8   Data Processing

This chapter explains how to perform data processing in the spectrum and time course basic analysis applications.

8.1   Manipulate

Change to the [Active] tab in the graph view.

The types of Manipulate are [Data Set], [Transformations], and [Arithmetic].

8.1.1   [Data Set] Operations

Data Operation (Data Set Calculation)

Item	Description
[Type]	Select the type of operation to perform for data set calculation. In data set calculation, select two data sets and an operator to perform an arithmetic operation (addition, subtraction, multiplication, or division) on the two data sets. For example, when [Subtraction] is selected for two spectrum data sets, the data of [Data Set B] is subtracted from the corresponding data in [Data Set A] for each of the same wavelengths. **NOTE** The data interval of the data set created in data set calculation is the same interval as [Data Set A]. If the data interval of the two data sets is different, [Data Set B] is interpolated to match the X-axis values of [Data Set A] before calculation is performed. (Interpolation is only performed internally and does not change [Data Set B] in memory.)

[Data Set A] [Data Set B]	Displays the name of the active spectrum (data set name) targeted for calculation. • [Data Set A]: Displays the active data set. • [Data Set B]: Select [Data Set] from the list.
[Operator]	Select an operator from addition, subtraction, multiplication, and division.
[Execute]	Execute the set calculation processing.

8.1.2   [Transformations] Operations

Data Operation (Transformations)

Item	Description
[Type]	Select the type of operation to perform for data transformation. In data transformation, transformation processing is performed according to the selected transformation method for the specified data set to create a different data set. **NOTE** The calculation for smoothing and derivatives is performed based on a convolution function that uses 17 data points. Because the used data points comprise the eight points each before and after the target data for calculation, both ends of the data range cannot be calculated.
[Data Set]	Displays the name of the active spectrum (data set name) targeted for calculation. **Hint** Set the active data set in the tree view.
[Transformation Method]	Select a transformation method from derivative, logarithm, reciprocal, power, square root, logarithm (ln), and exponential.
[Order]	This is displayed when [Derivative] is selected for [Transformation Method]. Select an order from smoothing, 1st, 2nd, 3rd and 4th.
[Delta Lambda]	This is displayed when [Derivative] is selected for [Transformation Method]. The derivative wavelength difference or derivative time difference is displayed. While the value of [Delta Lambda] varies according to the data interval of the data to transform, there are four levels that can be selected. **NOTE** Increasing the [Delta Lambda] value decreases noise and reduces fluctuations in the derivative spectrum. However, increasing this value too much will degrade spectrum resolution.
[Scaling Factor]	This is displayed when [Derivative] is selected for [Transformation Method]. Enter the scaling factor to use after transformation. This facilitates comparison with the data before transformation.
[Exponent]	This is displayed when [Power] is selected for [Transformation Method]. Enter the exponent for power calculation.
[Execute]	Execute the set calculation processing.

8.1.3   [Arithmetic] Operations

Data Operation (Arithmetic)

Item	Description
[Type]	Select the type of operation to perform for arithmetic calculation. In arithmetic calculation, addition, subtraction, multiplication, or division can be performed on data. For example, adding a constant of "2" to a data set creates a new data set with "2" added to all values on the Y axis.
[Data Set]	Displays the name of the active spectrum (data set name) targeted for calculation. **Hint** Set the active data set in the tree view.
[Operator]	Select an operator from addition, subtraction, multiplication, and division.
[Constant]	Enter the constant to use in calculation.
[Execute]	Execute the set calculation processing.

8.2   Data Print

Change to the [Overlay] tab in the graph view.

Hint   Only the spectrum (time course) data displayed on the [Overlay] tab is listed in the table.

Data Print

No.	Item	Description
		Select the display type of the data print table. • [See all the data] Display all the spectrum (time course) wavelengths and data shown on the [Overlay] tab. • [Fit the active data]

❶	Data print type	Use the active data to determine the data interval and range of the data print table. • [User Configuration] Set any data interval and range for the data print table. **Hint** When [See all the data] is selected, the smallest data interval value from among all open data files is selected for data print. For example, when a data file with a data interval of 0.2 nm and a data file with a data interval of 0.5 nm are open at the same time, 0.2 nm is selected. Therefore, in regard to the data with the 0.5 nm data interval, data of which the first decimal place is "0" (XXX.0) will be displayed, but data of which the first decimal place is "5" (XXX.5) will not. To display all data, select [User Configuration] and set the data interval to "0.1 nm".
❷	[Execute]	Update the data print table with the selected type and settings.
❸	[User Configuration] parameters	This field is enabled when [User Configuration] is selected. Click [Execute] to update the settings.
	[Start]	Set the start wavelength (time) of the data print table. Effective range: Minimum wavelength to maximum wavelength of the spectrum displayed on the [Overlay] tab
	[End]	Set the end wavelength (time) of the data print table. Effective range: Minimum wavelength to maximum wavelength of the spectrum displayed on the [Overlay] tab
	[Interval]	Select the data interval of the data print table.
❹	Data print table	Displays wavelengths (times) and fluorescence intensity. When changing the column width, move the mouse cursor to the column title boundary and when the cursor changes to ⊕ , drag to the side. **NOTE** Dragging the column when the cursor is in the ⊕ status will show a hidden column (e.g [RawData]). To return to the hidden state, click [Data Print] again.
	[Wavelength] /[Time]	Displays the item that corresponds to the X axis in the first column. Clicking on the column title row switches the display order to ascending or descending order of wavelengths (times).
	[Intensity]	Displays the fluorescence intensity values that correspond to the wavelengths (times) of the first column with respect to the spectrum (time course) data displayed on the [Overlay] tab. The data set name shown on the column title is displayed according to the data display format set via [User Settings] on the [Tools] menu. **Reference** • "[User Settings] window (spectrum application)" • "[User Setting] window (time course application)"

■**Right-click menu of the data print table**

Click the right mouse button on the data print table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Select All]	Select (highlight) all content in the table.
[Print]	Perform a quick print. Set the report file to use in the [User Setting] on the [Tools] menu. **Reference** "[User Setting] window (common)"

8.3   Point Pick

Change to the [Active] tab in the graph view.

| Point Pick | Wavlength(nm): | 586.0 | | Add | Template: | Open... | Save As... |

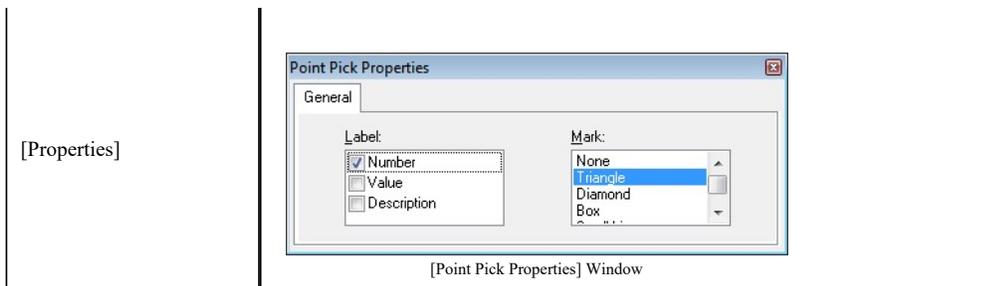| No.	Wavelength nm.	Intensity	Description
1	456.0	31.5	
2	559.0	185.0	
3	586.0	17.5	

Point Pick

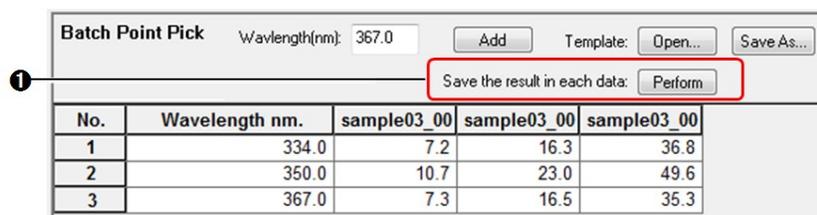| Item	Description
[Wavelength (nm)] ([Time])	Enter the wavelength (time) for extracting fluorescence intensity from the spectrum (time course) data.
[Add]	Execute point pick using the wavelength (time) entered for [Wavelength] ([Time]) and add one row to the table.
[Open]	Load an existing point pick template file (a file that stores the wavelengths (times) for extraction) in the [Open - Template File] window.
[Save As]	Save the wavelengths (times) in the current table as a template file in the [Save As - Template File] window.
Point pick table	Displays the fluorescence intensity for added wavelengths (times).
	[Wavelength nm.]/ [Time]	Displays the wavelengths (times) for which point pick was executed.
	[Intensity]	Displays the fluorescence intensity that corresponds to the wavelengths (times) that underwent point pick.
	[Description]	Enter a comment to describe an added point pick. (Character limit: 256 one-byte characters)

■**Right-click menu of the point pick table**

Click the right mouse button on the point pick table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Paste]	Paste the content on the clipboard to the [Description] column.
[Select All]	Select (highlight) all content in the table.
[Delete Point]	Delete the selected rows in the table. 💡 **Hint** Clicking [No.] in the point pick table selects (highlights) the corresponding row.
[Show Point Mark]	Indicate the position of data points in the point pick table on the spectrum (time course) graph using the specified mark.
[Print]	Perform a quick print. Set the report file to use via [User Setting] on the [Tools] menu. ▶▶ **Reference** "[User Setting] window (common)"
	Display the [Point Pick Properties] window and select the labels (number, value, description) and mark type (triangle, diamond, down arrow, etc.) to display on the graph.

[Properties]	 **Point Pick Properties** General Label: ☑ Number ☐ Value ☐ Description Mark: None Triangle Diamond Box [Point Pick Properties] Window

8.4   Batch Point Pick

Change to the [Overlay] tab in the graph view.

Batch Point Pick   Wavlength(nm): 367.0   [Add]   Template: [Open...] [Save As...]

❶ ⟶ Save the result in each data: [Perform]

No.	Wavelength nm.	sample03_00	sample03_00	sample03_00
1	334.0	7.2	16.3	36.8
2	350.0	10.7	23.0	49.6
3	367.0	7.3	16.5	35.3

Batch Point Pick

No.	Item	Description
-	[Wavelength] ([Time])	Enter the wavelength (time) for extracting fluorescence intensity from the spectrum (time course) data.
-	[Add]	Execute point pick using the wavelength (time) entered for [Wavelength] (Time]) and add one row to the table.
-	[Open]	Load an existing point pick template file (a file that stores the wavelengths (times) for extraction) in the [Open - Template File] window.
-	[Save As]	Save the wavelengths (times) in the current table as a template file in the [Save As - Template File] window.
❶	[Save the result in each data:]	Click [Execute] to update the results in the batch point pick table to the point pick table of each data set. When a point pick table already exists for a data set, the following confirmation message is displayed indicating the target table will be overwritten. **LabSolutions RF** Updates each spectrum point pick table with batch point pick results. Point pick table is overwritten. OK? ☐ Do not display this prompt in the future [Yes] [No] Confirmation Message **NOTE** If the message is closed with the [Do not display this prompt in the future] checkbox selected, the table will be overwritten without displaying this confirmation message from the next time [Execute] is clicked. To display this confirmation message again, set the relevant option via [User Settings] on the [Tools] menu. **Reference** • "[User Settings] window (spectrum application)"

				"[User Setting] window (time course application)"
-	Batch point pick table		Displays the fluorescence intensity for added wavelengths (times).	
		[Wavelength nm.]/[Time]	Displays the wavelengths (times) for which point pick was executed.	
		[Intensity]	Displays the fluorescence intensity of all loaded spectrum (time course) data. The data set name shown on the column title is displayed according to the data display format set via [User Settings] on the [Tools] menu. ▶▶ Reference • "[User Settings] window (spectrum application)" • "[User Setting] window (time course application)"	

■Right-click menu of the batch point pick table

Click the right mouse button on the batch point pick table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Select All]	Select (highlight) all content in the table.
[Delete Point]	Delete the selected rows in the table. 🔆 **Hint** Clicking [No.] in the point pick table selects (highlights) the corresponding row.
[Print]	Perform a quick print. Set the report file to use via [User Setting] on the [Tools] menu. ▶▶ **Reference** "[User Setting] window (common)"

8.5   Peak Pick

Change to the [Active] tab in the graph view.

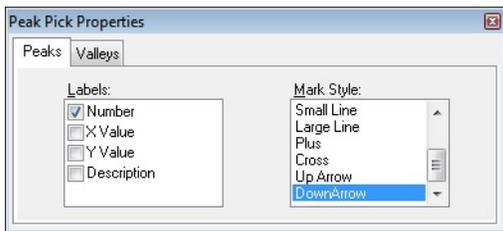| No.	P/V	Wavelength nm.	Intensity	Description
1	↑	327.5	4329.5	
2	↑	340.0	6044.1	
3	↑	435.0	71.9	
4	↑	444.0	52.5	
5	↑	473.5	26.9	
6	↓	329.5	4280.7	
7	↓	433.0	62.5	
8	↓	438.5	38.9	
9	↓	463.5	0.8	

Peak Pick: Threshold: 10   Points: 4   Execute

Peak Pick

Item	Description
[Threshold]	Set the threshold value (default of 10) used when detecting peaks. This value indicates the distance between the peak point and a line that connects the valley points (or provisional valley points) on each side of the peak point. Peaks with a distance shorter than the entered threshold value are excluded. The detection of unwanted peaks and noise can be avoided by adjusting the threshold value and number of points. Effective range: 0.01 to 10000
	Set the number of points (default of 5) used when detecting peaks. Peak detection occurs after the value consecutively increases for more than n points and then consecutively decreases for more than n points. The top of the peak (peak

[Points]		point) is taken as the point at which the value starts decreasing. Valley detection occurs when the opposite condition (value consecutively decreases for more than n points and then consecutively increases for more than n points) is satisfied. The number of points, n, can be changed. Effective range: 1 to 100
[Execute]		Perform peak detection using the threshold and number of points entered for [Threshold] and [Points].
Peak pick table		Displays information on detected peaks.
	[P/V]	Indicates whether the detected wavelength is a peak (🔼) or valley (🔽) using marks.
	[Wavelength nm.]/ [Time]	Displays the wavelength (time) of the detected peak or valley.
	[Intensity]	Displays the fluorescence intensity of the detected peak or valley.
	[Description]	Enter a comment to describe the peak or valley. (Character limit: 256 one-byte characters)

■**Right-click menu of the peak pick table**

Click the right mouse button on the peak pick table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Paste]	Paste the content on the clipboard to a [Description] cell.
[Select All]	Select (highlight) all content in the table.
[Graph]	Display or hide peak marks and valley marks on the graph.
[Show Peaks]	Display or hide peak information in the peak pick table.
[Show Valleys]	Display or hide valley information in the peak pick table.
[Print]	Perform a quick print. Set the report file to use via [User Setting] on the [Tools] menu. ▶▶ Reference "[User Setting] window (common)"
[Properties]	Display the [Peak Pick Properties] window and select the labels (number, value, description) and mark type (triangle, diamond, down arrow, etc.) for peaks and valleys displayed on the graph. [Peak Pick Properties] Window

8.6   Peak Area

Change to the [Active] tab in the graph view.

Peak Area

No.	Item	Description
-	[Start]	Enter the start wavelength (time) of the range for calculating area. Effective range: X-axis start value to X-axis end value of the active spectrum (time course)
-	[End]	Enter the end wavelength (time) of the range for calculating area. Effective range: X-axis start value to X-axis end value of the active spectrum (time course)
-	[Add]	Execute area calculation on the entered wavelength (time) range and add a result row to the table.
-	[Open]	Load an existing Peak Area template file (a file that stores the ranges for area calculation) in the [Open - Template File] window.
-	[Save As]	Save the range of wavelengths (times) in the current table as a template file in the [Save As - Template File] window.
❶	[Factor]	Enter the factor for multiplying the area under the data curve. This factor is used in the calculation of all table rows. Effective range: 0.0001 to 10000
❷	[Baseline to Zero]	Select this checkbox to perform area calculation from the zero line. This is used in the calculation of all table rows.
-	Peak Area table	Displays the conditions and results of area calculation.
	[Color]	Displays the color and style corresponding to each area calculation item. In order to differentiate between different areas on the graph, different colors and styles must be set in advance for each calculation item. A solid color style can also be selected.
	[Start]	Indicates the start wavelength or start time of the calculation region.
	[End]	Indicates the end wavelength or end time of the calculation region.
	[Divisor]	Indicates the divisor assigned to the area under the data curve. The default value is "1".
	[Area]	Indicates the area under the data curve in the set calculation region.
	[Result]	Indicates the result of the area column value divided by the divisor column value and then multiplied by the [Factor]. When both the divisor and [Factor] are "1" in the table, the area column value and the result column value are the same.
	[Description]	Enter any remarks or comments on the specified region.

■**Right-click menu of the Peak Area table**

Click the right mouse button on the Peak Area table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Paste]	Paste the content on the clipboard to a [Description] cell.
[Select All]	Select (highlight) all content in the table.

[Delete Region]	Delete the selected rows in the table. 💡 **Hint** Clicking [No.] in the point pick table selects (highlights) the corresponding row.
[Print]	Perform a quick print. Set the report file to use via [User Settings] on the [Tools] menu. ▶▶ **Reference** "[User Setting] window (common)"

8.7   Main Table

Change to the [Active] tab in the graph view.

Main Table   Start: 100.0   End: 200.0   [Calculation]

File	R	Activity	Initial Reading	SD	I/min	Factor	Correction Fator	Comment
TmcData_01	☐	161.4978	395.011	0.8793	-161.4978	1.0000	1.0000	

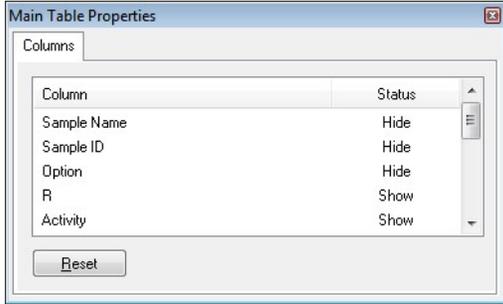Main Table (Display Columns in Default Configuration)

Item		Description
[Start]		Enter the start wavelength (time) of the range for calculating activity values. Effective range: X-axis start value to X-axis end value of the active time course
[End]		Enter the end wavelength (time) of the range for calculating activity values. Effective range: X-axis start value to X-axis end value of the active time course
[Calculation]		Execute activity value calculation on the entered wavelength (time) range and add a result row to the table.
Main table		Displays information (activity values in the specified region, etc.) on the time course data.
	[File]	Indicates the data set name of the time course data. The data display conforms to the format set via [User Settings] on the [Tools] menu. ▶▶ **Reference** "[User Setting] window (time course application)"
	[Sample Name]/ [Sample ID]/ [Option]	Indicates the sample information of the time course data.
	[R]	Select this checkbox to display the activity value calculation region on the graph. The calculation region is displayed with a dotted line.
	[Activity]	Indicates activity values. Activity values are calculated using first-order least-squares regression for each data entry in the activity value calculation region. The gradient is fluorescence intensity (I) per minute. Activity value calculation formula: Activity value = gradient × factor × correction factor
	[WL]	Indicates the wavelength during measurement.
	[Start]	Indicates the start time of the range in which activity values are calculated.
	[End]	Indicates the end time of the range in which activity values are calculated.
	[Initial Reading]	Indicates the fluorescence intensity at the start time of the activity value calculation region.
	[SD]	Indicates the standard deviation of [I/min].
	[I/min]	Indicates the rate of change in the fluorescence intensity (I) per minute.
	[Factor]	Indicates the factor used in activity value calculation.
	[Correction Factor]	Indicates the correction factor used in activity value calculation. This value is used to correct dilution and concentration factor errors.
	[Comment]	Displays the comment in the summary information of the data set. Entering or editing

	a comment here also updates the summary.

■Right-click menu of the main table

Click the right mouse button on the main table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Paste]	Paste the content on the clipboard to a [Description] cell.
[Select All]	Select (highlight) all content in the table.
[Print]	Perform a quick print. Set the report file to use via [User Setting] on the [Tools] menu. ▶▶ Reference "[User Setting] window (common)"
[Properties]	Display the [Main Table Properties] window and set whether to show or hide each column in the table. Click [Reset] to restore the default display settings. Main Table Properties Columns Column Status Sample Name Hide Sample ID Hide Option Hide R Show Activity Show Reset [Main Table Properties] Window

8.8   Intensity Difference Table

Change to the [Overlay] tab in the graph view.

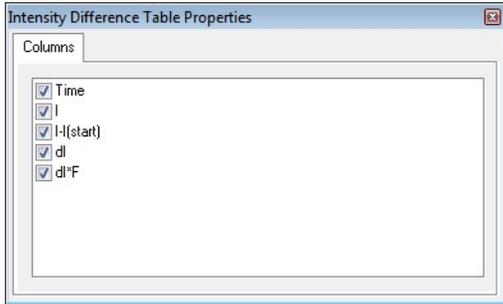Intensity Difference Table   Start: 80.000   End: 200.000   Calculation

Interval: 1.000   Factor: 1.000

	Tmc-01 - RawData				TmcData_01 - RawData			
Time	I	I-I(start)	dI	dI*F	I	I-I(start)	dI	dI*F
80.0	64.305	0.000			498.257	0.000		
81.0	63.915	-0.390	-0.390	-0.3900	494.670	-3.587	-3.587	-3.5875
82.0	63.173	-1.132	-0.742	-0.7420	492.277	-5.980	-2.393	-2.3928
83.0	62.454	-1.851	-0.719	-0.7190	487.021	-11.236	-5.256	-5.2560
84.0	61.986	-2.319	-0.468	-0.4680	477.319	-20.938	-9.702	-9.7021
85.0	61.350	-2.955	-0.636	-0.6360	468.521	-29.736	-8.798	-8.7976
86.0	61.287	-3.018	-0.063	-0.0630	466.682	-31.575	-1.839	-1.8390
87.0	60.589	-3.716	-0.698	-0.6980	458.924	-39.333	-7.758	-7.7583
88.0	60.292	-4.013	-0.297	-0.2970	456.562	-41.695	-2.362	-2.3621
89.0	59.630	-4.675	-0.662	-0.6620	453.271	-44.987	-3.291	-3.2913
90.0	58.337	-5.968	-1.293	-1.2930	449.492	-48.765	-3.778	-3.7785
91.0	58.074	-6.231	-0.263	-0.2630	444.966	-53.291	-4.526	-4.5265
92.0	57.863	-6.442	-0.211	-0.2110	429.572	-68.685	-15.393	-15.3934

Intensity Difference Table

Item	Description
[Start]	Set the start time of the intensity difference table.
[End]	Set the end time of the intensity difference table.
[Interval]	Set the display data interval of the intensity difference table.
[Factor]	Set the factor (F) used in calculating intensity differences.
[Calculation]	Calculate intensity differences using the entered data interval and factor and update the results to the intensity difference table.
Intensity difference table	Displays the fluorescence intensity for added wavelengths (times).
	[Time]	Indicates the times based on the set range and interval.
	Data set names	Displays the names of the loaded time course data sets. The data display conforms to the format set via [User Settings] on the [Tools] menu. ▶▶ Reference "[User Setting] window (time course application)"
		[I]	Indicates the fluorescence intensity values corresponding to the times in the first column.
		[I-I (start)]	Indicates the result of subtracting the fluorescence intensity at the start time displayed in the table from the fluorescence intensity at each time.
		[dI]	Indicates the amount of change from the previous fluorescence intensity for each data interval.
		[dI*F]	The value determined from the following calculation is displayed. $dI \times F$ （factor）

■**Right-click menu of the intensity difference table**

Click the right mouse button on the intensity difference table to display the following right-click menu.

Command	Description
[Copy]	Copy the content of the selected cells to the clipboard.
[Select All]	Select (highlight) all content in the table.
[Print]	Perform a quick print. Set the report file to use via [User Setting] on the [Tools] menu. ▶▶ Reference "[User Setting] window (common)"
[Properties]	Display the [Intensity Difference Table Properties] window and set whether to show or hide each column in the table. Intensity Difference Table Properties Columns ☑ Time ☑ I ☑ I-I(start) ☑ dI ☑ dI*F [Intensity Difference Table Properties] Window