

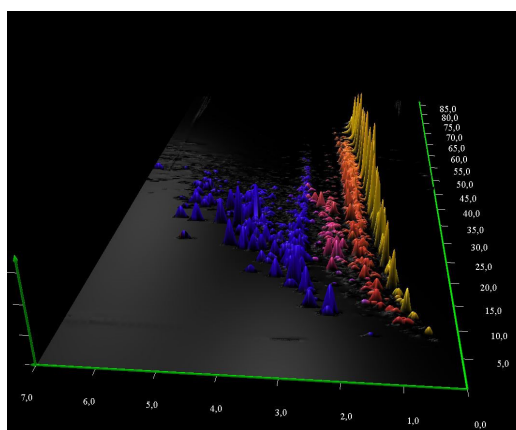
## Mass-based colorization for qualitative group analysis in GC×GC-MS

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### Introduction

GC×GC-MS, with its unmatched peak capacity and resolution, is the ideal tool for the detailed characterization of complex samples. The 2D chromatograms are organized, the position of a peak in the separation space being a strong indicator of its chemical/physical properties. This is particularly useful for group characterization, as different classes of compounds occupy distinct parts of the two-dimensional space.

The GC Image software allows simple and quick access to the 2D data. A very useful tool offered by this software package is the Spectra Color Map that allows 3D colorization of specific masses. When specific mass fragments are available, this provides a simple yet insightful visual overview of their distribution in the 2D space and can be used to visualize the group distribution.



3D view of a Spectra Color Map

### Instrumentation and software

Agilent 7890B GC equipped with a Zoex ZX2 cryogen-free thermal modulator and an Agilent 7200B QTOF detector. All 2D data were displayed and analyzed using the GC Image High Resolution software.

### Results

Fig. 1 shows the GC×GC chromatogram of a diesel oil with clear separation of several hundred compounds covering a wide range of boiling points (first dimension) and polarity (second dimension).

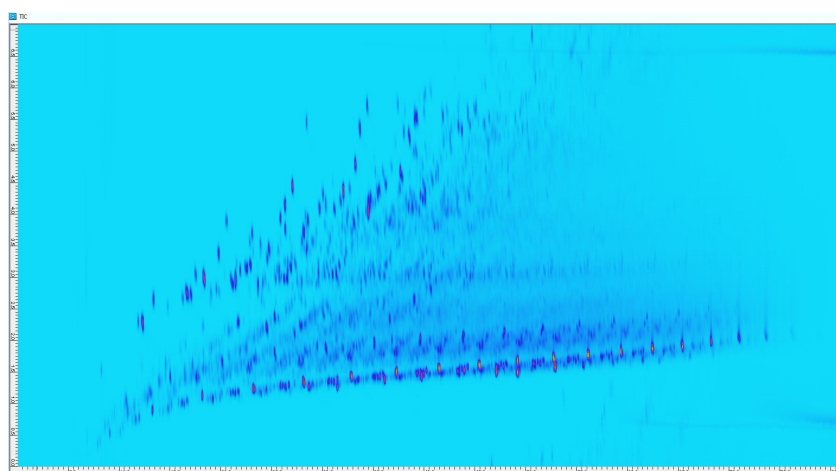


Fig. 1 - 2D plot of a diesel oil

Fig. 2 shows its counterpart colorized with the Spectra Color Map. In this example five fragments are selected and labeled with different colors. The color map obtained illustrates their distribution across the two-dimensional separation space, showing the position of potentially interesting groups like alkanes (yellow), alkenes and cyclic hydrocarbons (red) and substituted mono-aromatics (blue).

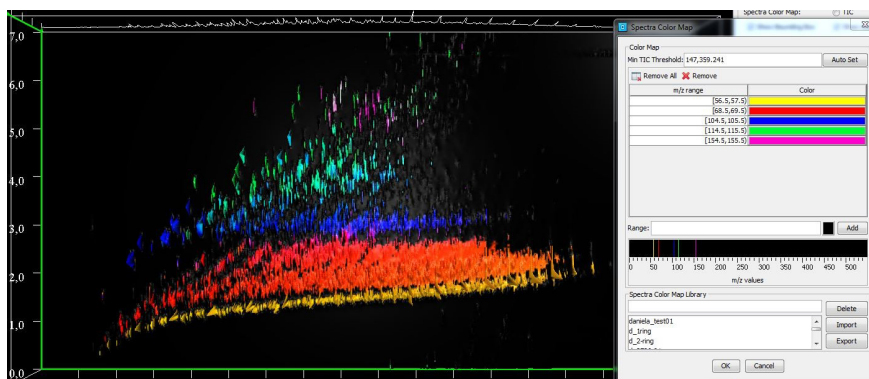


Fig. 2 - Example of spectra color map of different classes of compounds

The mass range of each fragment selected can be tuned. This becomes crucial in when using a high resolution mass spectrometer such as the Agilent QTOF. With a very narrow mass range the accurate mass information is not lost but exploited to the benefit of selectivity. This is shown, where the colorization for nominal mass 128 m/z and for the accurate mass  $128.0621 \pm 0.001$  m/z (C<sub>10</sub>H<sub>8</sub><sup>+</sup>) are compared. In the second case the target alkyl-substituted naphthalenes are displayed while the alkanes that contain mass 128.1521 m/z (C<sub>9</sub>H<sub>20</sub><sup>+</sup>) are filtered out.

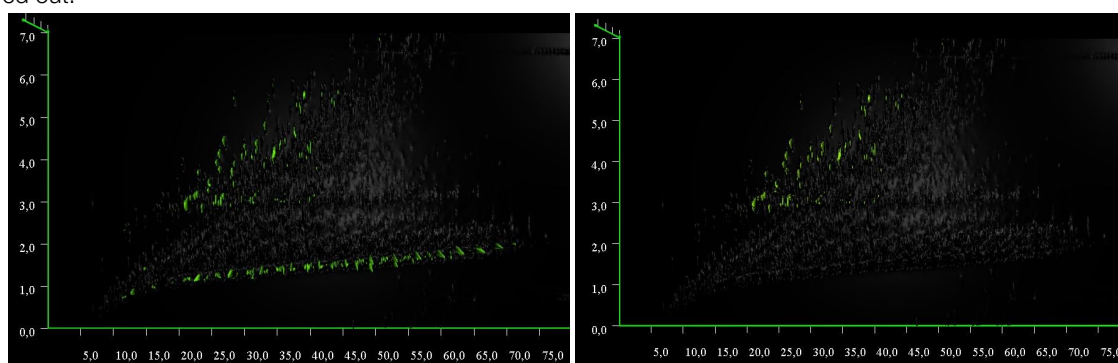


Fig. 3 - Colorization for the nominal mass  $128 \pm 0.5$  m/z (left) and for the accurate mass  $128.0621 \pm 0.001$  m/z (right)

## Conclusions

- GC×GC-MS can separate hundreds of components in complex matrixes in a single analysis. The two dimensions provide organized 2D separations based on polarity and volatility.
- The Spectra Color Map shows the 3D distribution of selected mass fragments in the separation space by colorization.
- When specific masses characteristic for individual group are known, these can be used to display a visual overview of the group separation.
- The excellent masses accuracy of the QTOF grants additional precision and selectivity.

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