OpenLAB CDS Match Compare

Software tool for OpenLAB CDS

Ideal for flavors/fragrance analysis

Problem / Solution

Problem
I need an automated process comparing a chromatogram against a reference, objectively to ensure the sample is the same composition as the reference.
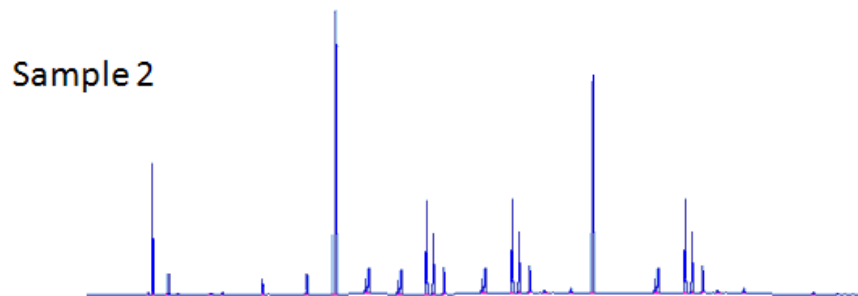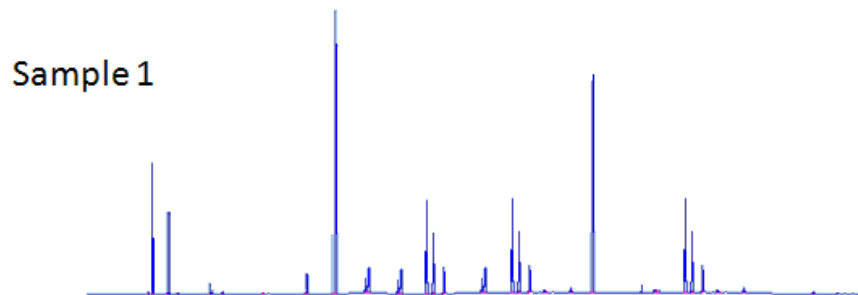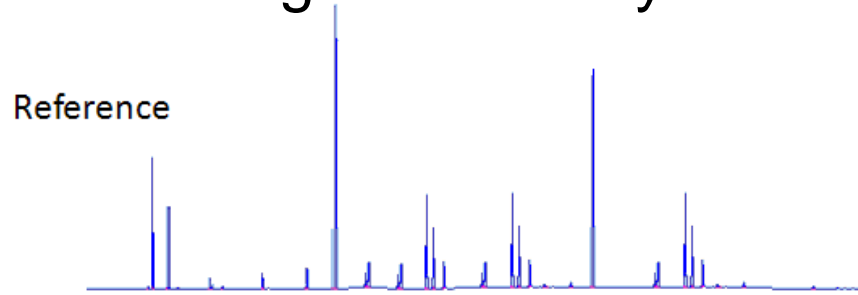
Solution
OpenLAB CDS MatchCompare Add-on Software

The Measure of Confidence

Agilent Technologies

Matching Chromatograms

Are the samples the same as the Reference?

One way: Analyst comparing chromatograms one by one

Reference

Sample 1

Sample 2

Automated way: Using OpenLAB CDS Match Compare

Similarity: 0.9711
79.17 % Identical
12.50 % Out of tolerance
4.17% Ref. only
4.17% Samp. only

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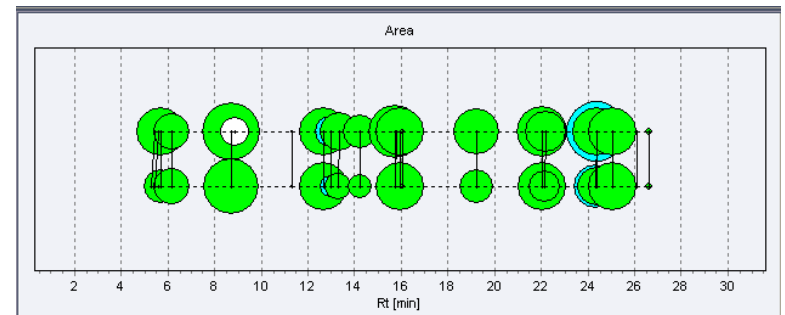
Problem / Solution

Problem

I would like to compare chromatograms within the OpenLAB CDS software.

Solution:

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Run the comparison against a reference chromatogram

Compare an unknown sample, by selecting the sample chromatogram, in data analysis within OpenLAB CDS.

To start the comparison, select "Compare current chromatogram" under the Match Compare menu item.

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Problem / Solution

Problem

I want a visual indicator and documentation of the comparison match of the sample chromatogram to the reference chromatogram.

Solution

A comparison summary gives a color coding of the match of retention time and area for the sample chromatogram.

Peak results

Comparison Summary


–the peak matches in sample and reference (Green)

–the peak appears in both sample and reference, but its area percent is out of tolerance (Cyan)

–the peak only appears in the reference (Gray)

–the peak only appears in the sample (White)

Area comparison

• Unknown on top, Reference on bottom

• Color circles indicate relative peak intensity of the peaks

•Color code as per the peak results table

• The displacement indicator line is the retention time difference between the sample chromatogram and the reference chromatogram.
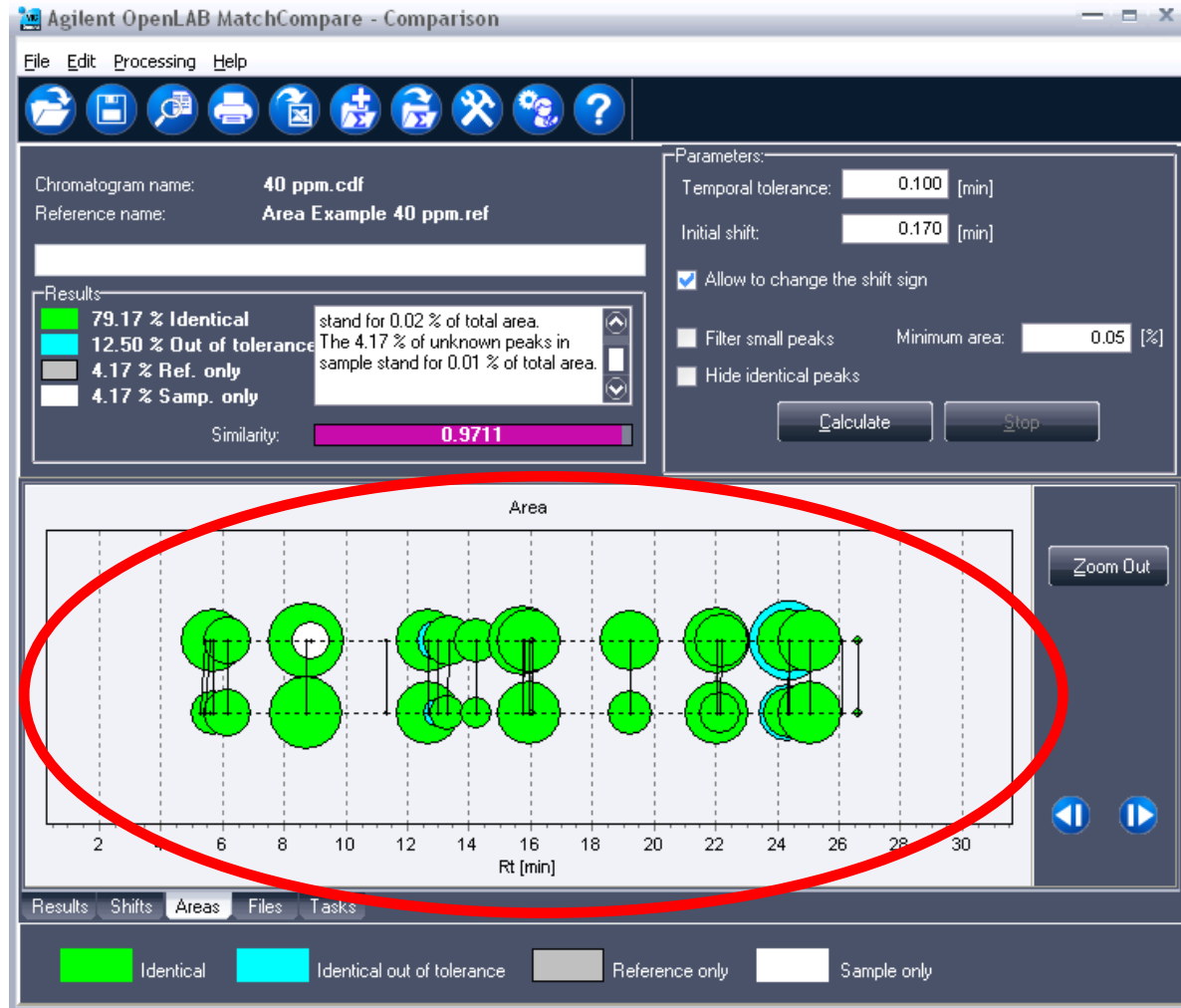
Problem / Solution

Problem

The chromatogram needs to be within a certain tolerance of a reference chromatogram.

Solution

Adjust the reference file parameters within
OpenLAB CDS MatchCompare Add-on Software

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Process of Adjusting the reference for Matching Chromatograms

Parameters to customized

- Area percent tolerance defined by each peak

- Retention Time (RI) tolerance defined in time or by Index

- Initial shift allows for injection delays

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Account for Retention time shifts

In order, to help the user determine the values to enter in the initial shifts and temporal tolerance, the points on the shifts tab show the retention time (index) variation and the temporal (time) limits.
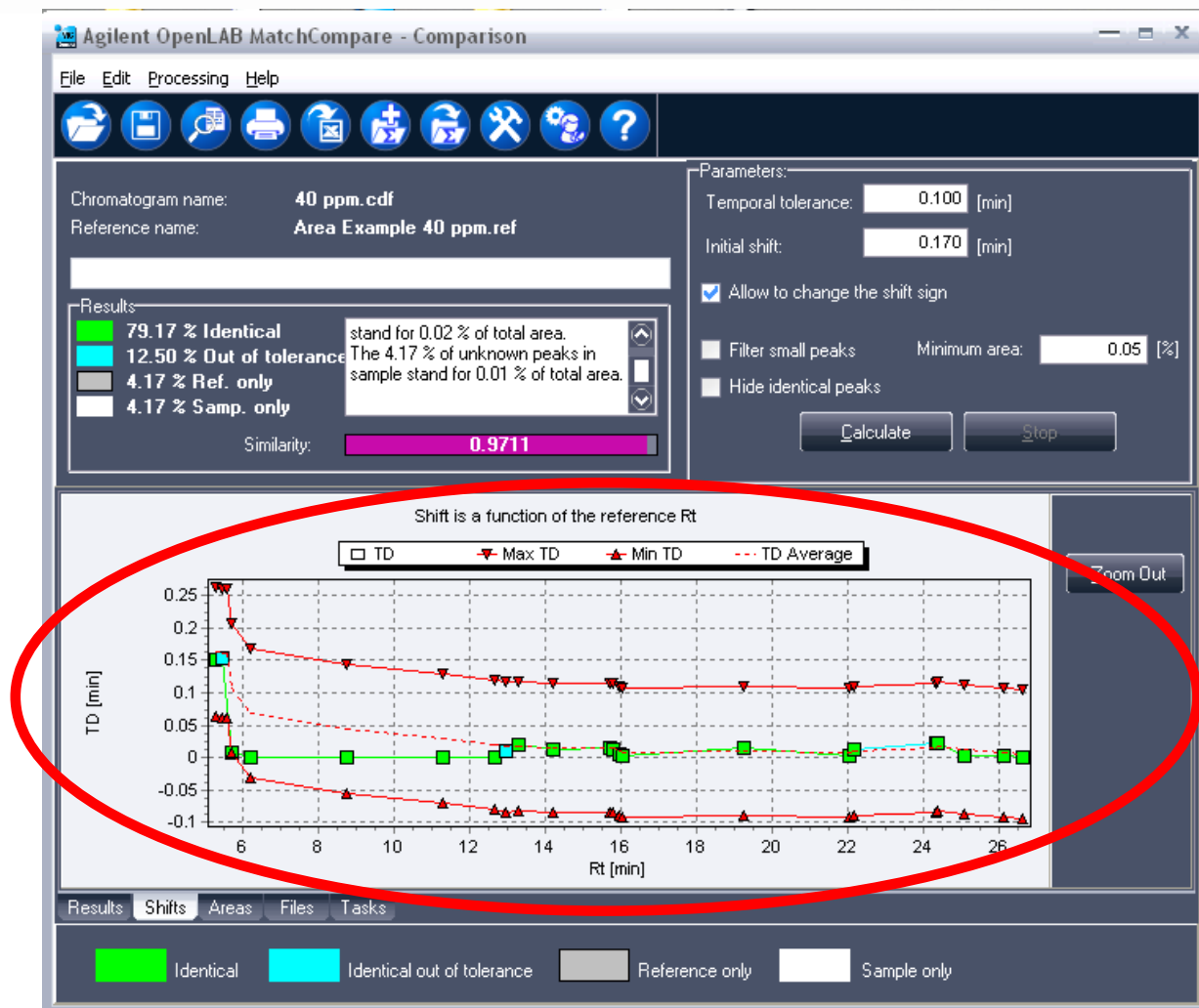
Problem / Solution

Problem

I need to document the similarity results and comparison of the sample and the reference.

Solution

OpenLAB CDS MatchCompare Comparsion Report

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OpenLAB CDS MatchCompare Reports

Comparison Report: The report documents the review and gives the similarity values.

Summary Report enables a user to save or export to .csv

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Principals of MatchCompare

- Comparison of two chromatograms
  - Pattern matching, not pattern recognition
  - Matching based on retention time (or retention index) and area percent

- Comparison parameters can be individually tailored

- Report can be on all peaks or just those falling outside the limits

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Reference

Refer to the OpenLAB CDS Match Compare User manual(available on the software media) for more information.