

Poster Reprint

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Workflow for Authenticity Testing of Plant Extract Using the High-Resolution LC/QTOF and Statistical Analysis

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Introduction

Interest in food authenticity testing is growing rapidly across the food manufacturing industry. Food manufacturers often encounter adulteration and false labeling in the complex food supply chain and consequently, there is a high demand for powerful, convenient, and easy-to-use analytical tools. High-resolution (HRMS) used in a non-targeted approach is gaining popularity in detecting food fraud and adulteration. This study used lavender essential oil to demonstrate a novel authenticity workflow. Lavender essential oil is often analyzed using GCMS (GC/TQ or GC/QTOF) for volatile compounds. The chemical composition of lavender extracts is also rich in secondary metabolites, such as phenolic acids and coumarins, which can produce unique fingerprints using LCMS. LC/QTOF with non-targeted data collection was utilized to profile and fingerprint complex lavender extracts, and to study composition differences and characterize unknown chemical components of lavender essential oil and its common adulterants. Agilent MassHunter Explorer was utilized for feature extraction, statistical analysis, and compound identification. The integration of Agilent curated libraries, NIST LCMS (MS/MS) Search, and SIRIUS into Explorer enhances accuracy and confidence in identifying unknown compounds.

Experimental

Agilent 1290 Infinity II UHPLC system was coupled with an Agilent Revident Q-TOF system in ESI positive mode for MS and MS/MS (data-dependent) acquisition. Spectra were analyzed using Agilent MassHunter Explorer and Qualitative Analysis. Explorer software processed LC-MS and LC-MS/MS data using tools that perform feature extraction and alignment to find and align compounds across samples.



Agilent 1290
Infinity II LC
with Revident
LC/Q-TOF
System

Experimental

Sample Information

Authentic Raw Ingredients for Lavender Essential Oil

Lavender Bulgarian (LB)

Lavender France (LF)

Lavender, China Blue Flower (LCB)

Lavender, China White Flower (LCW)

Commonly Used Lavender Oil Adulterants

A: Ho wood Crude Oil

B: Ho Leaf Crude Oil

C: Raw Clove Bud Oil

D: Eucalyptus

E: Rosewood oil

F: Potentially adulterated lavender essential oil from different vendor

G: Adulterated lavender oil by synthetic constituents

Chromatographic Conditions

UHPLC: Agilent 1290 Infinity II

Column: Agilent Poroshell SB-AQ 150 x 2.1 mm, 2.7 μ m

Column oven temperature: 40°C

Injection volume: 2 μ L

Autosampler: 5 \pm 2°C

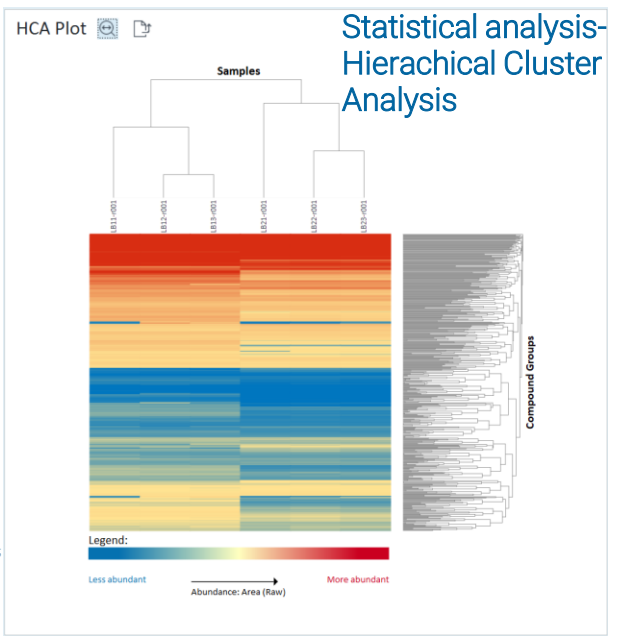
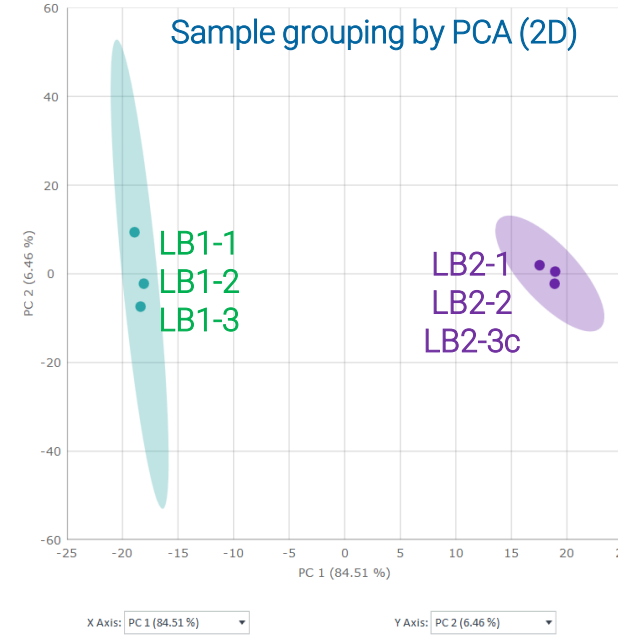
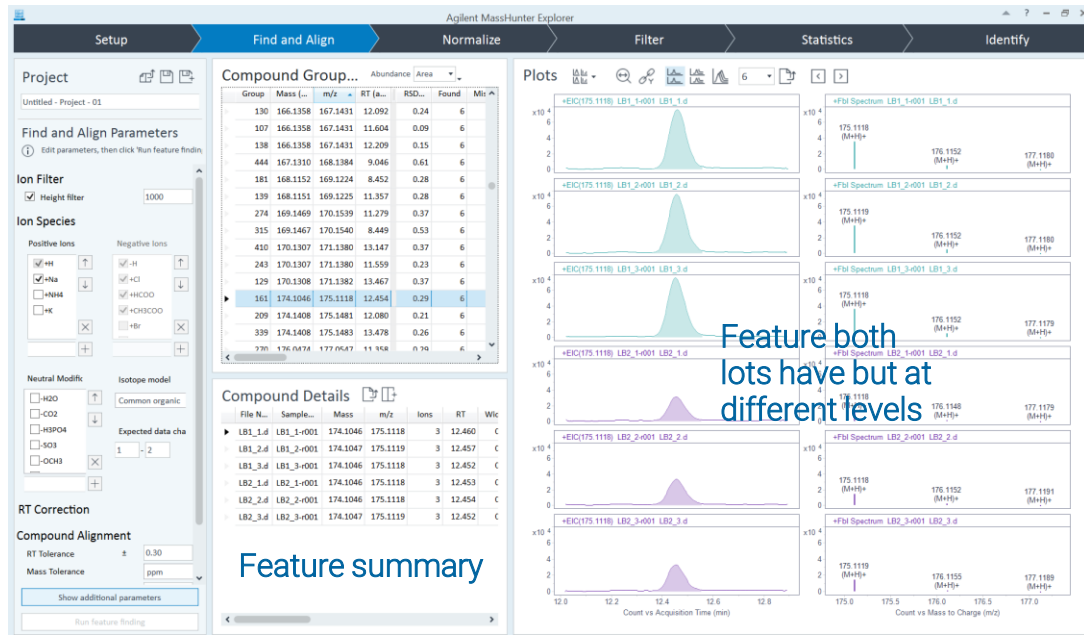
Mobile Phase A/B: 0.1% Formic Acid in Water/MeOH

Time, min	Flow Rate, mL/min	%B
0	0.25	10
10	0.25	60
15	0.25	80
22	0.25	100
25	0.25	100
26	0.25	10
30	0.25	10

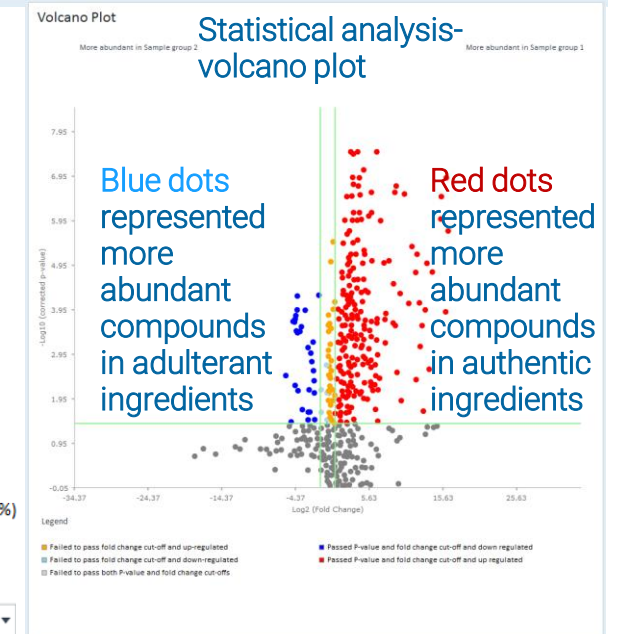
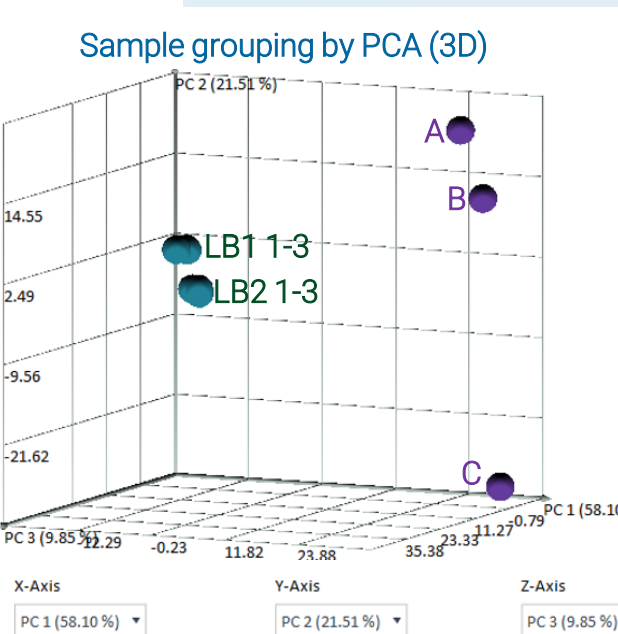
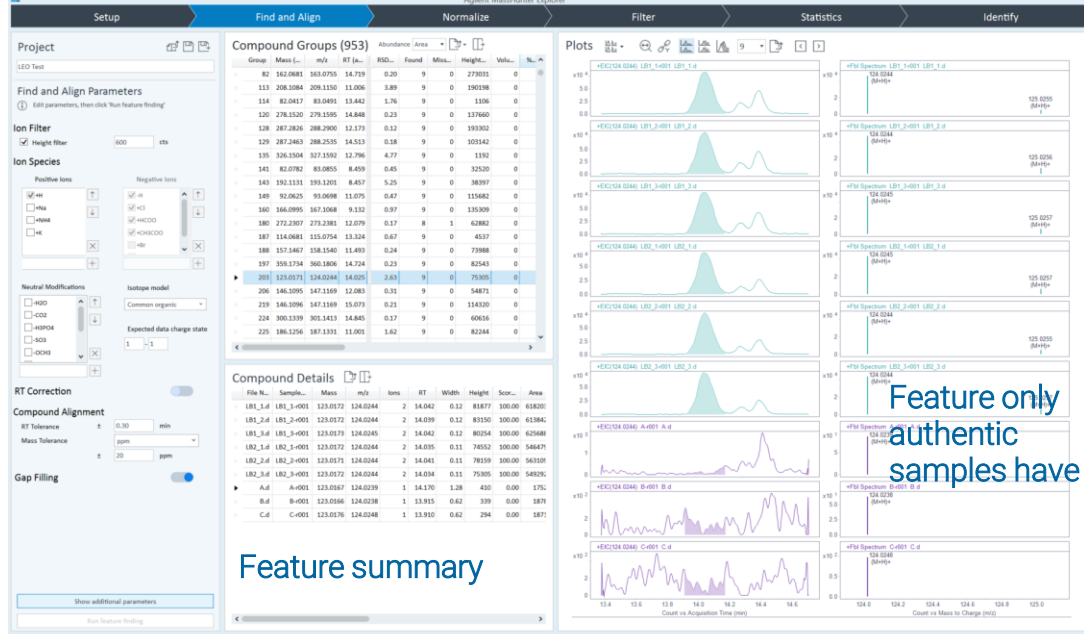
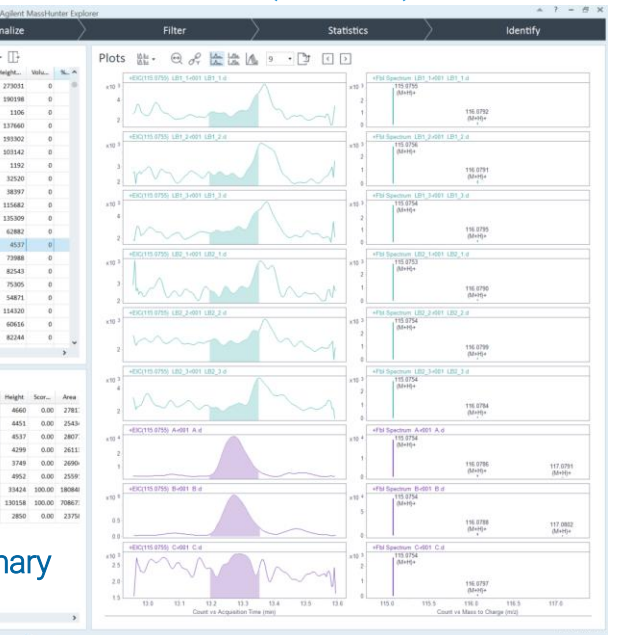
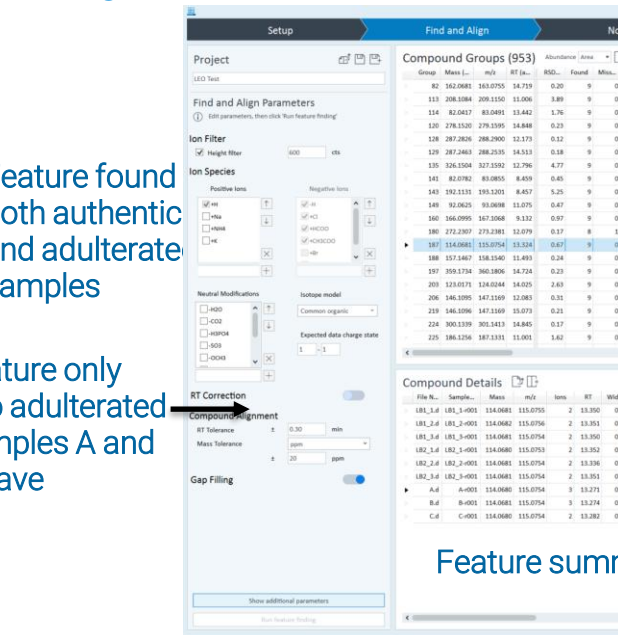
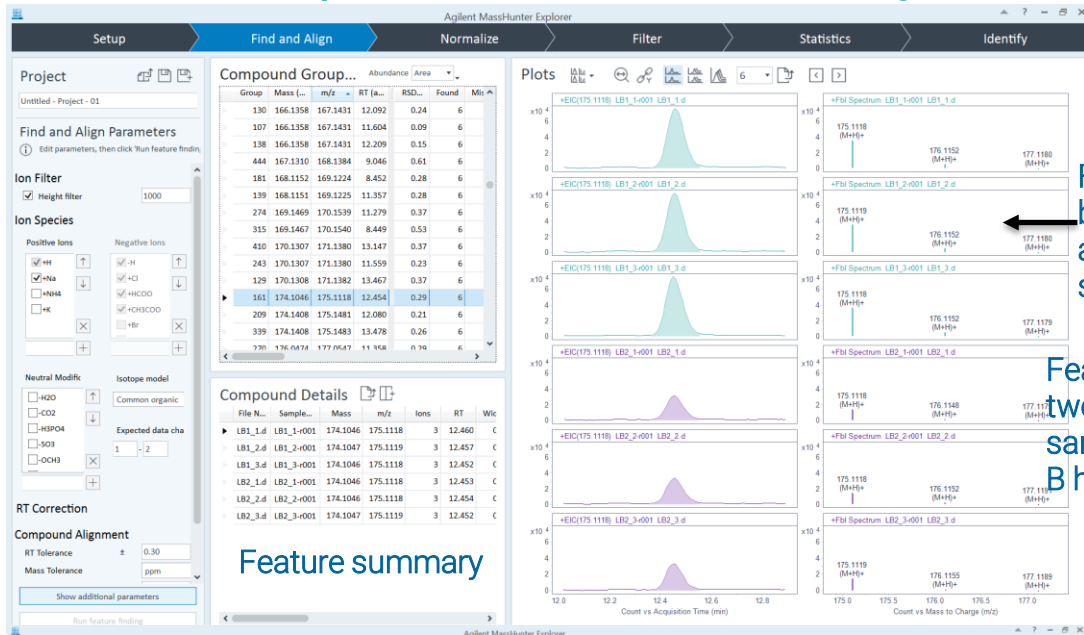
Optimized MS Conditions-Agilent Revident LC/Q-TOF

Parameters	
Drying gas temperature	275 °C
Drying gas flow	13 L/min
Nebulizer gas	30 psi
Sheath gas temperature	385°C
Sheath gas flow	12 L/min
Capillary voltage	4000 V
Nozzle voltage	1000 V
Ion mode	AJS ESI Positive
Fragmentor	125V
Skimmer	45V
MS acquisition	MS Scan and Auto MS/MS MS/MS: 40V CE
MS range	<i>m/z</i> 70-1100/25-1100 for MS/MSMS
Acquisition rate/Time	3 spectra/s

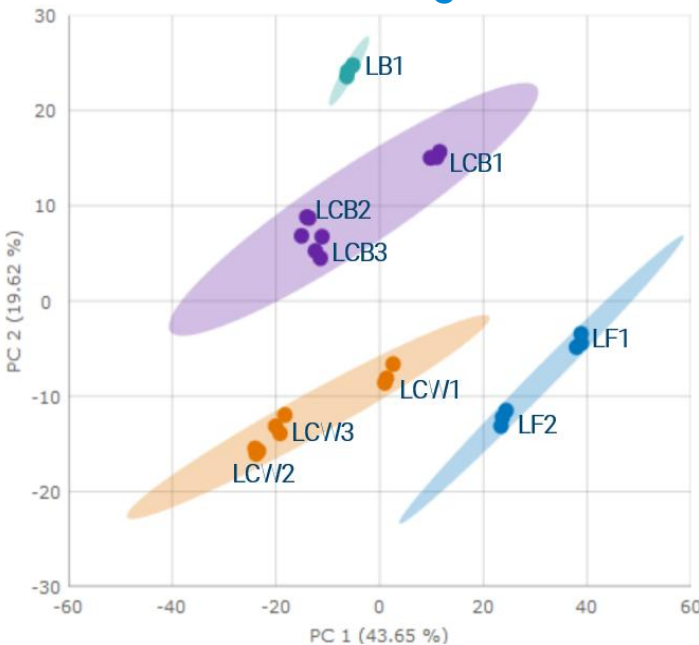
MH Explorer – Two Lots of Same Origin Authentic Ingredients



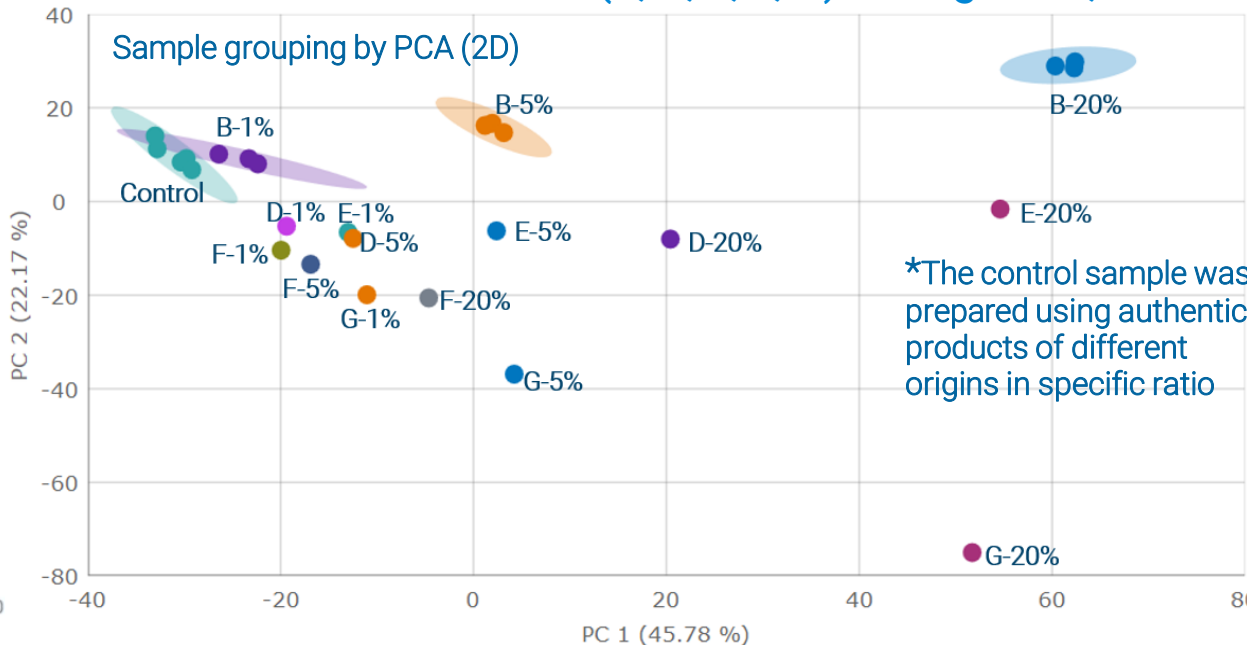
MH Explorer – Two Lots of Same Origin Authentic Ingredients vs. Three Common Adulterants (A, B, C)



MH Explorer – Different Origin Authentic Ingredients



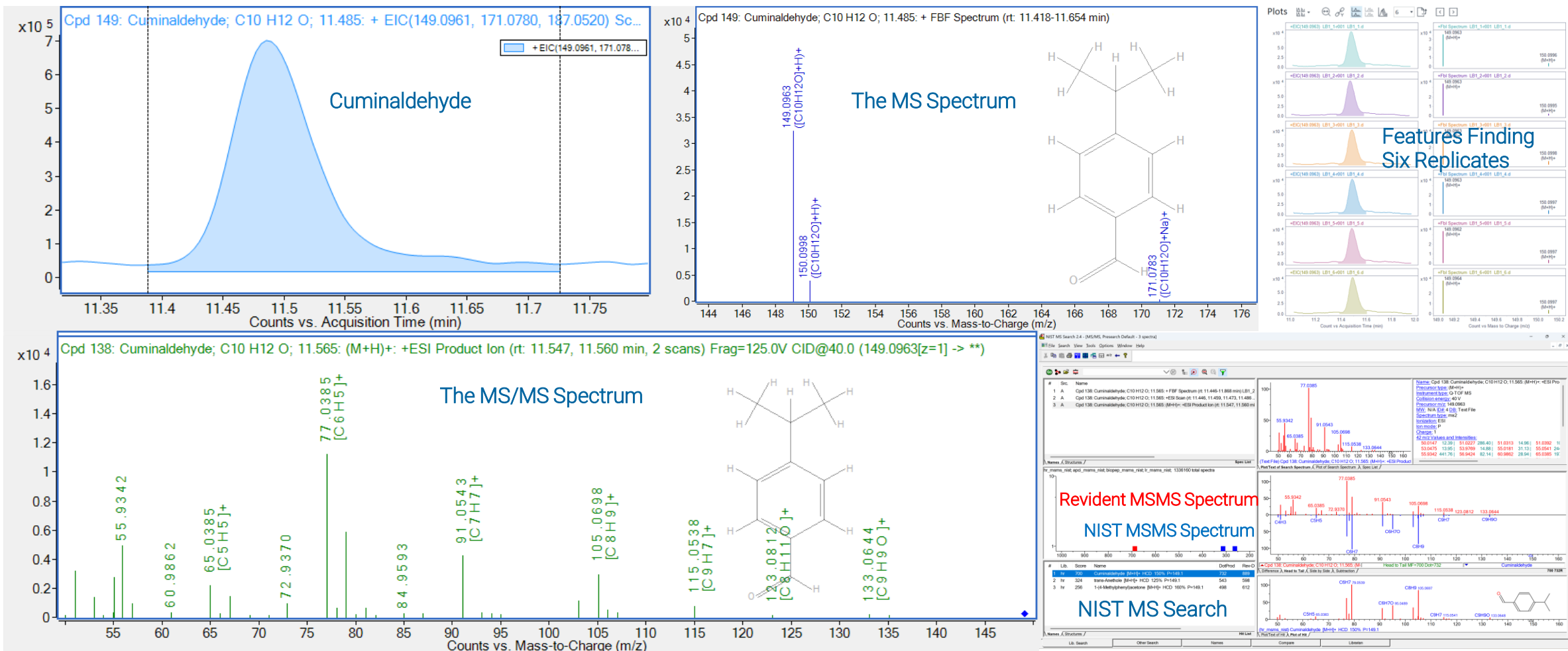
MH Explorer – Authentic product vs. Authentic Product with Adulterant (B, D, E, F, G) mixing in 1%, 5% and 20%



Sample groups	Replicates
Control*	5
B-1%	3
B-5%	3
B-20%	3
D-1%	1
D-5%	1
D-20%	1
E-1%	1
E-5%	1
E-20%	1
F-1%	1
F-5%	1
F-20%	1
G-1%	1
G-5%	1
G-20%	1

*The control sample was prepared using authentic products of different origins in specific ratio

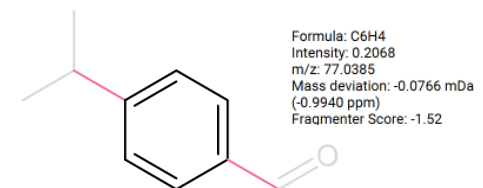
MH Explorer – Unknown Identification (Cuminaldehyde as an Example) with Agilent Database and NIST MS Search



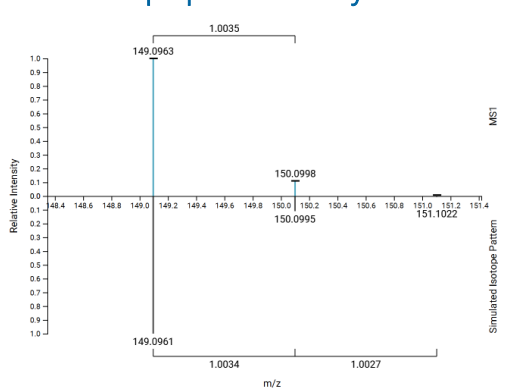
MH Explorer – Unknown Identification (Cuminaldehyde as an Example) with SIRIUS

Molecular formula generation

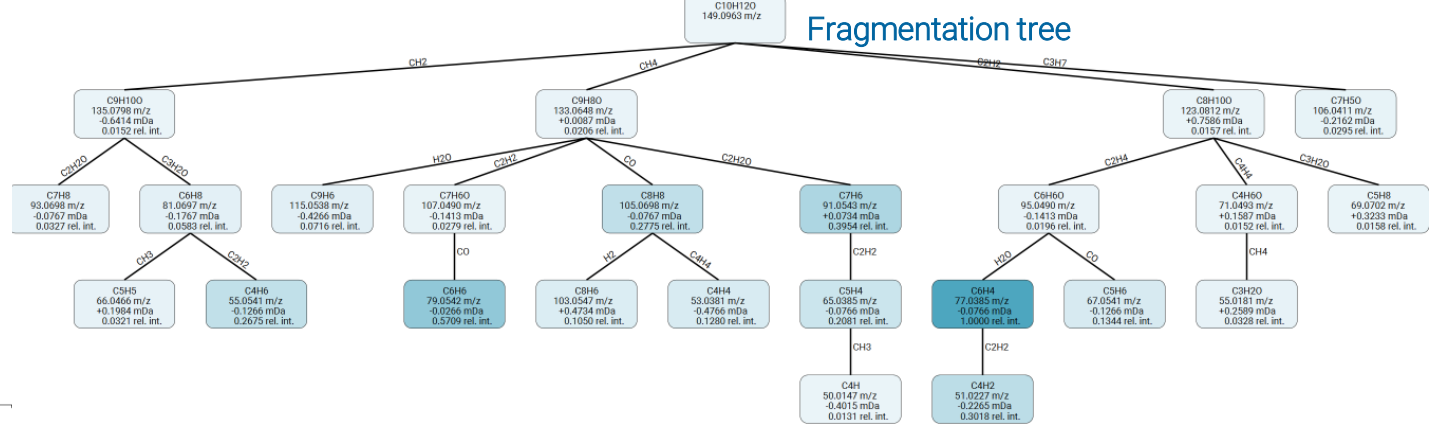
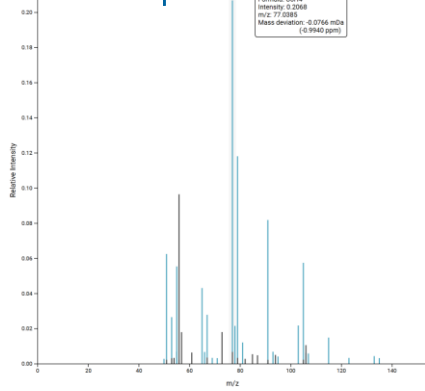
Rank	Molecular Formula	Adduct	Zodiac Score	Sirius Score (normalized) ▾	Isotope Score	Tree Score	Explained Peaks	Total Explained Intensity	Median Mass Error (ppm)	Median Mass Error (mDa)
1	C10H12O	[M + H] ⁺	NaN	100.000%	3.279	112.484	25/25	80.477%	-1.177	-0.077
2	C7H13FO2	[M + H] ⁺	NaN	0.000%	1.711	99.324	24/25	80.500%	-7.510	-0.573
3	C8H10N3	[M + H] ⁺	NaN	0.000%	1.479	76.346	22/25	78.355%	-0.534	-0.052
4	C7H15CIN	[M + H] ⁺	NaN	0.000%	0.000	68.666	21/25	70.590%	-2.180	-0.127
5	C4H12BN04	[M + H] ⁺	NaN	0.000%	0.000	39.327	19/25	57.438%	-7.485	-0.477
6	C3H9FN6	[M + H] ⁺	NaN	0.000%	0.000	35.715	17/25	63.254%	3.000	0.273
7	C5H14N3S	[M + H] ⁺	NaN	0.000%	0.261	18.095	15/25	26.389%	-1.177	-0.077



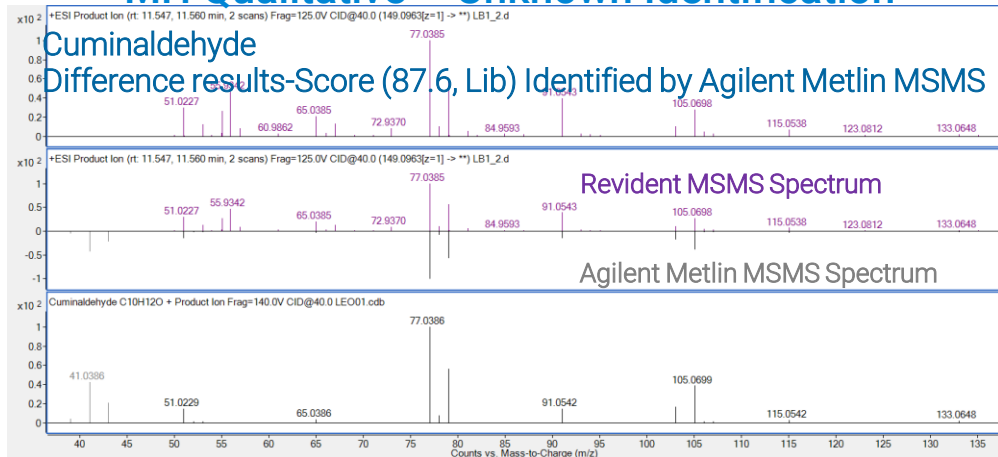
MS1 isotope pattern analysis



MSMS spectra



MH Qualitative – Unknown Identification



Conclusions

- The accurate mass LC/Q-TOF technique, combined with the advanced MassHunter Explorer differential analysis workflow, successfully analyzed and interpreted lavender essential oil profiling results, confirming adulteration and identifying unknown compounds.
- The workflow provides an efficient and accurate way for the quality control of lavender essential oils and other plant materials.

The authors declare no competing financial interest

<https://www.agilent.com/en/promotions/asms>

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