysis Result. Availability is additionally conditional on the relevant condition span and metadata. The advanced analyses operate on the stored member solutions and expose their own calculated outputs; they do not change the base fit parameters. A sequential result can still show its ordinary per-step ΔH, ΔG, –TΔS, Kd, and temperature-dependence presentation; it reports the Spolar Record method, protonation, and electrostatics as unsupported by that model rather than hiding the ordinary thermodynamic views.

Temperature

The **Temperature** view is available when member temperatures span more than the configured minimum temperature span. Its temperature-analysis controls expose **Folded mode** values **Globular** and **ID interaction**, together with **Temp mode** values **Isoentropic point**, **Mean temperature**, and **Reference temperature**.

The stored temperature-analysis output includes reference temperature, hydration contribution, conformational contribution, and residue estimate. These values describe the selected folded and temperature-evaluation modes under the fitted temperature dependence. They remain conditional estimates of the stored model and member series rather than direct structural measurements.



Temperature presents the stored temperature dependence together with its evaluation and folded-state analysis controls.

Salt

The **Salt** view requires a **Salt** attribute for every member and sufficient ionic-strength span across the member set. Its **Graph mode** values are **Affinity vs Salt**, **Debye-Huckel**, and **Counter Ion Release**. Counter-ion release is a salt analysis mode and is presented in the Salt view rather than as a separate advanced analysis.

The Salt output includes the extrapolated **Kd0** and **Counter ion** result when the analysis has a calculated fit. The graph mode determines whether the displayed dependence is expressed against salt, ionic strength using Debye-Huckel behavior, or ion activity for counter-ion release. The result is limited by the recorded salt identities, ionic-strength values, and the quality and span of the member affinity values.

CALCULATION:

$$\ln K_d(I) = \ln K_{d,0} + s\sqrt{I}$$

$$\ln K_d = b + n_{\text{ion}} \ln a_{\text{ion}}$$

I is ionic strength, s is the fitted sensitivity, a_{ion} is ion activity, and b is the fitted intercept. $K_{\text{d,0}}$ is the extrapolated value in the Debye–Hückel view. n_{ion} is the reported slope for Counter Ion Release; its sign is reported by the analysis and is not assigned an interpretation here.

Protonation

The **Protonation** view requires a **Buffer** attribute for every member and at least two distinct buffer identities. Its calculated output contains **Protons** and **Binding H**, with uncertainty when the stored analysis contains the corresponding uncertainty results.

The view relates the stored member binding enthalpies to the buffer protonation information associated with their conditions. The result is conditional on the recorded buffer identities, their temperature-dependent protonation enthalpies, and the model assumptions; it does not identify a particular residue or microscopic protonation event.

CALCULATION:

$$\Delta H_{\text{obs}} = \Delta H_{\text{bind}} + m \Delta H_{\text{buffer}}$$

The fitted slope is m. The application reports **Protons** as $-m$, while **Binding H** is the fitted intercept at zero buffer protonation enthalpy. This sign convention follows the application's protonation-enthalpy convention; it does not by itself assign a microscopic uptake or release mechanism.

Advanced-analysis values are supplemental views of a stored Analysis Result. Their availability and outputs are determined by the One-Set-Of-Sites model, member variation, metadata, selected graph or evaluation mode, and any completed uncertainty calculation. Result validity

remains a separate indication of whether the stored fit inputs match the current project state. Figure and table output is covered in Figures and export.

CHAPTER 09

Figures and export

Configure final and supporting figures, print active graphs, and export data, results, figures, and complete analysis reports.

Last verified: 2026-09-04

FT-ITC Analysis keeps publication figures, numerical data, and fitted result tables as separate output types. **Final Figure** is an Experiment Data workflow. An Analysis Result does not open directly as a Final Figure; **Export Associated Final Figures…** on a result exports figures for the experiment solutions associated with that result.

Final Figure

The **Final Figure** workspace renders the selected Experiment Data as a publication figure. Its preview and PDF output reflect the selected experiment, processing state, fitted solution, and figure options. An Analysis Result can supply fitted solutions for associated figure export, but the result itself is not the Final Figure workspace input.

The Export PDF controls contain three scopes:

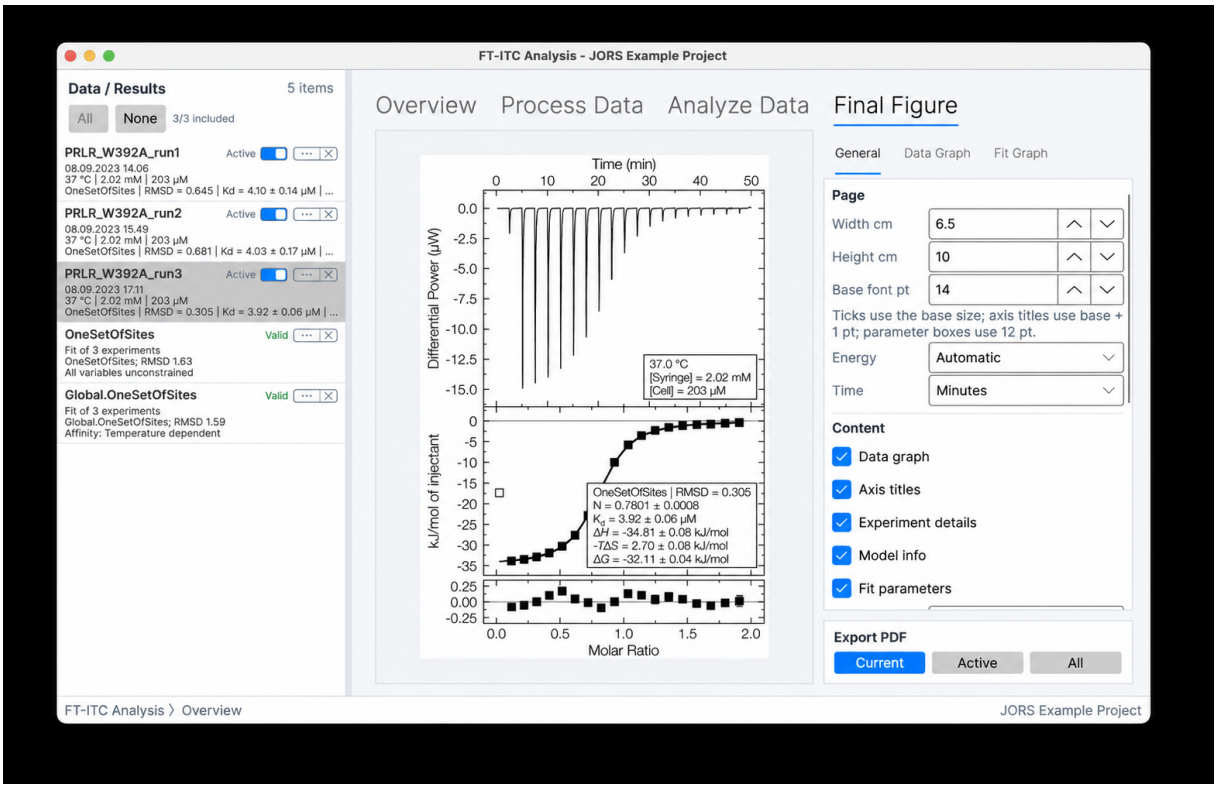
- **Current** exports the displayed experiment figure to one PDF.
- **Active** exports figures for Active Experiment Data.
- **All** exports figures for all Experiment Data in the project.

The result-list command **Export Associated Final Figures…** loads the result's member solutions into their experiments and writes one final-figure PDF per associated experiment. It is available for a result with exportable solutions. See Results and advanced analyses for result validity and stored member-solution behavior.

General

The **General** tab defines the page and common content. Page controls specify width and height in centimeters and the base font size. The **Energy units** selector provides **Automatic**, **J**, **kJ**, **cal**, and **kcal**. **Automatic** resolves one normal molar-energy unit from the figure's central plotted/result values; a fixed choice applies to all normal energy values. The selected family also controls thermogram units: differential power is **µW** or **µcal/s**, while integrated heat is **µJ** or **µcal**. Time controls set the displayed time unit. Content controls include the data graph, axis titles, experiment details, model information, fit parameters, and the information-box placement. The uncertainty selector provides **Automatic**, **SD**, **CI**, **SD + CI**, and **None**. **Automatic** uses the same per-quantity asymmetry rule described under Uncertainty and evaluation temperature.

The parameter controls determine which information appears in the information box: thermodynamic, derived, or offset parameters; temperature; concentrations; injection delay; instrument; and user-defined attributes. The information box is descriptive figure content and does not alter the underlying fit.



Final Figure combines a live publication preview with page, content, and PDF export controls.

Data Graph

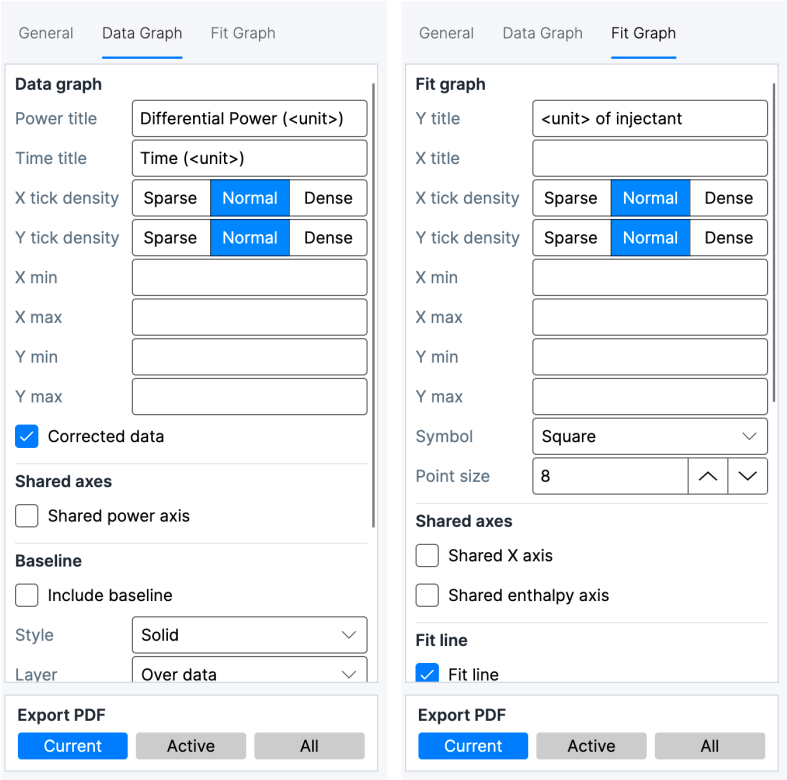
The **Data Graph** tab controls the differential-power trace. Power and time axis titles, tick density, and explicit minimum and maximum values define the axes. **Corrected data** selects the baseline-corrected trace when one is available. **Shared power axis** applies one power-axis range across the active experiments represented by a figure set.

Baseline controls expose the baseline, its **Solid** or **Dashed** style, **Under data** or **Over data** layer, and line width. **Integration ranges** displays the integration intervals as **Bar**, **Fill**, or **Endpoint lines**. These overlays describe processing and do not recalculate integration.

Fit Graph

The **Fit Graph** tab controls the integrated-heats and model panels. Enthalpy and molar-ratio axis titles, tick density, and explicit ranges define the axes. Symbols are **Square** or **Circle**, with an independent point size. **Shared X axis** and **Shared enthalpy axis** unify the corresponding ranges across active experiments; the residual-axis range follows the shared enthalpy setting when configured for unified residual axes.

Fit line displays the fitted binding curve with a selected width and **Smooth**, **Spline**, or **Linear** smoothness. **Show residuals graph** adds the residual panel, and **Residual gap** separates it visually from the fit panel. The display controls include the zero enthalpy line, confidence band, error bars, excluded points, excluded error bars, and offset-corrected heats. Error bars use processed injection uncertainties; confidence bands require bootstrap uncertainty in the fitted solution; fit lines and residuals require a fitted solution.



Data Graph and Fit Graph provide separate controls for the thermogram and fitted-heats panels.

Numerical data export

File > Export Data... opens the numerical export dialog. **Export Selected Data...** invokes the same export for the selected experiment. The data scope is one of **Selected experiment**, **Active experiments**, or **All experiments**.

The format list contains:

- **Thermogram Data** — a `.csv` file containing time and power samples, with the **Export baseline-corrected trace** option when baseline-corrected samples exist.
- **Integrated Peaks** — a `.csv` file containing injection-axis values, integrated heats, uncertainties, fitted values, and residuals when available, with **Export offset-corrected peaks** when a fitted solution is available.
- **Combined Data** — a `.csv` file placing thermogram samples and integrated-peak columns side by side; raw, corrected, fitted, and residual columns are included when available.
- **MicroCal / SEDPHAT** — a `.dat` file with MicroCal-style `DH`, `INJV`, `Xt`, `Mt`, `XMt`, `NDH`, `DY`, and `Fit` columns. `DH` is in µcal, `INJV` is in µL, concentrations are in mM, and `NDH`, `DY`, and `Fit` are in cal/mol. The first injection uses `--` for normalized heat and residual,

following the conventional excluded-first-injection layout.

- **pytc** — a `.dh` file containing the pytc-compatible injection and metadata fields.
- **ITCsim** — a `.csv` file containing ITCsim-compatible injection data and metadata, with offset-corrected peaks available when a fitted solution exists.

Output units are format-specific. Thermogram samples use seconds and watts; integrated-peak and combined-data enthalpy, model, and residual values use joules per mole; MicroCal/SEDPHAT, pytc, and ITCsim use their documented concentration, volume, temperature, and heat conventions. The application energy-family preference controls desktop presentation, not these raw/scientific interchange contracts. Fitted columns and correction controls are disabled when the selected data do not contain the corresponding processed or fitted state. Export defaults are described in Settings and defaults.

These exports are not project backups. General `.csv` and `.tsv` exports cannot be reopened through **File > Open...**. A MicroCal / SEDPHAT `.dat` export or pytc `.dh` export can be reopened as integrated-heat input, but doing so restores neither a thermogram nor the FT-ITC project state and requires choosing the source heat unit. Select **microcalorie** for the `DH` column when reopening a newly generated MicroCal / SEDPHAT export. Historical FT-ITC `.dat` exports may instead require **joule**, matching the unit used when they were created. Save an `.ftxtc` project when the analysis must remain editable.

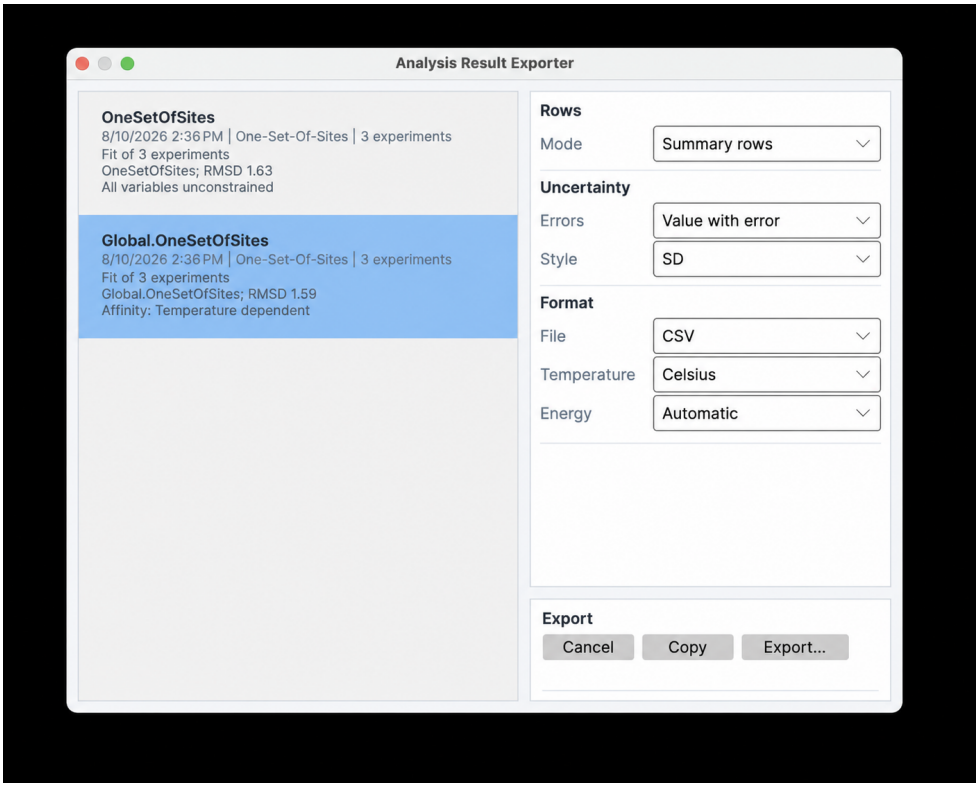
Analysis Result Exporter

Analysis Result Exporter... builds a table from one or more selected Analysis Results. **Summary rows** emits result-level rows; **All replicate rows** emits the individual fitted/member rows. Error layout is **Value with error** or **Separate columns**. Uncertainty style is **SD**, **CI**, or **SD + CI**. The file format is **CSV** or **TSV**. **Energy units** provides **Automatic**, **J**, **kJ**, **cal**, and **kcal**. Automatic chooses one stable molar-energy unit across all selected results and one independent unit for ΔCp columns; a fixed choice applies its normal energy numerator consistently. Temperature presentation is **Celsius** or **Kelvin**.

The configured table is available through **Copy** and **Export...**. Copy places the same delimited text on the clipboard; Export writes it to a file. Profile-likelihood SD columns use the equivalent display scale implied by their stored endpoints and are labeled as such in exported metadata; the exact lower/upper endpoints remain available in separate-column mode. The exporter does not include the parameter-correlation matrix, which is calculated for display rather than stored as a result-table field.

Result tables, clipboard output, final-figure metadata, and viewer output create thermodynamic columns from the fitted model shape. A sequential result therefore exports one Kd, ΔH, ΔG, and –TΔS value for every active step, including steps 3 and 4, rather than truncating the result to two interactions. The fixed step count is included as model information. Values remain in their displayed families; exporting does not convert macroscopic sequential constants into microscopic site constants.

Each affinity column chooses its concentration unit independently from its own magnitude. For example, Kd1 may be shown in nM while Kd4 is shown in µM. The column header and its values always use the same unit; this is display scaling only and does not change fitted or persisted values.



Analysis Result Exporter configures a delimited table for clipboard or file output.

Analysis Report

Tools > Analysis Report... creates a complete, printable report from one or more saved Analysis Results. The same tool is available as **Export Analysis Report...** in result-specific menus, where that result is initially selected. Use **Select report contents...** to choose results and optional supporting experiments together. The picker follows application order; applying the same ordered selection again restores its saved study context and approved interpretation. At least one result is required.

The report is a multipage A4 portrait PDF with print-safe margins. A single-result report retains its established structure. A report containing multiple results begins with a combined result index and concise table of contents on the first page, followed by the report-level interpretation and one self-contained chapter for each result. Results are referenced as **1**, **2**, and so on, and their experiments as **1A**, **1B**, **2A**, **2B**, and so on. These labels are derived from the persisted result and member order, so figures, captions, and interpretation evidence use the same stable references. No experiments or scientific estimates are merged across results. Each chapter overview uses the Supporting Figure composition pipeline to arrange every experiment as a compact, borderless publication panel titled with its reference and experiment name. The report automatically chooses three to five columns, centers incomplete rows, and suppresses repeated axis titles.

The analysis summary contains a compact grouped thermodynamic bar chart for every saved member and active binding step. Its whiskers show only the saved 95% confidence interval from the solution distribution or profile-likelihood calculation; the symmetric SD approximation remains available in report tables but is not superimposed on this plot. Each experiment section places a wider, baseline-focused view of the uncorrected thermogram—with its saved baseline and compact horizontal markers for the integration windows—beside a top-aligned, canonical-size Final Figure containing the complete thermogram, followed closely by fitted and derived parameters. When **Injection tables** is selected, a table records every saved injection, its inclusion state, volume, concentrations, analysis-axis value, integrated heat and uncertainty, fitted heat, and residual. This processing presentation is an automatic report preset and does not add another figure control. A concise notice replaces the processing graph when raw thermogram samples are unavailable. Selected shared correlations follow the analysis summary; selected member correlations follow that experiment’s parameter table, using a compact native matrix rather than a dedicated page.

Directly selected experiments that are not represented by a selected result appear once in a report-level **Supporting experiments** chapter after the result chapters and are labelled **S1**, **S2**, and so on. The report uses only saved content: a raw thermogram with any saved baseline and integration boundaries, finite integrated heats explicitly labelled as having no fit, experiment metadata, exception-only processing/correction notes, trusted dates, attributes, comments, and the report-wide optional injection table. Missing stages receive concise availability notices. Experiments already represented by a checked result remain visible but unavailable as supporting selections. Recorded buffer-subtraction references may be selected automatically according to the application setting, but remain ordinary optional selections; the report does not judge whether a reference is an appropriate blank. Report creation never fits, reintegrates, or performs subtraction.

Choose a title and optional subtitle, energy and temperature units, and **Uncertainties**. The subtitle appears as secondary, regular-weight text below the report title. Reports default to **SD + 95% CI**: SD is shown as the inner error mark and the 95% interval as the outer mark; **SD**, **95% CI**, and **None** restrict both tables and report plots accordingly. This selection is remembered only for the current application session. Final Figure injection errors and fitted confidence bands retain their established scientific meanings.

Optional content includes report-wide **Injection tables** and **Condense repeated experiments** switches together with the union of completed analysis types available across the selection. Each option applies to every eligible result chapter; chapters without that saved content simply omit it. The injection-table switch is on by default and applies consistently to every experiment. When the same experiment occurs in a later result, condensed mode retains both figures, comments, source file, trusted date, instrument, temperature, concentrations, and all result-specific fitted content, but replaces repeated secondary acquisition and processing details with a reference to its first occurrence. One **Parameter correlations** choice includes the saved shared matrix and all available member matrices at their inline report locations, avoiding repeated per-experiment controls. Available analyses are selected by default; **Select all** and **Clear** change that analysis list together. Temperature dependence is included once per eligible result with its saved fit and parameter summary, while saved electrostatics, protonation, and Spolar outputs are presented without recomputation. Report creation never reruns fitting or advanced analysis.

The builder opens in **Interpretation** mode with a large, wrapping editor for user remarks. Interpretation Markdown supports `##` section headings, `###` subsection headings, bullets, `**bold**`, and `*italic*` emphasis. Use the **Interpretation / Preview** control above the workspace to move between writing and the rendered report. Selecting **Preview** automatically builds the PDF when it has not yet been built or is out of date; a current preview is reused.

Update Preview forces a rebuild. Editing while a preview exists marks it as out of date without repeatedly rendering while you type. **Export PDF...** rebuilds stale content and writes the PDF atomically. Warning-bearing, stale, and partially invalid results remain exportable and carry a prominent notice. A structurally unusable result shows a validation error and cannot be previewed or exported.

The inspector's compact **Interpretation** section reports whether the text is manual, AI-generated, edited, or out of date. **Edit interpretation** returns focus to the large editor. **Generate with AI...** opens an optional **Main question** and **Additional context**. The question prioritizes the assessment; background helps interpret the ITC evidence without turning the output into a manuscript. Compressed thermograms are omitted by default to keep the model input compact. Administrators and Advanced capability-code users can opt in to **Include compressed thermograms**; standard and public access do not show the control.

Generation assesses all selected results and supporting experiments together, using the same references as the PDF. Results remain independent, including alternative fits of the same experiment. Supporting experiments contribute available observations and metadata without being assigned a fitted result or assumed control role. The package includes existing processing, integration, residual and uncertainty evidence where available; generation does not rerun integration, baseline fitting or model fitting. Compressed thermograms are omitted by default to keep the model input compact. Administrators and Advanced capability-code users can opt in to include them; standard and public access do not show that control. Thermograms use the `uniform-minmax-v1` encoding: one 15-second `[min, max]` value pair per interval in offset-relative µW, with timing stated once by the anchor and bin width. Pair order is not chronological; exact occurrence times, within-interval order and waveform are unavailable. A fitted baseline is retained as an independently calculated aligned array when available. If the request is too large, complete trace arrays may be omitted across the report while retaining summaries, injection tables and fit evidence; omissions are recorded. When multiple result members contain the same complete source and processing state, the compact model payload may place that evidence once under `experimentEvidence` and refer to it from each member. Fitted values, uncertainty, validity and constraints remain attached to their individual result. This reuse describes identical supplied evidence; it does not imply independent replication or equivalent fits.

One warning allows you to review stale or failed analyses before continuing. Historical fit-input snapshots and stored estimates are distinguished from current observations; diagnostics requiring a verified matching fit basis are unavailable when that basis cannot be established. An

interpretation can identify potential concerns, but it does not certify the experiment or establish a mechanism. Configured knowledge-base retrieval can support sparse paper-name, journal and year references; web search is disabled.

Interpretation troubleshooting: the application log records generation stages, request IDs, guidance revisions, instruction fingerprints, package sizes, timing, HTTP status and rejected contract fields. Full instructions, scientific context, generated text and credentials are not included in these diagnostic entries. An instruction fingerprint identifies exact text but cannot recreate it. Include the application log and visible error when reporting a generation failure. The desktop and MIST service use relay contract 5.0 together; the evidence package remains schema 2.0. MIST owns scientific guidance, while the app supplies output instructions matching its renderer. Output length and headings do not block accepting a nonempty response.

The returned text is a draft.

Use **Save AI package...** in the generation dialog to save a local ZIP with the complete evidence JSON, the compact model input (`model-package.json`), the actual application output instructions and a version/fingerprint manifest. Use the model-input file for AI evaluations; the complete evidence retains full precision for source review. The export uses the current selection, question, context and thermogram setting without a server request or new fits. This is a snapshot before transport; it never includes a purported copy of server scientific instructions. The archive contains your scientific data and context, so review it before sharing.

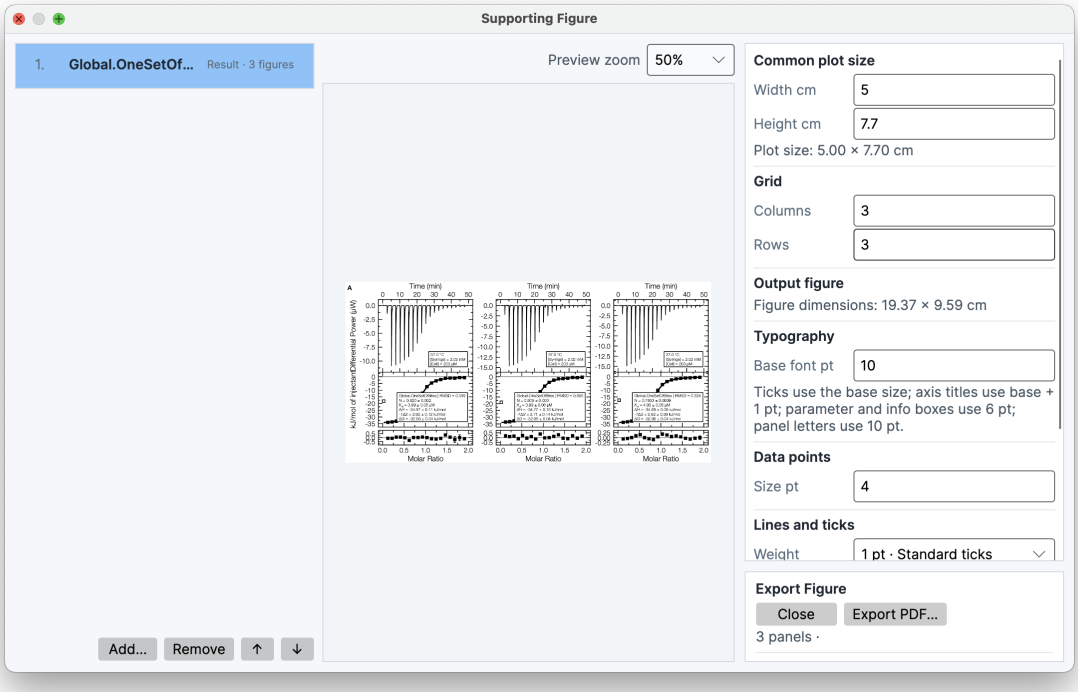
The compact model input keeps baseline diagnostics with each experiment. Landmark and spline-control arrays become shared-schema tables; spline control-point `locked`, `slopeLocked`, and `linear` flags are intentionally omitted, while unknown point fields remain in an explicit extension map. Segmented-baseline tables retain their boundaries, centres, injection scope and complete coefficient arrays. When source evidence is shared, `experimentEvidenceRef` points to the matching record and the fit table remains on each result member. Use `canonical-package.json` when those omitted control flags or full precision are needed for auditing.

The Analysis Report is distinct from the other output tools: **Analysis Result Exporter** writes CSV/TSV tables, **Final Figure** writes a publication figure, and **Supporting Figure** composes a multi-panel canvas.

Supporting Figure

Supporting Figure... composes figures from Experiment Data and Analysis Results into a multi-panel canvas. The **Figure order** list defines source order; **Add...**, **Remove**, **Up**, and **Down** change the composition. The source picker can filter available experiment and result figures by name or type.

Common plot size specifies width and height in centimeters. Grid controls specify columns and rows. Typography controls define base font size, point size, line weight, and tick style. **Panel letters** adds stable A, B, ... identifiers. **Panel titles** optionally adds the experiment name after that identifier (for example, **A. Experiment name**) and is off by default for existing Supporting Figure workflows. **Group result figures** and the parameter and information box control affect result grouping and annotations. The preview zoom shows the rendered canvas at 25%, 50%, 75%, or 100%. **Export PDF...** writes the composed supporting figure as a PDF.



Supporting Figure arranges the three member figures from an Analysis Result on a shared multi-panel canvas.

Printing

File > Print prints the active graph or figure through the operating system's print workflow. The active target can be the overview thermogram, processing graph, analysis graph, result graph—including an available **Correlation** matrix—or Final Figure, depending on the selected workspace. The operating-system print dialog supplies the available printer and PDF destinations; the graph content comes from the active application view.

CHAPTER 10

Tools

Design simulated titrations, subtract buffer controls, and merge standard or back-mixed tandem experiments.

Last verified: 2026-09-01

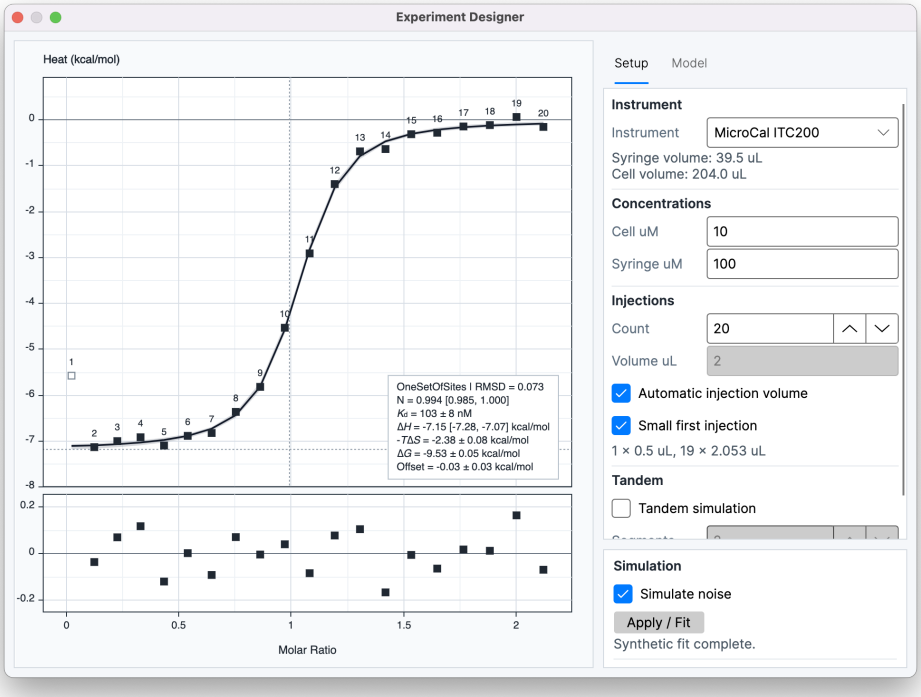
The **Tools** menu contains **Experiment Designer...**, **Buffer Subtraction...**, and **Experiment Merger...**. They have different output lifecycles: Experiment Designer keeps simulation and fitting inside its window, Buffer Subtraction stores a correction on target experiments, and Experiment Merger creates a new processed Experiment Data item. Source and target selection uses the project state described in Workspace.

Experiment Designer

Experiment Designer... creates a synthetic titration from instrument, concentration, injection, and model parameters. The graph updates as the design changes. The designer does not add the synthetic experiment or its fit as a project item.

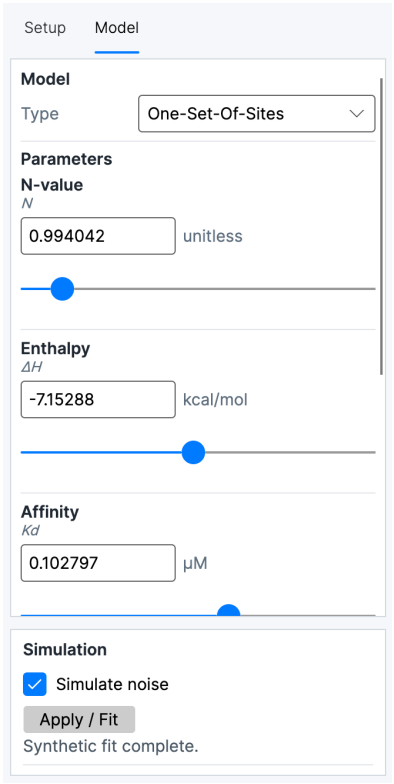
Setup and model controls

The **Setup** tab contains **Instrument**, **Cell uM**, **Syringe uM**, injection **Count**, and **Volume uL**. Count and volume define the injection schedule. **Automatic injection volume** derives the injection volume from the selected instrument's standard syringe volume and injection count. **Small first injection** gives the first injection of each load a smaller volume and marks it excluded. **Tandem simulation** creates consecutive loads, with **Segments** defining their count and the designer's tandem back-mixing model.



Setup defines the instrument, concentrations, injection schedule, tandem behavior, and simulation state.

The **Model** tab contains **Type**, exposed model **Parameters**, and model-specific **Options**. **Simulate noise** adds synthetic measurement noise. **Apply / Fit** fits the synthetic data in the designer window and reports the fit on its graph; neither the simulation nor this fit becomes an Analysis Result or Experiment Data entry.



Model exposes the synthetic model type and its parameter values.

Buffer Subtraction

BEFORE YOU BEGIN:

Process the reference experiment and every target experiment. Buffer subtraction operates on their integrated injection heats.

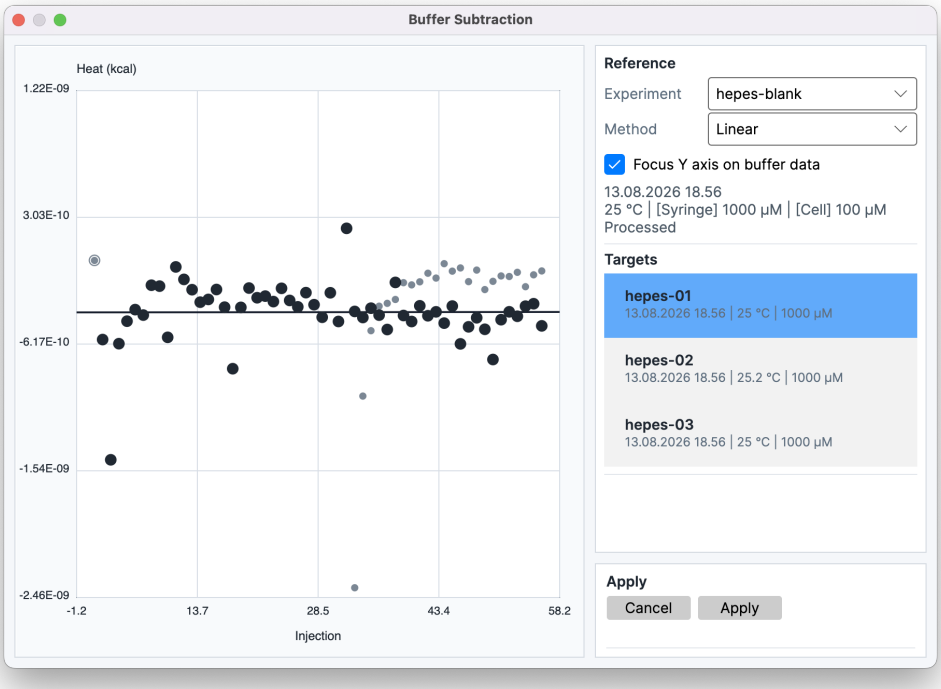
Buffer Subtraction... models background heat from one processed reference experiment and applies the resulting correction to one or more target experiments. The reference selector shows experiment metadata and a **Processed** or **Not yet processed** status. The target list excludes the selected reference and supports multiple targets. A processed reference is required; its processing state is described in Processing.

The **Method** selector contains **Matched**, **Linear**, and **Exp. decay**:

- **Matched** evaluates the reference heat at each target injection number, using nearby included reference injections when the matching injection is unavailable.
- **Linear** fits a line through valid, included reference injections and evaluates it across target injections.

- **Exp. decay** fits an exponential-decay model through valid, included reference injections when enough points are available.

The preview graph shows reference and target heats and the selected subtraction model. Reference-point inclusion changes the points available to the fitted methods. **Focus Y axis on buffer data** changes only the preview range. A continuous model line appears for **Linear** and **Exp. decay**; **Matched** is represented by injection-level reference values.



Buffer Subtraction previews the selected reference model and target experiments before storing the correction.

CALCULATION:

$$q_{i,\,\mathrm{corr}} = q_{i,\,\mathrm{target}} - q_{i,\,\mathrm{ref}}$$

The selected method determines the reference value evaluated for injection *i*. $q_{\mathrm{i,target}}$ is the target heat, $q_{\mathrm{i,ref}}$ is the corresponding reference value, and $q_{\mathrm{i,corr}}$ is the corrected heat used downstream.

Apply stores the reference and method on each target. The corrected heats are then used by downstream fitting and export while the original integrated heats remain unchanged. The reference Experiment Data becomes inactive. Changes in its processing or injection inclusion

update the target corrections. The subtraction is project data and can affect the validity of dependent results.

Experiment Merger

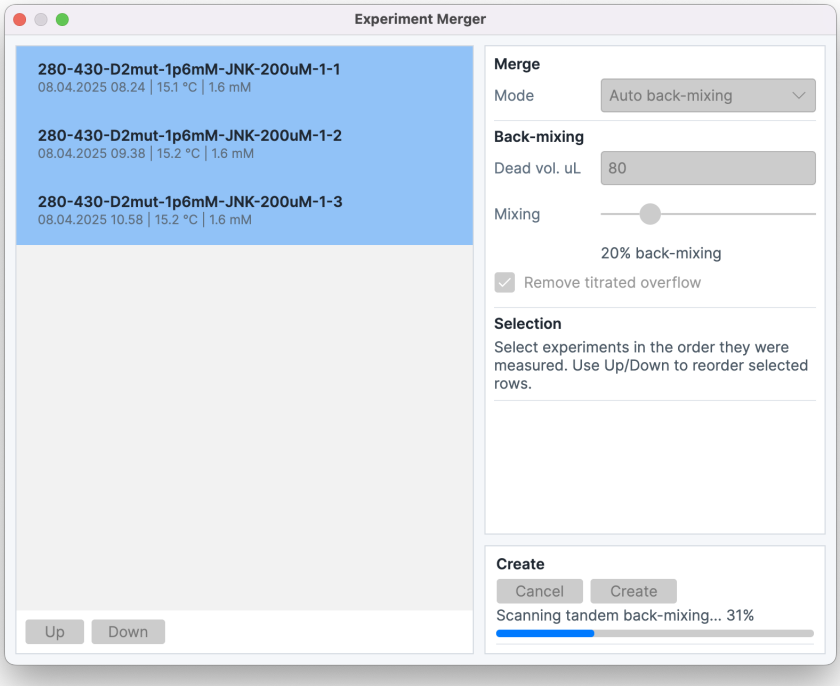
> **BEFORE YOU BEGIN:**
> Process each source experiment before merging. The merger uses its baseline-corrected thermogram when processing is available; otherwise, the application can fall back to the raw thermogram. The newly merged Experiment Data is processed automatically.

Experiment Merger... joins two or more eligible thermogram experiments from consecutive segments of a tandem titration. The source list contains thermograms that are not already tandem experiments. Selection order defines segment order; **Up** and **Down** reorder selected rows.

The merge **Mode** selector contains:

- **Simple tandem**, which concatenates the segments using the standard concentration progression without a user-selected back-mixing correction.
- **Fixed back-mixing**, which applies one configured mixing fraction at every segment transition. With three or four selected experiments, you can instead set an individual fraction for each reload.
- **Auto back-mixing**, which scans for a transition mixing fraction and is available for up to five source experiments. Its initial grid adapts to the number of sources (2%, 5%, 10%, and 20% steps for two through five experiments), followed by local pattern searches at smaller steps.

Back-mixing controls include **Dead vol. uL**, the **Mixing** fraction, and **Remove titrated overflow**. Dead volume represents the filling-stem or overflow volume above the active cell volume. The overflow control records whether titrated overflow was removed between segments. In Fixed mode, the shared slider supplies the fraction. With three or four experiments selected, enable the individual-fractions option to set **Reload 1**, **Reload 2**, and, for four experiments, **Reload 3** separately. In Auto mode, the scanner determines the transition values.



Auto back-mixing scans possible transition corrections for an ordered tandem experiment set.

Create produces a new processed Experiment Data item. Its thermogram samples are time-shifted and concatenated, its injection sequence retains segment boundaries, and its segment metadata stores the calculated starting active-cell and active-titrant concentrations. The merged item's comments record the selected tandem mode and back-mixing parameters. Source experiments remain separate and are not changed by creation; the new item is marked as a tandem experiment and is not eligible as a later merger source. It is a snapshot and does not update if its source experiments are subsequently edited. The resulting item can be fitted through Analyze Data.

INTERPRETATION:

A configured or automatically fitted back-mixing fraction is a model-based correction, not a direct measurement of liquid mixing that occurred between runs.

Tandem injection-displacement correction

The dilution-method preference selects either the **MicroCal** or **Exponential** injection-displacement correction for both simple concatenation and back-mixing modes. Let u be cumulative injected volume divided by active cell volume. The ordinary no-back-mixing reference curves are

$$A_M(u) = (1 - u/2) / (1 + u/2)$$
$$B_M(u) = u(1 - u/2)$$

for MicroCal, and

$$A_E(u) = \exp(-u)$$
$$B_E(u) = 1 - \exp(-u)$$

for the exponential method. A is the retained fraction of the original cell material and B is the cell concentration of syringe material relative to its syringe concentration.

For an injection advancing the history from u_0 to u_1, define

$$r = A(u_1) / A(u_0)$$
$$M_1 = rM_0$$
$$L_1 = rL_0 + C_s[B(u_1) - rB(u_0)]$$

Here M and L are the current active-cell concentrations and C_s is the syringe concentration. After a segment transition, the concentrations produced by the active/dead-volume mixing model are authoritative, while u retains the uninterrupted injection history. With no back-mixing, repeated application telescopes exactly to the ordinary reference curves.

The MicroCal reference curves are from Malvern Instruments, *MicroCal ITC Analysis Software Using Origin User Manual*, MAN0577-02-EN-00 (20 May 2015), section 12.3.1, equations 2 and 4. The arbitrary-state transition above is an FT-ITC Analysis extension derived from those curves; the Malvern manual does not specify a tandem back-mixing transition. Because $A_M(2) = 0$, stateful MicroCal advancement stops before cumulative injected volume reaches twice the

active cell volume: a later transition would divide by zero, and extending the approximation beyond that point would give negative retained concentrations. The exponential method has no corresponding finite-volume boundary.

CHAPTER 11

Settings and defaults

Configure shared defaults for display, processing, fitting, and export.

Last verified: 2026-08-27

Preferences... contains **General**, **Processing**, **Fitting**, and **Export**. Settings labelled as defaults provide starting values for new or reset work. Display settings affect presentation; export settings affect generated tables and figures. Project-specific values stored in a project remain distinct from application preferences. Project and recovery behavior is covered in Installation, files, and projects.

Both desktop applications use the same built-in values for first launch and Restore Defaults, including a **20,000-iteration optimizer limit** and **10% automatic concentration SD**. Saved custom values remain in effect, including values between or beyond the slider presets. Ordinary Apply also preserves settings that are not shown in that application's Preferences window.

Restore Defaults stages the built-in values in the window. **Apply** saves the staged values as application preferences. **Cancel** closes the window without saving staged edits.

General

SETTING	EFFECT
Energy units	Select **Joule** or **Calories**. Displayed values automatically use the base or kilo prefix from the finite central values being shown; empty groups default to kJ or kcal.
Concentration unit	Shared default unit for concentration entry, parameter display, and supported result-table concentration fields; format-specific data exports use their documented units.
Designer instrument	Shared default instrument for the Experiment Designer and its instrument-specific volumes.

Number precision	Controls numeric presentation: **Strict**, **Standard**, **Single decimal**, or **All decimals**. It does not set export decimal places.
Uncertainty display	Shared uncertainty presentation: **Automatic**, **Standard deviation**, **Confidence interval**, **SD + confidence interval**, or **None**. Automatic uses the confidence interval for a quantity whose stored 95% interval is materially asymmetric around its best-fit value; otherwise it uses SD. This changes presentation, not the underlying fit or calculated uncertainty.
Reference temperature (°C)	Temperature used where a result or derived quantity is evaluated at a reference temperature.
Minimum temperature span (°C)	Minimum temperature variation required for temperature-dependent result analyses.
Minimum salt span (mM)	Minimum ionic-strength variation required for salt-dependent result analyses.
Include buffer in ionic-strength calculation	Includes buffer contribution when ionic strength is calculated.
Check for updates and online resources on launch	Controls launch-time online checks; it does not disable local analysis.
Confirm remove/delete actions	Controls confirmation before remove or delete commands.
Automatically discard injections outside the thermogram range	Controls automatic removal of orphan injections when data are loaded.
Enable autosave	Enables periodic recovery copies.
Interval (minutes)	Sets the autosave interval. The built-in default is **5 minutes**.

Maximum files	Sets the number of autosave files retained. The built-in default is **10 files**.
Prompt to recover after an interrupted session	Controls whether the application presents an available autosave recovery after an interrupted session. Recovery prompting is enabled by default.
Open Autosave Folder	Opens the folder containing autosave recovery files.

Energy family, concentration unit, number precision, and uncertainty presentation are shared application settings where the corresponding control is available. The energy family does not change internal joule storage or format-specific interchange exports. Automatic display uses kJ or kcal when a value group is empty, zero, non-finite, or at/above the 100-unit threshold; fixed publication/result-export overrides are configured in their respective dialogs.

Processing

SETTING	EFFECT
Dilution method	Sets the default dilution correction model: **MicroCal** or **Exponential**.
Buffer subtraction	Sets the default buffer-subtraction model: **Matched**, **Linear**, or **Exp. decay**.
Discard integration regions for baseline	Controls whether existing integration regions are excluded from baseline construction.
Reprocess integrated heats on load	For `.dat` and `.aff` imports, recalculates the injection concentrations and ratios from the imported injection volumes and experiment concentrations. It does not create a thermogram or repeat baseline correction and peak integration.
Point density	Sets the default spline point density: **Sparse**, **Balanced**, or **Dense**.
Handle mode	Sets the default spline handle calculation: **Mean** or **Median** in the preferences window.
Allow spline point time dragging by default	Controls whether spline points can be moved in time by default.
Copy integration start with selected region	Controls whether copying an integration region also copies its start time.

Processing preferences provide defaults for new processors. Processing values already stored with an experiment are not replaced merely by changing a preference.

Fitting

SETTING	EFFECT
Default solver	Sets the starting optimizer: **Nelder-Mead [SIMPLEX]** or **Levenberg-Marquardt**.
Error estimation	Sets the default uncertainty method: **None**, **Bootstrap residuals**, **Leave-one-out**, or **Profile likelihood**. The built-in method is **Bootstrap residuals**.
Bootstrap iterations	Sets the number of residual-bootstrap refits. Leave-one-out uses one refit per deletion and profile likelihood does not use this count. The built-in count is **100**.
Optimizer tolerance	Sets the solver tolerance preset: **Fast**, **Relaxed**, **Balanced**, **Strict**, or **Very Strict**. The built-in default is **Balanced**.
Max iterations	Sets the maximum number of optimizer iterations. The built-in default is **20,000**, both at first launch and after Restore Defaults is applied.
Parameter limits	Sets the default parameter-limit policy: **Standard**, **Extended**, or **No limit**.
Use injection-error weighted fitting	Controls weighting of injection observations by their estimated errors.
Include concentration uncertainty in bootstrap	Includes concentration uncertainty in residual-bootstrap resampling. Leave-one-out keeps concentrations fixed.
Automatic concentration SD (%)	Sets the automatic fractional concentration SD used when concentration-uncertainty handling is enabled.
Create single-experiment analysis result	Controls creation of an Analysis Result after a usable single-experiment fit. Disabled in the built-in defaults.
Create global analysis result	Controls creation of a combined Analysis Result after a usable multiple-experiment fit. Enabled in the built-in defaults.
Auto-open new analysis result	Controls whether a newly created result is opened automatically.

Bootstrap method and count are shared fitting defaults; concentration sampling and parameter unlocking apply only to residual bootstrap. Profile updates retain the successful primary fit when profiling is cancelled or fails, and install partial output only under the stored replacement policy. Fit-specific settings captured in an Analysis Result remain part of that result. See Single-experiment fitting for model and uncertainty interpretation.

AI interpretation access

Without a code, AI interpretation uses the public **Default** depth. Enter a capability code and choose **Verify Access** to load the choices granted by that code. Standard and Advanced access show a single **Interpretation depth** selector populated by MIST; Administrator access instead shows model and reasoning controls. Preferences show the locally cached account status, label/name, email, access level, quota usage, total prompts, expiration, and most recent request when the service provides them. The cached account summary is displayed immediately and refreshed when Preferences opens; a temporary refresh failure leaves the cached values marked as cached. The code remains masked and is checked again whenever an interpretation is generated. If it expires or is revoked, generation is blocked until the code is replaced or removed to return to the Default setting.

Export

SETTING	EFFECT
Selection	Sets the default export scope: **Selected experiment**, **Active experiments**, or **All experiments**.
Decimals	Sets the number of decimal places in exported numeric tables.
Export baseline-corrected data	Includes baseline-corrected data in data exports.
Export fit points with peaks	Includes fitted peak points with exported peak data.
Molar ratio	Includes molar-ratio values in exported tables.
Injection info	Includes injection volume, delay, peak error, integration length, and temperature columns.

Concentrations	Includes cell and syringe concentration columns.
Included state	Includes the injection-inclusion state.
Peak heats	Includes integrated peak heats.
Fit values	Includes fitted values.
Width cm and **Height cm**	Set the default final-figure dimensions. The built-in dimensions are **6.5 × 10 cm**.
Publication font	Selects the publication figure font where the platform provides this selector.
Show residual graph	Includes the residual graph in final figures.
Show residual graph gap	Includes the gap separating residual and fit panels.
Unify residual graph axis	Uses a common residual-axis scale across applicable panels.
Fit line	Sets fit-line smoothing: **Smooth**, **Spline**, or **Linear**.
Show parameter box by default	Includes the parameter information box in new final figures.
Show experiment details by default	Includes experiment metadata in the figure information box.
Show model info by default	Includes model information in the figure information box.
Auto axes ignore excluded/bad points	Excludes points marked excluded or bad when automatic axes are calculated.
Thermodynamic parameters	Includes thermodynamic parameters in final-figure information.
Offset parameter	Includes the fit offset in final-figure information.
Derived parameters	Includes derived parameters in final-figure information.
Temperature	Includes temperature in final-figure information.
Concentrations	Includes concentrations in final-figure information.

Injection delay	Includes injection delay in final-figure information.
Instrument	Includes instrument information in final-figure information.
Attributes	Includes experiment attributes in final-figure information and limits their display to **Used in analysis**, **All**, or **None**.

Export preferences affect newly generated exports and figure defaults; they do not rewrite an existing export or a stored figure configuration. See Figures and export for output formats and units.

> **PLATFORM NOTE:**
> The **Publication font** selector is available on Windows and Linux, with choices of **Native**, **Inter**, and **Liberation Sans**. Some macOS releases use the native publication renderer and do not show this selector.

CHAPTER 12

Glossary and equations

Terminology, keyboard conventions, calculation symbols, equations, and references.

Last verified: 2026-09-01

Workspace terms

TERM	MEANING IN FT-ITC ANALYSIS
Experiment Data	One imported or application-created ITC dataset, including its details and analysis state.
Data / Results	The workspace list containing experiments and stored Analysis Results.
Selected	The item currently shown or targeted by a selection-specific command.
Active experiments	Experiments included in a multi-experiment operation.
Solution	A fitted model state for one experiment.
Analysis Result	A stored fit result with one or more member solutions and the fit state used to create it.
Attribute	Experiment metadata used for organization or analysis context.
Valid result	An Analysis Result whose recorded fit inputs still match the current project state.
Correlation view	Pearson correlations between fitted parameter coordinates across one listwise-complete residual-bootstrap ensemble, with finite-simulation precision diagnostics.
Pearson correlation	A value from –1 to +1 describing linear co-variation between two fitted coordinates.
Monte Carlo precision interval	Approximate Fisher-transformation interval describing how precisely the correlation coefficient *r* is estimated from the finite retained-refit ensemble; it is not uncertainty for either fitted parameter or a model-validity assessment.
AIC / AICc	Analysis-level criteria for comparing saved fits with the same observations, response definition, weighting mode, and likelihood convention; smaller values are preferred. Both modes estimate one residual-variance parameter; weighted criteria use integration errors as relative uncertainties. AICc uses the standard small-sample approximation for nonlinear fits and is preferred when available. Independently fitted members also show a per-member AICc / AIC column for same-experiment comparisons. Neither criterion establishes model adequacy.

Uncertainty terms

TERM	MEANING IN FT-ITC ANALYSIS
Best-fit value	Parameter value from the primary optimization. Resampling estimates uncertainty around this value but does not replace it with a resampling mean or median.
Standard deviation (SD)	Root-mean-square deviation of retained resampling values from the primary best-fit value.
95% confidence interval (CI)	The 2.5th and 97.5th percentiles of the retained resampling distribution. It can be asymmetric around the best-fit value.
Automatic uncertainty display	Shows CI for a materially asymmetric stored interval and SD otherwise. It selects a presentation separately for each reported quantity.
Displayed parameter uncertainty	Fitted-coordinate uncertainty after conversion or propagation into the quantity shown to the user. The Automatic display decision is applied to this displayed quantity.
Profile likelihood	Fixed-95% conditional profiling. Unweighted intervals use an F-calibrated RSS increment under independent Gaussian residual assumptions; weighted intervals use a one-degree-of-freedom chi-square increment conditional on supplied peak-area SDs. A parameter bound reached before crossing is censoring, not a confidence endpoint. The reported primary fit remains unchanged.
Profile equivalent SD	Symmetric `value ± SD` display scale computed from a complete asymmetric profile interval; it is a display equivalent, not a Gaussian sampling SD.

Keyboard conventions

The application command modifier is **Command** on macOS and **Ctrl** on Windows or Linux.

SHORTCUT	FUNCTION
Command/Ctrl + O	Open data or a project.
Command/Ctrl + S	Save the current project.
Command/Ctrl + Shift + S	Save the project under another name.
Command/Ctrl + E	Open data export.
Command/Ctrl + P	Print the active graph or figure.
Command/Ctrl + Z	Restore the most recently removed item.
Command/Ctrl + I	Invert the Active Experiment Data set.
Command/Ctrl + comma	Open Preferences.
Command/Ctrl + Q	Quit FT-ITC Analysis.
F1	Open **Help and Guide** on Windows and Linux. On macOS, open Help through the **?** menu command.
Enter	Open **Details** for the selected Data/Results item on Windows and Linux.
Left / Right	Change the selected injection in **Process Data**.
Space	Copy the selected integration length to the next injection in **Process Data**; the start is also copied when that processing option is enabled.

Thermodynamic symbols

SYMBOL	MEANING
N	Stoichiometry or site-number term under the selected model.
α	Syringe-side active-concentration correction when syringe correction is enabled.
K_a	Association constant.
K_d	Dissociation constant.
K_i	Macroscopic association constant for sequential transition i.
β_i	Cumulative sequential association product $\prod_{j=1\ldots i} K_j$.
F_i	Fraction of macromolecule in sequential state MX_i.
$\bar{\nu}$	Mean ligand occupancy in the sequential model.
ΔH	Binding enthalpy change.
ΔG	Gibbs free-energy change.
$-T\Delta S$	Entropic contribution reported by the application at the evaluation temperature.
ΔC_p	Heat-capacity change in a supported temperature-dependent analysis.
q	Integrated injection heat.
σ	Standard uncertainty or spread, according to context.
Offset	Energy-per-mole-of-injectant correction included in the modeled injection heat.

Calculation symbols

SYMBOL	MEANING
$P(t)$	Differential power at time t in a thermogram.
$b(t)$	Estimated baseline at time t.
n_i	Amount injected in injection i.
r_i	Residual for injection i: observed heat minus model heat.
r_{jk}	Pearson correlation between fitted parameter coordinates j and k.
θ_{bj}	Value of fitted coordinate j in complete bootstrap refit b.
σ_i	Processing-derived uncertainty for injection i.
R	Gas constant.
T	Absolute temperature, in kelvin, for thermodynamic relationships.
I	Ionic strength used in salt analysis.
a_{ion}	Ion activity used in Counter Ion Release analysis.
m	Fitted slope in the Protonation relationship; the application reports **Protons** as $-m$.
n_{ion}	Counter-ion slope reported by Counter Ion Release analysis.
RSS	Raw residual sum of squares, Σr_i^2, over included injections.
Q	Standardized residual sum of squares, $\Sigma(r_i/\sigma_i)^2$. Weighted AIC/AICc estimates a common variance multiplier as Q/n.
L	Gaussian likelihood used for AIC/AICc.
p	Number of free fitted parameters in the saved global model; shared coordinates count once and member coordinates count per member.
K	AIC/AICc likelihood parameter count: $p + 1$ in both weighting modes, including one estimated common residual variance or one estimated multiplier of the injection-error variances.

Equation index

RELATIONSHIP	LOCAL EXPLANATION
Integration and molar normalization	Processing
Monomer–dimer association	Dissociation
Sequential binding polynomial and ligand balance	Sequential Binding Sites
Thermodynamic conversion and **−TΔS**	Thermodynamic relationships
Fit residuals, RMSD, and weighting	Weight by injection error
AIC, AICc, Gaussian likelihood, and parameter counting	Information criteria
Temperature-dependent constraints	Multiple-experiment fitting
Parameter correlation (Pearson residual bootstrap)	Parameter correlation
Bootstrap SD and percentile confidence interval	Parameter uncertainty
Automatic uncertainty display	Uncertainty and evaluation temperature
Salt dependence	Salt
Protonation dependence	Protonation
Buffer correction	Buffer Subtraction
Tandem injection-displacement correction	Tandem injection-displacement correction

Units are those shown by the application or export.

References

- FT-ITC Analysis repository
- FT-ITC Analysis website
- FT-ITC Project Viewer
- Software DOI: 10.5281/zenodo.14832177
- Malvern Instruments, *MicroCal ITC Analysis Software Using Origin User Manual*, MAN0577-02-EN-00 (20 May 2015), section 12.3.1, equations 2 and 4.
- **Help > Citation** for the current paper citation, versioned software citation, and BibTeX

Scientific claims and model-specific methods require the primary literature appropriate to the experiment and analysis.