



Library Editor 2 — User Guide

Agilent ChemStation/MassHunter PBM (.L) mass spectral library editor · Leoson BV ·
October 2026

1. Overview

Library Editor 2 opens Agilent PBM libraries (.L folders), shows one tab per library with a fast grid of entries and a spectrum chart, and writes the library back together with its condensed spectra, index and sort files (no msda.exe or pbmdbsort.exe needed). Spectra can be imported from MSP, MSL, JCAMP, CID and MassHunter files and exported to the same formats.

The grid columns are: **#**, **On** (included in ChemStation searches), **Name**, **Formula**, **CAS**, **MW**, **RT**, **RI**, **User**, **BP**, **MP**, **Company**, **Info**, **Full** and **Cond** (number of peaks in the full and condensed spectrum), **Dirty** (condensed spectrum will be regenerated on save) and the search results **Match**, **Dot** and **PBM%**. The **Filter:** box above the grid (Ctrl+E) shows only entries whose Name, Formula, CAS, Info or Company contain the typed text (case-insensitive); Esc clears it. The internal condensed-record fields (HFM, Low, KV, SK2MI) are no longer shown; they are still read, computed and written.

2. Installation

Run `LibraryEditor2-<version>-setup.exe`. It installs into `C:\Program Files\Leoson BV\LibraryEditor2` (64-bit), installs the Microsoft .NET 10 Desktop Runtime first when it is missing, and creates Start menu shortcuts for Library Editor 2, its User Guide (this PDF) and the uninstaller; a desktop icon is optional. The guide is copied next to the program, so **Help > User guide (PDF)** or **F1** opens it in your PDF viewer. Uninstall via Windows Settings > Apps or the Start menu.

3. Menus

All menus use the FastSuite menu. Shortcuts are shown next to the items and work from anywhere in the window.

Menu	Items
File	New library (Ctrl+N), Open library (Ctrl+O), Open recent, Import spectra (Ctrl+Shift+I), Save (Ctrl+S), Save as, Reload from disk, Close library (Ctrl+W), Export > (CID, MSL, MSP, JCAMP-DX, MassHunter library, MassHunter Quant reference library, Retention index field), Exit
Edit	Undo (Ctrl+Z), Redo (Ctrl+Y), Copy cells (Ctrl+C), Copy cells with headers (Ctrl+Shift+C), Paste cells / fill selection (Ctrl+V), Fill down / increment (Ctrl+D), Filter rows (Ctrl+E), Find (Ctrl+F), Find next (F3), Find previous (Shift+F3), Replace (Ctrl+H)
Entries	Copy entries (Ctrl+Alt+C), Cut entries (Ctrl+Alt+X), Paste entries (insert) (Ctrl+Alt+V), Duplicate entries, Delete entries (Ctrl+Del), Move up (Alt+Up), Move down (Alt+Down), Copy selected entries to another library, Include in search (On), Exclude from search (Off), Clean up text fields, Calculate MW from formula

Menu	Items
Spectra	Search library with full spectrum, Search library with condensed spectrum, Compare spectra (Ctrl+K), Regenerate condensed spectra (selected / all)
Library	Protected (read-only in ChemStation) (check item), About protected libraries, Lock library (for other users), Clear lock, Show in Explorer
Lookup	Name / CAS in web database, Name in PubChem, Name in Google
Help	User guide (PDF) (F1), Import license..., License info, About protected libraries, About Library Editor 2

Grid context menu (right-click a cell). The first block is FastSuite's standard cell menu: Cut, Copy, Copy headers, Copy image, Paste, Select all, Find, Fill down (runs *Fill down / increment*), Increment down. Library Editor 2 adds: Undo, Replace, Filter rows; Search library with full / condensed spectrum, Compare spectra; Copy / Cut / Paste / Duplicate / Delete entries; *Entry fields* > (Include, Exclude, Clean up text fields, Calculate MW); *Look up* > (WebBook, PubChem, Google); Protected (read-only in ChemStation).

4. Editing cells

Copy cells / Paste cells. Cells are copied as tab-separated text (plus CSV). This is the format Excel, LibreOffice, Google Sheets and text editors exchange, so no special "Excel" mode is needed. Pasting puts the clipboard block at the selection; a single value or one row fills the whole selection. Each paste is one undo step; invalid values are skipped and reported in the status line. Match, Dot and PBM% are computed and cannot be pasted into.

Fill down / increment (Ctrl+D). Select the seed cell and the cells below it in one column. Numbers increase by 1 per row (100, 101, 102 ...). Text that contains a number increments its *last* number and keeps the text around it: Sample-007b → Sample-008b. When that number is zero-padded (a leading 0 or more than one digit), every value of the series, *including the first cell*, is padded to the width of the largest number: aa 01 filled over 120 rows gives aa 001, aa 002 ... aa 120 (the first cell becomes aa 001), 0099 gives 0099, 0100 ... , 01 over 12 rows gives 01 ... 12. Unpadded numbers stay unpadded: S1 gives S1, S2 ... S120, A9 → A10. Numeric columns (MW, RT, ...) just count up. Text without digits, and the On column, are copied. The whole fill, including the change to the first cell, is one undo step.

Clean up text fields. For the selected entries, in **Name, Info and Company** only: line breaks (CR/LF) and tabs are replaced by a space, runs of spaces are reduced to one space, and leading/trailing spaces are removed. Formula and CAS are not touched. The status line reports how many entries changed.

Calculate MW from formula sets MW to the nominal mass of the formula (only when it parses and differs).

Include in search (On) / Exclude from search (Off) set the On flag: excluded entries stay in the library but ChemStation skips them when searching.

Protected (read-only in ChemStation). A check item in the Library menu and the grid context menu. It is the same flag as the [protected] mark on the library tab, the Protected option in the Save as / New dialog and the status bar text Protected / Not protected. Protected is the style of large

commercial libraries (compact, variable-length text; msda reports the library as read-only and refuses to add or edit entries). *Not protected* writes the standard fixed-length 255-byte text fields that msda can edit (longer texts are clipped to 254 characters). See Library > About protected libraries. Library Editor 2 itself can always edit; the setting is applied when you save, and searching in ChemStation works either way.

Undo and redo

Every change is one undo step: typing in a cell, paste, cut cells, clear cells (Del), fill down / increment, Replace All, delete, cut, paste, duplicate and move of entries, import into an open library, copying entries into another open library, Include / Exclude, Clean up text fields, Calculate MW, Regenerate condensed spectra and the Protected setting. Ctrl+Z undoes and Ctrl+Y redoes the step; the Edit menu and the grid context menu name it (for example *Undo Delete 3 entries*) and the status bar reports what was undone. Undo restores deleted entries at their exact positions and restores the row order after a move. The last 100 steps are kept per library; deleted entries are kept by reference, so undo uses little memory even for very large libraries. Undoing back to the last saved state clears the *modified* mark. Save keeps the history; Reload clears it. Copying entries into a library that is not open writes that file directly and cannot be undone.

5. Searching and comparing spectra

Search library with a spectrum. Double-click the **Full** or **Cond** cell of an entry (or use the Spectra menu). Every entry in the library is scored against that spectrum, in parallel; the Match, Dot and PBM% columns are filled, the grid is sorted by PBM% and then Match (best first), the searched row stays selected, and the compare window opens with the searched spectrum as reference. Double-click any Match, Dot or PBM% cell to re-sort by that score. A new search replaces the previous scores.

- **Match** (0–1000): LibraryEditor 1's XCorr, $1000 - 1000 \cdot \Sigma |a-b| / \Sigma(a+b)$, peaks paired within 0.3 u.
- **Dot** (0–999): mass-weighted cosine, weight = $m/z \cdot \sqrt{\text{abundance}}$ (standard dot product).
- **PBM%** (0–100): McLafferty Probability Based Matching reliability, see below.

PBM%. A reverse search: the searched spectrum is the "unknown" (binned to nominal mass) and every library entry's **condensed** spectrum is the reference. Each kept condensed peak adds $K = U + A + W - D$, with U the uniqueness (1 below m/z 29, otherwise $\text{round}(1 + (m/z - 29)/130)$), A the abundance class 0–7 of the library peak (edges 0.24, 1, 3.4, 9, 19, 38 and 73 % of base), $W = 3$ and $D = \log_2(1/P_{\min})$ the dilution, $P_{\min}$ being the smallest unknown/library abundance ratio among the kept peaks (at least 0.10). Peaks above the abundance window (contamination) add nothing; up to three peaks may be flagged and the match retried. $\text{PBM\%} = 100 \cdot K/K_{\max}$, where $K_{\max}$ is the K of a perfect match to the same condensed peaks. Entries without a condensed spectrum stay empty. This is the same calculation as Quanto's PBM search.

Compare spectra (Ctrl+K, or Ctrl+double-click). Select two rows (Ctrl+click) and press Ctrl+K, or Ctrl+double-click the second row: the other selected row becomes the reference and the current row is compared, as a head-to-tail plot, a difference plot and an aligned peak table with Match and Dot. With one row selected it becomes the reference and the window follows whatever row you select next.

6. The role of molecular weight (MW)

In mass spectral searching in general. For electron-ionisation spectra the molecular ion (M^+ , at m/z = nominal MW) is the single most diagnostic peak: it fixes the size of the molecule, and the losses from it ($M-15$, $M-18$, ...) reveal the structure. Two compounds can share most fragment ions but never the same molecular ion unless they are isomers. A library entry with a missing or wrong MW is therefore harmful: the entry cannot be confirmed or ruled out on its molecular ion, MW-based filtering removes it (or keeps it wrongly), and software that derives anything from MW (condensing, constraints, reports) works from the wrong value. Common library search programs, for example, let you constrain a search to a molecular weight and can estimate the MW of an unknown from its hit list; both depend on correct MW values in the library.

In ChemStation PBM libraries (what the code shows). MW is stored in the header record of every entry and is an input of the PBM condensing step (msda's algorithm, reproduced in Library Editor 2's `MsdCondenser`):

- MW must be 1–9999, otherwise the entry gets no condensed spectrum ("Bad MW").
- Peaks above MW + an isotope allowance (2 per Cl/Br, +2, half the S/Si count) are discarded as impossible.
- The molecular-ion peak (MW, shifted for Cl/Br isotopes) is always kept and flagged; its position is stored in the condensed record (the MI index in the SK2MI field).
- Fragment peaks at chemically implausible losses from MW (1–38 u, depending on the formula's Si, P, O, F, Cl, Br) are removed when the formula allows an isotope check.
- The number of peaks kept in the condensed spectrum grows with MW (15 below MW 170 up to 26 above MW 600).

So a wrong MW changes the condensed spectrum that ChemStation's PBM search compares against, and with it the hit quality. That is why changing MW in Library Editor 2 marks the entry **Dirty**: its condensed spectrum is regenerated on save. Whether ChemStation's PBM scoring additionally weights the molecular ion via the stored MI index is not established by the code or the sources used here.

In Library Editor 2's own scores. Match, Dot and PBM% do **not** use MW: there is no MW filter, no molecular-ion weighting and no mass-range cut at MW in these three calculations. They compare peaks only. MW influences PBM% indirectly, because PBM% uses each entry's condensed spectrum, whose content depends on MW as described above. Library Editor 2 also uses MW when importing (from the formula, or the highest mass when missing) and when exporting (MSP/MSL/JCAMP/MassHunter MW fields). Use **Calculate MW from formula** to fix missing or wrong values.

7. Licensing

Without a license Library Editor 2 runs for a grace period of 30 days after installation (the earliest of the date the installer recorded and the first start of the program). During the grace period everything works, but Save, Save as, Copy to library and every export write at most 50 compounds: a larger library is refused with an explanation (nothing is ever cut off silently) and an offer to import a license. After the grace period the program is view-only: libraries open, filter, find, search and compare spectra, but editing, saving and exporting need a license. The window title shows *Unlicensed - N days left* or *Unlicensed - grace period expired*.

Installing a license. Leoson BV sends a license file (`.lic`). Choose **Help > Import license...** and select it. The file is checked and copied to

%ProgramData%\Leoson\LibraryEditor2\license.lic (or to %AppData%\Leoson\LibraryEditor2 when the ProgramData folder is not writable). The title then shows *Company license <company>* or *User license <user name>*; **Help > License info** and the About box show the details.

The license file is plain text that you can read: program, license type (Company or User), company, user, issue date, expiry date (or *never*) and an Id, followed by a signature. Any change to a value makes the signature invalid and the license is rejected. The file may be saved in any encoding (UTF-8 with or without BOM, UTF-16, ANSI) and with Windows or Unix line endings; names with accents such as *Société Générale* or *Müller GmbH* are shown and verified correctly either way.

```
# Library Editor 2 license - Leoson BV, www.waleson.eu
Program=LibraryEditor2
LicenseType=Company
Company=Example Lab GmbH
Issued=2026-10-15
Expires=never
Id=LE2-EXAMPLE
Signature=MEUCIQ...(base64)
```

Creating licenses (Leoson BV). The LicenseGen tool in the source folder (not installed with the program) signs license files with the private key in LicenseGen\Keys\ . Every new license is saved in the source folder's Licenses\ directory as <Company or User>_<Type>_<yyyyMMdd>_<Id>.lic (characters not allowed in file names become _; an existing file is never overwritten, a suffix (2), (3) ... is added) and registered as one line in Licenses\licenses-log.csv (date, type, company, user, expires, id, file name). The form's save dialog starts in that folder; on the command line - -out is optional. The key and the Licenses\ folder are kept out of git.

8. Shortcuts at a glance

Action	Shortcut / gesture
Search library with full / condensed spectrum	Double-click Full / Cond cell
Compare two selected rows	Ctrl+K, Ctrl+double-click
Fill down / increment	Ctrl+D
Clear cells (empty the selected cells)	Del
Delete the selected entries	Ctrl+Del
Copy / paste cells	Ctrl+C / Ctrl+V (Ctrl+Shift+C with headers)
Copy / cut / paste entries	Ctrl+Alt+C / X / V
Filter, Find, Replace	Ctrl+E, Ctrl+F (F3, Shift+F3), Ctrl+H
Undo / redo	Ctrl+Z / Ctrl+Y
New, Open, Save, Close library	Ctrl+N, Ctrl+O, Ctrl+S, Ctrl+W
Import spectra	Ctrl+Shift+I
User guide (this PDF)	F1