

# 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

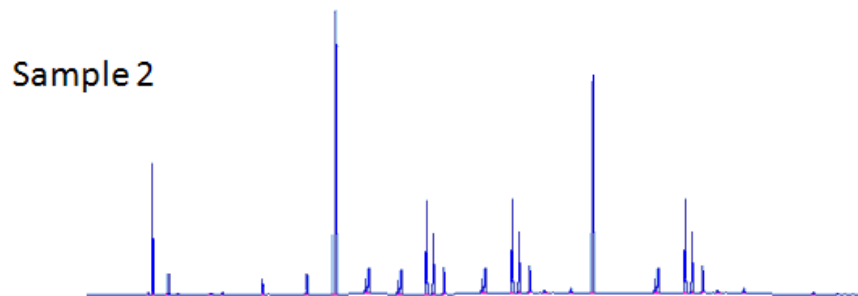
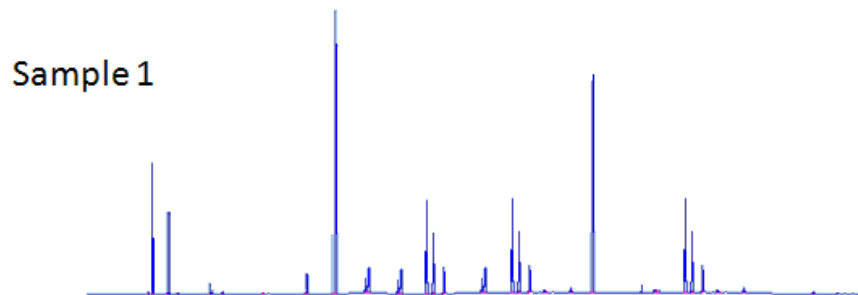
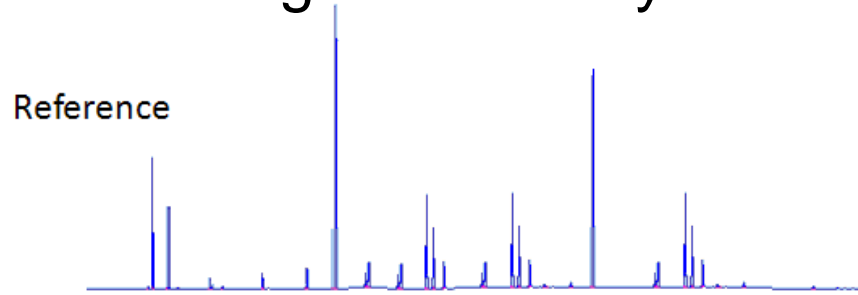
OpenLAB CDS MatchCompare Add-on Software

# Matching Chromatograms

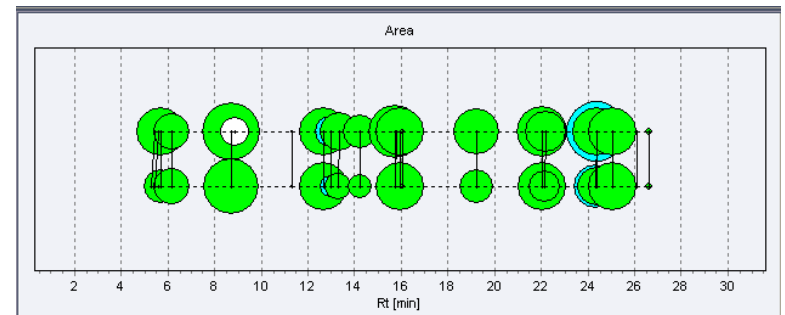
Are the samples the same as the Reference?

One way: Analyst comparing chromatograms one by one

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*



# Problem / Solution

## Problem

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

## Solution:

OpenLAB CDS MatchCompare Add-on Software

# 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.

The screenshot displays the OpenLAB CDS MatchCompare interface. The main window shows a comparison between a sample chromatogram (40 ppm.cdf) and a reference chromatogram (Area Example 40 ppm.ref). The results summary indicates a similarity of 0.9711. The results table shows the following data:

Retention Time (min)	Sample Area (%)	Reference Area (%)	Comparison Status
7.917	79.17	79.17	Identical
12.50	12.50	0.00	Out of tolerance
4.17	4.17	0.00	Ref. only
4.17	0.00	4.17	Samp. only

The interface also includes a chromatogram plot showing peaks at various retention times, with a legend indicating the comparison status for each peak. The legend shows: Green circle for Identical, Cyan circle for Identical out of tolerance, Grey circle for Reference only, and White circle for Sample only.

# 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

Agilent OpenLAB MatchCompare - Comparison

File Edit Processing Help

Chromatogram name: 40 ppm.cdf  
Reference name: Area Example 40 ppm.ref

Parameters:  
Temporal tolerance: 0.100 [min]  
Initial shift: 0.170 [min]  
 Allow to change the shift sign  
 Filter small peaks Minimum area: 0.05 [%]  
 Hide identical peaks

Calculate Stop

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

stand for 0.02 % of total area.  
The 4.17 % of unknown peaks in sample stand for 0.01 % of total area.

Similarity: 0.9711

Name	Rt Samp	Rt Ref [min]	DT	% Samp	% Ref	% Error	Tol [%]	Info
	5.44	5.29	0.15	0.0000	0.0000	13.18	100.00	Id.
	5.60	5.44	0.15	0.0001	0.0000	140.73	100.00	Id. OT
	-----	5.60	-----	-----	0.0001	0.00	100.00	Ref.
analyte 32al	5.73	5.72	0.01	0.0211	0.0107	97.03	100.00	Id. , Tall peak
	6.19	6.20	0.00	0.0120	0.0114	5.34	100.00	Id.
analyte 32	8.75	8.75	0.00	0.0304	0.0283	7.29	100.00	Id. , Tall peak
	8.88	-----	-----	0.0075	-----	-----	-----	Samp.
	11.30	11.30	0.00	0.0001	0.0001	10.37	100.00	Id.
32al	12.66	12.66	0.00	0.0212	0.0201	5.57	100.00	Id. , Tall peak
	12.98	12.97	0.01	0.0083	0.0041	103.85	100.00	Id. OT

Results Shifts Areas Files Tasks

Identical Identical out of tolerance Reference only Sample only

—the peak matches in sample and reference (Green)

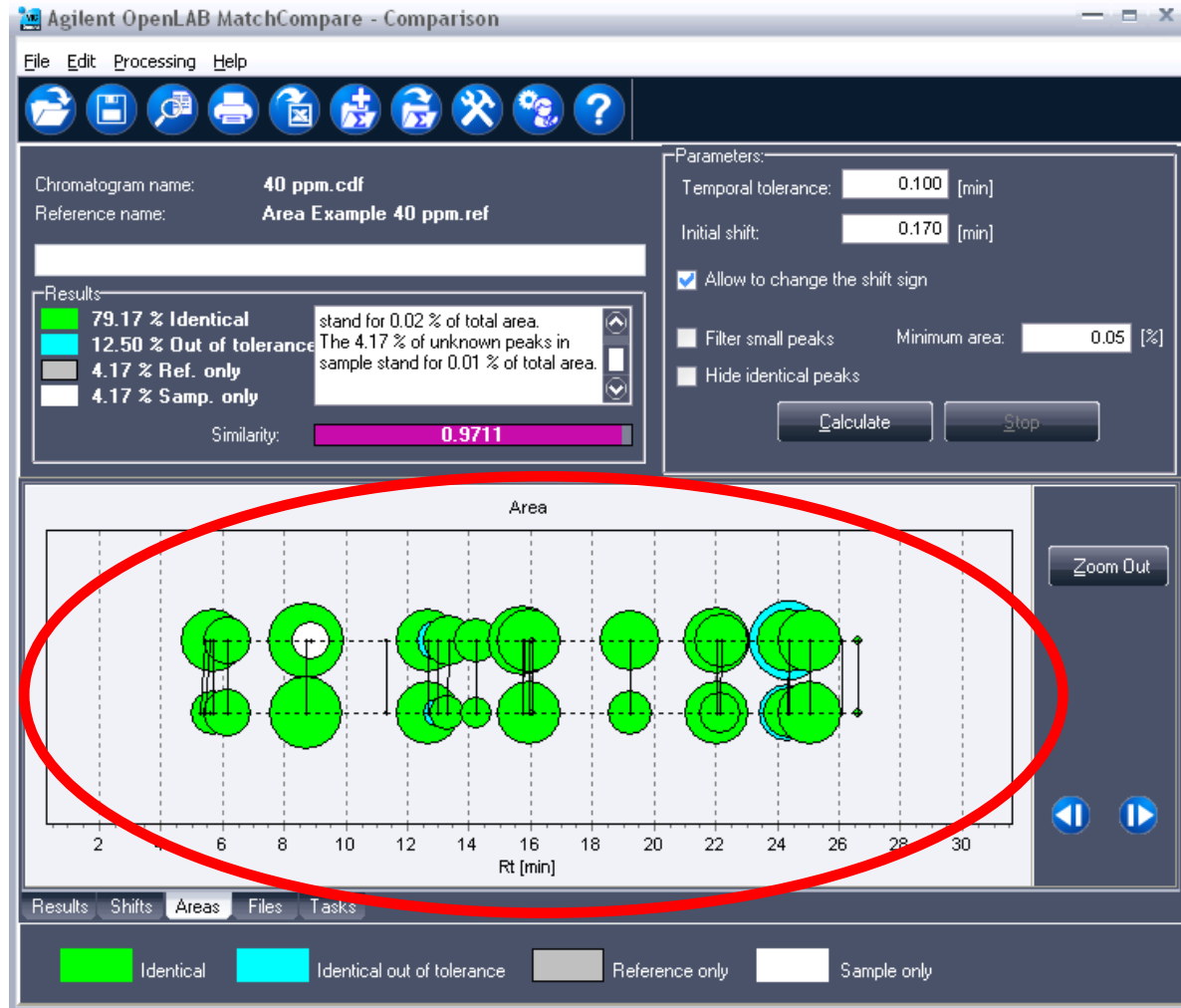
—the peak appears in both sample and reference, but its area percent is out of tolerance (Cyan)

—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

# 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

Area Example 40 ppm.ref		40 ppm.cdf			
#	Components	Ref Time	Ref Area	Time	Area
9		5.44	0.00	5.60	0.00
10		5.60	0.00		
11		5.72	0.01	5.73	0.02
12		6.20	0.01	6.19	0.01
13		8.75	0.03	8.75	0.03
14				8.88	0.01
15		11.30	0.00	11.30	0.00
16	analyte 4ds	12.66	0.02	12.66	0.02
17		12.97	0.00	12.98	0.01
18		13.31	0.01	13.33	0.01
19		14.23	0.01	14.24	0.01
20		15.72	0.01	15.74	0.03
21		15.77	0.00	15.78	0.01
22	analyte 32al	15.96	0.02	15.97	0.02
23		16.05	0.00	16.05	0.00
24		19.24	0.01	19.25	0.02
25	analyte 34ai	22.03	0.02	22.03	0.02
26		22.17	0.01	22.18	0.02
27	analyte 231	24.34	0.02	24.36	0.03
28		24.38	0.01	24.41	0.02
29		25.06	0.02	25.06	0.02
30		26.10	0.00	26.10	0.00
31		26.62	0.00	26.62	0.00

Reference name: Area Example 40 ppm.ref Nb of peaks:30

A comparison will be successful if and only if:

- The sum of the missing or additional peaks area is under  %
- and all errors are under  %

Success criterion | Tolerances

Parameters:

Temporal tolerance:  [min]

Initial shift:  [min]

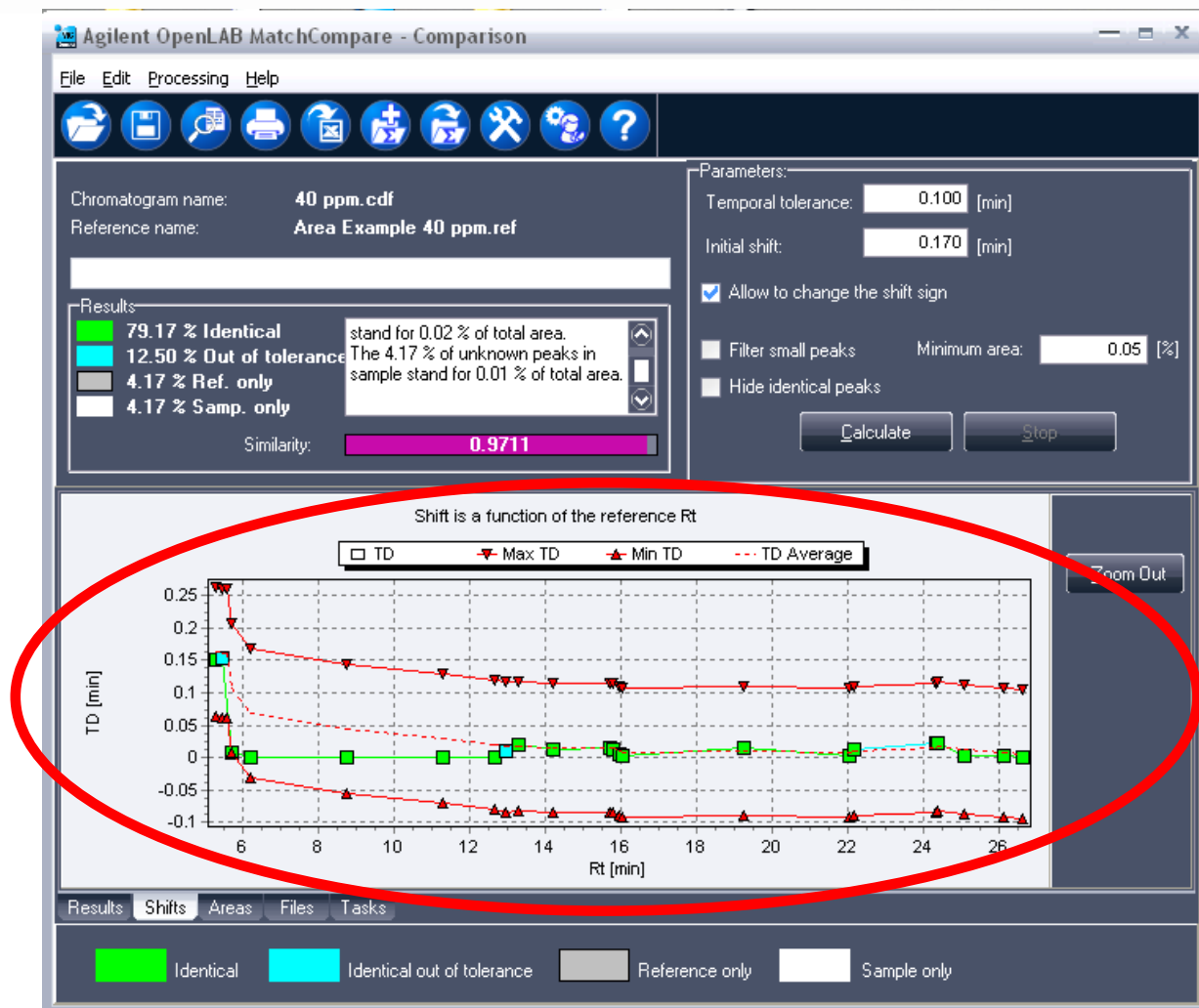
Allow to change the shift sign

Filter small peaks Minimum area:  [%]

Hide identical peaks

# 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 Comparison Report

# 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

## Comparison Report

Comparison between Area Example 40 ppm.ref and SIGNAL01.cdf

Similarity: 0.9781  
87.50% identical  
4.17% Out of tolerance  
4.17% in reference  
4.17% in sample

4.17 % of peaks out of tolerance represents 0.00 % of total area

4.17 % of unknown peaks represents 0.00 % of total area

Validated by: \_\_\_\_\_ Signature: \_\_\_\_\_

### Results table

Code	Name	Rt Samp [min]	Rt Ref [min]	DT	% Samp	% Ref	% Error	Tol (%)	Info
0.00	5.29	---	---	---	0.0000	---	---	---	Samp
0.00	5.44	5.29	0.15	0.0000	0.0000	25.72	100.00	id	
0.00	5.60	5.44	0.15	0.0001	0.0000	163.05	100.00	id_OT	
0.00	---	---	---	---	0.0001	0.0000	---	100.00	Ref
0.00	5.72	5.72	0.00	0.0107	0.0107	0.00	100.00	id_Tall peak	
0.00	6.20	6.20	0.00	0.0114	0.0114	0.00	100.00	id_Tall peak	
0.00	8.75	8.75	0.00	0.0283	0.0283	0.00	100.00	id_Tall peak	
0.00	11.30	11.30	0.00	0.0001	0.0001	0.00	100.00	id	
0.00	12.66	12.66	0.00	0.0021	0.0021	0.00	100.00	id_Tall peak	
0.00	12.97	12.97	0.00	0.0041	0.0041	0.00	100.00	id	
0.00	13.31	13.31	0.00	0.0065	0.0065	0.00	100.00	id	
0.00	14.23	14.23	0.00	0.0052	0.0052	0.00	100.00	id	
0.00	15.72	15.72	0.00	0.0130	0.0130	0.00	100.00	id_Tall peak	
0.00	15.77	15.77	0.00	0.0035	0.0035	0.00	100.00	id	
0.00	15.96	15.96	0.00	0.0024	0.0024	0.00	100.00	id_Tall peak	
0.00	16.05	16.05	0.00	0.0001	0.0001	0.00	100.00	id	
0.00	19.24	19.24	0.00	0.0100	0.0100	0.00	100.00	id_Tall peak	
0.00	22.03	22.03	0.00	0.0028	0.0028	0.00	100.00	id_Tall peak	
0.00	22.17	22.17	0.00	0.0082	0.0082	0.00	100.00	id_Tall peak	
0.00	24.34	24.34	0.00	0.0163	0.0163	0.00	100.00	id_Tall peak	
0.00	24.38	24.38	0.00	0.0126	0.0126	0.00	100.00	id_Tall peak	
0.00	25.06	25.06	0.00	0.0002	0.0002	0.00	100.00	id_Tall peak	
0.00	26.10	26.10	0.00	0.0001	0.0001	0.00	100.00	id	
0.00	26.62	26.62	0.00	0.0003	0.0003	0.00	100.00	id	

Summary - Area Example 40 ppm.merg

#	Area Example 40 ppm.ref	40 ppm.cdf			
Components	Ref Time	Ref Area	Time	Area	
9	5.44	0.00	5.60	0.00	
10	5.60	0.00			
11	5.72	0.01	5.73	0.02	
12	6.20	0.01	6.19	0.01	
13	8.75	0.03	8.75	0.03	
14			8.88	0.01	
15	11.30	0.00	11.30	0.00	
16	analyte 4ds	12.66	0.02	12.66	0.02
17		12.97	0.00	12.98	0.01
18		13.31	0.01	13.33	0.01
19		14.23	0.01	14.24	0.01
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22	analyte 32al	15.96	0.02	15.97	0.02
23		16.05	0.00	16.05	0.00
24		19.24	0.01	19.25	0.02
25	analyte 34ai	22.03	0.02	22.03	0.02
26		22.17	0.01	22.18	0.02
27	analyte 231	24.34	0.02	24.36	0.03
28		24.38	0.01	24.41	0.02
29		25.06	0.02	25.06	0.02
30		26.10	0.00	26.10	0.00
31		26.62	0.00	26.62	0.00

# 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

# Reference

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