HISTORICAL OVERVIEW JSB RELEASE NOTES UNTIL THE CURRENT *GC IMAGE* SOFTWARE VERSION

NEW *GC IMAGE* SOFTWARE RELEASES SINCE 2017

Since the release of *GC Image v2.7* software package in June 2017, which was subject to major developments, JSB decided to build release notes with our own brief introduction to the new versions after evaluation by our specialists.

This document is a historical overview of these notes and will be extended after each new release, to give guidance to users with older versions and indicate why they should update/upgrade to more recent releases. Please notice that it is only possible to upgrade to the current software version.

WHAT'S NEW IN V2.7 (RELEASED JUNE 2017-FEBRUARY 2018)?

- A new, default MS mode that opens MS View for point, blob, or area spectra based on the specific area the user clicks on.
- MS Library Search for Area objects.
- New Library Search features.
- Quantifier ions can be set as internal standard for isotope dilution.
- A new quantification interface that allows for full optimization. This includes:
  - A new menu for convenient creation and modification of calibration tables directly from other images.
  - A new Calibration Table interface for easy tuning of each calibrant.
  - More calibration functions.
  - More settings and options that can be saved as methods for later use.

- New improvements for Peak Detection, Identification, and Review
- Several new features dedicated to High Resolution MS data, such as:

  - Much faster import and open times for very large data.
  - Possibility to export centroid data extracted from profile data to a .GCI file.
  - Mass calibration of centroid data, with or without profile data.

WHY UPGRADE?

The quantification interface has been significantly improved: the new features and tools make calibration fully controlled and tunable in an easy fashion. A must-have for any user interested in quantitative analysis!

Additionally, the much faster operational speed and new features make this version a very interesting step forward for HRMS data processing.

WHAT'S NEW IN V2.8 (RELEASED JULY 2018)?

- A new and improved ion peak detection.
  - A new algorithm for spectral deconvolution similar to AMDIS.
  - A Review Mode allows to easily examine the extracted ion peaks with their characteristic ions and deconvoluted spectra.
- A new Side-by-Side comparison tool.
  - Two images can be visualized next to each other and compared within *GC Image*.
  - Interactive review for the blob features in the two chromatograms.
  - Access to direct spectral comparison for the compounds of interest.
- Easier *Image Investigator* workflow to find common compounds and/or unique markers across many samples.

WHY UPGRADE?

The possibility to perform full deconvolution in a fast, easy way allows for more detailed and accurate peak integration and identification.

In addition, the image comparison possibilities have been greatly improved. The new *GC Image* and *Image Investigator* tools make comparison, from simple one-on-one to large sample batches, more accessible and efficient.

WHAT'S NEW IN V2.9 (RELEASED JULY 2019)?

- Improved baseline correction and signal-noise estimation.
  - A new algorithm for better automated noise estimation.
  - A new tool that supports detailed customization of noise estimation for specific areas.

- A new Blob Detection cursor tool.
  - Easy and optimal manual blob detection.
  - Accessible optimization of local integration parameters.

- New *Image Investigator* features.
  - PCA analysis runs in the background, making it possible to continue working during processing.
  - New compounds distribution view with bar charts to assess feature behaviors (amount, response etc.) across samples/classes in a simple, graphical way.
  - New spectral view for easy comparison of compounds MS patters across sample images.

WHY UPGRADE?

GC Image v2.9 brings improvements for precise noise estimation and manual integration compared to the previous versions.

In addition, image comparison with *Investigator* is more informative and efficient.

For a full overview of all *GC Image* announcements please visit www.gcimage.com/forum/ and click on "announcements".

SHARPER PEAKS, BETTER SEPARATIONS