



Applying statistical data processing tools for GC×GC differentiation of alternative aviation fuels

Christina Kelly, LECO SepSci Application Chemist

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LECO Corporation – Our Beginning



- The Laboratory Equipment Company was founded in 1936 by Carl Schultz, when he introduced the first rapid carbon analyzer for use in the steel industry.
- LECO followed this with the Rapid Sulphur Determinator and many more pioneering innovations.
- In the 1970s LECO won the “E” Award for Exports from President Nixon, received by Robert Warren who became President of LECO Corp.
- In 1980s the age of the computer: self-calibration, microprocessors etc

LECO Corporation, St Joseph, Michigan



- LECO's HQ, is located in Saint Joseph, MI on the shores of Lake Michigan.
- An established, global organisation, serving 75 countries around the world and still privately owned, actively run by 3rd generation family.



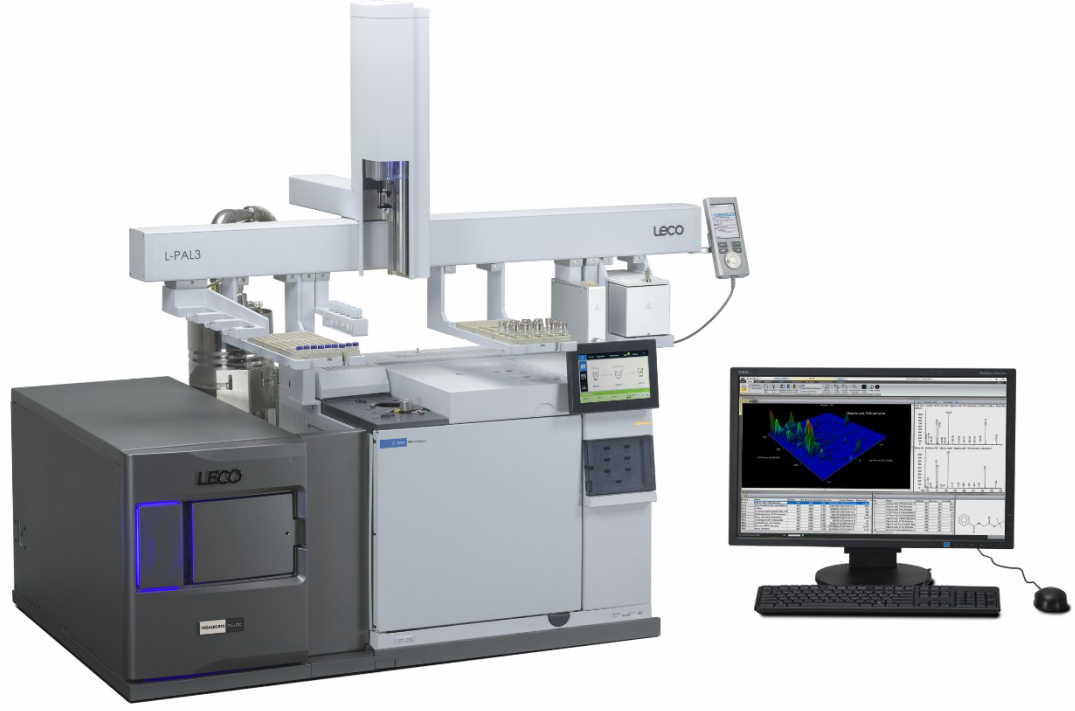
LECO Corporation – A Leader in Separation Science

- Innovation of the first fast GC-MS based on time-of-flight (ToF) technology at Pittcon in 1995.
- One year later, introduction of the world's first commercial GC-TOFMS, the Pegasus
- In the next decade, a move into modulation technology sees LECO become industry leaders in comprehensive 2D GCxGC solutions
- 2011 - introduction of a fast acquisition high resolution platform – the Pegasus HRT
- Best of class, full mass range, fast data acquisition is the hallmark of LECO Pegasus TOFMS products
- 2016-2020 Introduction of highly sensitive benchtop TOFMS product range - the Pegasus BT






Introducing the next-generation benchtop TOFMS: BTX

Detector:	Scintillator – Photomultiplier Tube with extended lifetime
Mass Analyzer:	Time-of-Flight Mass Analyzer with Dual Stage single Reflectron
Mass Range:	10 – 1500 m/z
Mass Resolution:	> 1,100 at m/z 219
Spectral Acquisition Rate:	1-500 spectra/second
Detection Limit:	10fg OFN with Quant S/N > 10 (Helium carrier gas) 10fg OFN with Quant S/N > 10 (Hydrogen carrier gas)
IDL:	< 4fg for 8 replicates of 10fg OFN injected
Precision:	< 5% RSD for 15 injections of 100fg OFN
Linear Dynamic Range:	5 orders of magnitude



With new more-rugged detector, BTX is our most sensitive TOFMS to date!

Comparison of Software Offerings

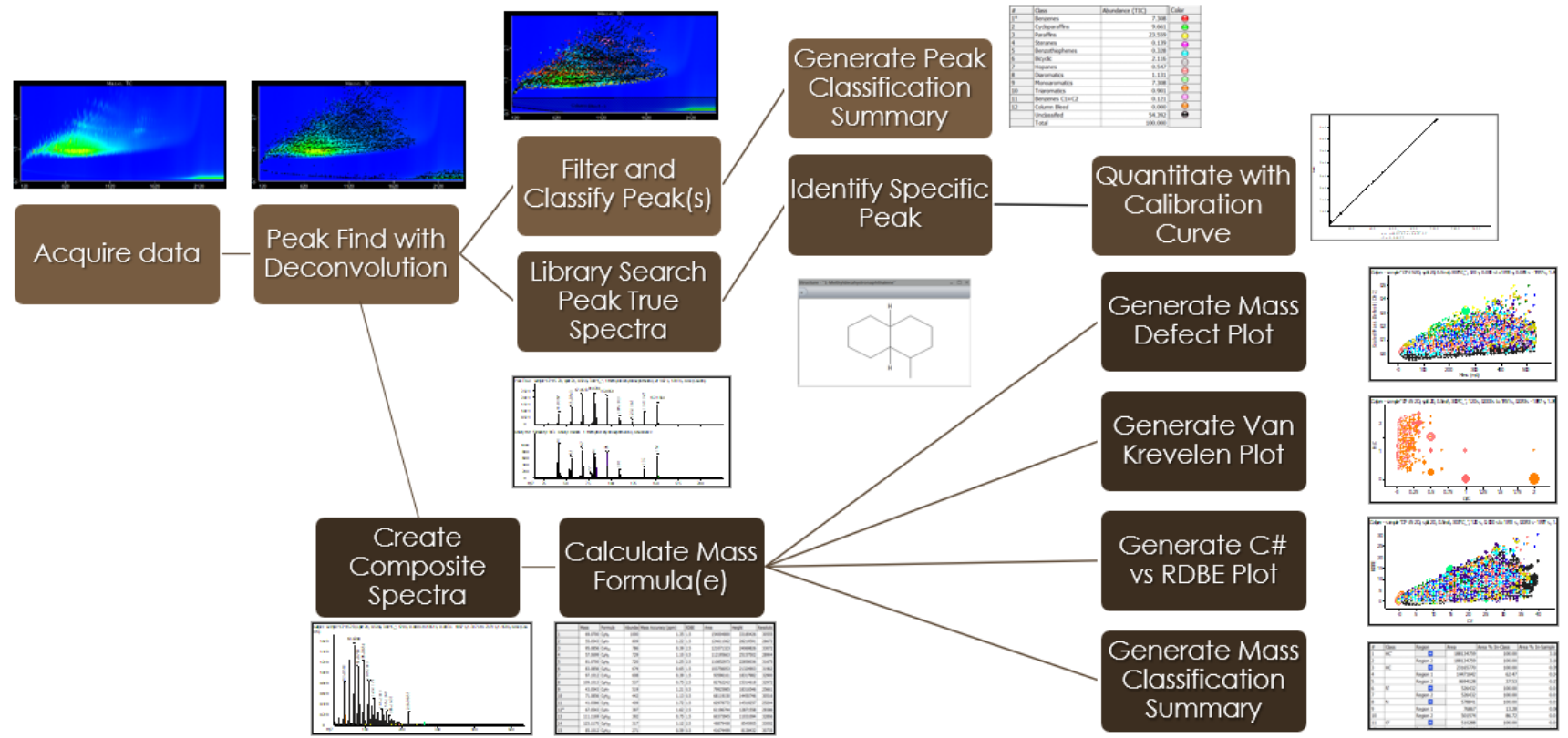
Software Option			
Objective	Detailed sample acquisition & characterization	Find differences between samples or groups of samples	Detailed batch interrogation
Features	<ul style="list-style-type: none"> • Single-sample deconvolution • Target Analyte Find • Quantitation • Classifications 	Statistical comparisons using: <ol style="list-style-type: none"> 1. Fisher Ratio 2. CoV 3. Fold-Change 	<ul style="list-style-type: none"> • Deconvolution performed over a set of samples • Aligned Peak Table • Statistical trends

Complementary approaches for a variety of experimental design needs!

See Liz Humston-Fulmer's poster this afternoon for more on ChromaTOF Sync!

ChromaTOF Data Acquisition & Processing

- Full AS, GC, MS acquisition control
- NonTarget Deconvolution
- Target Analyte Find
- Classification Summaries
- Quantitation
- Spectral Analysis Tools (for High-Resolution MS data)



ChromaTOF Data Acquisition & Processing

Application Note

Instrument: Pegasus® BTX 4D

Characterization of Fischer-Tropsch Synthetic Paraffinic Kerosene and Traditional Aviation Turbine Fuel

LECO Corporation, Saint Joseph, Michigan USA

Key Words: Petroleum, GCxGC, Thermal Modulation, Aviation Fuels, SAF



Introduction

The synthetic aviation fuels (SAF) market provides an alternative to traditional fossil-based aviation fuels derived from crude oil by using renewable and sustainable feedstock. This market is expected to grow significantly in the next decade due to regulations like the EU's ReFuelEU proposal and the United States' Sustainable Aviation Fuel Grand Challenge that promote the use of sustainable aviation fuels to reduce air quality impacts and greenhouse gas emissions. Many of the existing certified SAF processing pathways reduce or eliminate the total aromatics and sulfur content, reducing particulate and sulfur-oxide emissions. However, a certain amount of aromatic content is still necessary to maintain the proper freeze points, viscosity, and polymer sealing properties in a jet fueling system, making it important to balance understanding of not only the physical properties, energy content, and emissions profiles of a new fuel, but also the individual components in its chemical makeup that affect these bulk properties. For new fuels to gain approval for use, detailed characterization is required to meet regulatory requirements such as ASTM D7566 and ASTM D1655, which provide specifications for fuels allowed in co-processing and blending for commercial use in the United States. With a combination of comprehensive two-dimensional gas chromatography (GCxGC) and time-of-flight mass spectrometry (TOFMS), the high-quality information necessary for deeper understanding of the composition of synthetic aviation fuels can be produced and utilized to expedite the certification process.

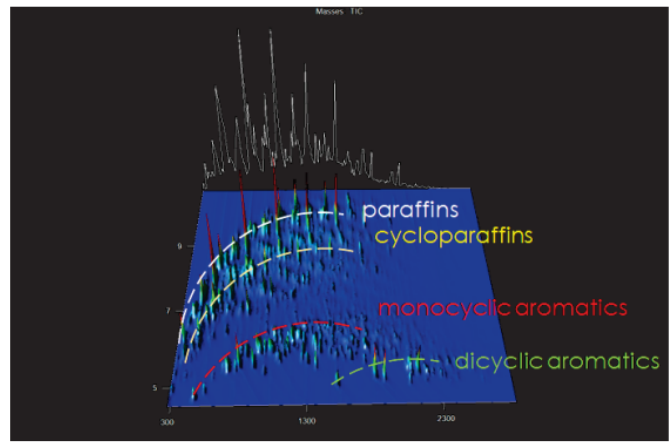
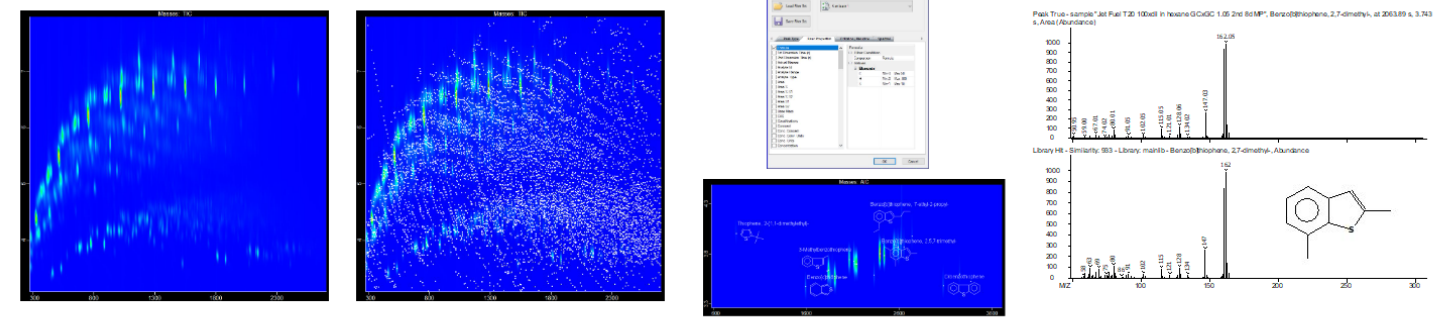
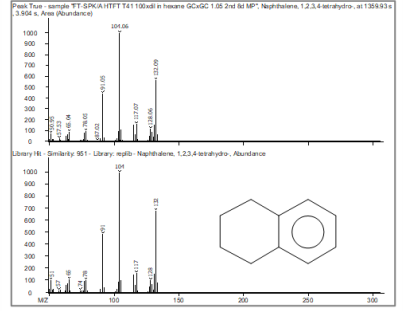
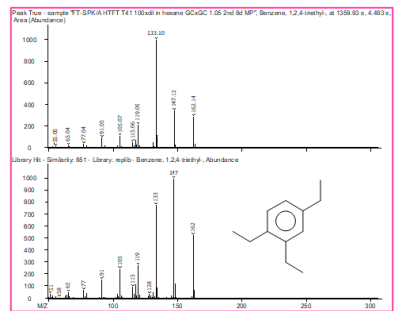
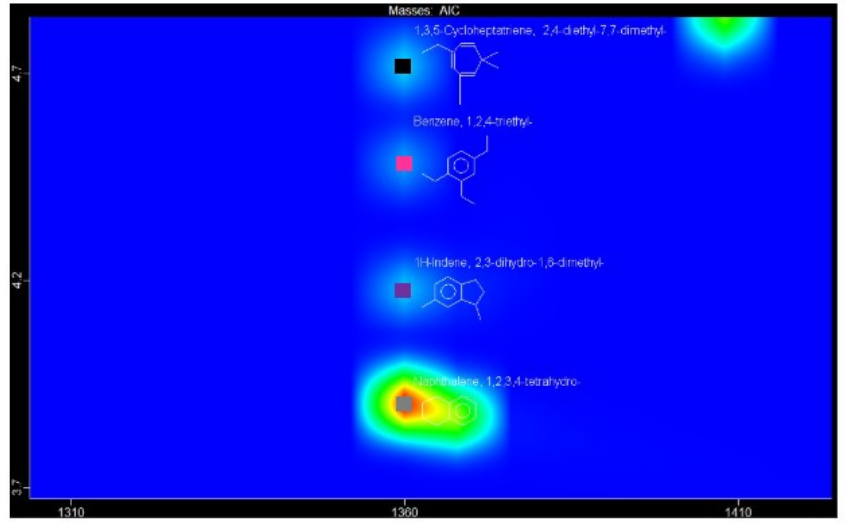
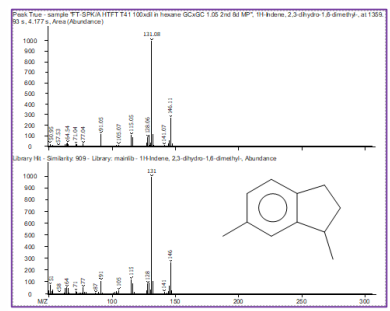
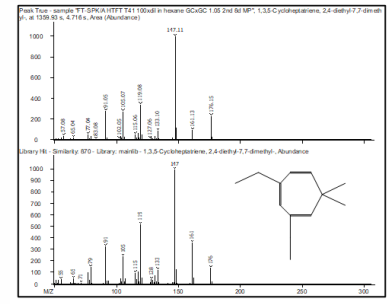


Figure 1. GCxGC 3D surface plot of commercial aviation turbine fuel with Total Ion Chromatogram (TIC) shown. Reconstructed trace of what a single dimension of GC separative would have looked like is shown in white. Elution bands of paraffins (white), cycloparaffins (yellow), monocyclic aromatics (red), and dicyclic aromatics (green) are indicated by dotted lines.



ChromaTOF Data Acquisition & Processing

Application Note

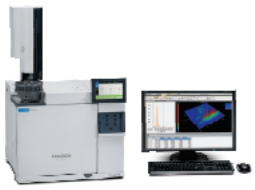


Instrument: Paradigm™ GCxGC-FID

Satisfying ASTM D8396 Requirements

LECO Corporation, Saint Joseph, Michigan USA

Key Words: Petroleum, GCxGC, Flow Modulation, Aviation Fuel, Diesel, Gasoline, Routine



Introduction

In response to the need for standardized compositional characterization of emerging aviation fuels, ASTM Method D8396— "Standard Test Method for Group Types Quantification of Hydrocarbons in Hydrocarbon Liquids with a Boiling Point between 36 °C and 343 °C by Flow Modulated GCxGC-FID"— was first approved in 2022. This application note describes how to use a simple workflow with the LECO Paradigm system to fulfill the requirements of the ASTM D8396 test method to quantitatively determine mass % of total n-paraffins, iso-paraffins, naphthenes, 1-ring aromatics, and 2-ring aromatics using reverse-fill flush flow modulated comprehensive two-dimensional gas chromatography-flame ionization detection (GCxGC-FID). Understanding of bulk composition is crucial for fast-track certification of synthetic aviation fuels as outlined in ASTM D4054, and the more accurate group-type analysis results provided by GCxGC assist with streamlining the acceptance process. GCxGC clearly resolves aliphatic regions from aromatic ones, creating bands of similar compounds which allow for general classification of chemical components based on structural elements and boiling point behavior with only a single-channel detector. When FID is used, area % values from groups of peaks can be used to quantify mass % composition of a sample.

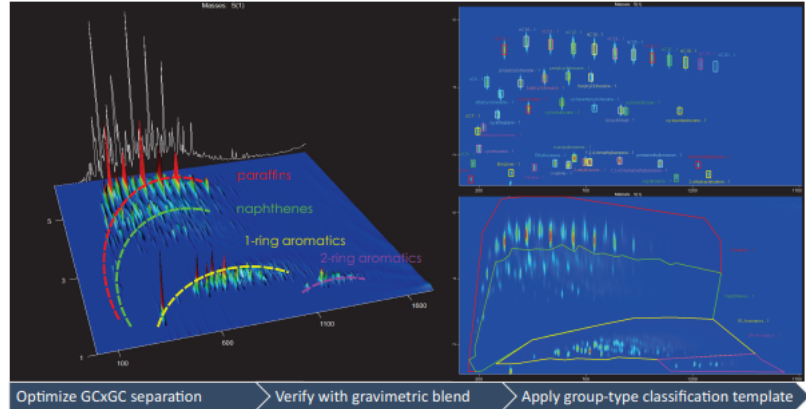
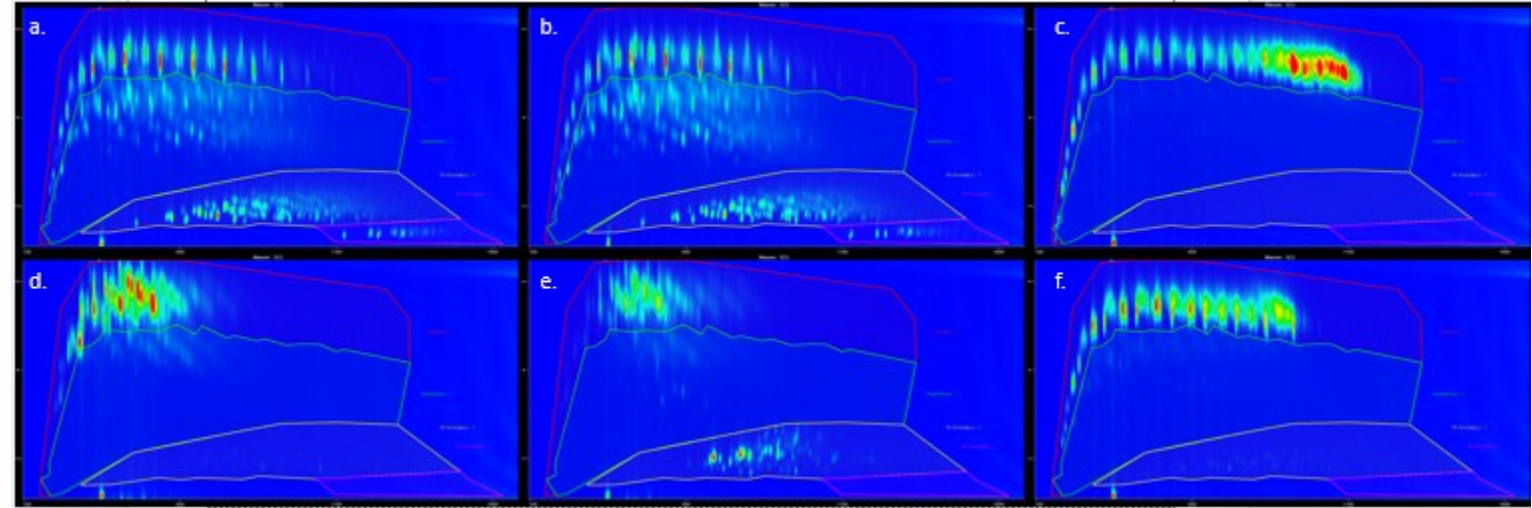
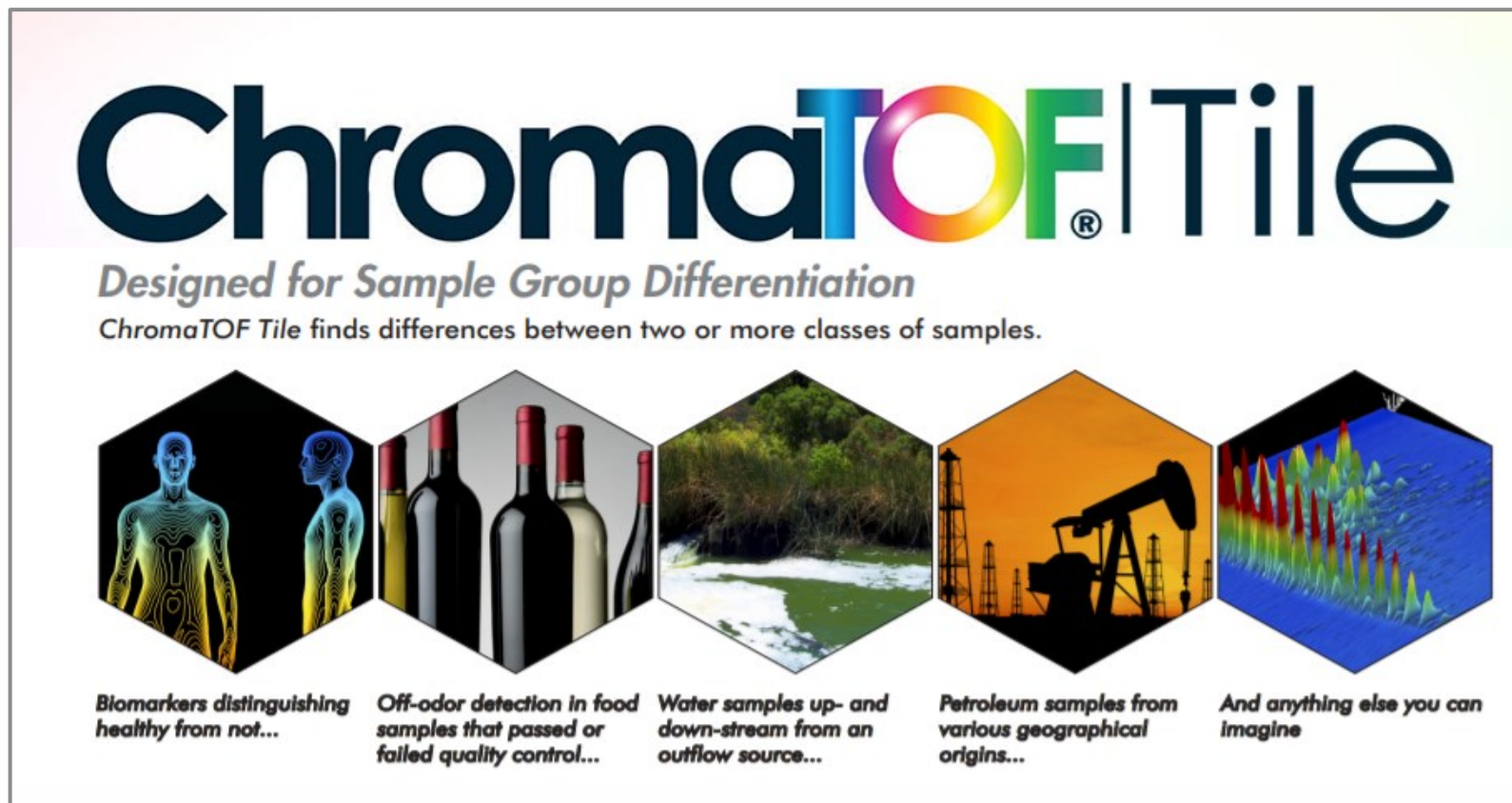


Figure 1. Left: 3D surface plot of aviation fuel showing benefit of GCxGC for improvement of chromatographic resolution, with white reconstructed trace of the 1D GC separation. Compound groups are visually apparent, with the tallest peaks in the back corresponding to paraffins and the short band of analytes at the front corresponding to 2-ring aromatic. Right top: Classification identifying components of the gravimetric standard mix used to verify quantitation method. Right bottom: Contour plot of aviation reference fuel showing classification regions used to generate summary compound class information for ASTM D8396.



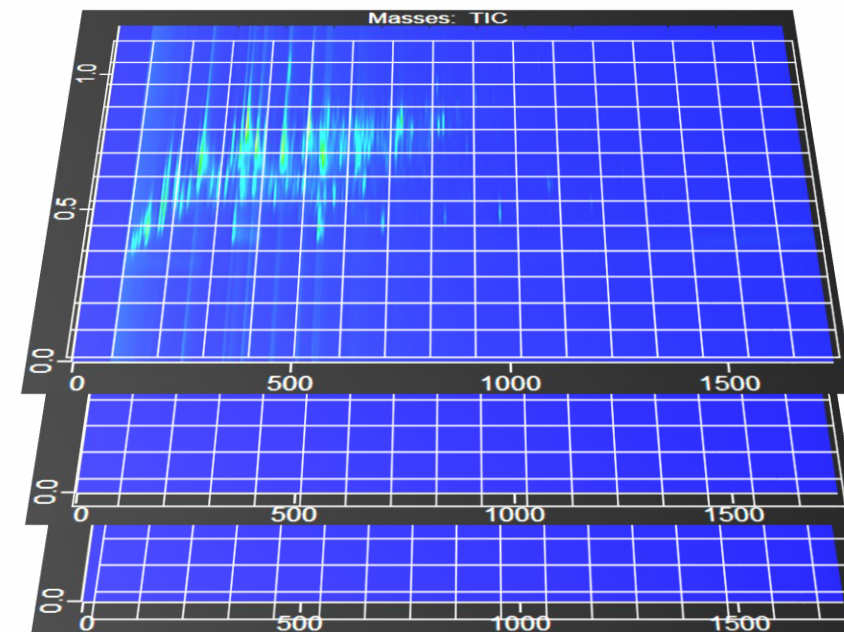
Mass % per Hydrocarbon Group-type Class by FID						
	AVTUR	Jet A	SATF	FT-SPK	FT-SPK/A	HEFA-SPK
n-Paraffins	21.0	18.0	34.0	2.2	5.6	22.3
Iso-Paraffins	26.1	25.2	64.7	92.7	69.1	74.6
Naphthenes	31.8	37.3	0.8	4.4	6.8	2.1
1-Ring Aromatics	19.0	17.7	0.3	0.4	18.3	0.7
2-Ring Aromatics	2.1	1.8	0.2	0.2	0.2	0.3

ChromaTOF TILE Sample Differentiation Tool



ChromaTOF|Tile
Designed for Sample Group Differentiation
ChromaTOF Tile finds differences between two or more classes of samples.

Biomarkers distinguishing healthy from not...
Off-odor detection in food samples that passed or failed quality control...
Water samples up- and down-stream from an outflow source...
Petroleum samples from various geographical origins...
And anything else you can imagine



connects samples with chromatographic tiling approach that links the data set and compares raw data **to find differences**

ChromaTOF TILE Simple Workflow



Click here to auto-calculate suggested tile size
Samples must be selected first

Tile size D1 (modulations):

Tile size D2 (spectra):

S/N threshold:

D1 signal to base threshold:

D2 signal to base threshold:

Samples that must exceed S/N threshold:

Mass F-ratios to average:

Statistical threshold type to apply:

F-ratio threshold:

Relative change threshold type to apply:

Minimum masses per tile:

Minimum mass:

Maximum mass:

Masses to ignore:

Perform one-point normalization:

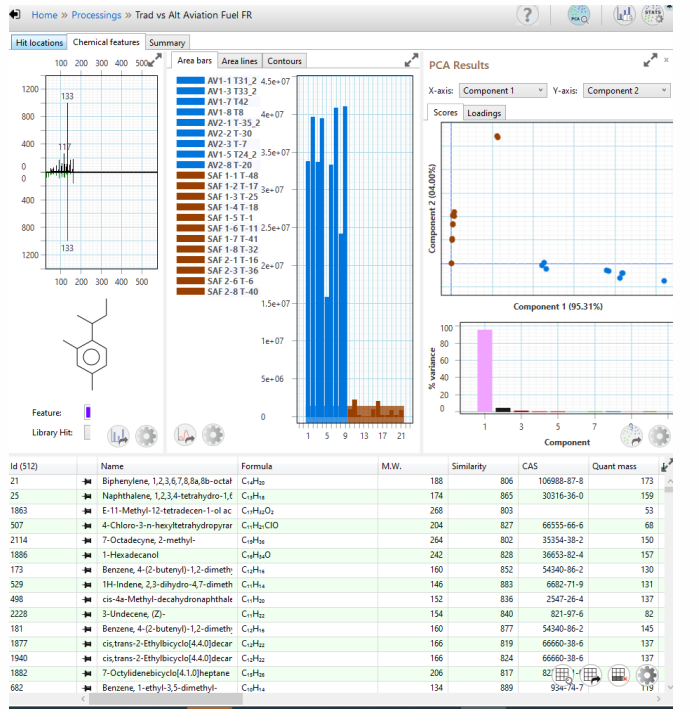
Home » Processings » Trad vs Alt Aviation Fuel FR

All selected tiles: Reject | Unreviewed




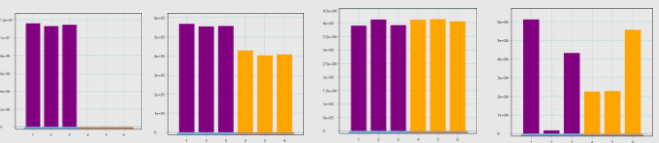
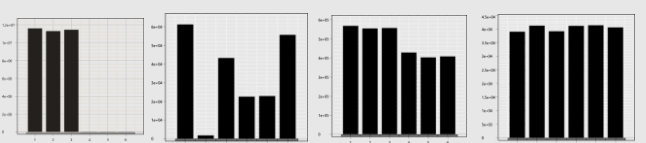
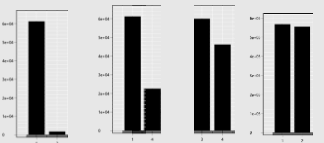
Hit locations	Chemical features	Summary
#	Avg F-ratio	Avg Relative Top mass RT1 RT2 Masses A S
001	730.80	0.00 94 880.20 4.18 2 Accept Reject
002	559.94	0.00 179 880.20 3.58 9 Accept Reject
003	492.79	0.00 145 988.20 1.91 9 Accept Reject
004	484.91	0.00 173 1112.40 2.02 3 Accept Reject
005	429.77	0.00 144 1058.40 1.94 9 Accept Reject
006	396.51	0.00 150 880.20 3.70 2 Accept Reject
007	375.56	0.00 59 955.80 3.60 18 Accept Reject
008	373.34	0.00 119 869.40 3.69 2 Accept Reject
009	373.75	0.00 160 950.40 1.96 53 Accept Reject
010	367.49	0.00 92 955.80 3.61 28 Accept Reject
011	355.49	0.00 148 982.60 3.09 21 Accept Reject
012	341.46	0.00 192 907.20 3.47 5 Accept Reject
013	339.63	0.00 171 1101.60 2.03 10 Accept Reject
014	334.27	0.00 146 966.60 1.89 2 Accept Reject
015	333.52	0.00 158 1051.40 1.87 26 Accept Reject
016	328.03	0.00 144 880.20 2.05 5 Accept Reject
017	327.39	0.00 112 972.00 1.98 73 Accept Reject
018	322.92	0.00 159 1015.20 2.03 12 Accept Reject
019	320.19	0.00 163 961.20 3.22 2 Accept Reject
020	317.55	0.00 131 847.80 1.94 8 Accept Reject
021	311.37	0.00 143 1090.80 1.94 13 Accept Reject
022	300.04	0.00 134 820.80 1.79 61 Accept Reject
023	297.21	0.00 157 1144.80 1.96 17 Accept Reject
024	296.66	0.00 119 869.40 3.40 2 Accept Reject
025	294.13	0.00 196 1231.20 1.74 6 Accept Reject
026	291.75	0.00 92 1004.40 2.73 7 Accept Reject
027	291.44	0.00 134 1004.40 1.93 9 Accept Reject
028	289.07	0.00 80 884.00 3.62 4 Accept Reject
029	288.71	0.00 126 856.60 1.78 61 Accept Reject
030	287.93	0.00 171 1053.00 2.12 2 Accept Reject
031	282.54	0.00 127 856.60 1.87 7 Accept Reject
032	282.04	0.00 138 907.20 3.54 8 Accept Reject
033	280.50	0.00 138 723.60 3.28 5 Accept Reject

Mass hits for selected tile:

#	Mass	F-ratio	Relative Cha	RT1	RT2	Area diff	Accept	Reject	A	S
3	179	689.52	0.00	880.20	3.58	2070763.59	Accept	Reject		
4	110	587.83	0.00	880.20	3.57	1074092.94	Accept	Reject		
5	90	402.47	0.00	880.20	3.57	100710.64	Accept	Reject		
6	149	297.66	0.00	880.20	3.53	177808.57	Accept	Reject		
7	63	189.59	0.00	880.20	3.53	210819.87	Accept	Reject		
8	130	127.19	0.00	880.20	3.53	53772.93	Accept	Reject		
9	188	98.77	0.00	880.20	3.53	9944.57	Accept	Reject		
10	158	10.38	0.00	880.20	3.54	6802.61	Accept	Reject		
11	186	11.57	0.00	880.20	3.53	4254.94	Accept	Reject		



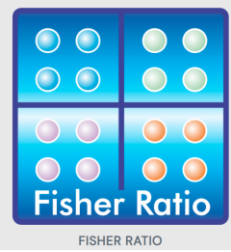
ChromaTOF TILE Comparison of Statistical Methods

Comparison Option	 <small>FISHER RATIO</small>	 <small>COEFFICIENT OF VARIATION</small>	 <small>FOLD CHANGE</small>
Objective	Find differences between samples or groups of samples		
Calculation	$FR = \frac{\textit{class to class variation}}{\textit{within class variation}}$	$CV = \frac{\textit{St Dev of Tile Areas}}{\textit{Mean of Tile Areas}}$	$FC = \frac{\textit{Max response}}{\textit{Min response}}$ <p style="font-size: small; margin-top: 5px;">*reported as Log2(FC) and generalized to compare > 2 values</p>
Experimental design requirements	<ul style="list-style-type: none"> Classes required Replicates required 	<ul style="list-style-type: none"> Classes are not used 	<ul style="list-style-type: none"> Classes optional Only 2 samples needed
Differences that are found			

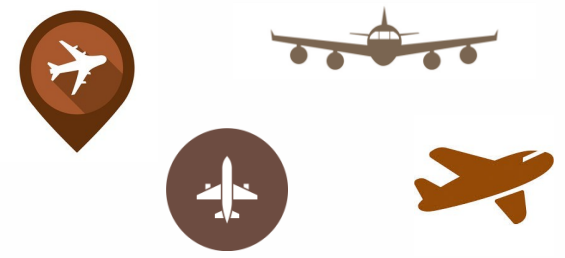
Applications for Each Statistical Method

<p>Comparison Option</p>			
<p>Application Example</p>	<div style="display: flex; flex-direction: column; align-items: center;"> <div style="display: flex; justify-content: space-around; width: 100%;">  </div> <p>Traditional Aviation Fuel</p> <div style="display: flex; justify-content: space-around; width: 100%;">  </div> <p>Synthetic Aviation Fuel</p> </div>	<p>Alternative Aviation Fuels (Multiple Production Methods)</p> 	<p>Pinpointing Components in Aromatics Additive Package</p> 

Experimental Setup: Comparison of Traditional and Synthetic Aviation Fuel



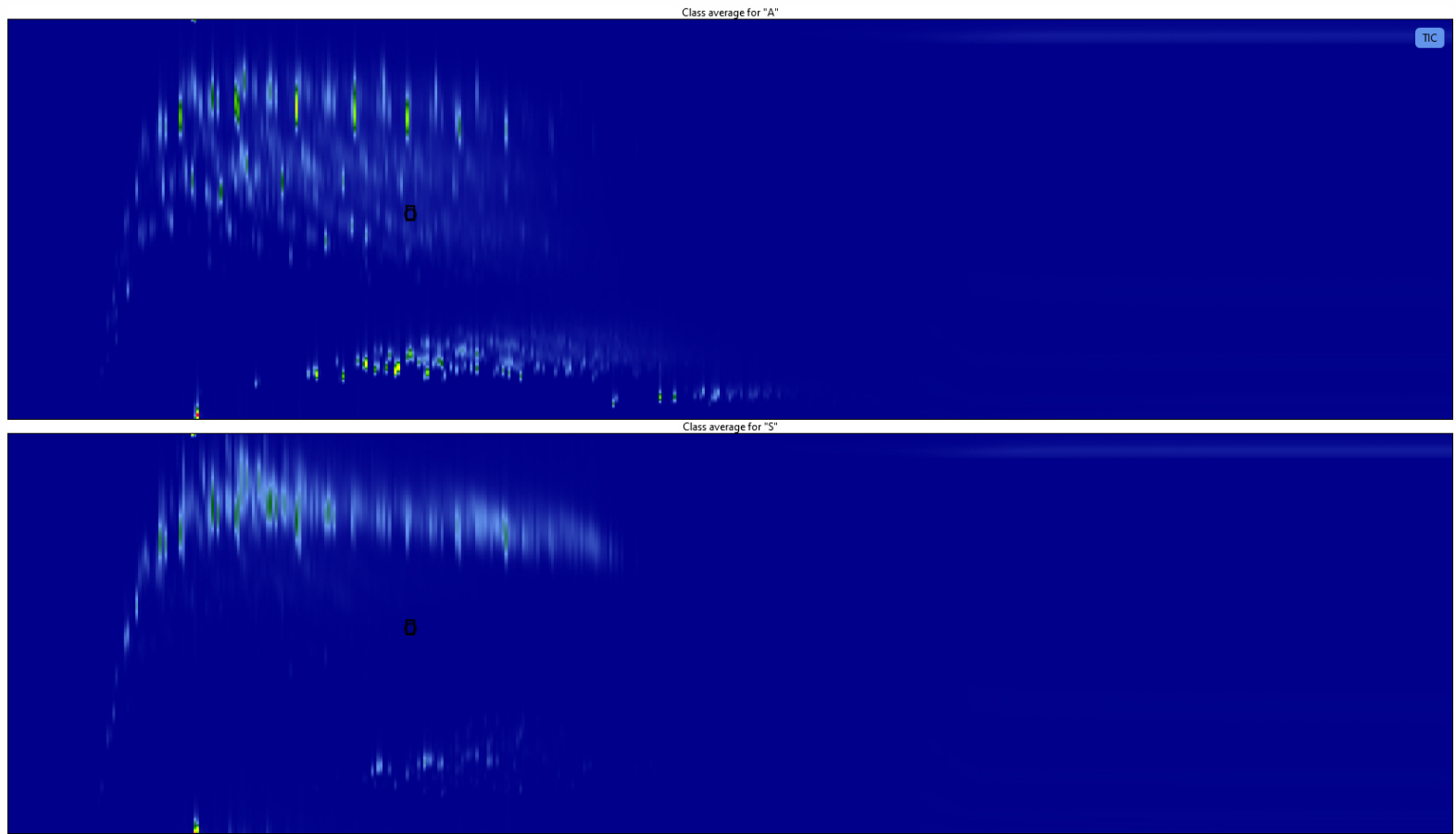
Driving question: What are the most statistically significant differences between these sets of traditional and synthetic aviation fuels?



Traditional Aviation Fuel

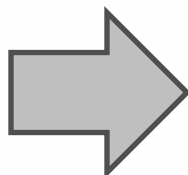


Synthetic Aviation Fuel



Curation of Tile and Mass Hits into Feature Table

- Method
 - Tile size D1 (modulations): 3
 - Tile size D2 (spectra): 20
 - S/N threshold: 5
 - D1 signal to base threshold: 2
 - D2 signal to base threshold: 2
 - Samples that must exceed S/N threshold: 1
 - Mass F-ratios to average: 3
 - Statistical threshold type to apply: F-ratio
 - F-ratio threshold: 10
 - Relative change threshold type to apply: None
 - Minimum masses per tile: 2
 - Minimum mass: 35
 - Maximum mass: 600
 - Masses to ignore:
 - Perform one-point normalization:



The screenshot shows a software interface with a 'Library search' dialog box. The dialog includes the following settings:

- Automatically perform library search on accepted hits
- Library Identity Search Mode:
 - Normal
 - Quick
- Library Search Mode:
 - Forward
 - Reverse
- Rank hits by:
 - Probability
 - Similarity
 - Reverse Similarity
- Maximum number of hits: 10
- Minimum mass to library search: 0
- Maximum mass to library search: 1000
- Minimum molecular weight allowed: 0
- Maximum molecular weight allowed: 1000
- Relative abundance threshold (0-998): 10
- Minimum similarity for matches (0-999): 500
- Minimum similarity before hit is assigned (0-999): 700
- Retrieve retention indices
 - Semi-standard non-polar
 - Standard non-polar
 - Polar
- Filter hits that are at least 30 units out of tolerance with computed retention index

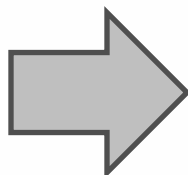
Below the dialog, there is a 'Libraries to search:' section with the following options:

- biomarkers_rkn
- ddt
- fames
- mainlib
- naphs & phens
- nist_msms
- nist_msms2
- nist_ri
- pashs
- replib

At the bottom of the dialog, it says '16 Landmark(s) (Edit)' and 'Close'.

Curation of Tile and Mass Hits into Feature Table

- Method
 - Tile size D1 (modulations): 3
 - Tile size D2 (spectra): 20
 - S/N threshold: 5
 - D1 signal to base threshold: 2
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 - Relative change threshold type to apply: None
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 - Minimum mass: 35
 - Maximum mass: 600
 - Masses to ignore:
 - Perform one-point normalization:



Home > Processings > Trad vs Alt Aviation Fuel FR

All selected tiles: Reject | Unreviewed

Hit locations | Chemical features | Summary

Tile hits:

#	Avg F-ratio	Avg Relative	Top mass	RT1	RT2	Masses
1081	21.65	0.00	104	664.20	2.58	2
436	94.80	0.00	68	399.60	3.11	11
294	131.62	0.00	96	880.20	3.01	4
1249	16.19	0.00	117	664.20	2.83	2
1131	19.96	0.00	117	556.20	3.64	2
859	35.29	0.00	127	1123.20	1.30	8
169	184.09	0.00	105	745.20	3.46	3
817	39.05	0.00	96	496.80	3.31	3
328	119.57	0.00	120	664.20	3.50	4
1163	18.69	0.00	128	1123.20	3.63	4
661	54.20	0.00	155	1409.40	1.55	3
213	160.40	0.00	120	664.20	3.93	2
879	33.62	0.00	82	432.00	3.51	16
536	73.70	0.00	78	432.00	4.09	8
1014	25.15	0.00	103	664.20	2.73	4
500	80.32	0.00	170	1431.00	1.42	80
874	33.85	0.00	128	1123.20	3.24	3
952	28.85	0.00	120	664.20	2.92	3
311	125.13	0.00	80	966.60	3.60	4
207	163.02	0.00	179	891.00	3.62	2
587	65.52	0.00	182	1441.80	1.38	3
001	1206.28	0.00	173	1258.20	1.84	21
033	344.49	0.00	193	1020.60	3.31	15
303	127.07	0.00	149	799.20	3.21	4
986	26.74	0.00	54	442.80	3.48	10
023	378.16	0.00	179	880.20	3.58	10
104	234.37	0.00	121	847.80	3.07	3
670	53.41	0.00	181	1452.60	1.41	24
690	51.40	0.00	128	1123.20	3.11	3
025	369.36	0.00	54	955.80	3.61	32
219	157.24	0.00	135	853.20	3.03	4
209	162.31	0.00	67	993.60	3.72	2
372	109.16	0.00	81	556.20	3.19	11
891	27.74	0.00	106	496.80	3.36	14

Class average for "A"

Hit filtration

Retention time ?

Exclusion regions (sec): (none)

Inclusion regions (sec): (none)

Edit these settings

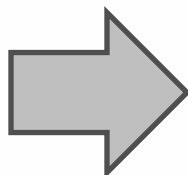
Apply filters

Mass hits for selected tile:

#	Mass	F-ratio	Relative Cha	RT1	RT2	Area diff
11174	104	27.02	0.00	664.20	2.58	112331.00
11175	115	16.28	0.00	664.20	2.58	109661.39

Curation of Tile and Mass Hits into Feature Table

- Method**
- Tile size D1 (modulations): ? 3
 - Tile size D2 (spectra): ? 20
 - S/N threshold: ? 5
 - D1 signal to base threshold: ? 2
 - D2 signal to base threshold: ? 2
 - Samples that must exceed S/N threshold: ? 1
 - Mass F-ratios to average: ? 3
 - Statistical threshold type to apply: ? F-ratio
 - F-ratio threshold: ? 10
 - Relative change threshold type to apply: ? None
 - Minimum masses per tile: ? 2
 - Minimum mass: ? 35
 - Maximum mass: ? 600
 - Masses to ignore: ?
 - Perform one-point normalization: ?



Home > Processings > Trad vs Alt Aviation Fuel FR

All selected tiles: Reject | Unreviewed

Hit locations | Chemical features | Summary

Tile hits:

#	Avg F-ratio	Avg Relative	Top mass	RT1	RT2	Masses	Accept	Reject
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294	131.62	0.00	96	880.20	3.01	4	Accept	Reject
1249	16.19	0.00	117	664.20	2.83	2	Accept	Reject
1131	19.96	0.00	117	556.20	3.64	2	Accept	Reject
859	35.29	0.00	127	1123.20	1.30	83	Accept	Reject
169	184.09	0.00	105	745.20	3.46	3	Accept	Reject
817	39.05	0.00	96	496.80	3.31	3	Accept	Reject
328	119.57	0.00	120	664.20	3.50	4	Accept	Reject
1163	18.69	0.00	128	1123.20	3.63	4	Accept	Reject
661	54.20	0.00	155	1409.40	1.55	3	Accept	Reject
213	160.40	0.00	120	664.20	3.93	2	Accept	Reject
879	33.62	0.00	82	432.00	3.51	16	Accept	Reject
536	73.70	0.00	78	432.00	4.09	8	Accept	Reject
1014	25.15	0.00	103	664.20	2.73	4	Accept	Reject
500	80.32	0.00	170	1431.00	1.42	80	Accept	Reject
874	33.85	0.00	128	1123.20	3.24	3	Accept	Reject
952	28.85	0.00	120	664.20	2.92	3	Accept	Reject
311	125.13	0.00	80	966.60	3.60	4	Accept	Reject
207	163.02	0.00	179	891.00	3.62	2	Accept	Reject
587	65.52	0.00	182	1441.80	1.38	3	Accept	Reject
001	1206.28	0.00	173	1258.20	1.84	21	Accept	Reject
033	344.49	0.00	193	1020.60	3.31	15	Accept	Reject
303	127.07	0.00	149	799.20	3.21	4	Accept	Reject
986	26.74	0.00	54	442.80	3.48	10	Accept	Reject
023	378.16	0.00	179	880.20	3.58	10	Accept	Reject
104	234.37	0.00	121	847.80	3.07	3	Accept	Reject
670	53.41	0.00	181	1452.60	1.41	24	Accept	Reject
690	51.40	0.00	128	1123.20	3.11	3	Accept	Reject
025	369.36	0.00	54	955.80	3.61	32	Accept	Reject
219	157.24	0.00	135	853.20	3.03	4	Accept	Reject
209	162.31	0.00	67	993.60	3.72	2	Accept	Reject
372	109.16	0.00	81	556.20	3.19	11	Accept	Reject
831	27.74	0.00	106	496.80	3.36	14	Accept	Reject

Class average for "A"

Autocuration

For:

- All tile hits
- Selected tile hits

Auto-accept the mass with the maximum:

- Area difference between classes
- Relative change
- F-ratio

If its F-ratio is at least:

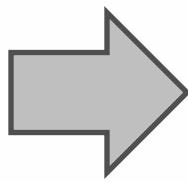
Autocurate

Mass hits for selected tile:

#	Mass	F-ratio	Relative Cha	RT1	RT2	Area diff	Accept	Reject
11174	104	27.02	0.00	664.20	2.58	112331.00	Accept	Reject
11175	115	16.28	0.00	664.20	2.58	109661.39	Accept	Reject

Curation of Tile and Mass Hits into Feature Table

- Method**
- Tile size D1 (modulations): 3
 - Tile size D2 (spectra): 20
 - S/N threshold: 5
 - D1 signal to base threshold: 2
 - D2 signal to base threshold: 2
 - Samples that must exceed S/N threshold: 1
 - Mass F-ratios to average: 3
 - Statistical threshold type to apply: F-ratio
 - F-ratio threshold: 10
 - Relative change threshold type to apply: None
 - Minimum masses per tile: 2
 - Minimum mass: 35
 - Maximum mass: 600
 - Masses to ignore:
 - Perform one-point normalization:



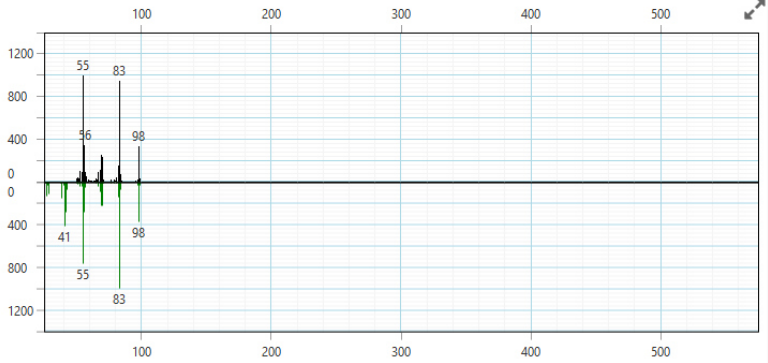
The screenshot shows the LECO software interface with the following components:

- Table of Mass Hits:** A table with columns for Hit #, Avg F-ratio, Avg Relative, Top mass, RT1, RT2, and Masses. The table lists various mass hits with their corresponding F-ratios and relative values.
- Spectrum Plots:** Two mass spectra are displayed. The top plot is titled "Caliper spectra at 1263.60, 1.85 sec" and shows peaks at m/z 77, 91, 105, 117, 143, 145, 159, and 186. The bottom plot is titled "SAF 1-1 T-48" and shows peaks at m/z 55, 78, 114, and 141.
- Configuration Dialog Box:** A dialog box is open, showing options for zooming the x-axis (Collected mass range, Library search parameters' mass range, Do not zoom), stick labeling threshold (set to 250), samples per page (set to 0), and baseline subtraction level.

Feature Table to Statistical Plots

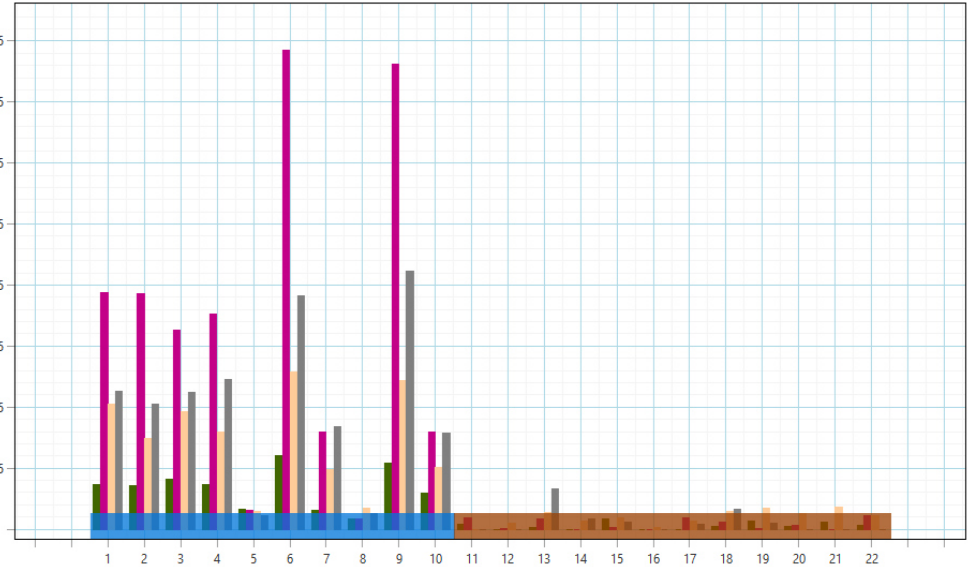
Home » Processings » Trad vs Alt Aviation Fuel FR

Hit locations | Chemical features | Summary



Area bars | Area lines | Contours

- Cyclohexane, methyl-
- Cyclohexane
- Cyclopentane, 1,2-dimethyl-, cis-
- Cyclobutane, ethyl-



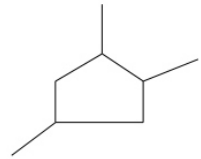
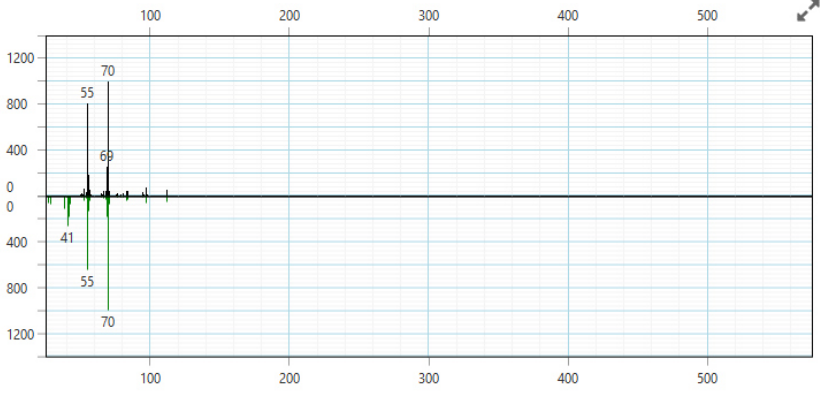
Feature: Cyclohexane, methyl-

Library Hit: 899/901/59.29 Cyclohexane, methyl- Unassign

Id (530)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
10809	Cyclobutane, ethyl-	C ₆ H ₁₂	84	911	4806-61-5	70	659	692	-33	183.6	1.91	27.50	225672.67	204905.95	223672.31	2453
10456	Cyclopentane, 1,2-dimethyl-, cis-	C ₇ H ₁₄	98	930	1192-18-3	99	718	N.A.	N.A.	199.8	2.52	31.24	204865.83	148278.98	192391.81	1596
11538	Cyclohexane	C ₆ H ₁₂	84	932	110-82-7	59	718	736	-18	199.8	2.18	18.30	387644.72	385299.16	325360.66	3520
10356	Cyclopentane, 1,1,3-trimethyl-	C ₈ H ₁₆	112	885	4516-69-2	95	732	N.A.	N.A.	205.2	3.03	32.08	151369.16	114725.73	172219.11	1218
10835	Cyclopentane, 1,2,4-trimethyl-	C ₈ H ₁₆	112	892	2815-58-9	95	745	N.A.	N.A.	210.6	3.26	27.17	574842.63	423155.53	589017.25	3934
10681	Heptane, 4-methylene-	C ₈ H ₁₆	112	833	15918-08-8	76	758	N.A.	N.A.	216.0	3.36	36.09	125639.94	75113.52	118521.48	793
12068	Hexane, 2,2,5-trimethyl-	C ₈ H ₁₈	128	908	3522-94-9	72	760	N.A.	N.A.	216.0	4.14	12.22	50514.34	71307.16	53565.26	565
10046	Cyclohexane, methyl-	C ₇ H ₁₄	98	899	108-87-2	93	769	780	-11	221.4	2.85	37.72	72861.49	70699.19	81711.26	737
11194	Cyclopentane, 1,3-dimethyl-	C ₇ H ₁₄	98	851	2453-00-1	81	770	N.A.	N.A.	221.4	3.21	34.06	273051.97	186692.03	268743.84	1810
11441	Cyclohexane, methyl-	C ₇ H ₁₄	98	899	108-87-2	76	769	780	-11	221.4	2.94	20.75	105840.47	47861.14	75603.55	788
12038	Heptane, 3-methyl-	C ₈ H ₁₈	114	816	589-81-1	298	773	768	5	221.4	4.51	13.00	1129.97	603.05	1169.47	28
9836	2-Heptene, 6-methyl-	C ₈ H ₁₆	112	890	73548-72-8	79	795	N.A.	N.A.	232.2	3.40	42.52	74919.83	82937.02	94138.08	739
8785	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆	112	894	591-21-9	108	811	837	-26	243.0	3.67	71.42	46386.74	43898.16	60863.52	382
8256	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆	112	893	591-21-9	108	811	837	-26	243.0	3.62	70.44	50289.03	49672.55	326297.63	11
9668	1α,2β,3α,4β-Tetramethylcyclopenta	C ₈ H ₁₈	126	865	2532-67-4	126	812	N.A.	N.A.	243.0	4.16	47.25	334705.31	225433.44	326297.63	2493

Feature Table to Statistical Plots

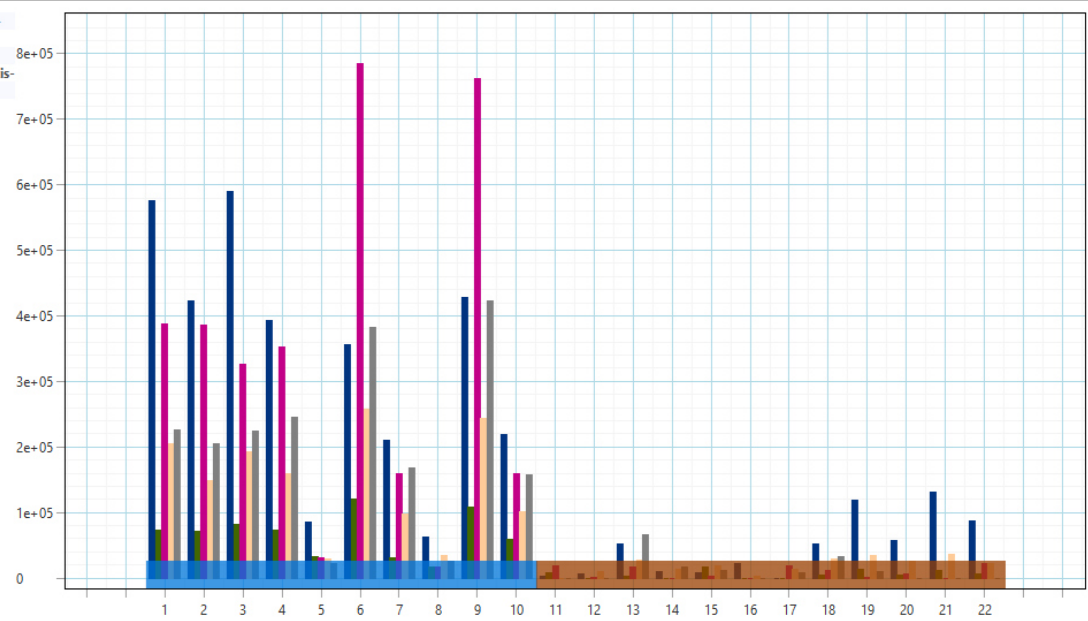
Hit locations Chemical features Summary



Feature: ■ Cyclopentane, 1,2,4-trimethyl-
 Library Hit: ✓ 892/892/27.18 Cyclopentane, 1,2,4-trimethyl-

Area bars Area lines Contours

- Cyclopentane, 1,2,4-trimethyl-
- Cyclohexane, methyl-
- Cyclohexane
- Cyclopentane, 1,2-dimethyl-, cis-
- Cyclobutane, ethyl-



Feature table

Features:
[Pin all](#) | [Unpin all](#)

Samples:
[Pin all](#) | [Unpin all](#) | [Fit Columns To Content](#)

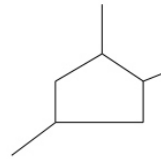
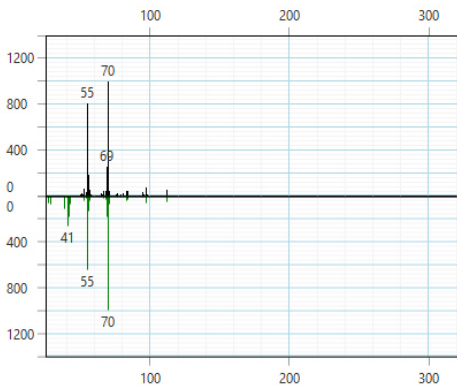
Filters...
[Use suggested quant mass](#)
[Adjust the integration boundary...](#)
[Edit user field values...](#)
[Import user field values...](#)
[Edit feature colors...](#)
[Copy rows](#)

Id (530)	Name	Formula	M.W.	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio		
10809	Cyclobutane, ethyl-	C ₄ H ₈		70	659	692	-33	183.6	1.91	27.50		
10456	Cyclopentane, 1,2-dimethyl-, cis-	C ₇ H ₁₄		99	718	N.A.	N.A.	199.8	2.52	31.24		
11538	Cyclohexane	C ₆ H ₁₂		59	718	736	-18	199.8	2.18	18.30		
10356	Cyclopentane, 1,1,3-trimethyl-	C ₈ H ₁₆		95	732	N.A.	N.A.	205.2	3.03	32.08		
10835	Cyclopentane, 1,2,4-trimethyl-	C ₈ H ₁₆		95	745	N.A.	N.A.	210.6	3.26	27.17		
10681	Heptane, 4-methylene-	C ₈ H ₁₆	112	833	15918-08-8	76	758	N.A.	N.A.	216.0	3.36	36.09
12068	Hexane, 2,2,5-trimethyl-	C ₈ H ₁₆	128	908	3522-94-9	72	760	N.A.	N.A.	216.0	4.14	12.22
10046	Cyclohexane, methyl-	C ₇ H ₁₄	98	899	108-87-2	93	769	780	-11	221.4	2.85	37.72
11194	Cyclopentane, 1,3-dimethyl-	C ₇ H ₁₄	98	851	2453-00-1	81	770	N.A.	N.A.	221.4	3.21	34.06
11441	Cyclohexane, methyl-	C ₇ H ₁₄	98	899	108-87-2	76	769	780	-11	221.4	2.94	20.75
12038	Heptane, 3-methyl-	C ₈ H ₁₆	114	816	589-81-1	298	773	768	5	221.4	4.51	13.00
9836	2-Heptene, 6-methyl-	C ₈ H ₁₆	112	890	73548-72-8	79	795	N.A.	N.A.	232.2	3.40	42.52
8785	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆	112	894	591-21-9	108	811	837	-26	243.0	3.67	71.42
8256	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆	112	893	591-21-9	108	811	837	-26	243.0	3.62	70.44
9668	1α,2β,3α,4β-Tetramethylcyclopenta	C ₈ H ₁₆	126	865	2532-67-4	126	812	N.A.	N.A.	243.0	4.16	47.25

Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
70	659	692	-33	183.6	1.91	27.50	225672.67	204905.95	223672.31	2453...
99	718	N.A.	N.A.	199.8	2.52	31.24	204865.83	148278.98	192391.81	1596...
59	718	736	-18	199.8	2.18	18.30	387644.72	385299.16	325360.66	3520...
95	732	N.A.	N.A.	205.2	3.03	32.08	151369.16	114725.73	172219.11	1218...
95	745	N.A.	N.A.	210.6	3.26	27.17	574842.63	423155.53	589017.25	3934...
76	758	N.A.	N.A.	216.0	3.36	36.09	125639.94	75113.52	118521.48	793...
72	760	N.A.	N.A.	216.0	4.14	12.22	50514.34	71307.16	53565.26	565...
93	769	780	-11	221.4	2.85	37.72	72861.49	70699.19	81711.26	737...
81	770	N.A.	N.A.	221.4	3.21	34.06	273051.97	186692.03	268743.84	1810...
76	769	780	-11	221.4	2.94	20.75	105840.47	47861.14	75603.55	788...
298	773	768	5	221.4	4.51	13.00	1129.97	603.05	1169.47	2...
79	795	N.A.	N.A.	232.2	3.40	42.52	74919.83	82937.02	94138.08	739...
108	811	837	-26	243.0	3.67	71.42	46386.74	43898.16	60863.52	382...
108	811	837	-26	243.0	3.62	70.44	50289.03	49672.55		
126	812	N.A.	N.A.	243.0	4.16	47.25	334705.31	225433.44		

Feature Table to Statistical Plots

Hit locations Chemical features Summary



Feature: Cyclopentane, 1,2,4-trimethyl-
 Library Hit: 892/892/27.18 Cyclopentane, 1,2,4-trimethyl-

Id (530)	Name	Formula
10809	Cyclobutane, ethyl-	C ₆ H ₁₂
10456	Cyclopentane, 1,2-dimethyl-, cis-	C ₇ H ₁₄
11538	Cyclohexane	C ₆ H ₁₂
10356	Cyclopentane, 1,1,3-trimethyl-	C ₈ H ₁₆
10835	Cyclopentane, 1,2,4-trimethyl-	C ₈ H ₁₆
10681	Heptane, 4-methylene-	C ₈ H ₁₆
12068	Hexane, 2,2,5-trimethyl-	C ₉ H ₂₀
10046	Cyclohexane, methyl-	C ₇ H ₁₄
11194	Cyclopentane, 1,3-dimethyl-	C ₇ H ₁₄
11441	Cyclohexane, methyl-	C ₇ H ₁₄
12038	Heptane, 3-methyl-	C ₈ H ₁₆
9836	2-Heptene, 6-methyl-	C ₈ H ₁₆
8785	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆
8256	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆
9668	1 α ,2 β ,3 α ,4 β -Tetramethylcyclopenta	C ₈ H ₁₆

Feature filter settings

Show only features that satisfy the following conditions:

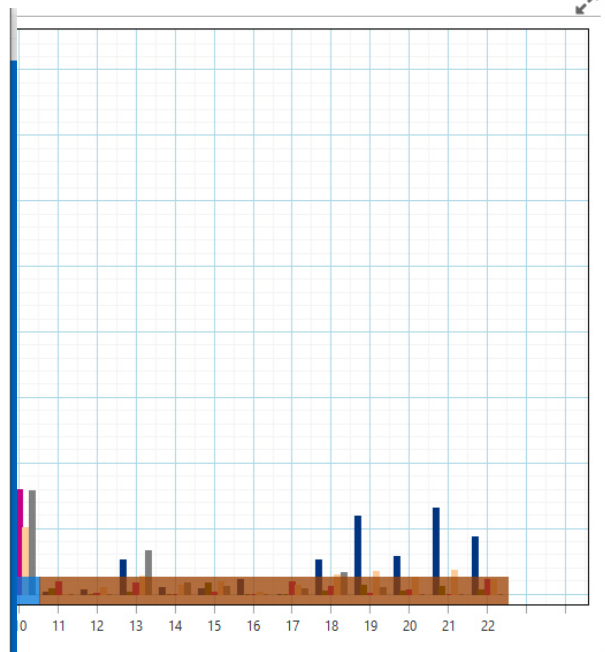
Simple Rules **Advanced Rules**

Similarity

AND

Formula

[Add rule](#) | [Remove all rules](#)

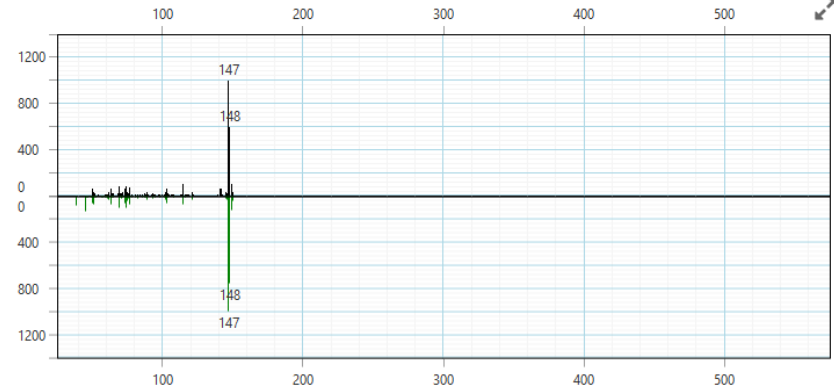


F-ratio	1	2	3	4	
91	27.50	225672.67	204905.95	223672.31	2453
52	31.24	204865.83	148278.98	192391.81	1596
18	18.30	387644.72	385299.16	325360.66	3520
03	32.08	151369.16	114725.73	172219.11	1218
26	27.17	574842.63	423155.53	589017.25	3934
36	36.09	125639.94	75113.52	118521.48	793
14	12.22	50514.34	71307.16	53565.26	565
85	37.72	72861.49	70699.19	81711.26	737
21	34.06	273051.97	186692.03	268743.84	1810
94	20.75	105840.47	47861.14	75603.55	788
51	13.00	1129.97	603.05	1169.47	2
40	42.52	74919.83	82937.02	94138.08	739
67	71.42	46386.74	43898.16	60863.52	382
62	70.44	50289.03	49672.55		
16	47.25	334705.31	225433.44	326	7.63

Feature Table to Statistical Plots

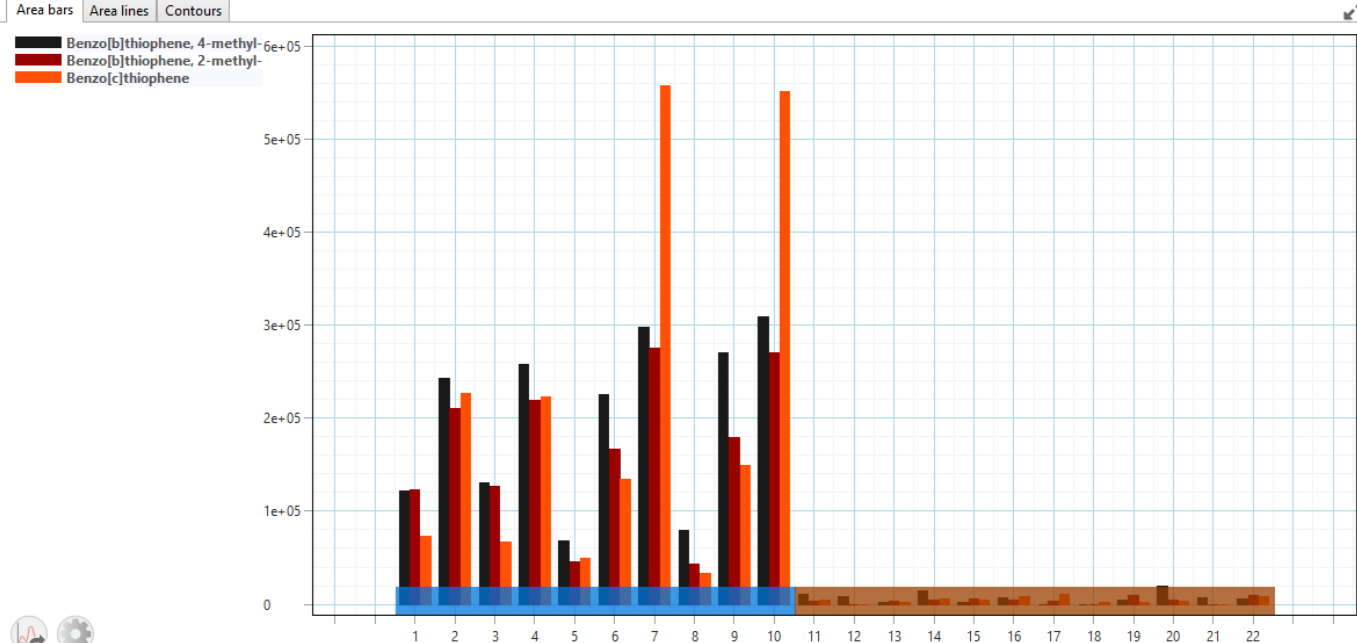
Home » Processings » Trad vs Alt Aviation Fuel FR

Hit locations | Chemical features | Summary



Area bars | Area lines | Contours

- Benzo[b]thiophene, 4-methyl-
- Benzo[b]thiophene, 2-methyl-
- Benzo[c]thiophene



Feature:

Library Hit: 841/841/22.38 Benzo[b]thiophene, 4-methyl- [Unassign](#)

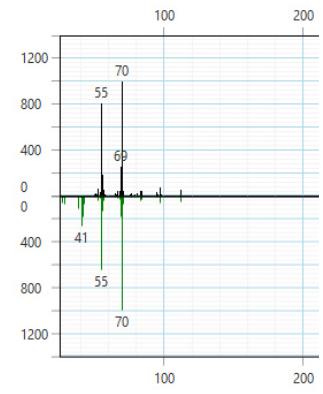
Id (3)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
12032	Benzo[c]thiophene	C ₉ H ₆ S	134	823	270-82-6	134	1809	N.A.	N.A.	1171.8	1.26	12.98	73475.75	225941.92	67311.59	22316
9633	Benzo[b]thiophene, 2-methyl-	C ₉ H ₈ S	148	849	1195-14-8	149	1887	N.A.	N.A.	1225.8	1.39	43.21	123378.24	210630.89	127095.57	2192
10101	Benzo[b]thiophene, 4-methyl-	C ₉ H ₈ S	148	841	14315-11-8	115	1933	N.A.	N.A.	1258.2	1.33	49.96	121499.85	243377.89	131065.05	2571

Feature Table to Statistical Plots

Home >> Processings >> Trad vs Alt Aviat

Feature filter settings

Hit locations Chemical features Summary



Show only features that satisfy the following conditions:

Simple Rules Advanced Rules

BaseMass()=105 Or BaseMass()=120

Feature: Cyclopentane, 1,2,4-trimethyl
Library Hit: 892/892/27.18 Cyclopent

Id (530)	Name
10809	Cyclobutane, ethyl-
10456	Cyclopentane, 1,2-dimethyl
11538	Cyclohexane
10356	Cyclopentane, 1,1,3-trimethyl
10835	Cyclopentane, 1,2,4-trimethyl
10681	Heptane, 4-methylene-
12068	Hexane, 2,2,5-trimethyl-
10046	Cyclohexane, methyl-
11194	Cyclopentane, 1,3-dimethyl
11441	Cyclohexane, methyl-
12038	Heptane, 3-methyl-
9836	2-Heptene, 6-methyl-
8785	Cyclohexane, 1,3-dimethyl-
8256	Cyclohexane, 1,3-dimethyl-
9668	1 α ,2 β ,3 α ,4 β -Tetramethylcyc

Operators: -- := + - * / = <> < <= > >= () "" Contains Between() And Or Not

Fields: [User field 1] [User field 2] [User field 3] [User field 4] [User field 5] [ID] [Name] [Formula] [M.W.] [Similarity] [Reverse] [Probability (%)] [CAS] [Quant mass] [R.I. calc] [R.I. lib] [R.I. Δ] [Min RT1] [Min RT2] [Mean RT1] [Mean RT2] [Med RT1] [Med RT2] [Max RT1] [Max RT2] [%RSD RT1] [%RSD RT2] [F-ratio] [Relative Change] [Samples] [Tile#] [Area - AV1-1 T31_2] [Area - AV1-3 T33_2] [Area - AV1-7 T42] [Area - AV1-8 T8]

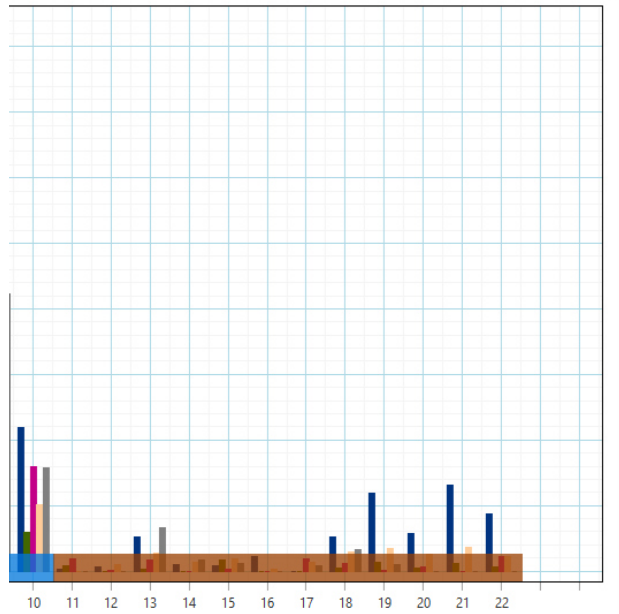
Functions: Sin() Cos() Tan() Sinh() Cosh() Tanh() Asin() Acos() Atan() Abs() Sqrt() Log() Log10() Exp() Round() Square() Cube() Pow() Max() Min() Mod() IIF() Intensity() BaseMass() NumOfMasses()

Others: Any() Count() m

Load rules | Save rules

Cancel OK

Close ? PCA Q LISTS

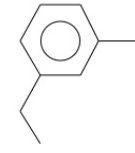
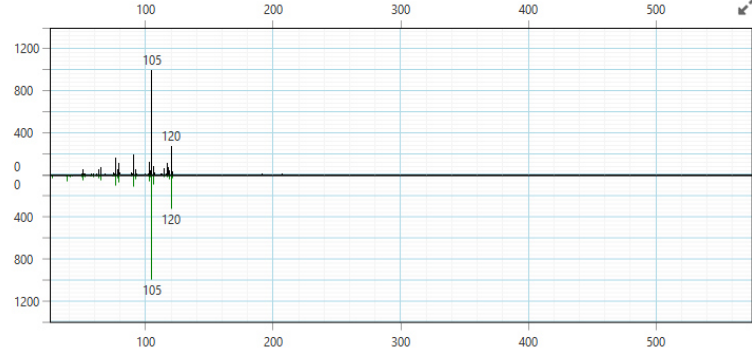


F-ratio	1	2	3	4
1.91	27.50	225672.67	204905.95	223672.31
2.52	31.24	204865.83	148278.98	192391.81
2.18	18.30	387644.72	385299.16	325360.66
3.03	32.08	151369.16	114725.73	172219.11
3.26	27.17	574842.63	423155.53	589017.25
3.36	36.09	125639.94	75113.52	118521.48
4.14	12.22	50514.34	71307.16	53565.26
2.85	37.72	72861.49	70699.19	81711.26
3.21	34.06	273051.97	186692.03	268743.84
2.94	20.75	105840.47	47861.14	75603.55
4.51	13.00	1129.97	603.05	1169.47
3.40	42.52	74919.83	82937.02	94138.08
3.67	71.42	46386.74	43898.16	60863.52
3.62	70.44	50289.03	49672.55	32627.63
4.16	47.25	334705.31	225433.44	25493.44

Feature Table to Statistical Plots

Home » Processings » Trad vs Alt Aviation Fuel FR

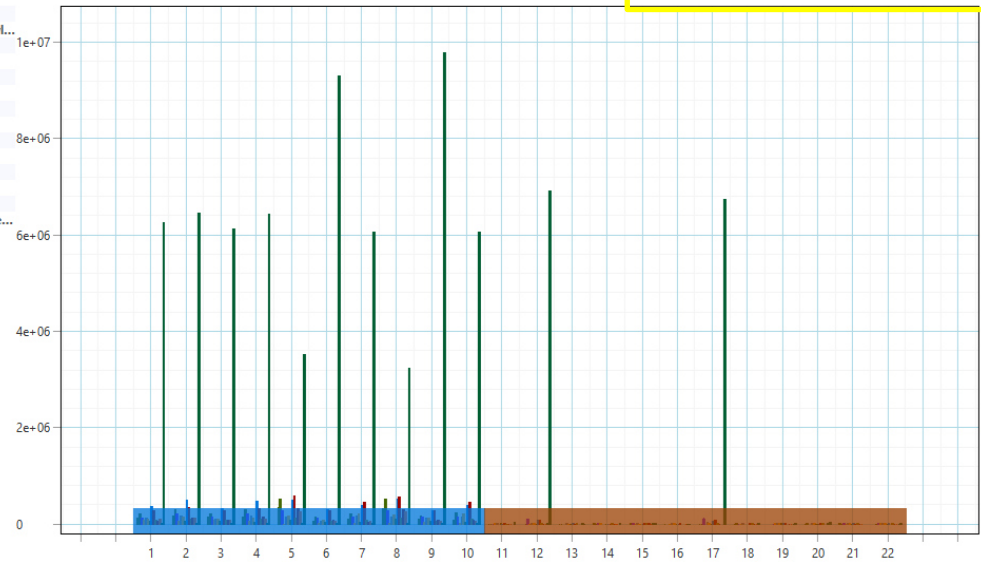
Hit locations Chemical features Summary



Feature: Benzene, 1-ethyl-3-methyl-
Library Hit: 853/855/21.84 Benzene, 1-ethyl-3-methyl-

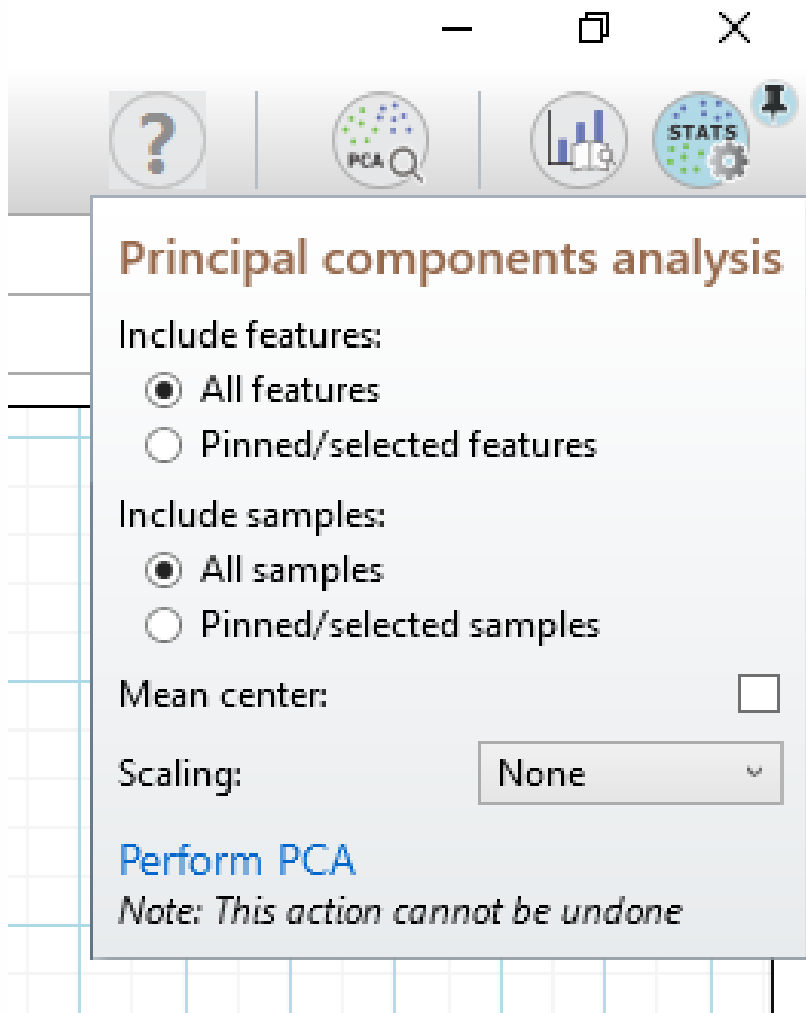
Area bars Area lines Contours

- Benzene, 1-ethyl-3-methyl-
- 1,3-Cyclopentadiene, 5-(1-methyl-...
- Benzene, 1-ethyl-3-methyl-
- Benzene, (1-methylethyl)-
- Benzene, 1,2,4-trimethyl-
- Benzene, 1,2,4-trimethyl-
- Benzene, 1-ethyl-3-methyl-
- Benzene, 1-ethyl-2-methyl-
- Benzene, 1,2,3-trimethyl-
- 2,4-Nonadiyne
- Benzene, 1,2,4-trimethyl-
- Benzene, 1-ethyl-2-methyl-
- Benzene, 1-ethyl-4-methyl-
- Benzene, 1-(1-ethylpropyl)-4-me...



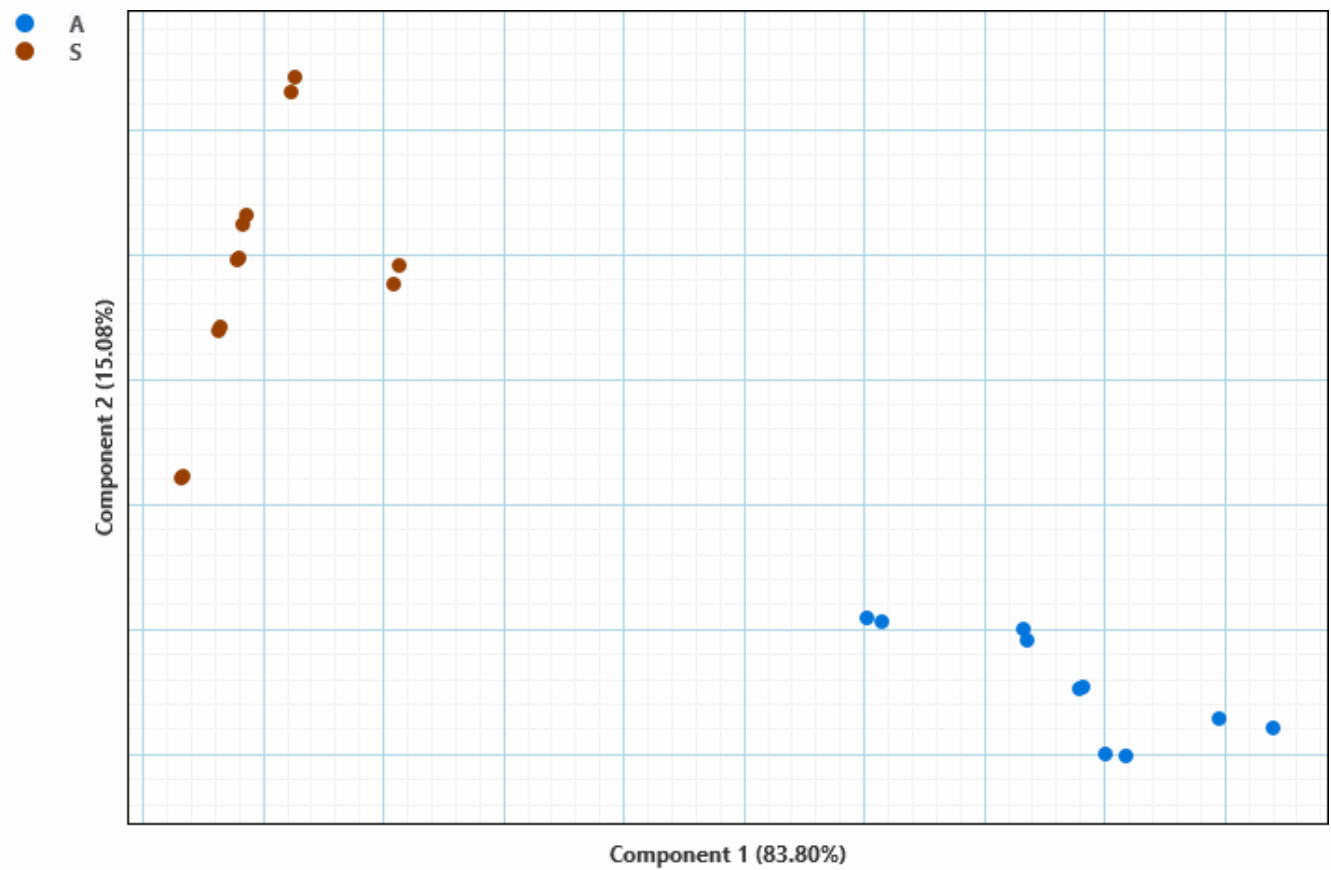
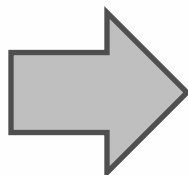
Id (21)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
3698	Benzene, (1-methylethyl)-	C ₉ H ₁₂	120	924	98-82-8	122	1172	1178	-6	610.2	1.87	173.58	51744.52	74971.77	48382.73	626
4826	2,4-Nonadiyne	C ₉ H ₁₂	120	836	63621-15-8	140	1224	N.A.	N.A.	664.2	1.85	143.74	83864.81	101691.47	81844.10	9813
10640	1,3-Cyclopentadiene, 5-(1-methylp	C ₆ H ₁₂	120	832	3141-02-4	120	1225	N.A.	N.A.	664.2	2.92	53.39	218161.05	301961.69	201791.06	3043
10926	Benzene, 1-ethyl-3-methyl-	C ₉ H ₁₂	120	853	620-14-4	103	1225	1225	0	664.2	2.73	34.97	131204.72	155031.84	139470.75	1450
10938	Benzene, 1-ethyl-4-methyl-	C ₉ H ₁₂	120	912	622-96-8	160	1224	1226	-2	664.2	1.90	32.44	12886.76	12863.40	8476.33	1518
11174	Benzene, 1-ethyl-2-methyl-	C ₉ H ₁₂	120	863	611-14-3	104	1225	1258	-33	664.2	2.58	27.02	102155.15	121958.95	69086.88	946
11723	Benzene, 1,2,4-trimethyl-	C ₉ H ₁₂	120	802	95-63-6	117	1225	1283	-58	664.2	2.83	20.29	66595.23	114368.31	77262.80	1352
11870	Benzene, (1-methylethyl)-	C ₉ H ₁₂	120	834	98-82-8	144	1225	1178	47	664.2	2.22	16.93	68865.80	57044.92	83200.86	547
6597	Benzene, 1,2,3-trimethyl-	C ₉ H ₁₂	120	890	526-73-8	111	1241	1340	-99	680.4	1.76	102.67	265380.81	330513.28	266930.72	3134
2442	Benzene, 1-ethyl-2-methyl-	C ₉ H ₁₂	120	909	611-14-3	108	1263	1258	5	702.0	1.79	207.04	355588.53	499923.47	325075.06	4780
8950	Benzene, 1-ethyl-3-methyl-	C ₉ H ₁₂	120	816	620-14-4	120	1264	1225	39	702.0	2.61	75.75	120134.71	200888.78	144615.06	2094
2999	Benzene, 1,2,4-trimethyl-	C ₉ H ₁₂	120	889	95-63-6	126	1280	1283	-3	718.2	1.74	208.11	122219.63	162535.25	109643.55	1661
3314	Benzene, 1-ethyl-3-methyl-	C ₉ H ₁₂	120	848	620-14-4	133	1286	1225	61	723.6	2.19	184.34	59289.22	47535.18	48030.02	353
7492	Benzene, 1,2,4-trimethyl-	C ₉ H ₁₂	120	901	95-63-6	125	1285	1283	2	723.6	1.86	113.80	103368.23	140555.98		66
11322	Benzene, 1,2,4-trimethyl-	C ₉ H ₁₂	120	852	95-63-6	158	1286	1283	3	723.6	2.36	22.37	68572.77	55434.98		6233

Feature Table to Statistical Plots



A software dialog box for Principal Component Analysis (PCA). It features a toolbar with icons for help, PCA, a bar chart, and a 'STATS' button. The main area contains the following settings:

- Principal components analysis**
- Include features:**
 - All features
 - Pinned/selected features
- Include samples:**
 - All samples
 - Pinned/selected samples
- Mean center:**
- Scaling:** None (dropdown menu)
- Perform PCA** (button)
- Note: This action cannot be undone*



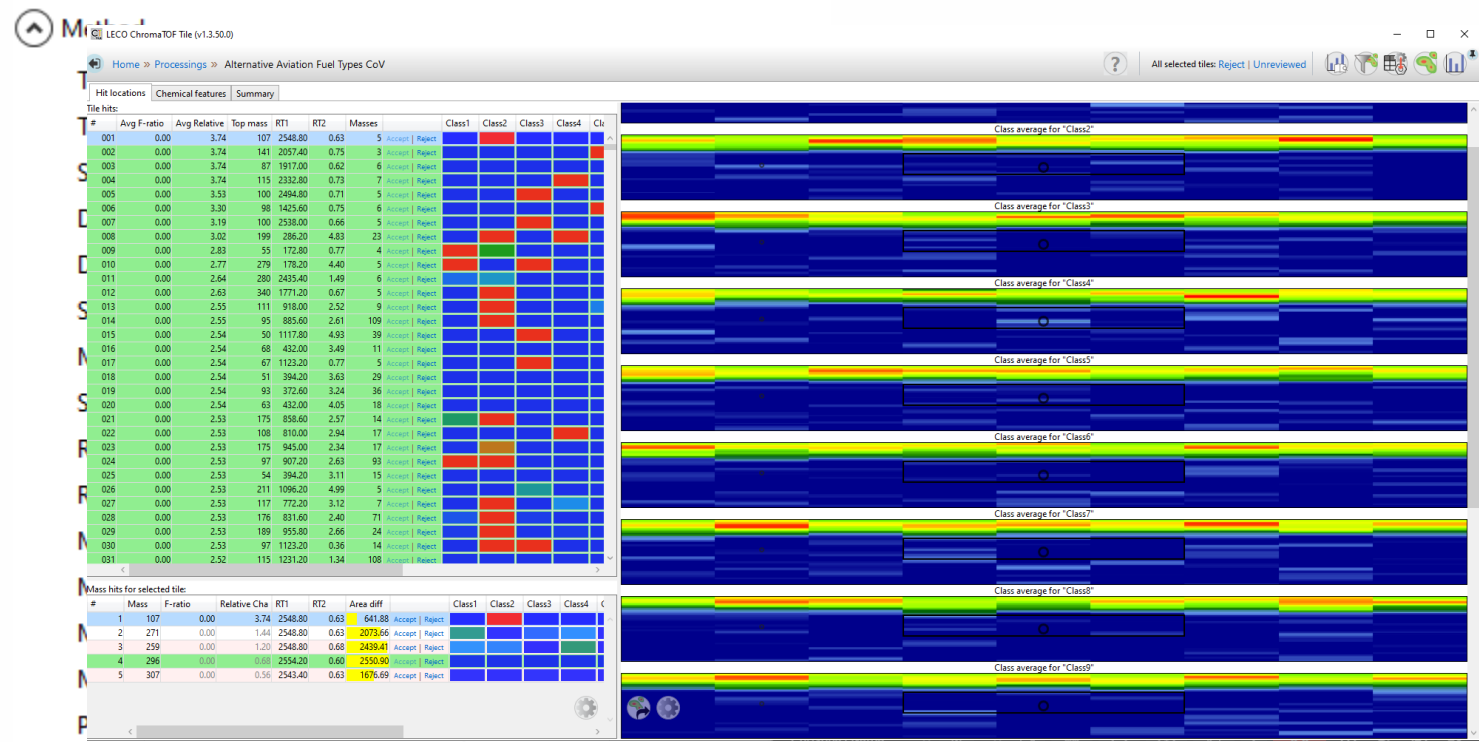
Experimental Design: Tracking Differences between Alternative Fuel Types



Driving Question: What kinds of major chemical variation can we see between these processes? Can PCA reveal clusters of similar processes?



- Variety of alternative fuel processes represented for a set of unlabelled samples:
- Low-temperature Fischer-Tropsch Synthetic Paraffinic Kerosene (LT-FTSPK)
 - High-temperature Fischer-Tropsch Synthetic Paraffinic Kerosene (HT-FTSPK)
 - Hydrotreated Esters and Fatty Acids (HEFA)
 - Synthesized Isoparaffins (SIP)
 - Alcohol-to-Jet (ATJ)
 - Catalytic Hydrothermolysis (CHJ)
 - Blends with aromatics packages (-A)

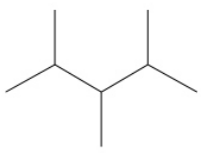
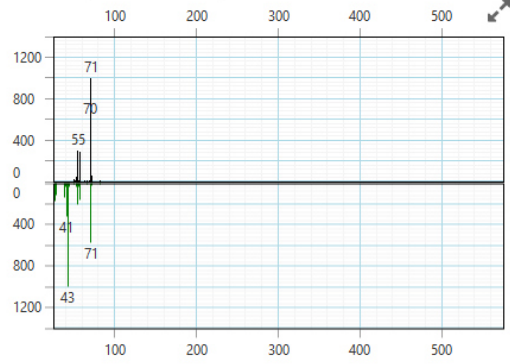


Tracking Differences between Alternative Fuel Types

Home >> Processings >> Alternative Aviation Fuel Types CoV



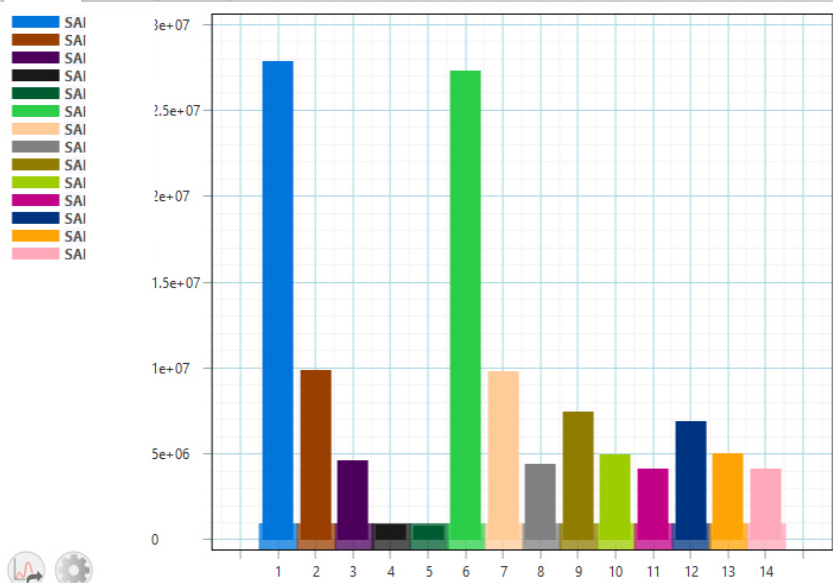
Hit locations Chemical features Summary



Feature: ■ Pentane, 2,3,4-trimet...

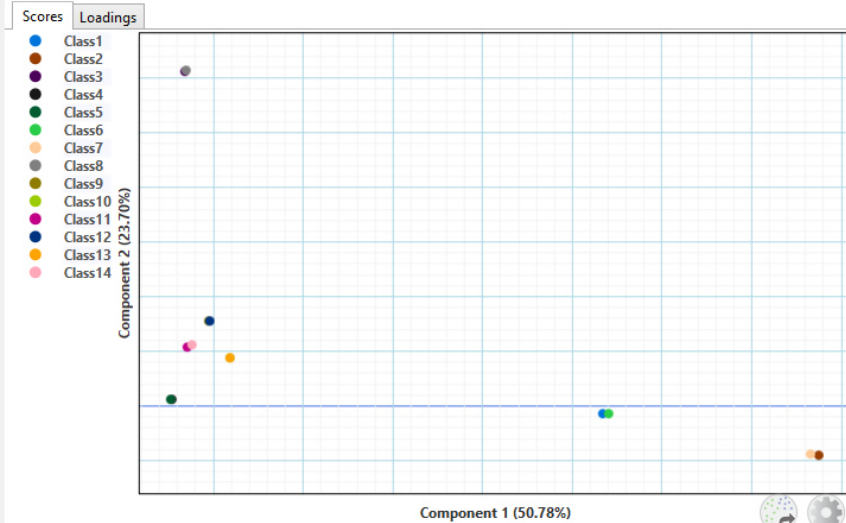
Library Hit: 866/869/35.42 P... Unassign

Area bars Area lines Contours



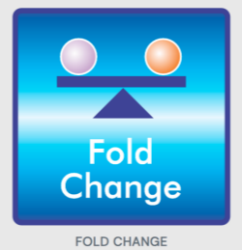
PCA Results

X-axis: Component 1 Y-axis: Component 2



Id (535)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	
20536	Pentane, 2,3,4-trimethyl-	C ₈ H ₁₈	114	114	866	565-75-3	71	758	N.A.	216.0	3.38	0.00	27843426.00	9830900.00	460474	
20419	Tetradecane, 3-methyl-	C ₁₅ H ₃₂	212	212	893	18435-22-8	120	1474	N.A.	896.4	4.84	0.00	1010.87	3688.18	19200	
20373	Heptane, 3,4,5-trimethyl-	C ₁₀ H ₂₂	142	142	892	20278-89-1	139	955	762	193	372.6	5.17	0.00	210551.98	167147.59	730
20168	10-Heneicosene (c,t)	C ₂₁ H ₄₂	294	294	820	95008-11-0	211	1333	N.A.	766.8	4.84	0.00	2646.57	4619.58	16	
19982	Hexane, 3-ethyl-2,5-dimethyl-	C ₁₀ H ₂₂	142	142	854	52897-04-8	75	961	N.A.	383.4	0.61	0.00	433696.00	419767.47	1799	
19960	1-Dodecanol, 3,7,11-trimethyl-	C ₁₅ H ₃₂ O	228	228	820	6750-34-1	199	990	N.A.	410.4	4.97	0.00	2386.68	3799.42	16	
19881	Octane, 2,4,6-trimethyl-	C ₁₁ H ₂₄	156	156	864	62016-37-9	114	961	1058	-97	383.4	0.63	0.00	336962.34	349015.88	2104
19622	Tridecane	C ₁₃ H ₂₈	184	184	898	629-50-5	89	1305	1300	5	739.8	5.06	0.00	0.00	28788.46	19098
19519	Octadecane, 2-methyl-	C ₁₉ H ₄₀	268	268	895	1560-88-9	233	1728	1862	-134	1107.0	5.30	0.00	0.00	540.12	145
19367	Cyclooctane, methyl-	C ₈ H ₁₆	126	126	847	1502-38-1	260	1065	N.A.	491.4	4.97	0.00	0.00	959.53	29	
18957	10-Heneicosene (c,t)	C ₂₁ H ₄₂	294	294	823	95008-11-0	205	1505	N.A.	923.4	4.44	0.00	5698.80	6814.85	16	
18460	10-Heneicosene (c,t)	C ₂₁ H ₄₂	294	294	820	95008-11-0	167	1283	N.A.	718.2	4.63	0.00	131522.88	175865.88	666	
18437	Cyclohexane, 1,3-dimethyl-	C ₈ H ₁₆	112	112	903	591-21-9	148	811	837	-26	243.0	3.75	0.00	4925.64	0.00	39
18302	Tetradecane	C ₁₄ H ₃₀	198	198	916	629-59-4	173	1406	1400	6	837.0	4.78	0.00	1647.43	0.00	624

Finding Components of Aromatics Additive Package



Driving Question: With only 2 samples (one sample with aromatics additive and one similar one without), can I quickly identify which compounds make up an aromatics additive package?



- Method
- Tile size D1 (modulations): ? 3
 - Tile size D2 (spectra): ? 25
 - S/N threshold: ? 2
 - D1 signal to base threshold: ? 2
 - D2 signal to base threshold: ? 5
 - Samples that must exceed S/N threshold: ? 1
 - Mass F-ratios to average: ? 1
 - Statistical threshold type to apply: ? None
 - Relative change threshold type to apply: ? LOG (base2) fold...
 - Relative change threshold: ? 1
 - Minimum masses per tile: ? 3
 - Minimum mass: ? 35
 - Maximum mass: ? 600
 - Masses to ignore: ?
 - Perform one-point normalization: ?

Home » Processings » Aromatics Package Log2FC

Hit locations | Chemical features | Summary

File hits:

#	Avg F-ratio	Avg Relative	Top mass	RT1	RT2	Masses	Class1	Class2
001	0.00	34.14	50	772.20	2.06	121	Accept	Reject
002	0.00	34.06	68	588.60	3.49	86	Accept	Reject
003	0.00	33.87	79	891.00	2.06	81	Accept	Reject
004	0.00	33.86	57	858.60	2.57	31	Accept	Reject
005	0.00	33.29	91	831.60	2.40	96	Accept	Reject
006	0.00	33.20	55	869.40	2.15	134	Accept	Reject
007	0.00	33.00	93	739.80	1.88	110	Accept	Reject
008	0.00	32.96	79	707.40	1.96	108	Accept	Reject
009	0.00	32.95	51	891.00	2.24	109	Accept	Reject
010	0.00	32.84	57	907.20	2.62	72	Accept	Reject
011	0.00	32.71	58	804.60	1.63	64	Accept	Reject
012	0.00	32.59	81	664.20	3.21	45	Accept	Reject
013	0.00	32.53	103	950.40	2.44	18	Accept	Reject
014	0.00	32.42	54	523.80	3.29	53	Accept	Reject
015	0.00	32.40	105	950.40	1.69	91	Accept	Reject
016	0.00	32.39	64	853.20	2.16	52	Accept	Reject
017	0.00	32.29	105	885.60	2.62	132	Accept	Reject
018	0.00	32.18	91	831.60	1.77	58	Accept	Reject
019	0.00	32.17	66	675.00	1.93	113	Accept	Reject
020	0.00	32.13	65	750.60	1.94	23	Accept	Reject
021	0.00	32.01	67	464.40	3.51	21	Accept	Reject
022	0.00	31.89	79	831.60	1.95	48	Accept	Reject
023	0.00	31.63	115	820.80	2.19	24	Accept	Reject
024	0.00	31.46	78	907.20	2.08	131	Accept	Reject
025	0.00	31.30	80	761.40	2.03	122	Accept	Reject
026	0.00	31.26	128	918.00	2.28	33	Accept	Reject
027	0.00	31.17	67	604.80	3.43	24	Accept	Reject
028	0.00	31.13	77	1069.20	1.98	139	Accept	Reject
029	0.00	31.11	64	901.80	1.72	58	Accept	Reject
030	0.00	31.05	57	982.80	2.65	70	Accept	Reject
031	0.00	31.05	57	928.80	2.73	11	Accept	Reject
032	0.00	31.04	66	761.40	1.86	73	Accept	Reject
033	0.00	31.03	86	345.60	5.29	16	Accept	Reject
034	0.00	30.82	127	842.40	2.09	69	Accept	Reject

Mass hits for selected tile:

#	Mass	F-ratio	Relative Cha	RT1	RT2	Area diff	Class1	Class2
1	50	0.00	34.14	772.20	2.06	8447129.81	Accept	Reject
2	56	0.00	33.04	772.20	2.06	8623624.80	Accept	Reject
3	86	0.00	32.15	772.20	2.06	4662367.53	Accept	Reject
4	101	0.00	32.03	772.20	2.05	4289513.60	Accept	Reject
5	68	0.00	31.79	772.20	2.06	3632376.78	Accept	Reject
6	69	0.00	31.62	772.20	2.06	322073.54	Accept	Reject
7	114	0.00	31.39	772.20	2.05	2757368.66	Accept	Reject
8	97	0.00	31.23	772.20	2.05	2468019.71	Accept	Reject
9	144	0.00	28.68	772.20	2.06	421264.46	Accept	Reject

Class average for "Class1"

Class average for "Class2"

Finding Components of Aromatics Additive Package

Hit locations | Chemical features | Summary

Feature: Benzene, 1-eth...
Library Hit: 923/939/21.35 B. Unassign

Area bars | Area lines | Contours

PCA Results

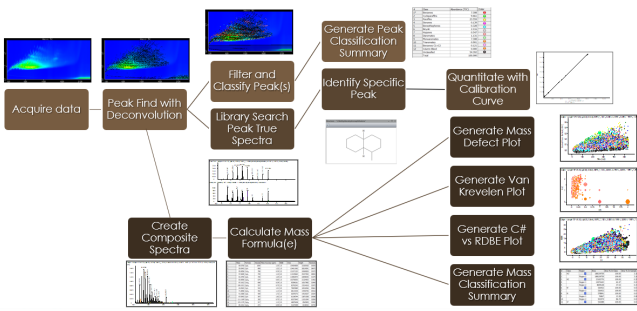
X-axis: Component 1 | Y-axis: Component 2

Scores | Loadings

d (8807)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2
!001	→ Benzene, 2-(2-butenyl)-1,3,5-trimet	C ₁₂ H ₁₈	174	741	63435-25-6	77	1676	N.A.	N.A.	1069.2	1.98	0.00	0.00	2275523.50
!140	→ 1H-Indene, 2,3-dihydro-4-methyl-	C ₁₀ H ₁₂	132	915	824-22-6	64	1477	1468	9	901.8	1.72	0.00	0.00	2259636.75
!198	→ Benzene, 1,2,4-tripropyl-	C ₁₈ H ₂₄	204	791	41898-97-9	57	1572	N.A.	N.A.	982.8	2.65	0.00	0.00	2178223.50
!268	→ Benzene, 1-ethyl-3,5-diisopropyl-	C ₁₄ H ₂₂	190	766	15181-13-2	57	1509	N.A.	N.A.	928.8	2.73	0.00	0.00	2170850.50
!279	→ Benzene, 1-ethyl-3,5-dimethyl-	C ₁₀ H ₁₄	134	885	934-74-7	66	1324	1319	5	761.4	1.86	0.00	0.00	1886563.00
!352	→ Undecane, 5-methyl-	C ₁₂ H ₂₆	170	771	1632-70-8	86	930	1157	-227	345.6	5.29	0.00	3862357.00	1431653.00
!368	→ Benzene, 1-(1,1-dimethylethyl)-3,5-	C ₁₂ H ₁₈	162	890	98-19-1	127	1409	1388	21	842.4	2.09	0.00	0.00	1850288.50
!437	→ 1,3,5-Cycloheptatriene, 2,4-diethyl-	C ₁₃ H ₂₀	176	854		79	1453	N.A.	N.A.	880.2	2.32	0.00	0.00	1641474.13
!497	→ Benzene, 1-ethyl-3,5-diisopropyl-	C ₁₄ H ₂₂	190	831	15181-13-2	79	1497	N.A.	N.A.	918.0	2.45	0.00	0.00	1522238.50
!553	→ Benzeneacetaldehyde, α-ethyl-	C ₁₀ H ₁₂ O	148	886	2439-43-2	94	1308	N.A.	N.A.	745.2	2.15	0.00	0.00	1466991.50
!574	→ 2,4-Dimethylstyrene	C ₁₀ H ₁₂	132	824	2234-20-0	65	1385	1440	-55	820.8	1.80	0.00	0.00	1229449.13
!624	→ 9-Methylbicyclo[3.3.1]nonane	C ₁₀ H ₁₈	138	836	25107-01-1	66	1079	N.A.	N.A.	507.6	3.84	0.00	0.00	1299523.25
!638	→ Benzene, 1,4-dimethyl-2,5-bis(1-m	C ₁₄ H ₂₂	190	828	10375-96-9	57	1571	1607	-36	982.8	2.24	0.00	0.00	1296057.3
!672	→ 1H-Indene, 2,3-dihydro-1,1,2,3,4-tetra	C ₁₂ H ₁₈	188	837	1203-17-4	91	1826	N.A.	N.A.	1182.6	1.97	0.00	0.00	1288219.75

Choose the right processing method to simplify answering your question!

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Off-odor detection in food samples that passed or failed quality control...
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ChromatOF|SYNC ChromatOF|SYNC 2D

ChromatOF Sync and Sync 2D – Capture Every Clue

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<p>Traditional Aviation Fuel</p>  <p>Synthetic Aviation Fuel</p> 	<p>Alternative Aviation Fuels (Multiple Production Methods)</p> 	<p>Pinpointing Components in Aromatics Additive Package</p> 



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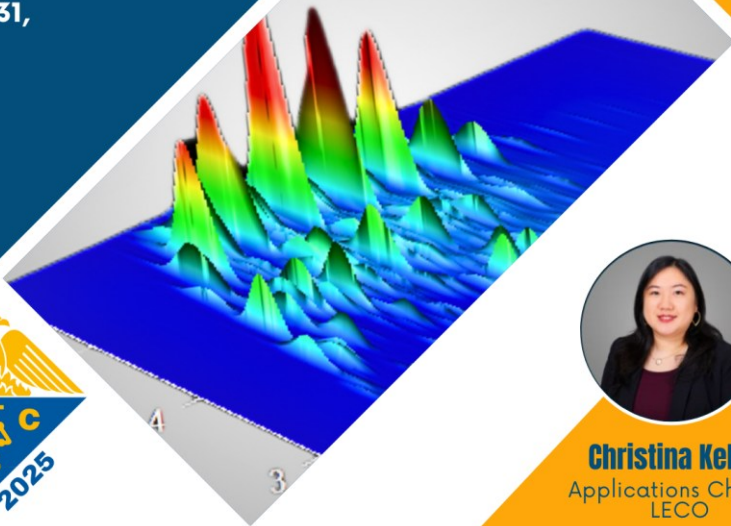
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EMPOWERING RESULTS

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**MARCH 31,
2025**



Christina Kelly
Applications Chemist
LECO



**Katelynn Perrault
Uptmor, PhD**
Assistant Professor
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