

Applying Computer Vision to Automate Routine GCxGC Analysis

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Introduction

Routine analysis of comprehensive two-dimensional gas chromatography (GCxGC) data, such as ASTM D8396 and UOP 990, frequently involves complex group-type assignments. To avoid recreating these assignments, they are typically stored in templates. However, retention time shifts require adjusting these templates manually with repetitive processing steps. We demonstrate the use of computer-vision-driven workflows to make this routine analysis faster, more consistent, and easier to automate.

Types of Misalignment

This work looks at three different sources of chromatographic misalignment:

Phase Shift Offsets

Different chromatograms may have different timing offsets or slightly varying chromatographic conditions resulting in visible shifts and sometimes peak wrapping in the second dimension.

Retention Time Drift

Retention times may vary run-to-run due to system variations, such as pressure and temperature fluctuations, and due to column aging.

Different Instruments/Detectors

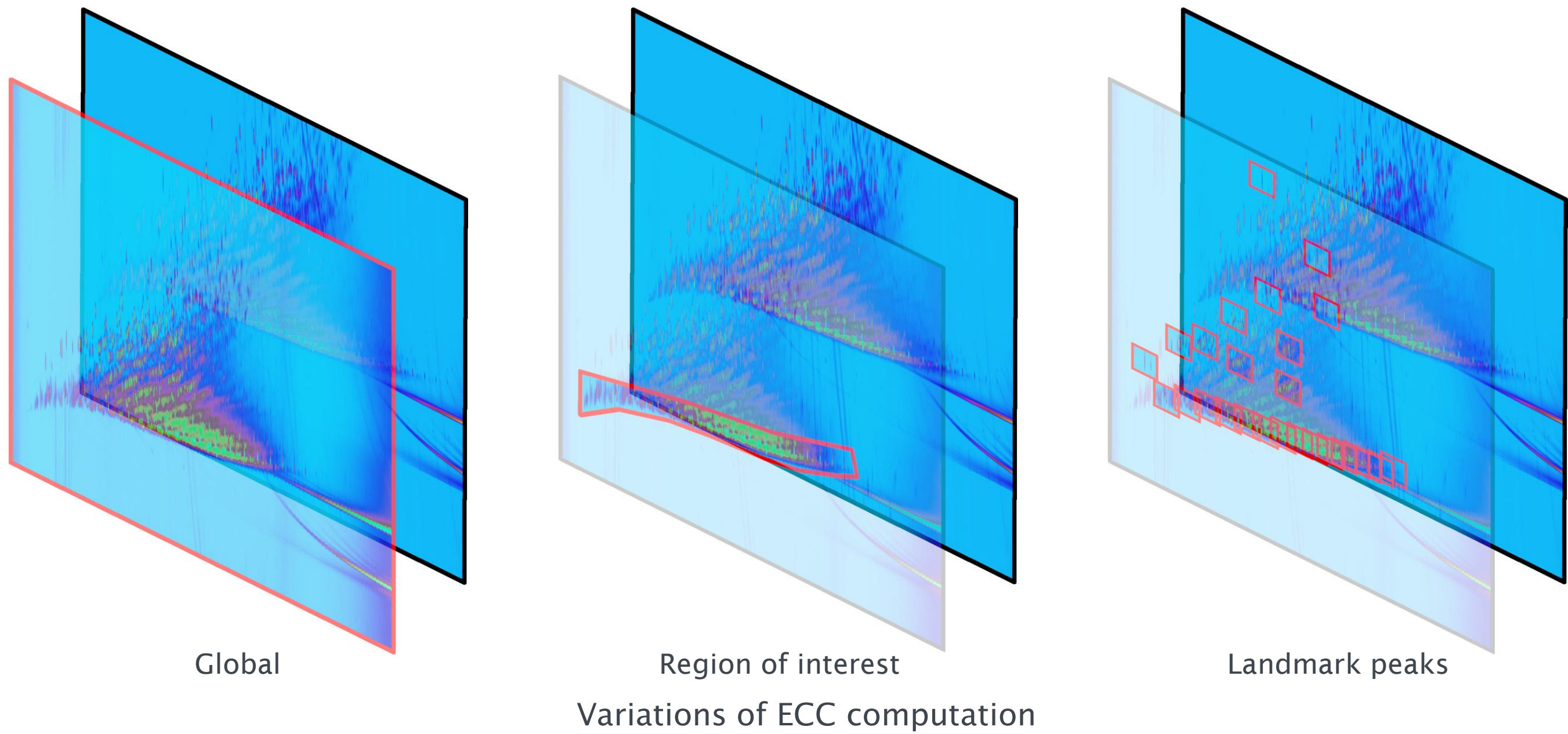
Chromatograms obtained from different instruments or detectors (e.g. MS/FID data fusion) may have significantly different retention times.

Correcting with Computer Vision

In the absence of MS data, correcting these various types of misalignment can be a challenging task. We apply computer vision techniques to identify corresponding visual features between chromatograms.

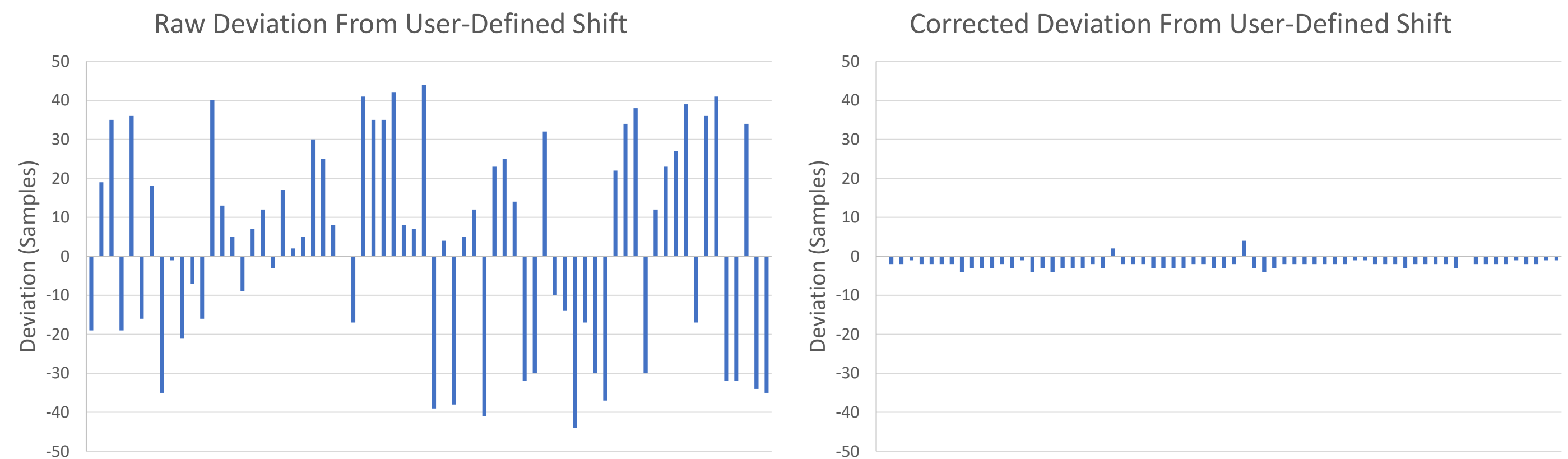
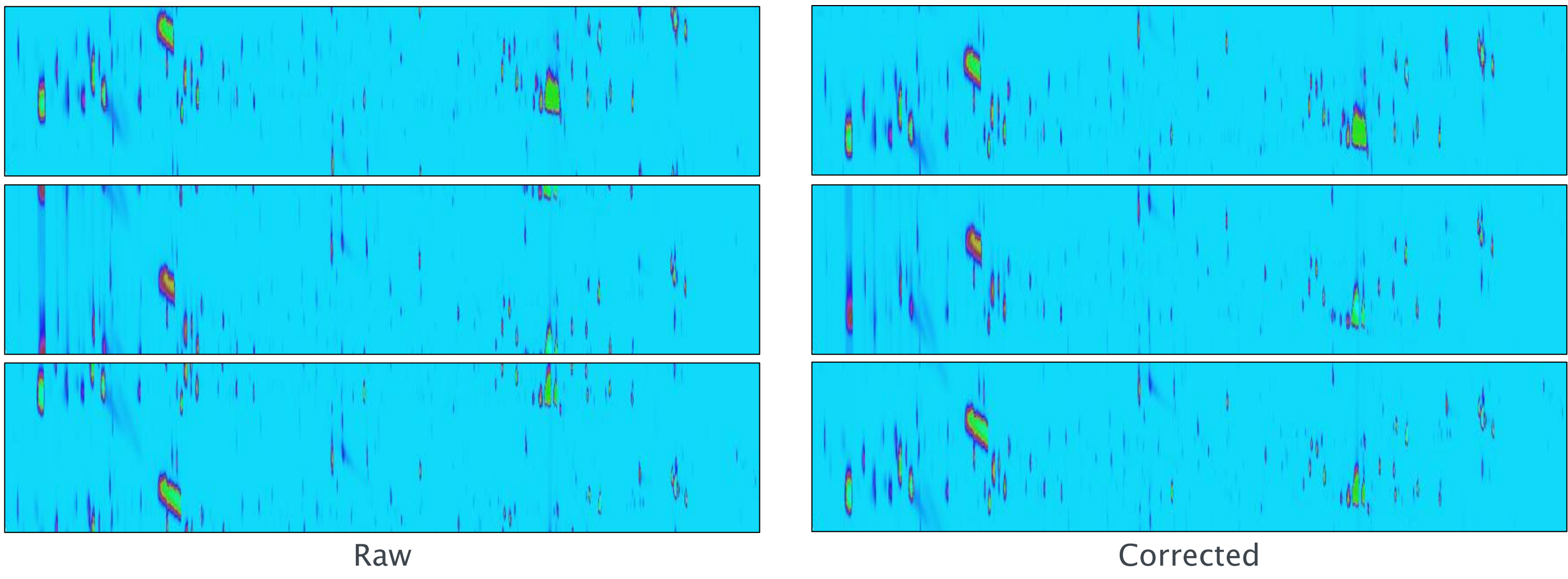
Visual similarity can be computed in several ways:

- Globally, using the entire chromatogram
- Locally, using a single user-specified region of interest
- Locally, using a set of user-specified landmark peaks



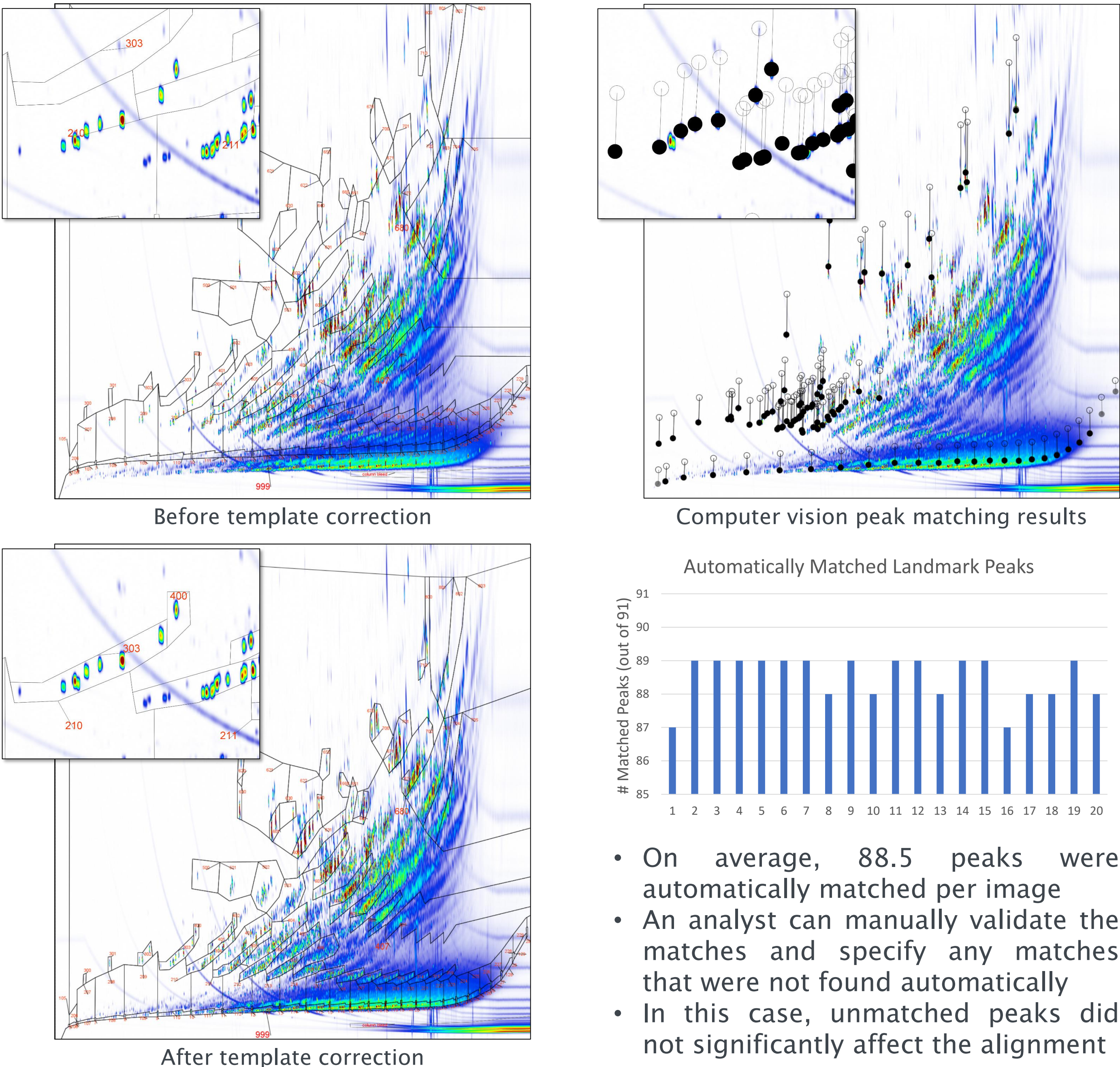
Application 1: Phase Shift Correction

- ❖ Data Set: GCxGC-HRTOF-MS data set for untargeted serum metabolic profiling [1]
- ❖ Instruments: JMS-T100GCVV GCxGC-TOF-MS using an Agilent 6890 GC coupled to a CTC Autosampler
- ❖ Data Processing:
 - Manually correct shift on one reference image
 - Automatically correct shift using computer vision, computed globally against the reference



Application 2: Landmark Peak Matching for UOP 990

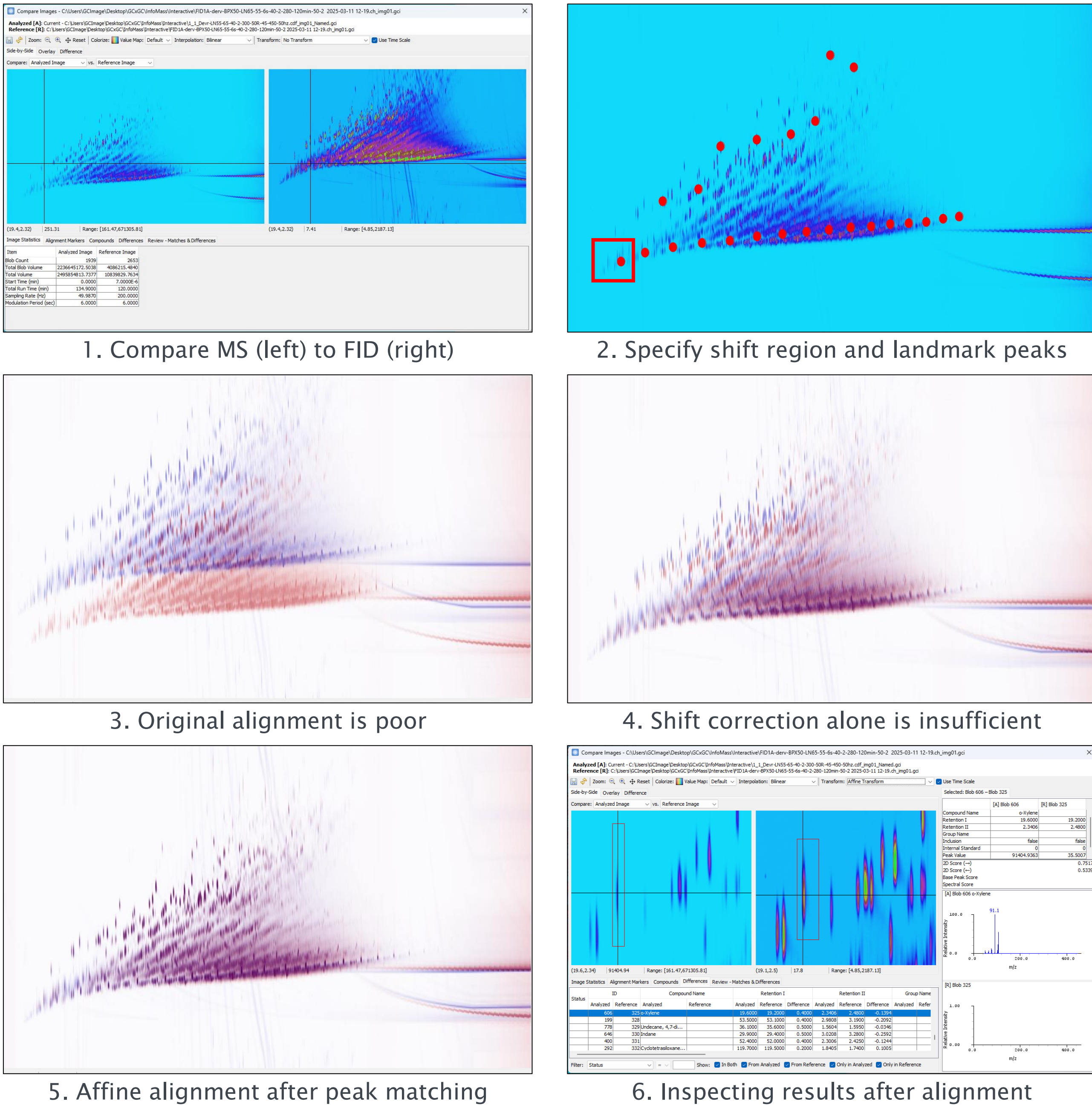
- ❖ Data Set: Single distillate diesel sample run 20 times on the same GCxGC system over a short period of time [3]
- ❖ Instruments: LECO GCxGC-FID system, Agilent 6890 GC. Run conditions in accordance with UOP 990
- ❖ Data Processing:
 - Select reference, manually process and apply the UOP 990 template
 - Template has 91 landmark peaks, 138 groups
 - Each image is automatically shift-corrected then has peaks matched using computer vision; template is transformed based on the matching



- On average, 88.5 peaks were automatically matched per image
- An analyst can manually validate the matches and specify any matches that were not found automatically
- In this case, unmatched peaks did not significantly affect the alignment

Application 3: RT Alignment for MS/FID Data Fusion

- ❖ Data Set: GCxGC data of a diesel fuel sample
- ❖ Instruments: Agilent 7890A GC/InfoMass L10 thermal modulator/Hexin TOFMS
 - Detectors: FID (350 °C, 200 Hz), MS (45-450 m/z, 50 Hz)
 - Modulation: 6 seconds with programmable cold jet gas flow (15 L/min to 6 L/min)
- ❖ Data Processing:
 - Manually correct shift on reference, specify landmark peaks, specify shift correction region of interest (if needed)
 - Paired image automatically shift-corrected, then has peaks matched using computer vision



GC Image

Software for Multidimensional Chromatography

References

1. N. Di Giovanni. (2019). "Untargeted Serum Metabolic Profiling by GCxGC-HRTOF-MS". <https://doi.org/10.7910/DVN/E95BO5>, Harvard Dataverse.
2. D. W. Rempe, S. E. Reichenbach, Q. Tao, C. Cordero, W. E. Rathbun, C. A. Zini. (2016). "Effectiveness of global, low-degree polynomial transformations for GCxGC data alignment". *Analytical Chemistry*, 88(20), 10028-10035.

Data processes and screenshots for this publication are from an alpha version of GC Image v2026. Visit www.gcimage.com for current v2025 releases.



Animated Examples