

DETECTING CONTAMINATION IN FRAGRANCES



Technology Advantage: Agilent Intuvo 9000 GC with
OpenLAB CDS version 2 and MatchCompare



Introduction

The fragrance industry uses gas chromatography throughout its manufacturing process. Complex products such as fragrances are typically made from hundreds of ingredients, and present an unusual challenge to manufacturers desiring consistency from sample to sample. Individual ingredients can change, and the possibility of contamination exists from processing steps and airborne ingredients.

Two examples of possible contaminants include limonene, an ingredient from orange oil that is very volatile and found throughout a fragrance facility, and diethyl phthalate (DEP), frequently found as a plasticizer in polymeric processing equipment. DEP can be leached into fragrances if inadequate replacements are used in processing equipment.

Ensuring that the final fragrance is the same from batch to batch, and free of possible contaminants requires time-consuming, careful analyses of each region of the gas chromatogram.

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The Agilent Intuvo 9000 GC provides a unique solution for fragrance analysis with additional advantages over conventional gas chromatographs.

- Smaller footprint
- Increased stability
- Easier maintenance

At only 27 cm, the Intuvo 9000 GC is approximately half the size of a conventional GC. A proprietary flow path and connection paradigm yields a more robust analysis while enabling faster column changes for method development, if needed.

Agilent OpenLAB CDS MatchCompare is an add-on software enhancement that automates the time-consuming task of comparing quality control chromatograms. An important feature is the ability to compare both major components and trace compounds, making it an ideal tool for any screening application where consistency is important.

Methodology

A commercially available perfume sample was spiked with small unknown quantities of diethyl phthalate and orange oil (95 % limonene). These samples were mixed into a sequence of unspiked perfume and analyzed on the Intuvo 9000 GC using conditions typical to the industry. Processing was performed using Agilent OpenLAB CDS 2.1 with Match Compare A.01.03.

Results and Discussion

Figure 1 shows that processing was completed using Agilent OpenLAB CDS 2.1. Roughly a dozen chromatograms of the same fragrance are overlaid in the central window. Typically, a chromatographer would have to examine the overlaid chromatograms in close detail, ensuring that they all match. OpenLAB CDS 2.1 has features such as the Peak Explorer window (offering primarily a qualitative comparison) that can help with this comparison.

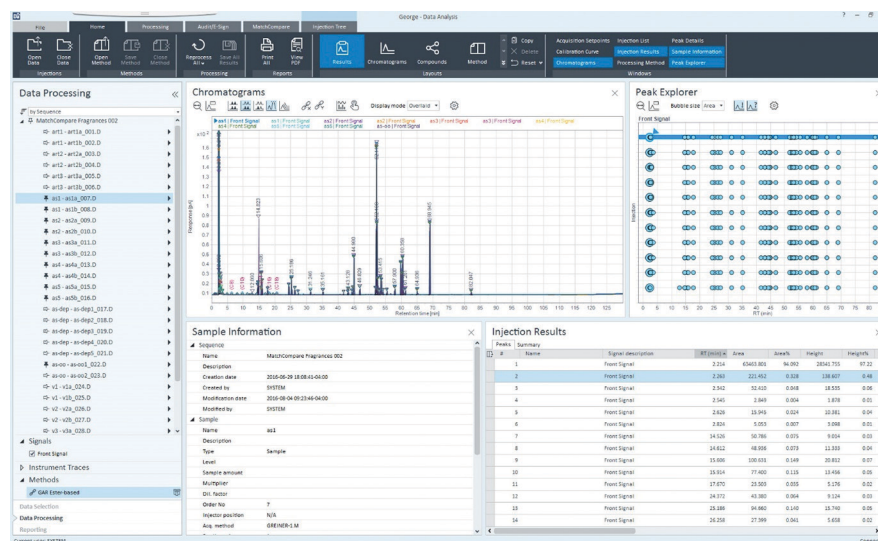


Figure 1, Agilent OpenLAB 2 Data Analysis screen showing overlaid fragrance chromatograms and the associated Peak Explorer window.

OpenLAB MatchCompare adds the ability to quantitatively compare two chromatograms in terms of peak area and retention time. A standard chromatogram is chosen, and tolerances can be set up for each of its peaks. Figure 2 presents a comparison of the standard and a sample chromatogram. This clearly shows peaks where the two chromatograms match (green), where peaks are present in both but out of tolerance (blue), and peaks present in the reference only (grey) or sample only (white). A printed or electronic report of this window is available.

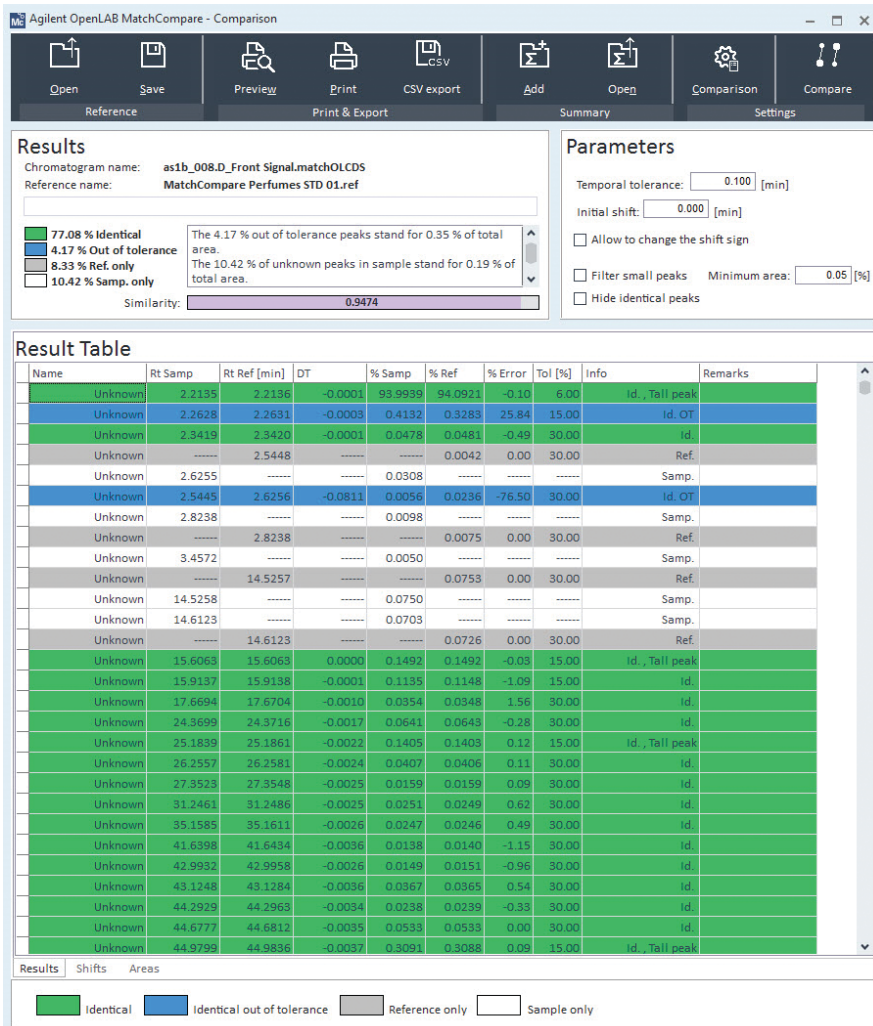


Figure 2. Agilent OpenLAB MatchCompare comparison window showing peaks where the two chromatograms match (green), where peaks are present in both but out of tolerance (blue), and peaks present in the reference only (grey) or sample only (white).

Figures 3, 4, and 5, present OpenLAB MatchCompare area plots showing a perfect match (Figure 3), severe DEP contamination (Figure 4), and mild limonene contamination (Figure 5). The color coding is the same as in Figure 2. A chromatographer can quickly zero in on where problem areas are in the chromatogram, allowing efficient use of time in the quality control laboratory.

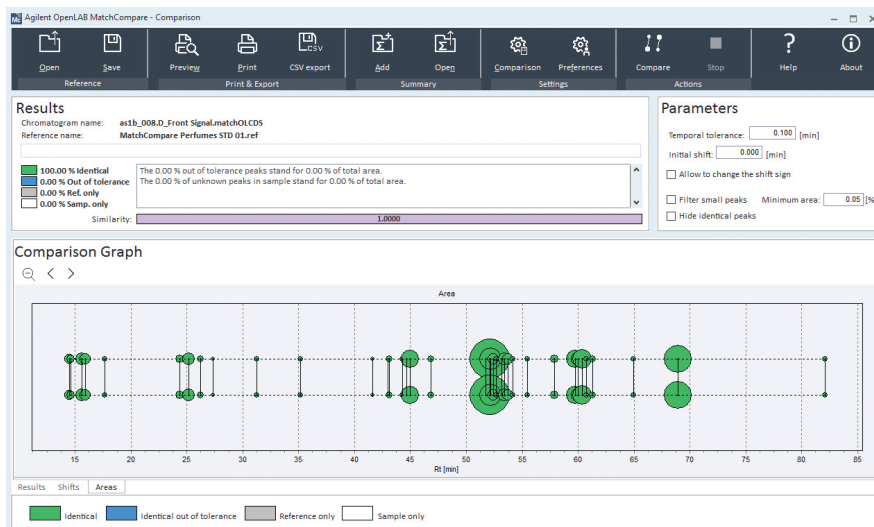


Figure 3. Agilent OpenLAB MatchCompare comparison area window showing a perfect match between the reference and sample.

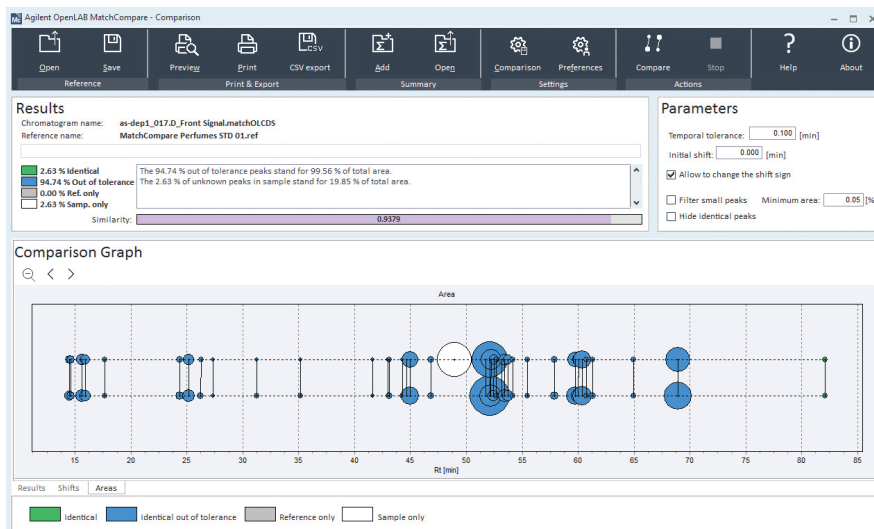


Figure 4. Agilent OpenLAB MatchCompare comparison area window showing severe contamination from DEP (tr = 49 minutes). The contamination throws all the other peaks out of tolerance in terms of peak area.

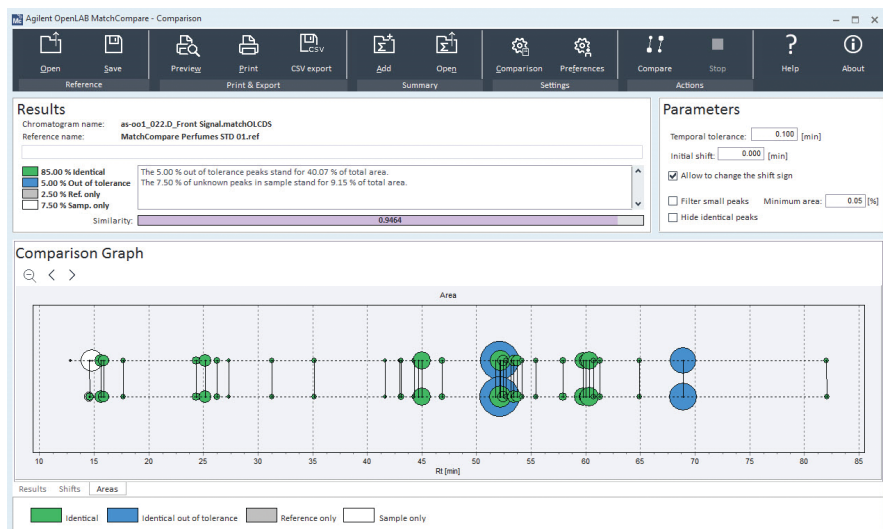


Figure 5. Agilent OpenLAB MatchCompare comparison area window showing mild limonene ($t_r = 15$ minutes) contamination. A smaller amount of limonene is actually present in the reference, and many ingredients are still within tolerance in terms of peak area.

Conclusion

The Agilent Intuvo 9000 GC, when paired with Agilent OpenLAB CDS 2 and MatchCompare, provides a powerful way to quickly and quantitatively compare complex samples such as fragrances in a quality control environment. This critical application from the fragrance industry demonstrates the analytical capability of the Intuvo 9000 GC, and illustrates the power of combining this innovative instrument with Agilent state-of-the-art software products such as OpenLAB CDS 2 and MatchCompare.

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