

NEW AND IMPROVED GC IMAGE FEATURE: ION PEAK DETECTION FOR COMPREHENSIVE CHROMATOGRAPHIC DECONVOLUTION

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A new version of the GC Image software package released this year, **GC Image v2.8**, advances software capability and user-friendliness with improvements and new features. The new and improved **Ion Peak Detection (Extract Ion Peaks as Area Objects)** replaces the *Extract Ion Peak to Areas* functionality of version 2.7 in order to provide faster and easier comprehensive chromatographic deconvolution.

Brief overview of possibilities

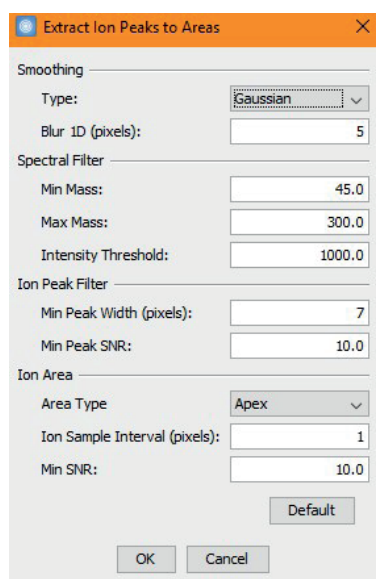
The tool applies an algorithm adapted to detect 2D chromatographic peaks of individual ions, combines peaks for multiple ions of the same analyte and performs spectral deconvolution.

The process steps involve:

1. Determination of each 2D ion peak with slight variations in different spectra;
2. Collection of 2D ion peaks into components based on retention times and peak-shape;
3. Deconvolution of each component based on combination of co-eluting components;
4. Generation of an area object for each component.

For each area object the most abundant ion is set as the first quantifier and the deconvoluted spectrum is set to as Reference MS. The process can be controlled and fine-tuned through a number of settings as shown in the option dialog window in Fig. 1. The Ion Area determines the type of objects created by the deconvolution process and can be set, for instance, to Apex or 2D Bounding Box.

Fig. 1
 The Extract Ion Peaks to
 Areas options dialog.



Deconvolution improves characterization through more precise and detailed detection and identification of co-eluting compounds. This does not apply only to partially eluting blobs easy to spot due to poor peak shape (Fig. 2), but also to seemingly pure blobs characterized by fair, symmetric shape that are in fact composed of closely-eluting compounds (Fig. 3).

Fig. 2
 Example of blob with relative spectrum and results of deconvolution into 3 objects (apex mode) with relative MS spectra.

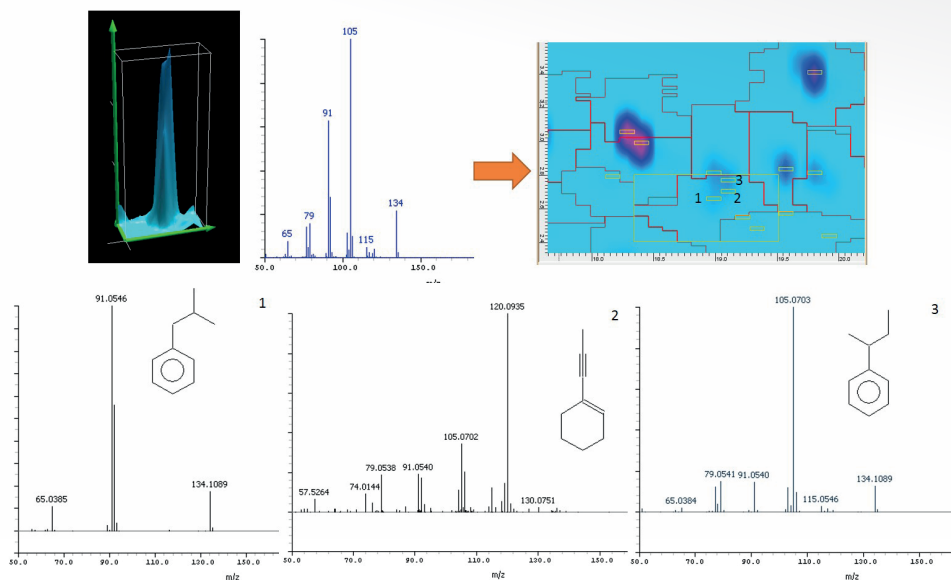
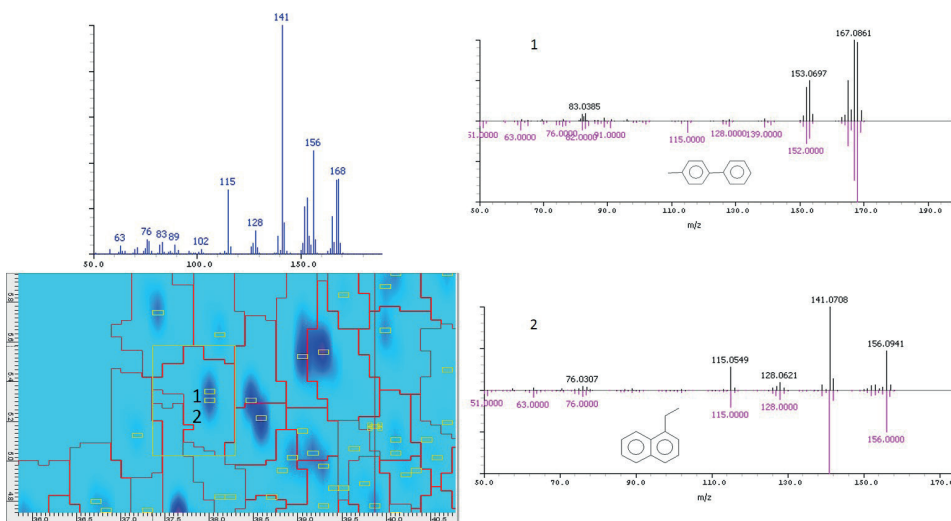


Fig. 3
 Example of seemingly pure blob (blue spectrum) deconvoluted to two objects (apex mode) with their corresponding spectra (black, NIST library search match in pink).




CONCLUSIONS

- The new Ion Peak Detection tool performs deconvolution of the entire 2D chromatogram.
- The deconvoluted analytes are extracted as area objects with corresponding MS spectra that can be easily evaluated through an interactive review mode.
- It is possible to perform more detailed and accurate chemical profiling also for highly complex matrices.

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