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

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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 Robbert Warren who became President of LECO Corp.
- In 1980s the age of the computer: self-calibration, microprocessors etc

LECO Corporation, St Joseph, Michigan

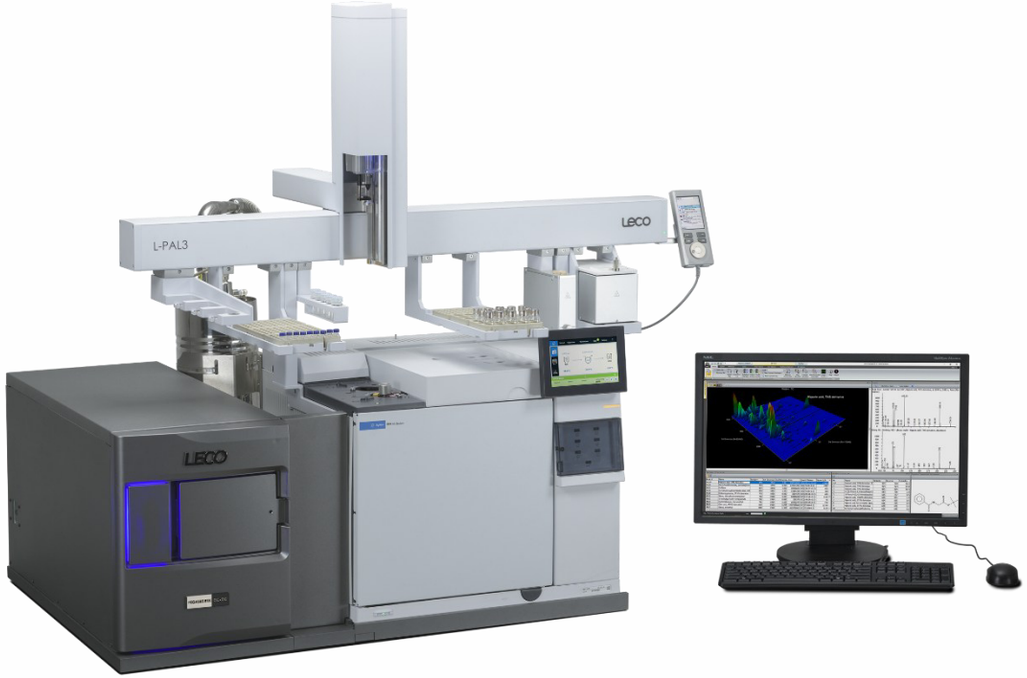
- LECO's HQ, is located in Saint Joseph, MI on the shores of Lake Michigan.
- An established, global organisation, serving 75 countries around the world and still privately owned, actively run by 3rd generation family.

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

Introducting 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	ChromaTOF®	ChromaTOF® Tile	ChromaTOF® SYNC
Objective	Detailed sample acquisition & characterization	Find differences between samples or groups of samples	Detailed batch interrogation
Features	• Single-sample deconvolution • Target Analyte Find • Quantitation • Classifications	Statistical comparisons using: 1. Fisher Ratio 2. CoV 3. Fold-Change	• Deconvolution performed over a set of samples • Aligned Peak Table • Statistical trends

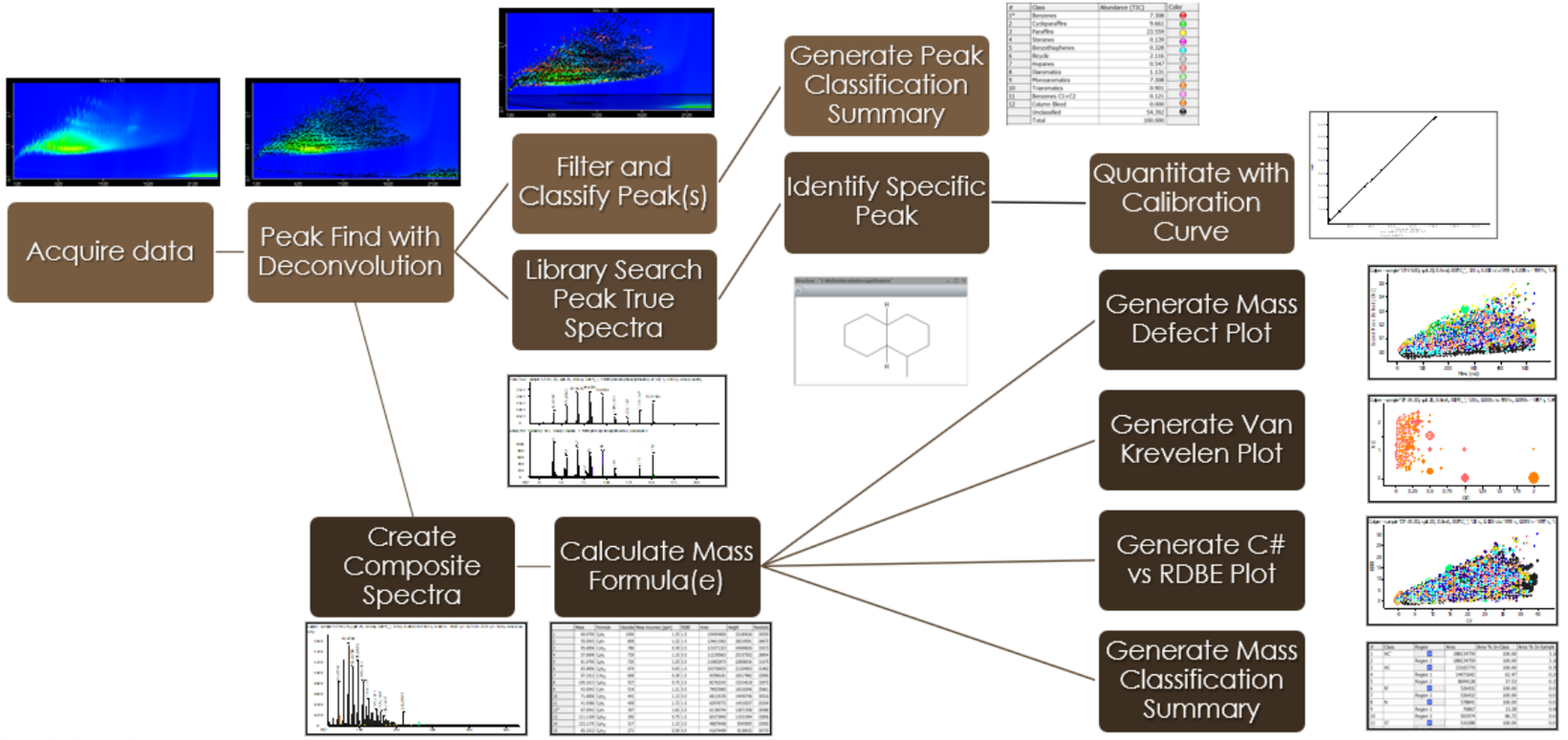
Complementary approaches for a variety of experimental design needs!

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®



ChromaTOF Data Acquisition & Processing

Application Note

LECO
EMPOWERING RESULTS
Elemental Analysis | GC Mass Spectrometry | Metallography

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 polymeric 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.

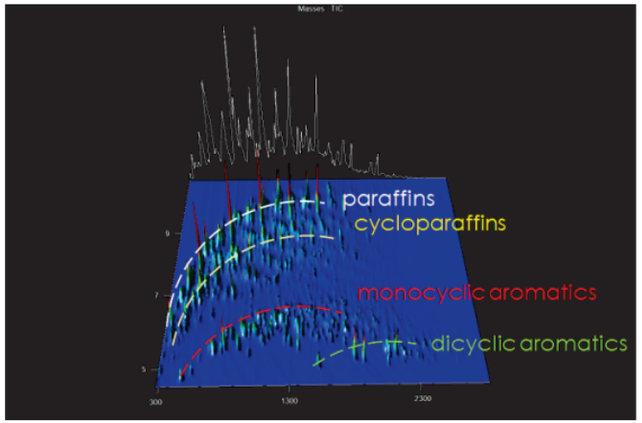
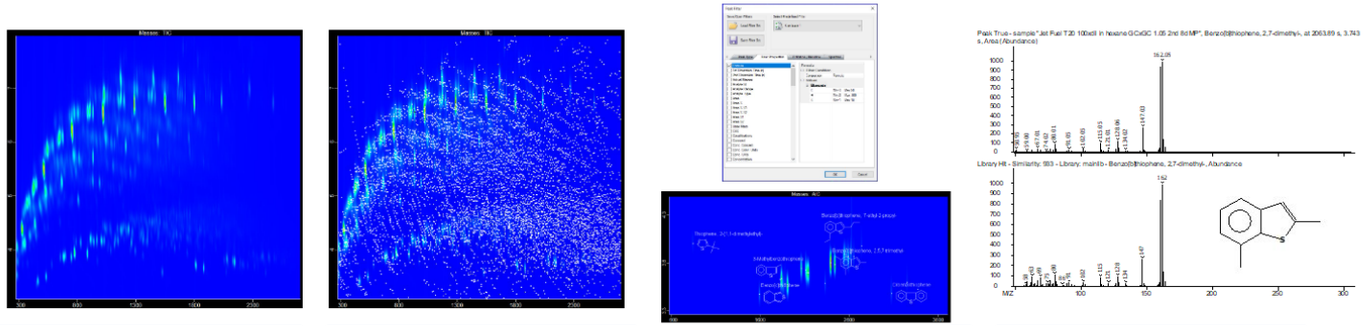
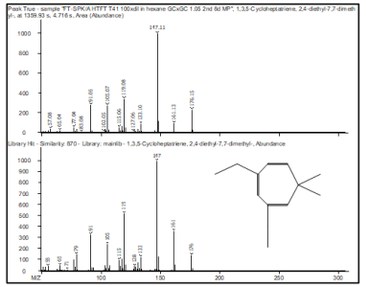
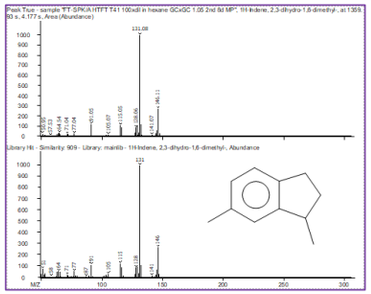


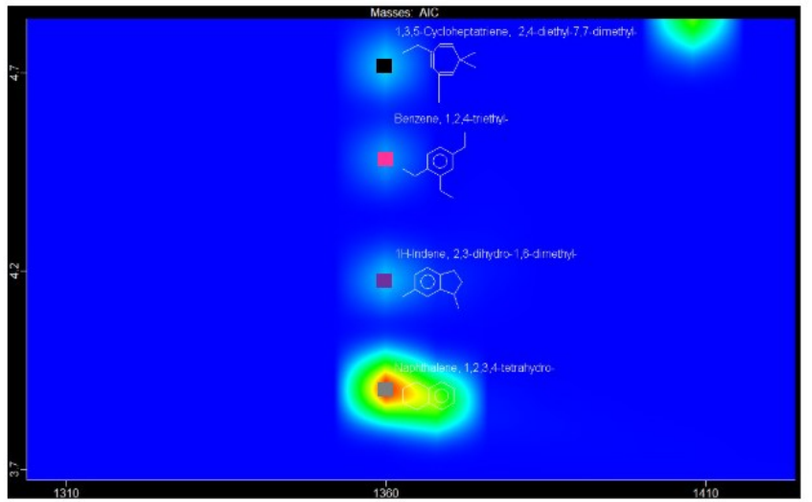
Figure 1. GCxGC 3D surface plot of commercial aviation turbine fuel with Total Ion Chromatogram (TIC) shown. Reconstructed trace of what a single dimension of GC separation would have looked like is shown in white. Elution bands of paraffins (white), cycloparaffins (yellow), monocyclic aromatics (red),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

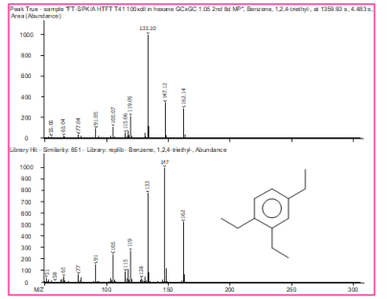


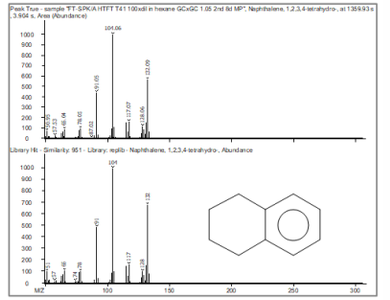
Acquire Data → Automated Peak Find & Library Search → Apply Custom Filters → Identify Analytes of Interest











ChromaTOF Data Acquisition & Processing

Application Note

LECO
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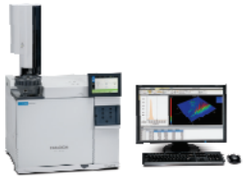
Elemental Analysis | GC Mass Spectrometry | Metallography

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.

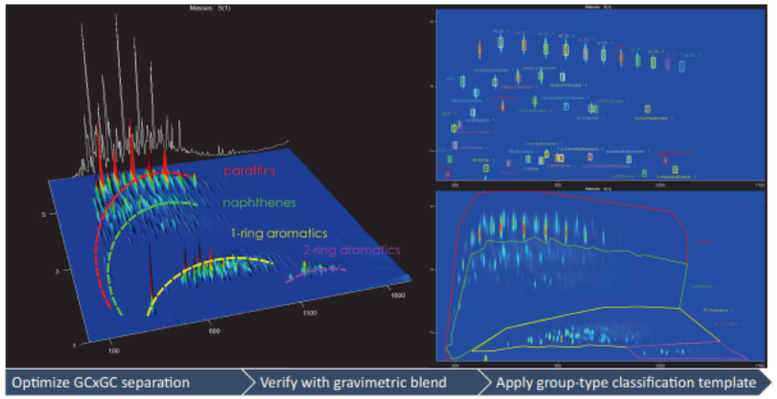
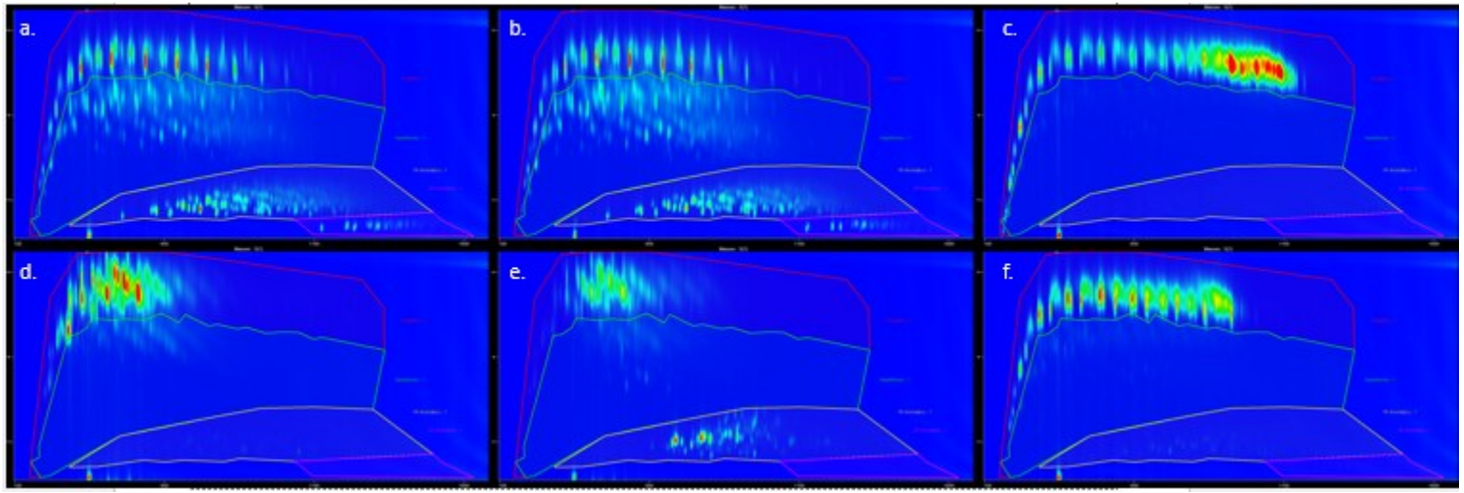


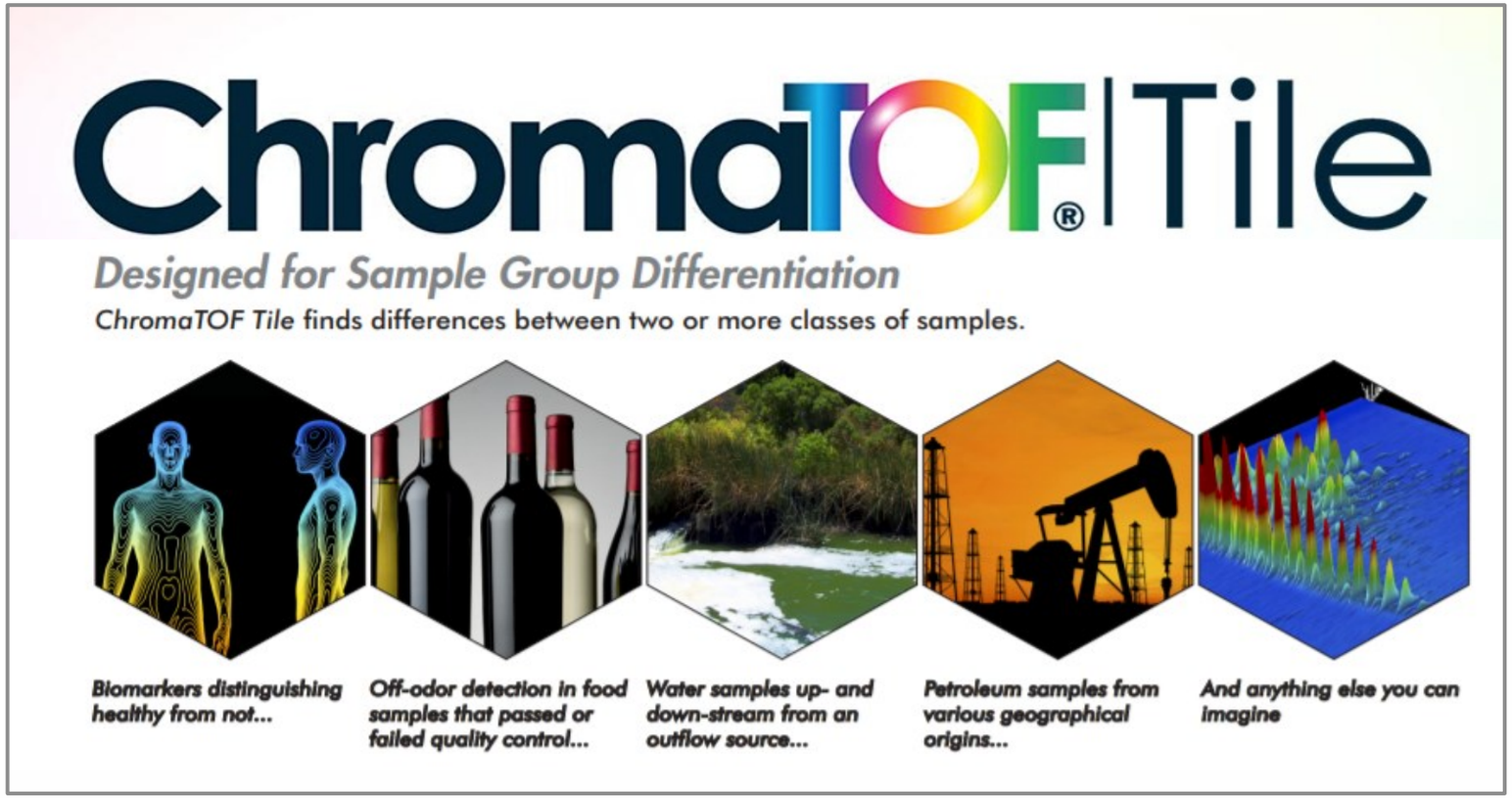
Figure 1. Left: 3D surface plot of aviation fuel showing benefit of GCxGC for improvement of chromatographic resolution, with white reconstructed trace of the 1D GC separation. Compound groups are visually apparent, with the tallest peaks in the back corresponding to paraffins and the short band of analytes 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.

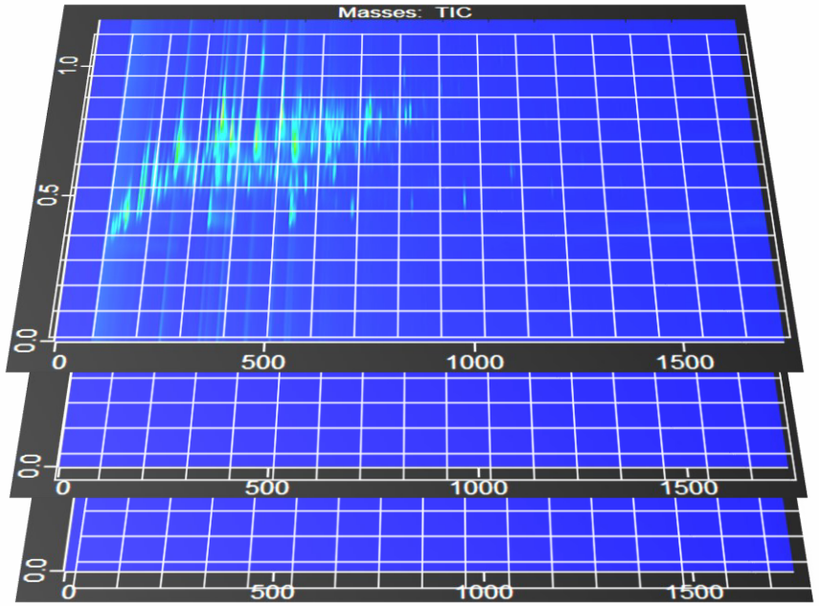


Mass % per Hydrocarbon Group-type Class by FID

	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





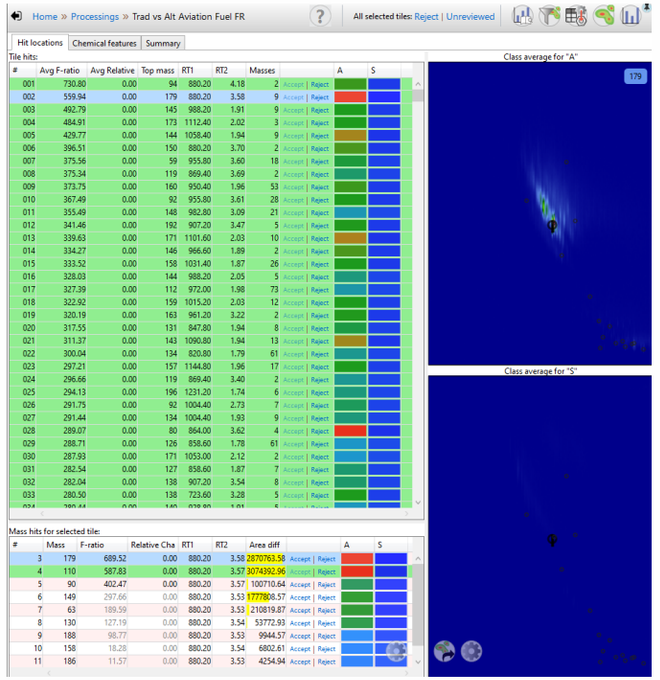
connects samples with chromatographic tiling approach that links the data set and compares raw data **to find differences**

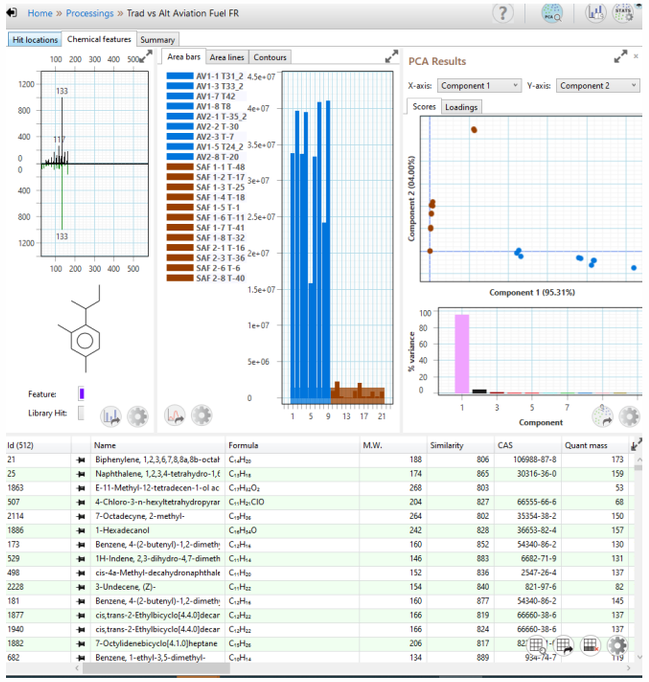
ChromaTOF TILE Simple Workflow

Click here to auto-calculate suggested tile size

Samples must be selected first

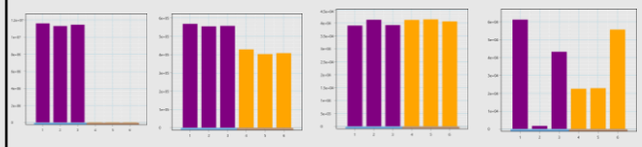
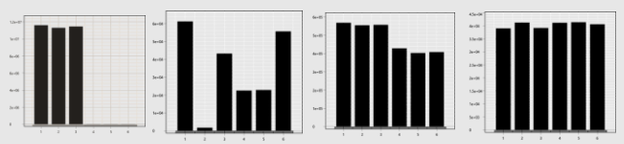
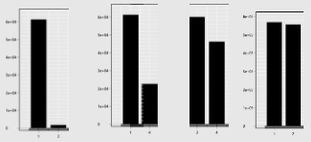
Tile size D1 (modulations):	0
Tile size D2 (spectra):	0
S/N threshold:	10
D1 signal to base threshold:	1
D2 signal to base threshold:	3
Samples that must exceed S/N threshold:	1
Mass F-ratios to average:	1
Statistical threshold type to apply:	F-ratio
F-ratio threshold:	20
Relative change threshold type to apply:	None
Minimum masses per tile:	3
Minimum mass:	0
Maximum mass:	10000
Masses to ignore:	
Perform one-point normalization:	☐



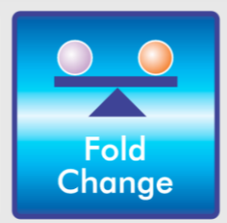


Import Data → Setup Processing Parameters → Compile Hits in Feature Table → Review Statistical Results

ChromaTOF TILE Comparison of Statistical Methods

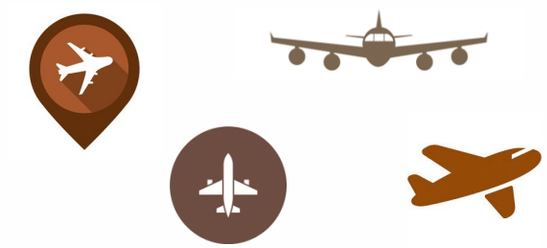
Comparison Option	 FISHER RATIO	 COEFFICIENT OF VARIATION	 FOLD CHANGE
Objective	**Find differences between samples or groups of samples**		
Calculation	$FR = \frac{class\ to\ class\ variation}{within\ class\ variation}$	$CV = \frac{St\ Dev\ of\ Tile\ Areas}{Mean\ of\ Tile\ Areas}$	$FC = \frac{Max\ response}{Min\ response}$ *reported as Log2(FC) and generalized to compare > 2 values
Experimental design requirements	• Classes required • Replicates required	• Classes are not used	• Classes optional • Only 2 samples needed
Differences that are found			

Applications for Each Statistical Method

Comparison Option	 FISHER RATIO	 COEFFICIENT OF VARIATION	 FOLD CHANGE
Application Example	 Traditional Aviation Fuel  Synthetic Aviation Fuel	Alternative Aviation Fuels (Multiple Production Methods) 	Pinpointing Components in Aromatics Additive Package 

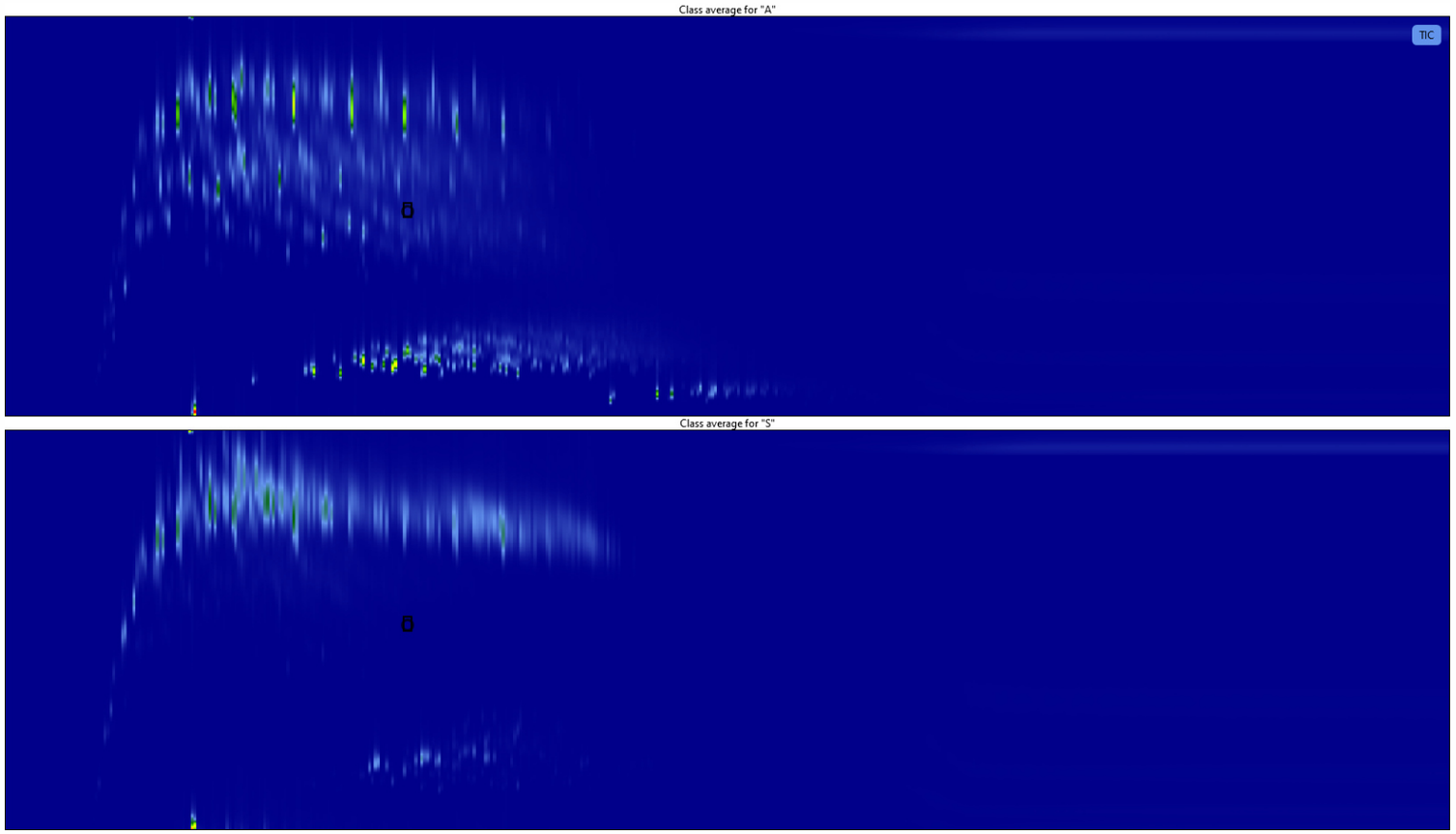
Experimental Setup: Comparison of Traditional and Synthetic Aviation Fuel

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



Traditional Aviation Fuel

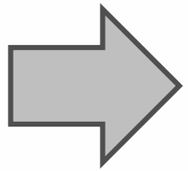
Synthetic Aviation Fuel

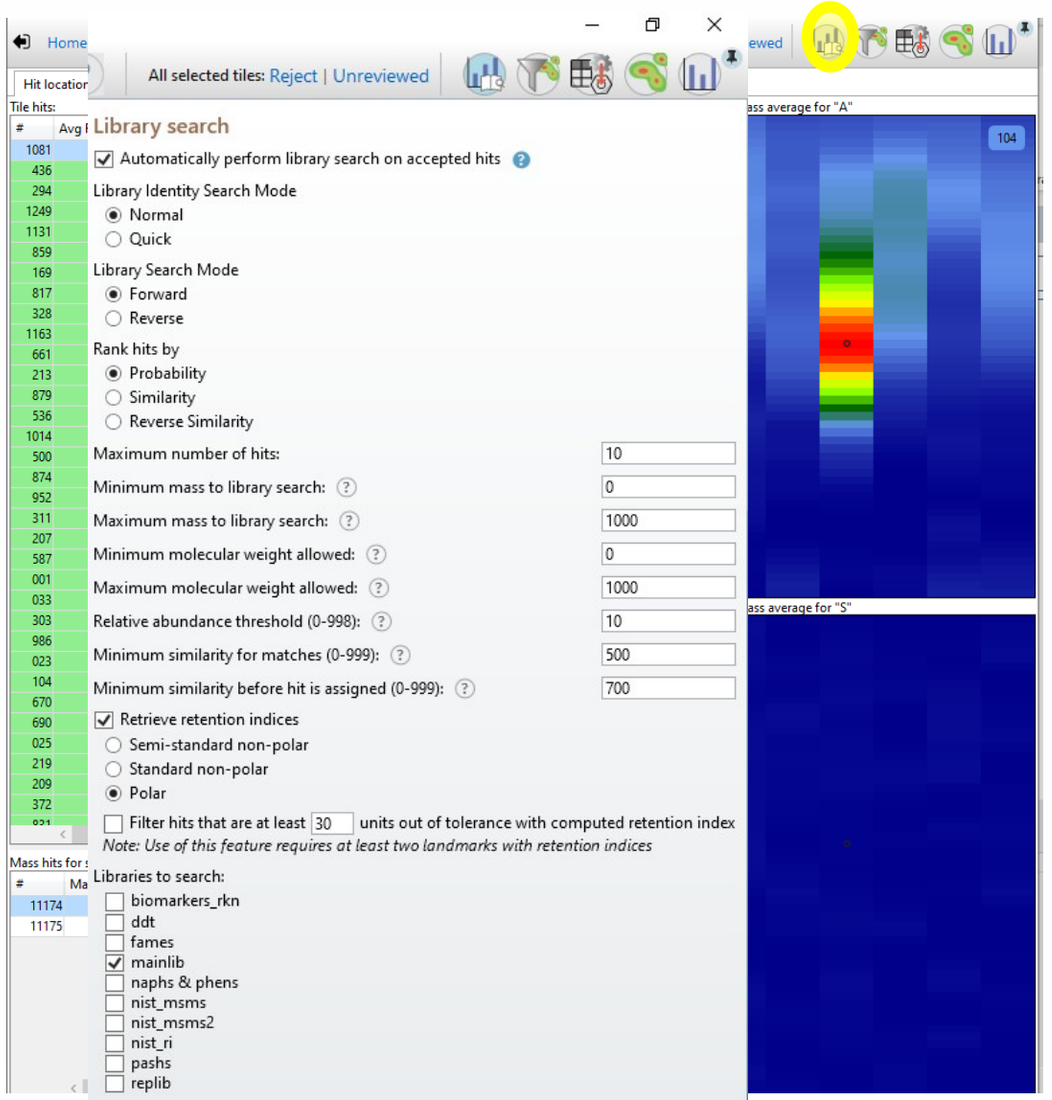


Curation of Tile and Mass Hits into Feature Table

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:	☐





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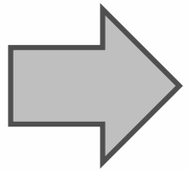

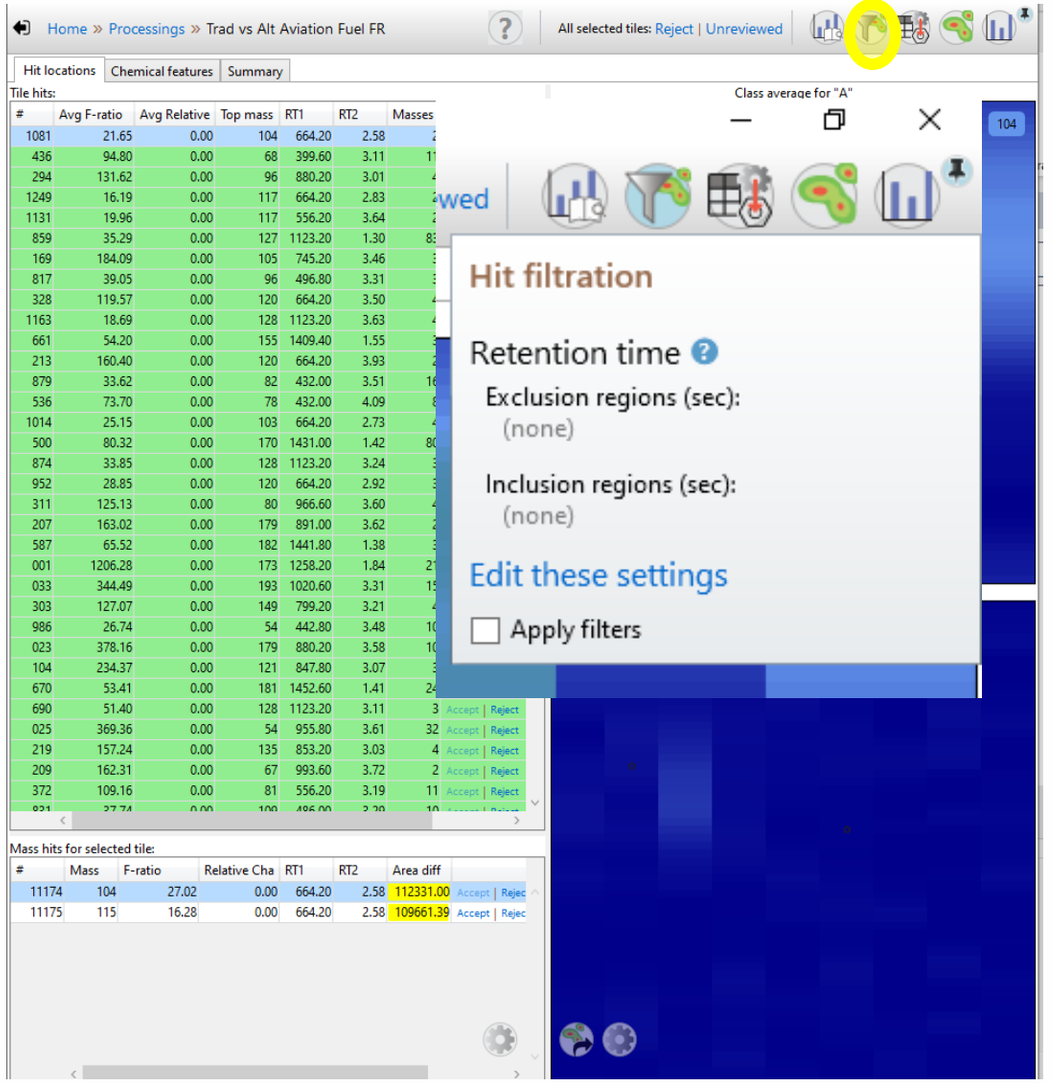

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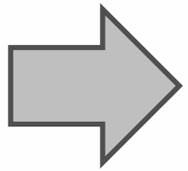

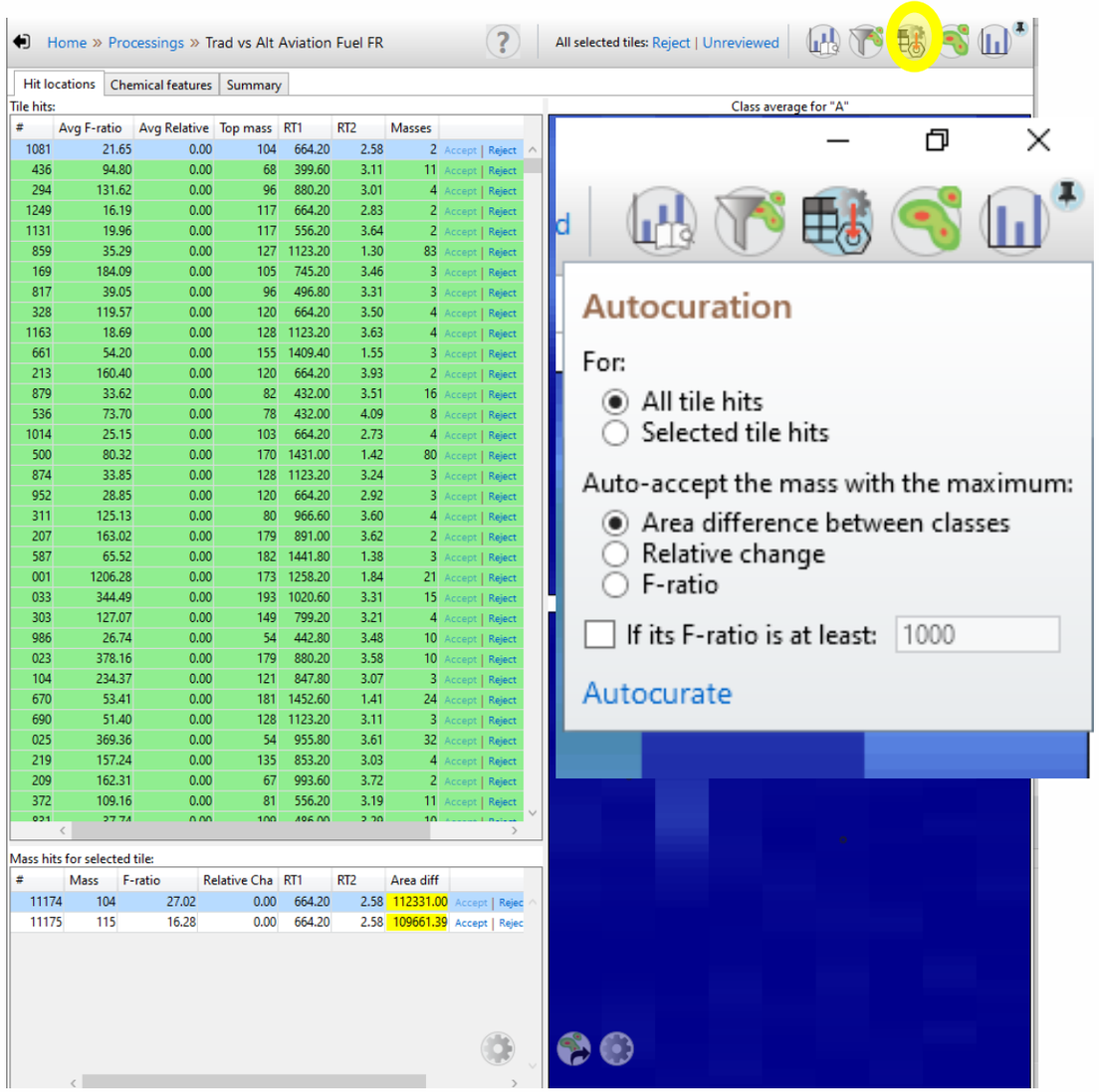

Curation of Tile and Mass Hits into Feature Table

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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
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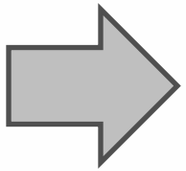
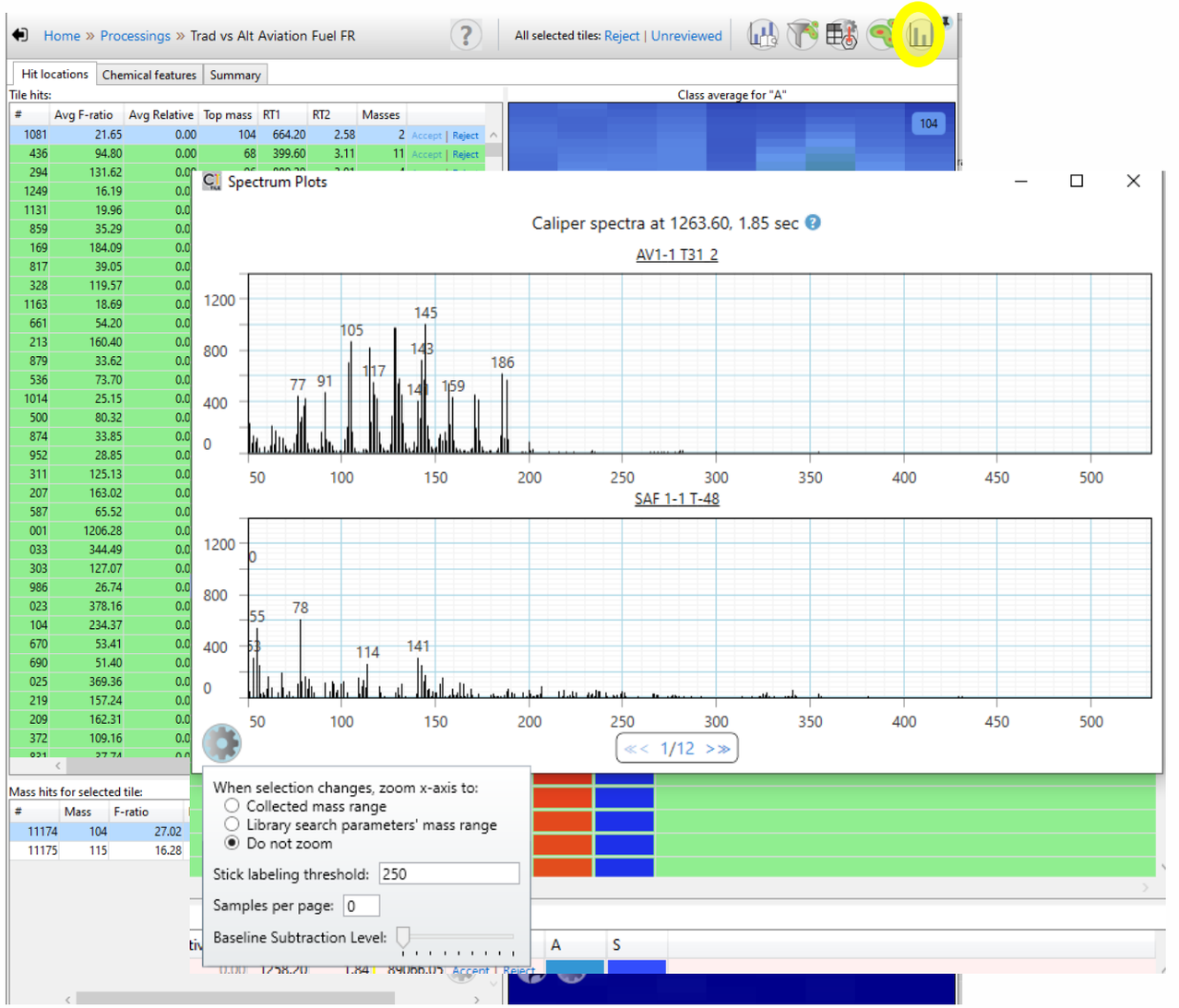
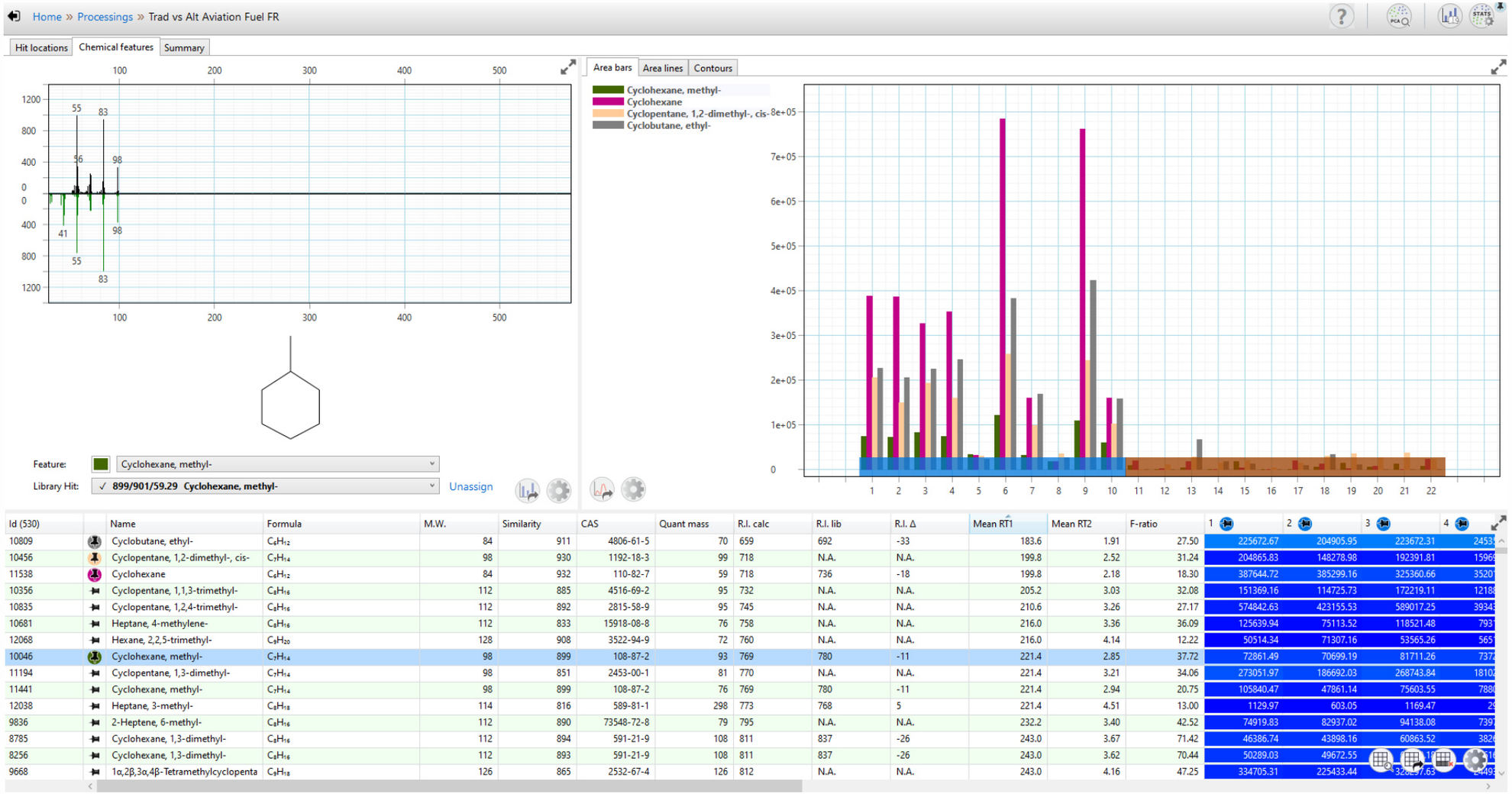


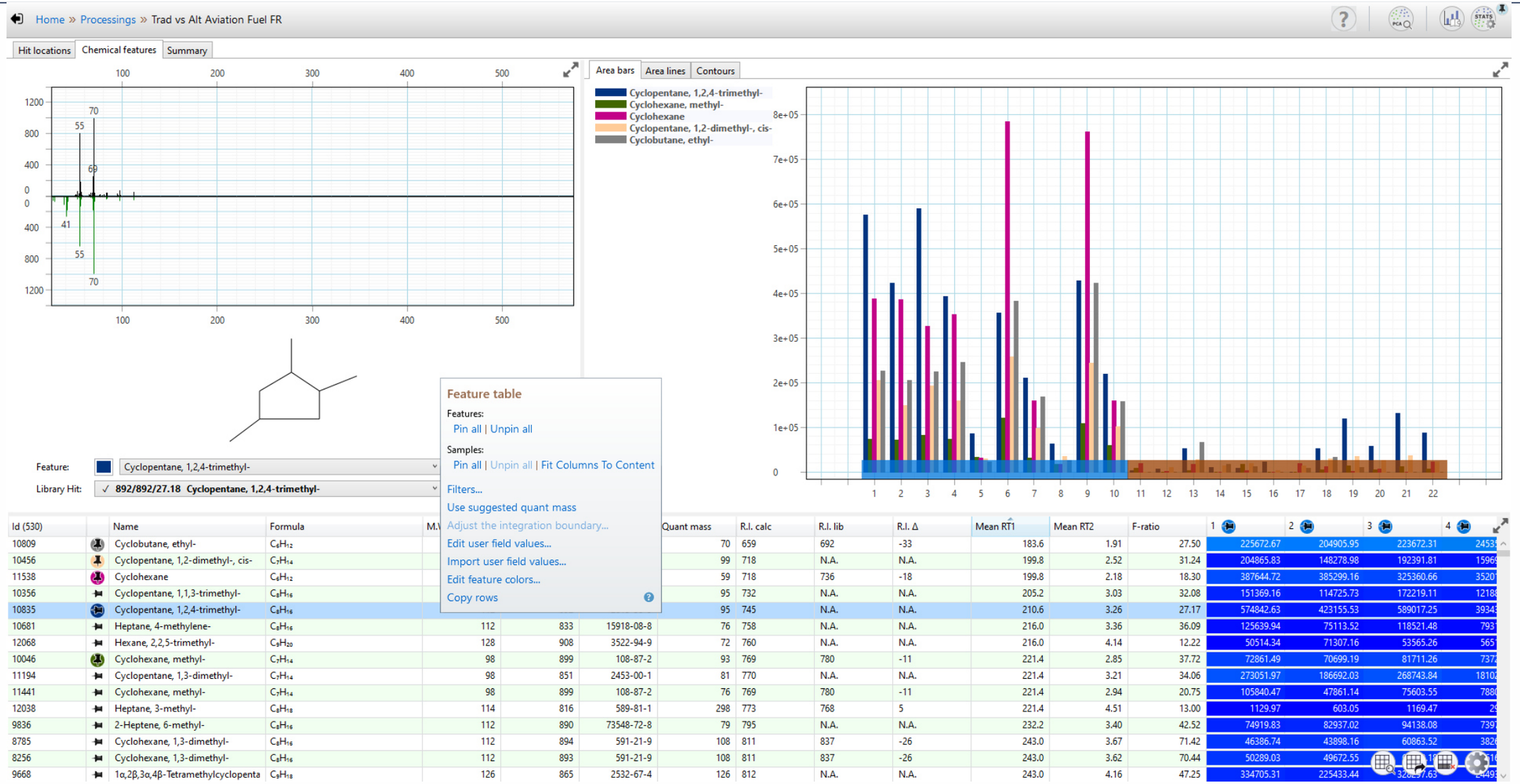


Feature Table to Statistical Plots



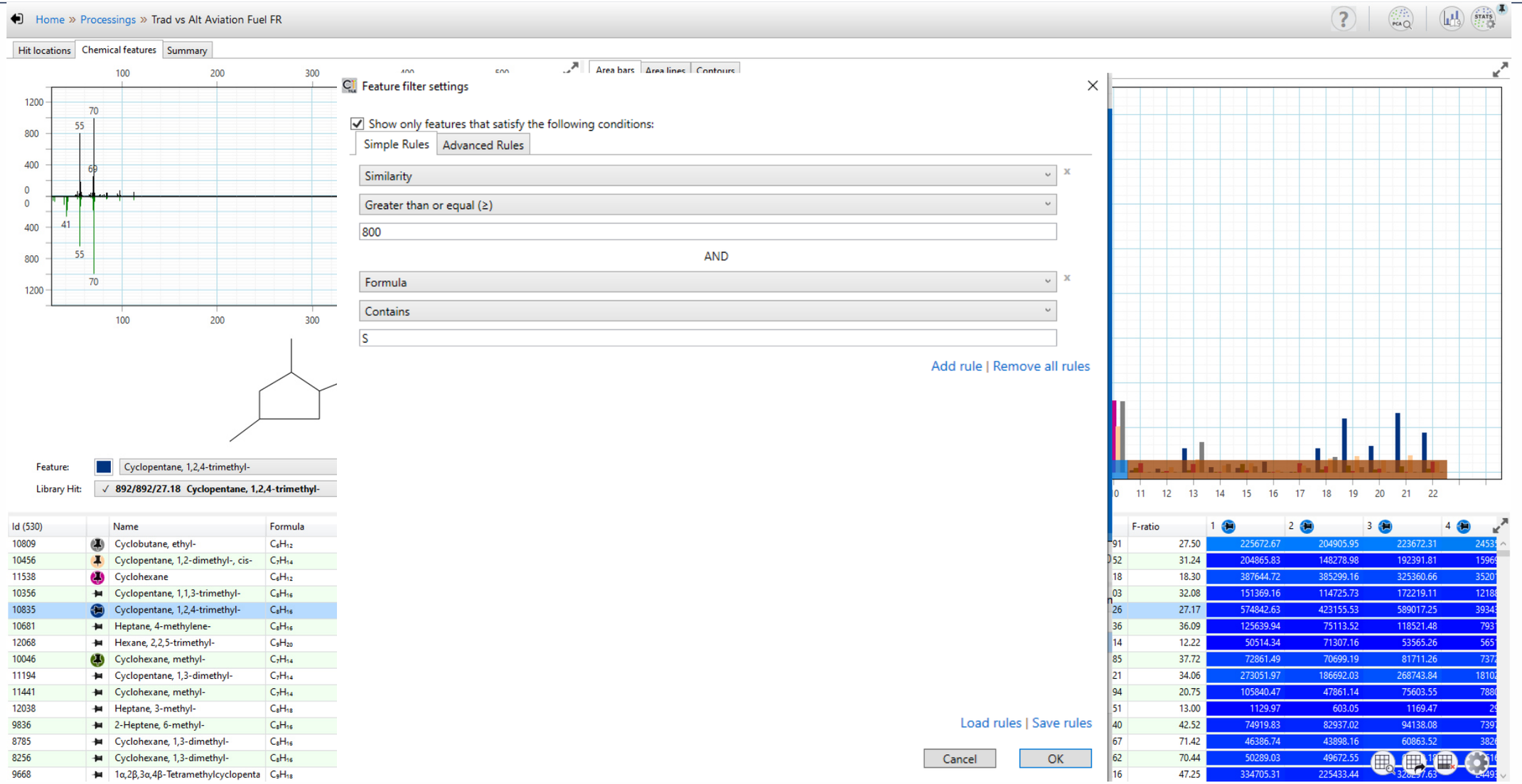
Id (530)		Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
10809		Cyclobutane, ethyl-	C_6H_{12}	84	911	4806-61-5	70	659	692	-33	183.6	1.91	27.50	225672.67	204905.95	223672.31	2453
10456		Cyclopentane, 1,2-dimethyl-, cis-	C_7H_{14}	98	930	1192-18-3	99	718	N.A.	N.A.	199.8	2.52	31.24	204865.83	148278.98	192391.81	1596
11538		Cyclohexane	C_6H_{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_8H_{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_8H_{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_8H_{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_9H_{20}	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_7H_{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_7H_{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_7H_{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_8H_{18}	114	816	589-81-1	298	773	768	5	221.4	4.51	13.00	1129.97	603.05	1169.47	2
9836		2-Heptene, 6-methyl-	C_8H_{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_8H_{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_8H_{16}	112	893	591-21-9	108	811	837	-26	243.0	3.62	70.44	50289.03	49672.55	1	51
9668		1α,2β,3α,4β-Tetramethylcyclopenta	C_8H_{18}	126	865	2532-67-4	126	812	N.A.	N.A.	243.0	4.16	47.25	334705.31	225433.44	32	2493

Feature Table to Statistical Plots



Id (530)	Name	Formula	M.W			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_6H_{12}				70	659	692	-33	183.6	1.91	27.50	225672.67	204905.95	223672.31	24535
10456	Cyclopentane, 1,2-dimethyl-, cis-	C_7H_{14}				99	718	N.A.	N.A.	199.8	2.52	31.24	204865.83	148278.98	192391.81	15969
11538	Cyclohexane	C_6H_{12}				59	718	736	-18	199.8	2.18	18.30	387644.72	385299.16	325360.66	35207
10356	Cyclopentane, 1,1,3-trimethyl-	C_8H_{16}				95	732	N.A.	N.A.	205.2	3.03	32.08	151369.16	114725.73	172219.11	12188
10835	Cyclopentane, 1,2,4-trimethyl-	C_8H_{16}				95	745	N.A.	N.A.	210.6	3.26	27.17	574842.63	423155.53	589017.25	39343
10681	Heptane, 4-methylene-	C_8H_{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_9H_{20}	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_7H_{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_7H_{14}	98	851	2453-00-1	81	770	N.A.	N.A.	221.4	3.21	34.06	273051.97	186692.03	268743.84	18102
11441	Cyclohexane, methyl-	C_7H_{14}	98	899	108-87-2	76	769	780	-11	221.4	2.94	20.75	105840.47	47861.14	75603.55	7880
12038	Heptane, 3-methyl-	C_8H_{18}	114	816	589-81-1	298	773	768	5	221.4	4.51	13.00	1129.97	603.05	1169.47	29
9836	2-Heptene, 6-methyl-	C_8H_{16}	112	890	73548-72-8	79	795	N.A.	N.A.	232.2	3.40	42.52	74919.83	82937.02	94138.08	7397
8785	Cyclohexane, 1,3-dimethyl-	C_8H_{16}	112	894	591-21-9	108	811	837	-26	243.0	3.67	71.42	46386.74	43898.16	60863.52	3826
8256	Cyclohexane, 1,3-dimethyl-	C_8H_{16}	112	893	591-21-9	108	811	837	-26	243.0	3.62	70.44	50289.03	49672.55	1	516
9668	1α,2β,3α,4β-Tetramethylcyclopenta	C_8H_{18}	126	865	2532-67-4	126	812	N.A.	N.A.	243.0	4.16	47.25	334705.31	225433.44	328297.63	24493

Feature Table to Statistical Plots



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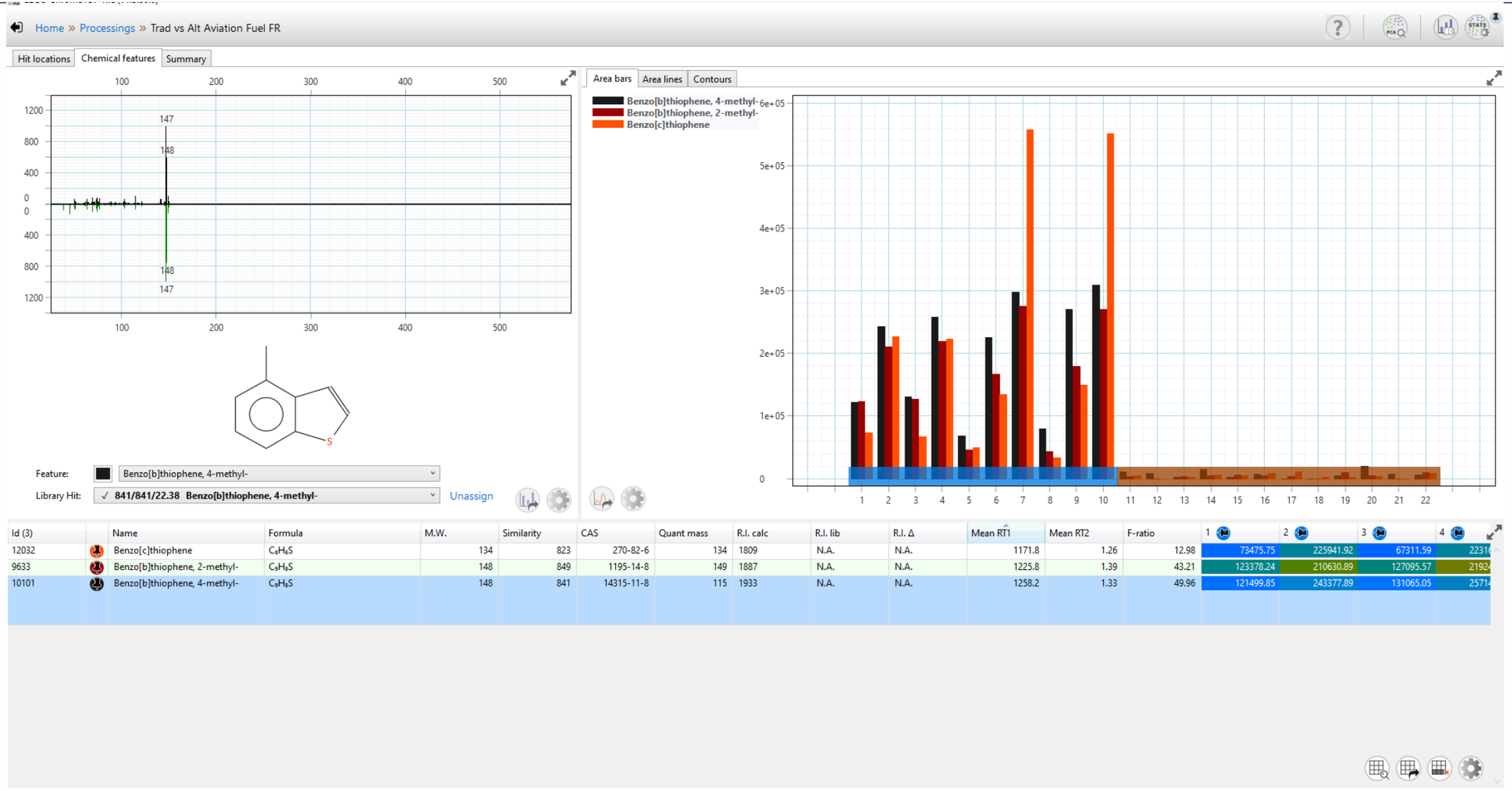
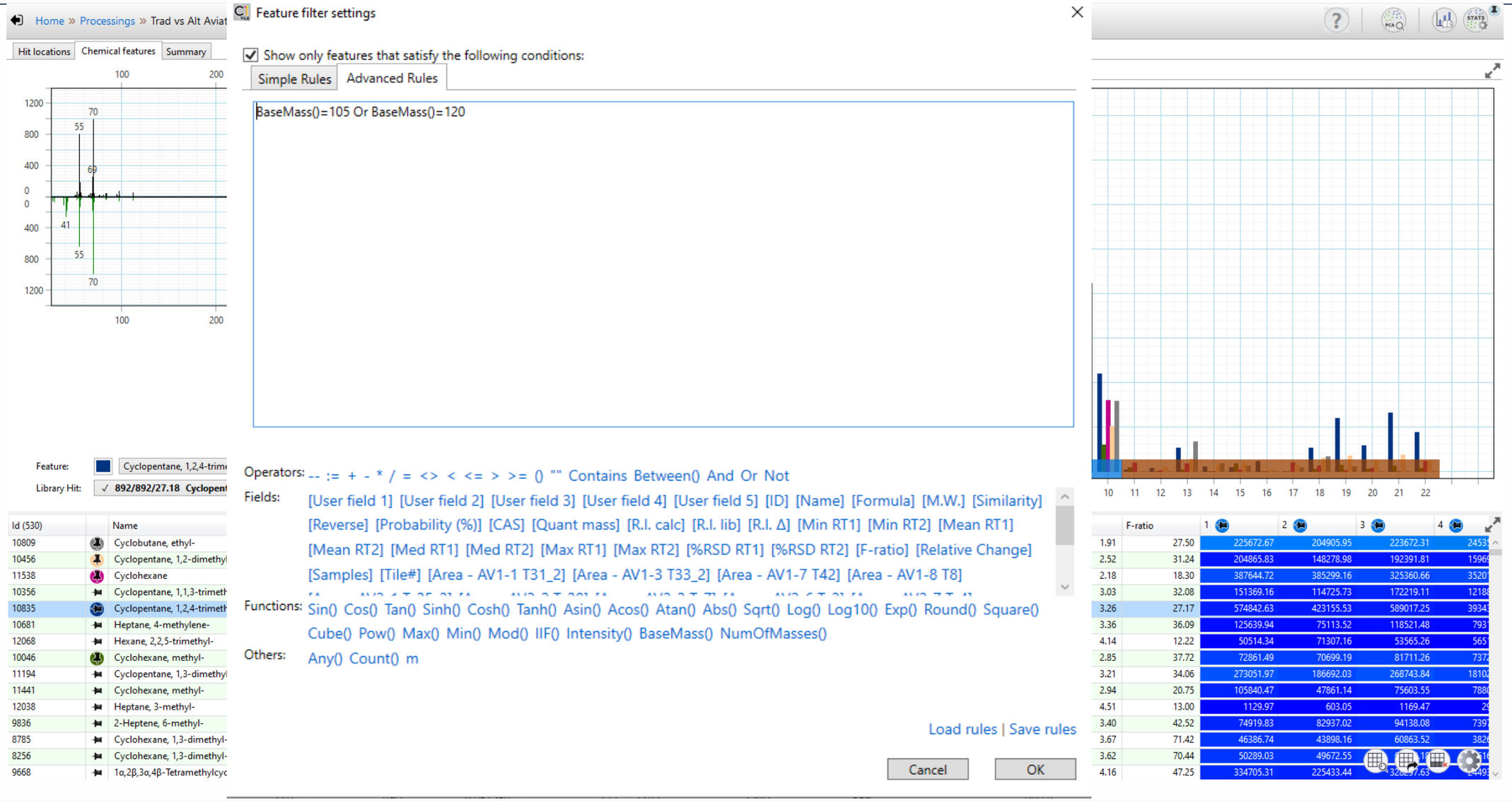


Id (3)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
12032	Benzo[c]thiophene	C_8H_6S	134	823	270-82-6	134	1809	N.A.	N.A.	1171.8	1.26	12.98	73475.75	225941.92	67311.59	22316
9633	Benzo[b]thiophene, 2-methyl-	C_9H_8S	148	849	1195-14-8	149	1887	N.A.	N.A.	1225.8	1.39	43.21	123378.24	210630.89	127095.57	21924
10101	Benzo[b]thiophene, 4-methyl-	C_9H_8S	148	841	14315-11-8	115	1933	N.A.	N.A.	1258.2	1.33	49.96	121499.85	243377.89	131065.05	25714

Feature Table to Statistical Plots



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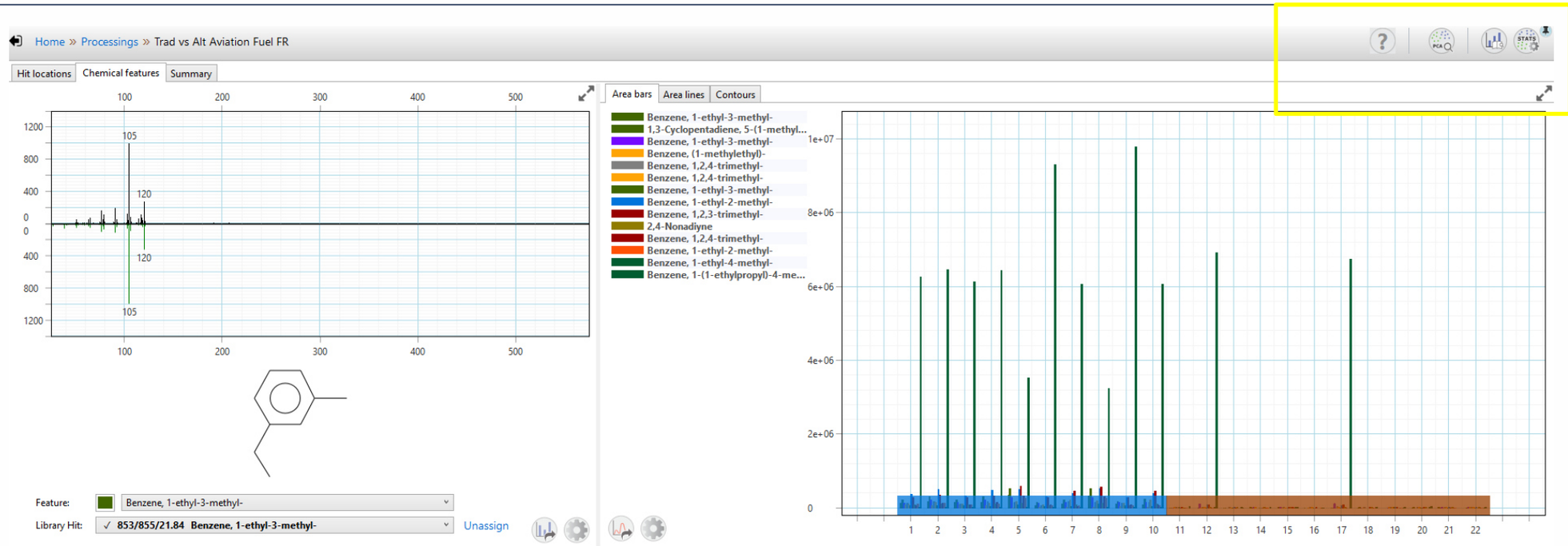
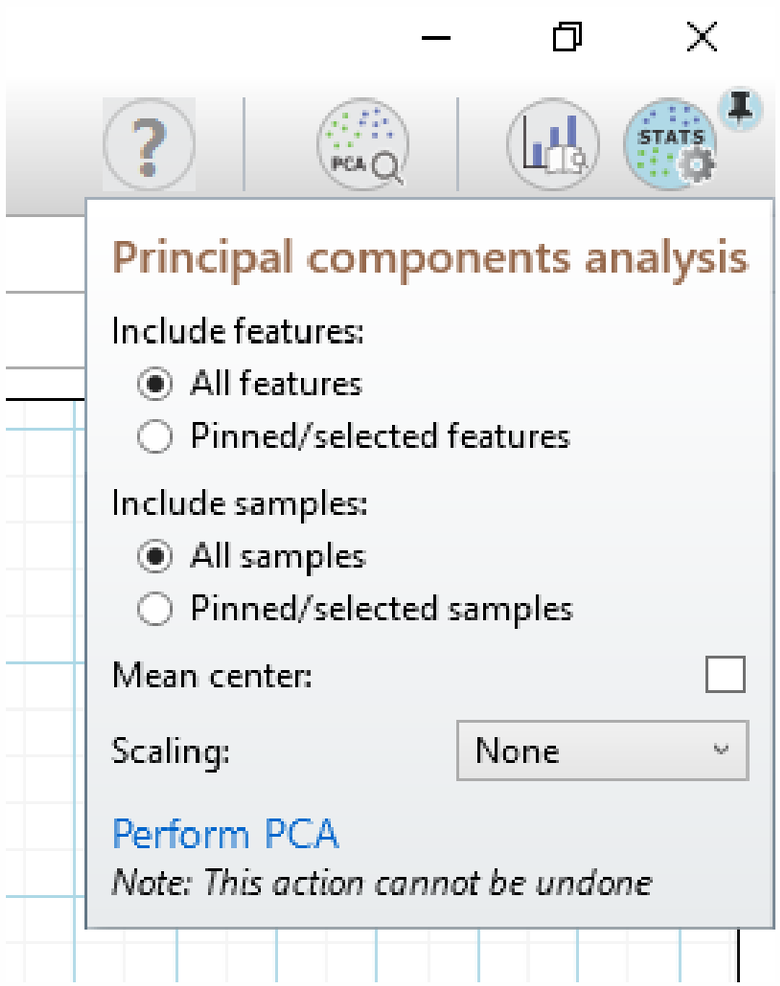
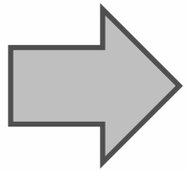
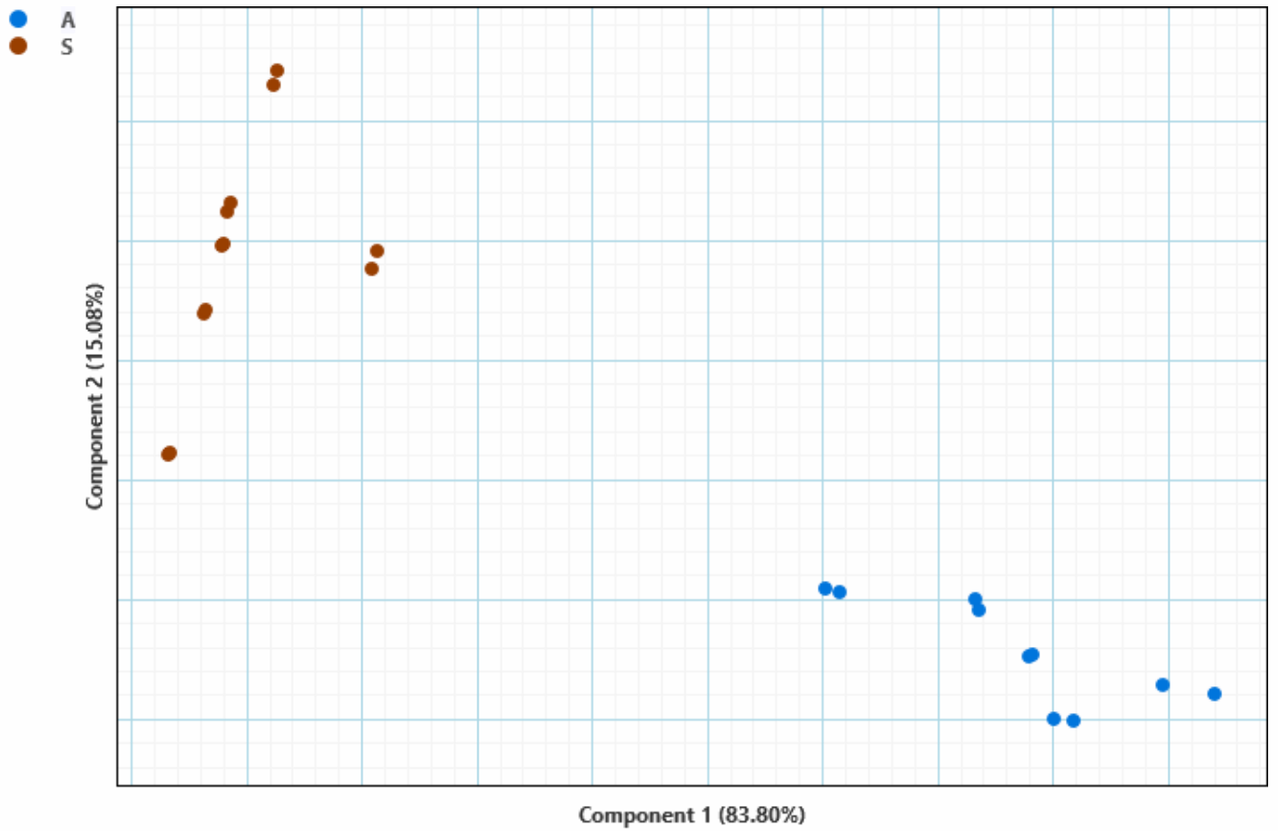


Id (21)	Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3	4
3698	Benzene, (1-methylethyl)-	C_9H_{12}	120	924	98-82-8	122	1172	1178	-6	610.2	1.87	173.58	51744.52	74971.77	48382.73	626
4826	2,4-Nonadiyne	C_9H_{12}	120	836	63621-15-8	140	1224	N.A.	N.A.	664.2	1.85	143.74	83864.81	101691.47	81844.10	981
10640	1,3-Cyclopentadiene, 5-(1-methylp	C_9H_{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_9H_{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_9H_{12}	120	912	622-96-8	160	1224	1226	-2	664.2	1.90	32.44	12886.76	12863.40	8476.33	151
11174	Benzene, 1-ethyl-2-methyl-	C_9H_{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_9H_{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_9H_{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_9H_{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_9H_{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_9H_{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_9H_{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_9H_{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_9H_{12}	120	901	95-63-6	125	1285	1283	2	723.6	1.86	113.80	103368.23	140555.98	1	6
11322	Benzene, 1,2,4-trimethyl-	C_9H_{12}	120	852	95-63-6	158	1286	1283	3	723.6	2.36	22.37	68572.77	55434.98	7	623

Feature Table to Statistical Plots







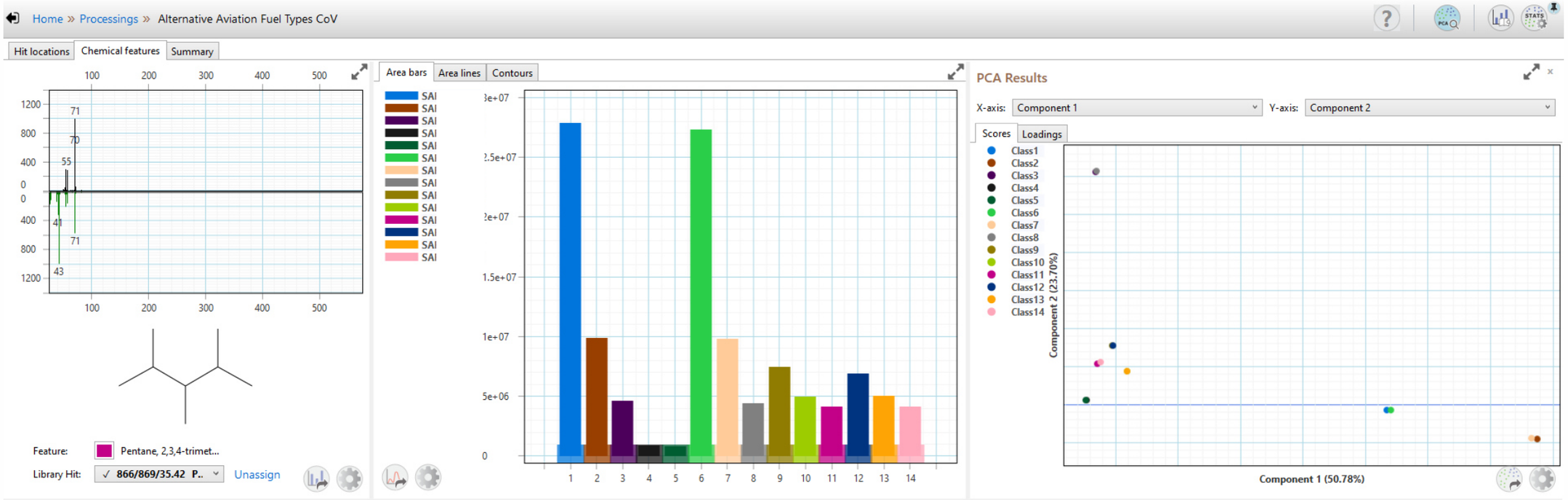
Experimental Design: Tracking Differences between Alternative Fuel Types

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:

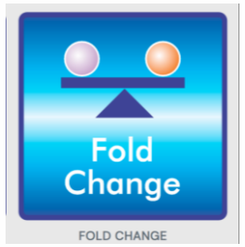
- Low-temperature Fischer-Tropsch Synthetic Paraffinic Kerosene (LT-FTSPK)
- High-temperature Fischer-Tropsch Synthetic Paraffinic Kerosene (HT-FTSPK)
- Hydrotreated Esters and Fatty Acids (HEFA)
- Synthesized Isoparaffins (SIP)
- Alcohol-to-Jet (ATJ)
- Catalytic Hydrothermolysis (CHJ)
- Blends with aromatics packages (-A)

Tracking Differences between Alternative Fuel Types

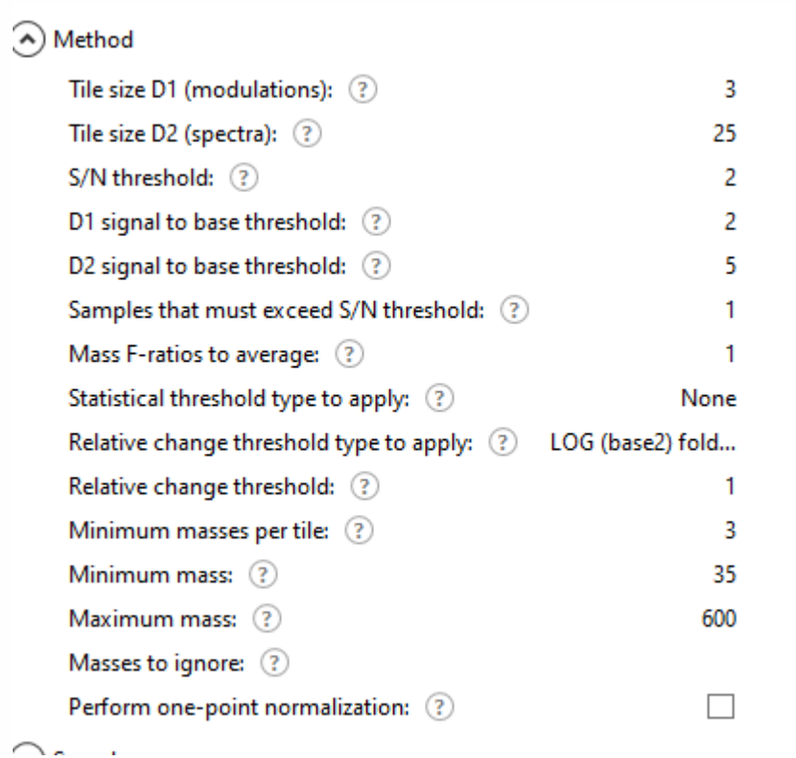


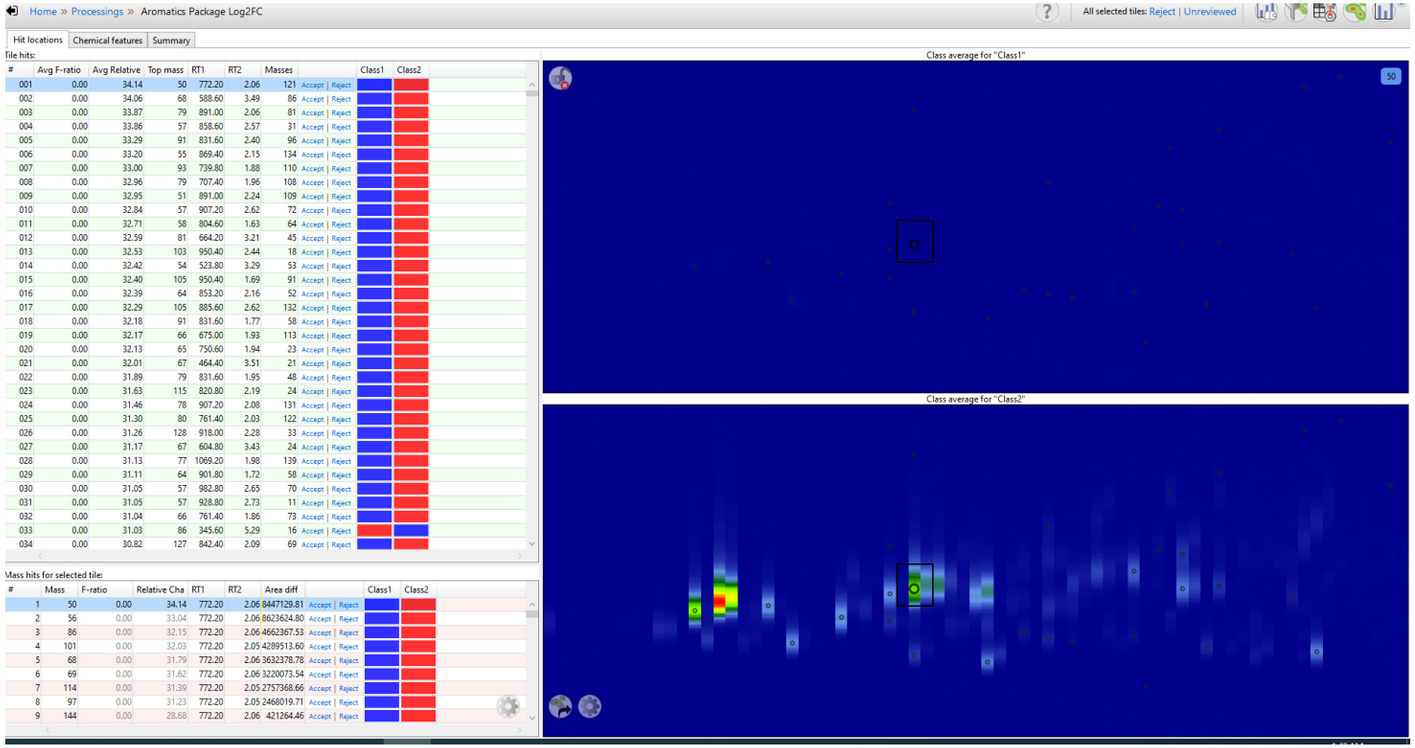
Id (535)		Name	Formula	M.W.	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	R.I. Δ	Mean RT1	Mean RT2	F-ratio	1	2	3
20536		Pentane, 2,3,4-trimethyl-	C_8H_{18}	114	866	565-75-3	71	758	N.A.	N.A.	216.0	3.38	0.00	27843426.00	9830900.00	460474
20419		Tetradecane, 3-methyl-	$C_{15}H_{32}$	212	893	18435-22-8	120	1474	N.A.	N.A.	896.4	4.84	0.00	1010.87	3688.18	19200
20373		Heptane, 3,4,5-trimethyl-	$C_{10}H_{22}$	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	820	95008-11-0	211	1333	N.A.	N.A.	766.8	4.84	0.00	2646.57	4619.58	
19982		Hexane, 3-ethyl-2,5-dimethyl-	$C_{10}H_{22}$	142	854	52897-04-8	75	961	N.A.	N.A.	383.4	0.61	0.00	433696.00	419767.47	1795
19960		1-Dodecanol, 3,7,11-trimethyl-	$C_{15}H_{32}O$	228	820	6750-34-1	199	990	N.A.	N.A.	410.4	4.97	0.00	2386.68	3799.42	16
19881		Octane, 2,4,6-trimethyl-	$C_{11}H_{24}$	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	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	895	1560-88-9	233	1728	1862	-134	1107.0	5.30	0.00	0.00	540.12	145
19367		Cyclooctane, methyl-	C_9H_{18}	126	847	1502-38-1	260	1065	N.A.	N.A.	491.4	4.97	0.00	0.00	959.53	29
18957		10-Heneicosene (c,t)	$C_{21}H_{42}$	294	823	95008-11-0	205	1505	N.A.	N.A.	923.4	4.44	0.00	5698.80	6814.85	
18460		10-Heneicosene (c,t)	$C_{21}H_{42}$	294	820	95008-11-0	167	1283	N.A.	N.A.	718.2	4.63	0.00	131522.88	175865.88	666
18437		Cyclohexane, 1,3-dimethyl-	C_8H_{16}	112	903	591-21-9	148	811	837	-26	243.0	3.75	0.00	4925.64		89
18392		Tetradecane	$C_{14}H_{30}$	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

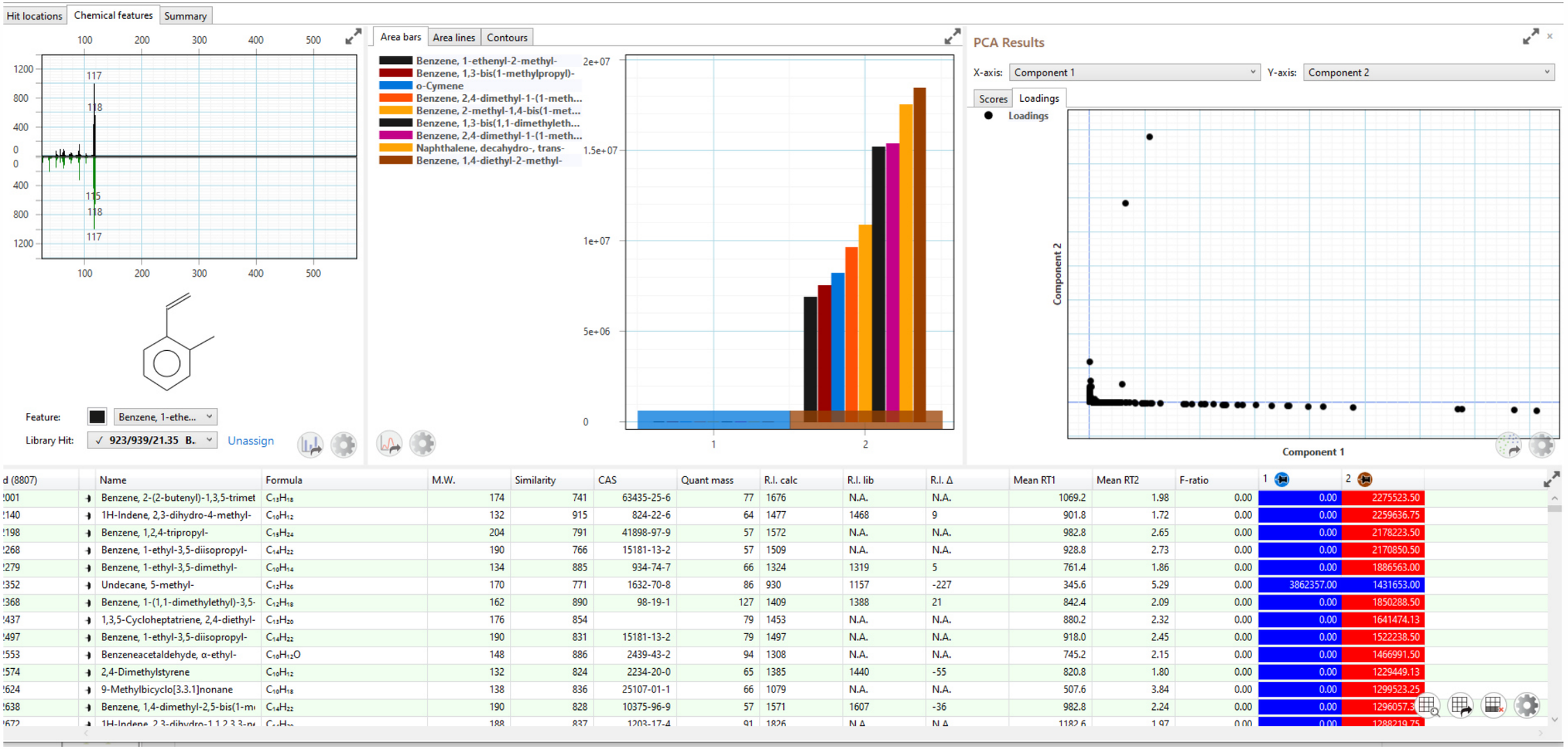


Driving Question: With only 2 samples (one sample with aromatics additive and one similar one without), can I quickly identify which compounds make up an aromatics additive package?





Finding Components of Aromatics Additive Package



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	$C_{13}H_{18}$	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-	$C_{15}H_{24}$	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-1,1,2,3,3-pr	$C_{14}H_{20}$	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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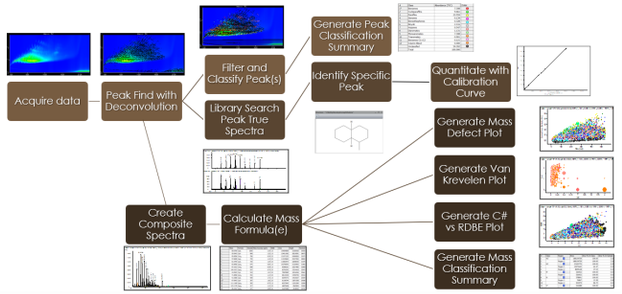

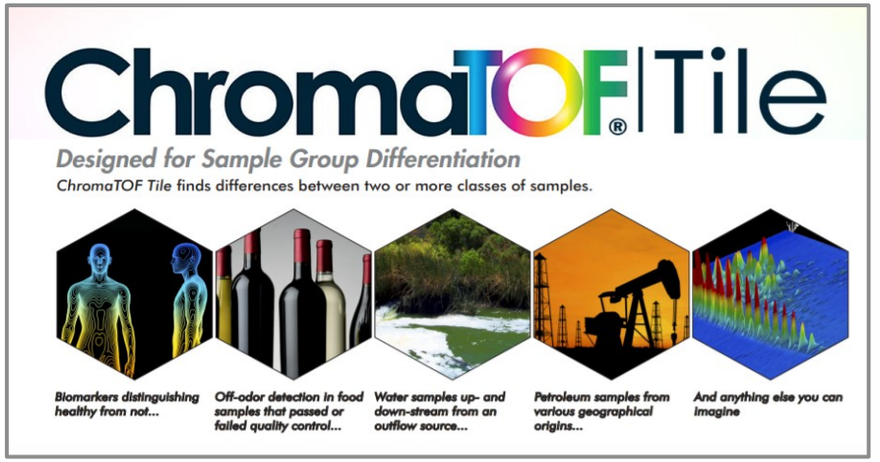

Fisher Ratio	CoV	Fold Change
Traditional Aviation Fuel Synthetic Aviation Fuel	Alternative Aviation Fuels (Multiple Production Methods)	Pinpointing Components in Aromatics Additive Package

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ChromaTOF® SYNC 2D

ChromaTOF Sync and Sync 2D — Capture Every Clue

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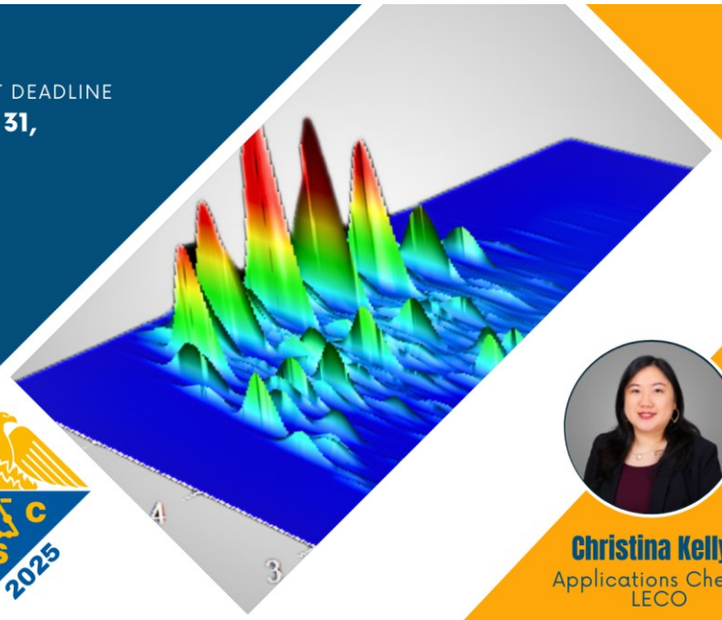
ABSTRACT DEADLINE
MARCH 31, 2025



ACS FALL 2025

Multidimensional Gas Chromatography:
FROM PETROLEUM TO BEYOND
Symposium

AUGUST 17-21, 2025

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