

Technical Report

Usability Enhancements to the LabSolutions Manual Integration Function

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Abstract:

Manual peak integration is an essential feature for chromatograms when the peak cannot be integrated as desired using the automatic peak integration function based on parameter settings alone.

As manual peak integration must be performed on each data set, the ease of use of the user interface has a substantial effect on operating efficiency and the reliability of results.

This report introduces the LabSolutions manual peak integration function, which makes manual peak integration simple, error-free, and quick.

Keywords: data processing, manual peak integration, usability

1. Introduction

Since manual peak integration requires various types of processing depending on peak shape, it needs many features in the software as well as a user interface that allows interactive peak integration to be performed appropriately.

The relationship between multi-functionality and usability is normally that of a trade-off. To satisfy both requirements, it is important to design a system that accommodates multiple requirements simultaneously, in order to improve operating efficiency, enhance work quality, and reduce the time to system familiarization.^{1), 2)}

For these reasons, we performed a usability evaluation³⁾ with the main objective of enhancing system ease-of-use. Results show an improved manual peak integration function with LabSolutions.

This improvement reduced the average number of clicks in a workflow by half compared to the existing system design.

2. Requirements and Solutions for Usability Enhancement

A user interface is required that facilitates a simple, error-free, and fast interactive system. Improvements to the manual peak integration function were made based on a new concept and design that meet these demands.

2-1. Simple

Peak integration of the target peak can be performed simply using features that allow for intelligent peak integration according to peak shape and cursor position on the chromatogram view.

- Auto mode (Automatic processing command selection)

Peak shape is recognized automatically and an appropriate command is selected based on the cursor position, whereupon manual peak integration can be performed.

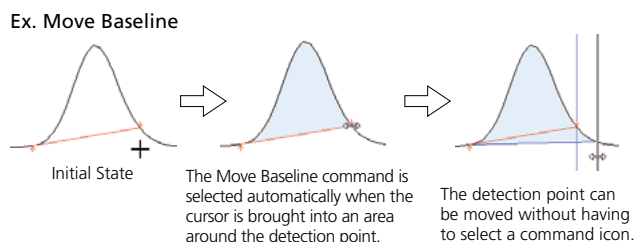


Fig. 1 Automatic Processing Command Selection in Auto Mode

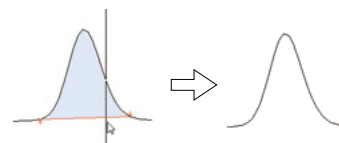
- Drag and click operation

Baseline movement and peak insertion can now be performed by performing a dragging operation with the mouse, or by clicking twice to specify the start and destination points of a movement or the peak start and end points. This provides more intuitive processing.

As for peak integration and peak rejection, single peaks can be processed with a click, and multiple peaks can be processed by dragging the mouse. Appropriate use of the click-and-drag operation has allowed for various command icons to be consolidated.

Ex. Reject Peak

- A single peak is rejected with a mouse click.



- Multiple peaks are deleted by dragging the mouse.

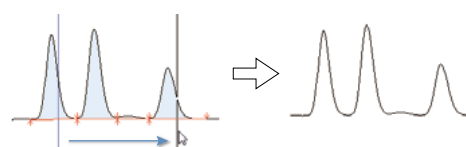


Fig. 2 Simplified User Interaction by a Mouse Drag Operation

- Baseline guide

A baseline guide function has been added. This function restricts movement of the detection point to a location on the chromatogram and to a position that gives a horizontal baseline.

This removes the need for fine mouse operation, and makes it easier to specify the target position of the detection point.

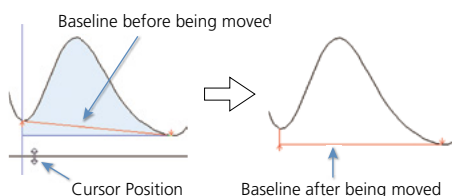


Fig. 3 Moving the Detection Point to a Position That Creates a Horizontal Baseline (left: during movement, right: after movement)

2-2. Error-Free

The following functions allow even a novice user to perform manual peak integration without hesitation.

- Pop-up hints and target objects highlighting

Pop-up hints describing the current operation are displayed next to the cursor as a guide. Also, during processing, the relevant peaks are highlighted by hatching (fill-in shading). These features were added so that important information stands out.

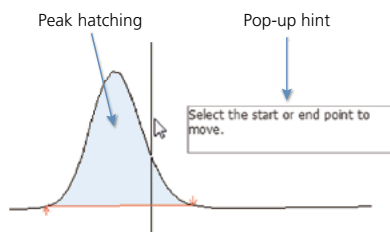


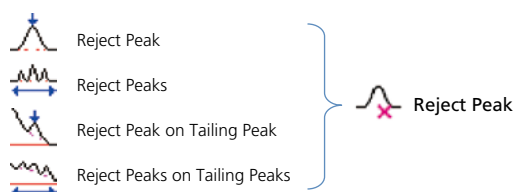
Fig. 4 Pop-up Hints and Target Objects Highlighting

- Consolidation/Splitting of Icons

Icons with similar functions and icons that represent single peak processing and multiple peak processing are consolidated, simplifying command selection.

Changing the workflow from one where the processing commands had to be selected from branch commands during processing results in a more consistent operation.

Consolidated icons



Split icons

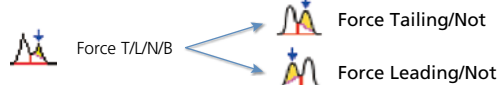


Fig. 5 Consolidation/Splitting of Icons

- Addition of new commands

New commands allow for implementation of complicated processing with a single command. This feature allows the user to implement a desired workflow with a single operation.

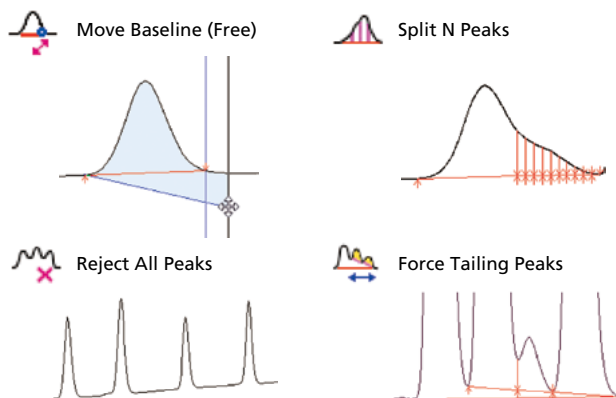


Fig. 6 New Command examples

2-3. Quick

Support functions allow for the implementation of faster peak integration with LabSolutions.

- Peak integration with keyboard shortcuts

Keyboard shortcuts such as Redo/Undo, and combining keys with click/drag operation, allow the user to select the processing they want without the need for command icon selection or moving the cursor near a chromatogram.

Table 1 Shortcuts

Command	Key
Insert Peak	I
Insert Peak (Free)	D
Split Peak	S
Unify Peaks	U
Reject Peak	R
Baseline Separation	B
Vertical Division	V
Tailing Processing	T
Leading Processing	L

- Deletion of unnecessary peaks

In addition to using the tool bar, peaks can now be deleted using the [Delete] key or the right click menu on the peak table or in the Chromatogram View.

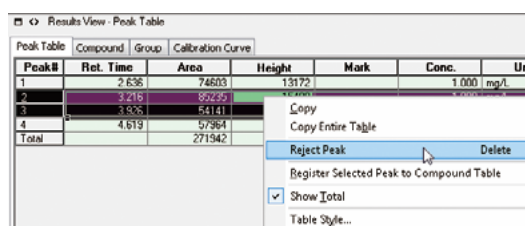


Fig. 7 Deleting Unnecessary Peaks from the Peak Table

- Screen Scrolling Using the Mouse Scroll Wheel

Peaks can be displayed in the desired position using the mouse scroll wheel to scroll left/right or up/down, and zoom in/out on the screen.

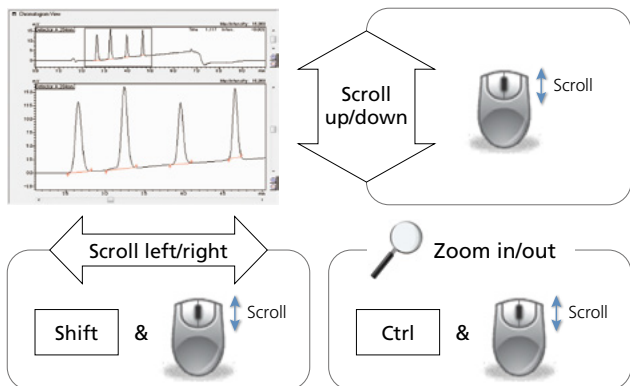


Fig. 8 Screen Scrolling Using the Mouse Scroll Wheel

3. Improvements Made to Enhance Usability

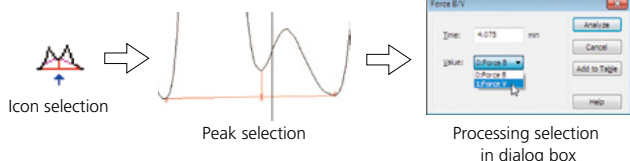
Ease-of-use improvements were made by evaluating system usability in terms of operability, recognition, and amenity, then improving the workflow accordingly.

3-1. Operability

The workflow was reviewed and improved to make implementation of a desired peak integration simpler to perform. This was achieved by reducing the number of operation steps, adding dragging operation, consolidating and separating commands, and adding new commands.

Ex. Baseline Separation (Number of mouse clicks reduced from 4 to 2.)

- Before Improvement



- After Improvement

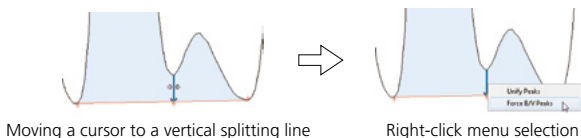


Fig. 9 Comparison of Old and New Workflows

3-2. Recognition

Recognition was improved by adding labeled icons, redesigning the user interface graphically, and changing the terminology used for naming commands so they can be more easily associated with their effect.

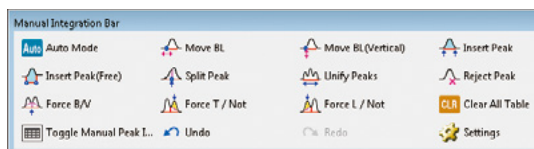


Fig. 10 Labeled Icons Added

3-3. Amenity

Auto mode and pop-up hints assist users in completing work even if they have forgotten a specific workflow.

The manual peak integration interface can also be customized. This includes changing the auto mode cursor detection area to the user's preferred size.

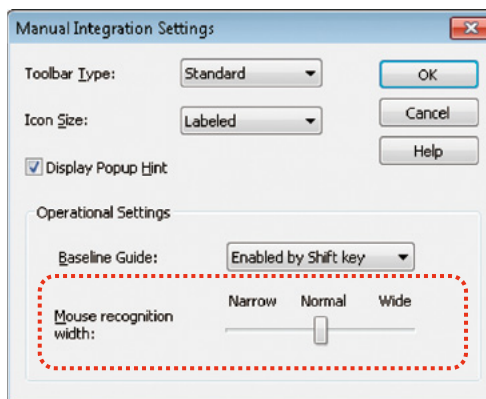


Fig. 11 Customization of the Manual Peak Integration Interface

These improvements enhance the usability of the interactive system and reduce the average number of clicks in a workflow by half compared to the existing manual peak integration function.

4. Legal and Regulatory Requirements

Regulatory compliant laboratories that must comply with PIC/S GMP or ER/ES guidelines are required to record and control records of all operations that affect analysis results.

The LabSolutions manual peak integration function records all manual peak integration operations in a command table of a data file, which allows reproduction of the same operations at any time. In addition, an audit trail function of peak integration history is an essential function for users that must be regulatory compliant.

The LabSolutions audit trail function allows the user to record change history and the reasons for changes made.

Annex 11: Computerised Systems – 9. Audit Trails

Consideration should be given, based on a risk assessment, to building into the system the creation of a record of all GMP-relevant changes and deletions (a system-generated "audit trail"). For change or deletion of GMP-relevant data, the reason should be documented. Audit trails need to be available and convertible to a generally intelligible form and regularly reviewed.

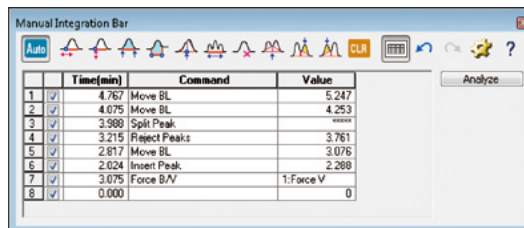


Fig. 12 PIC/S Guideline User Requirements and Management of Manual Peak Integration History

Table 2 Improvements to Manual Peak Integration Commands

Command	Improvements
General	<ul style="list-style-type: none"> • Addition of Auto Mode • Addition of shortcut keys (for each command, undo, redo, cancel selection) • Addition of highlighted display of relevant peaks and processes • Addition of pop-up hint labels • Removal of the selection between single processing and consecutive processing, and change to consecutive processing only • Removal of confirmation dialog box for processing commands • Addition of scrolling left/right, up/down on the screen, and zoom in/out via the mouse scroll wheel • Addition of the display state hold function of manual peak integration tool bar
Move Baseline Move Baseline (Vertical) Move Baseline (Free)	<ul style="list-style-type: none"> • Addition of drag operation • Addition of baseline guide function (movement along intensity axis and free direction movement only) • Addition of the [Move Baseline (Free)] command
Insert Peak Insert Peak (Free)	<ul style="list-style-type: none"> • Addition of drag operation • Name change (from [Insert Peak Start/End] to [Insert Peak (Free)])
Split Peak Split N Peaks	<ul style="list-style-type: none"> • Change of specification to split at a valley if there is a valley near to a specified time • Addition of the [Split N Peaks] command
Unify Peaks	<ul style="list-style-type: none"> • Consolidation of the processing icons for the single peak processing, multiple peak processing, and tailing/leading peak processing
Reject Peak Reject All Peaks	<ul style="list-style-type: none"> • Consolidation of the processing icons for the single peak processing, multiple peak processing, and tailing/leading peak processing • Addition of the [Reject All Peaks] command • Addition of peak deletion command to the [Peak Table] and [Zoom Chromatogram]
Force B/V Force B Peaks Force V Peaks	<ul style="list-style-type: none"> • Consolidation of icons for main peak processing and tailing/leading peak processing • Addition of drag operation (for multiple peak processing only)
Force T/Not Force L/Not Force T Peaks Force L Peaks Force N Peaks	<ul style="list-style-type: none"> • Separation of command icons for tailing processing and leading processing, and removal of processing selection in the dialog box • Addition of multiple peak processing
Clear All Table	<ul style="list-style-type: none"> • Addition of new commands

5. Conclusion

The design goal of this work was to develop a user interface that is simple, error-free, and quick. As shown, the LabSolutions manual peak integration function was improved and its usability enhanced. The key points of the changes are:

- Make it easier to learn how to use LabSolutions to reduce training costs and support costs.
- Relieve user stress to prevent user error.
- Improve the operating and practical efficiency of the system.

Usability enhancements contribute toward enhanced reliability and improved operating efficiency.

The new user interface is expected to increase workflow efficiency and enhance the reliability of analysis work.

References

- [1] ISO 13407:1999 "Human-Centred Design Process for Interactive Systems" (JIS Z8530 "Human-centred design processes for interactive systems" Japanese Standards Association)
- [2] ISO 9241-210: Human-Centred Design Process for Interactive Systems (2010)
- [3] Masaaki Kurosu, Masamori Sugizaki, Sachiyo Matsuura (1997) "Usability Evaluation Technique with High Efficiency —1. Structured Heuristic Evaluation (sHEM)—" Human Interface Symposium 481–488