



Application of GC×GC for the investigation of fermented beverages



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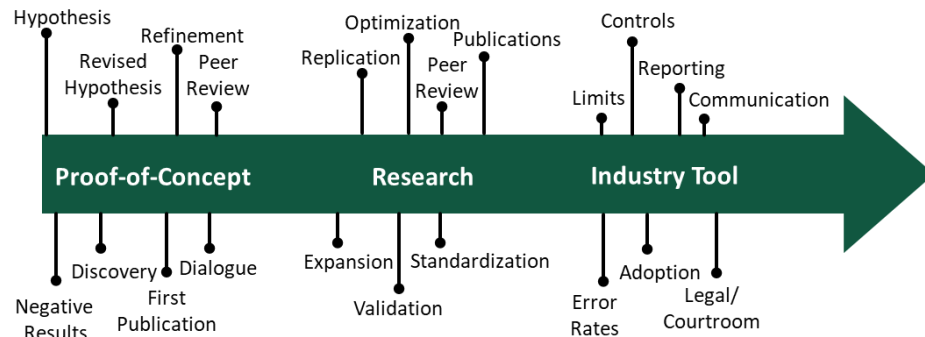
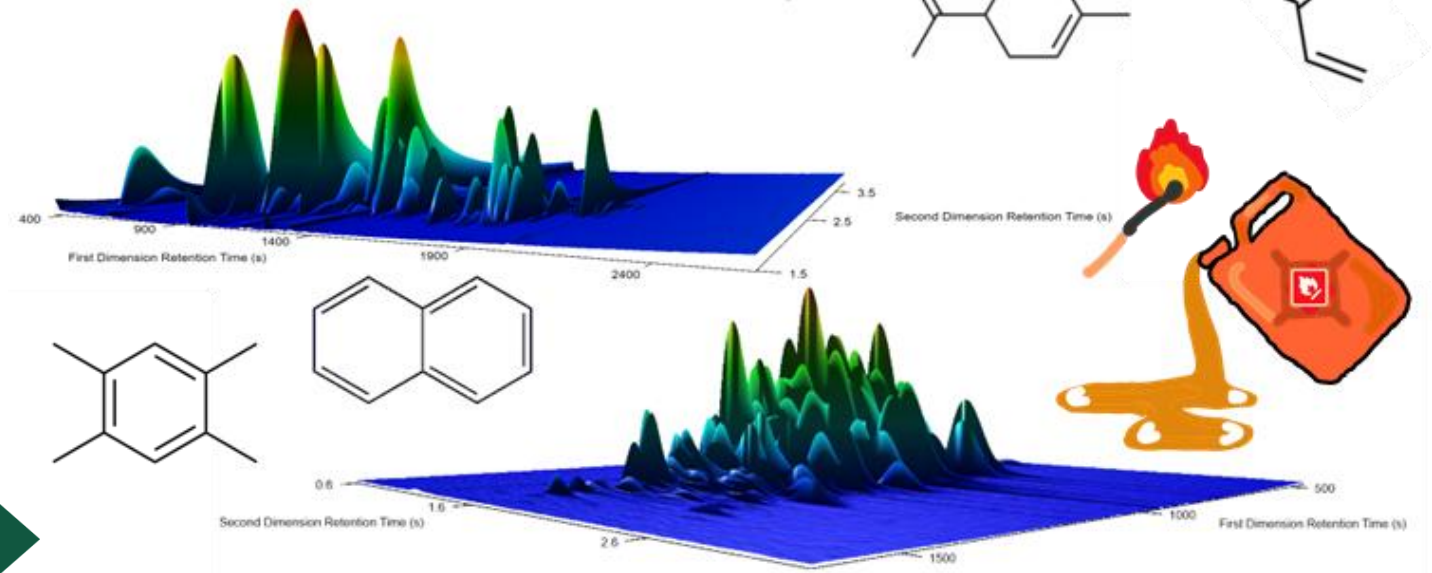
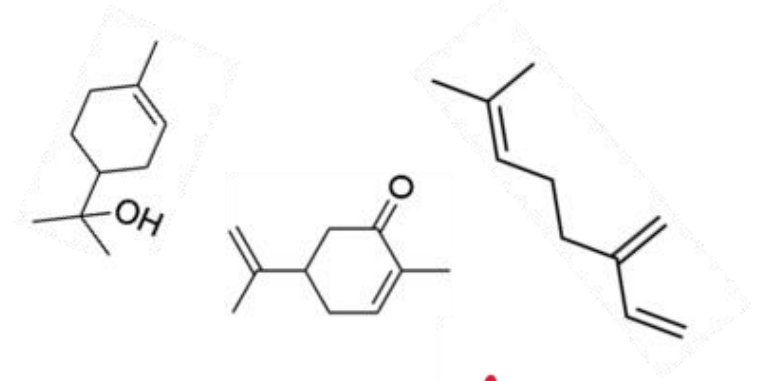
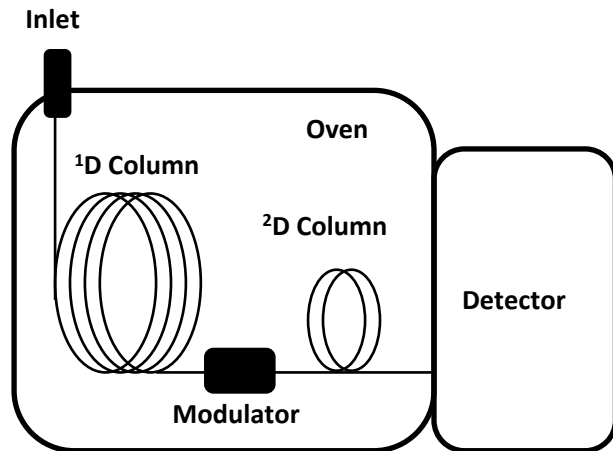
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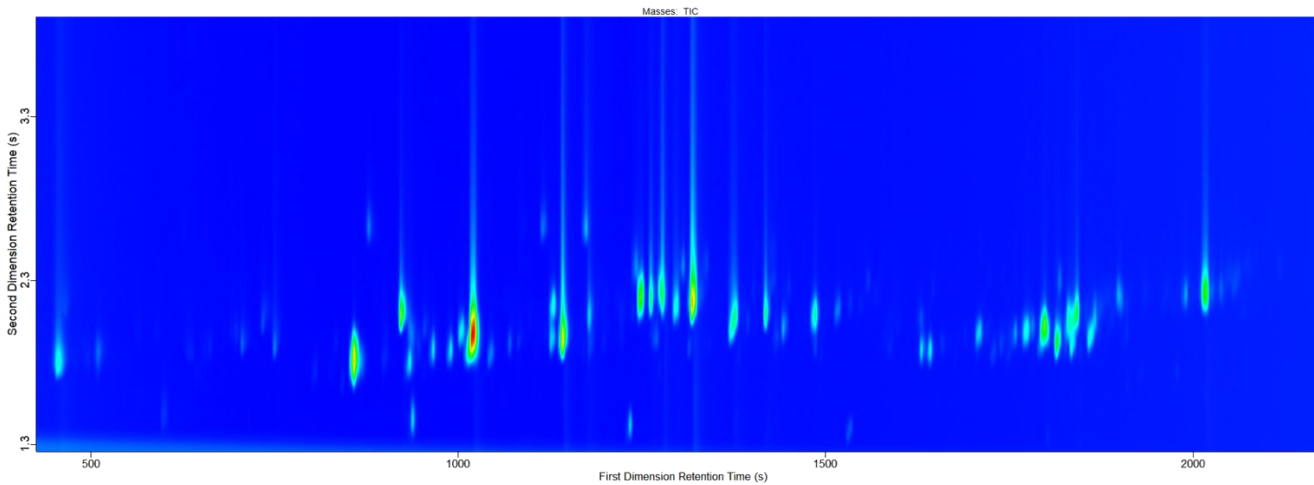
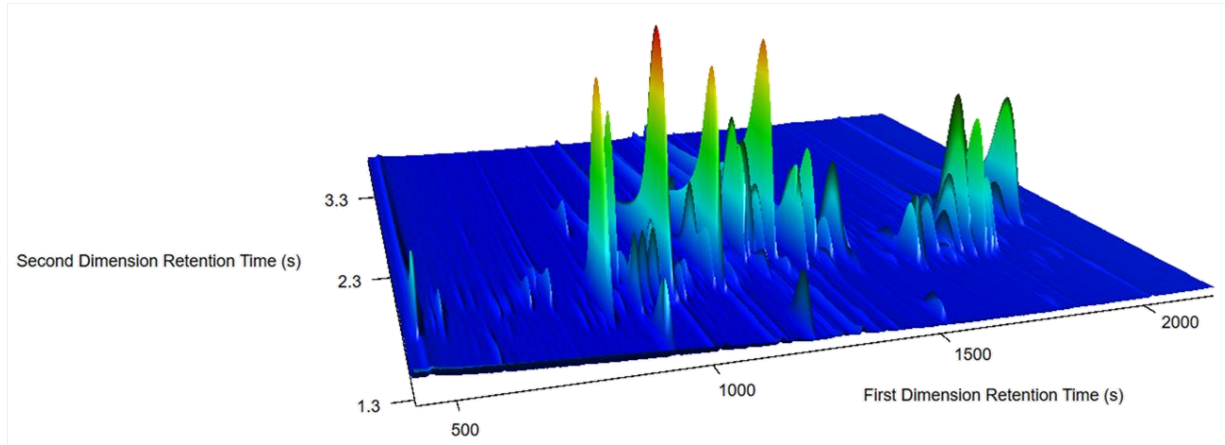
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Comprehensive Two-Dimensional Gas Chromatography (GC×GC)





Challenges in Data Analysis

- Resolving of complex co-elutions
- Increase in number of features
- Increase in compound classes
- Can compare subtle differences between samples
- Abundance no longer dictates importance

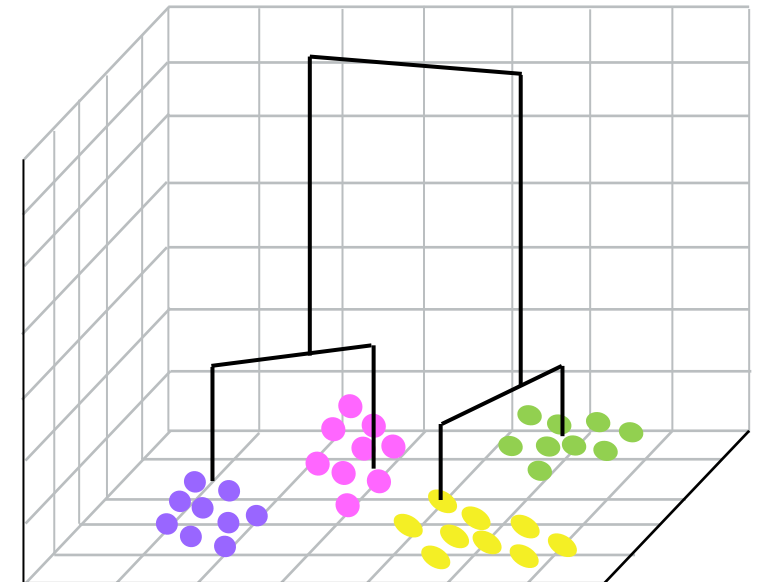
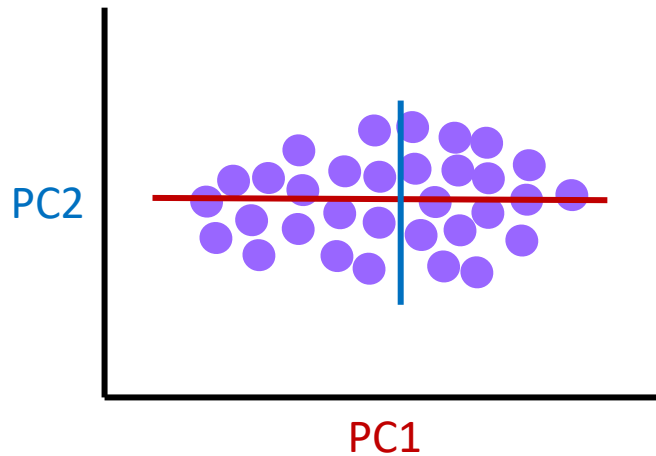
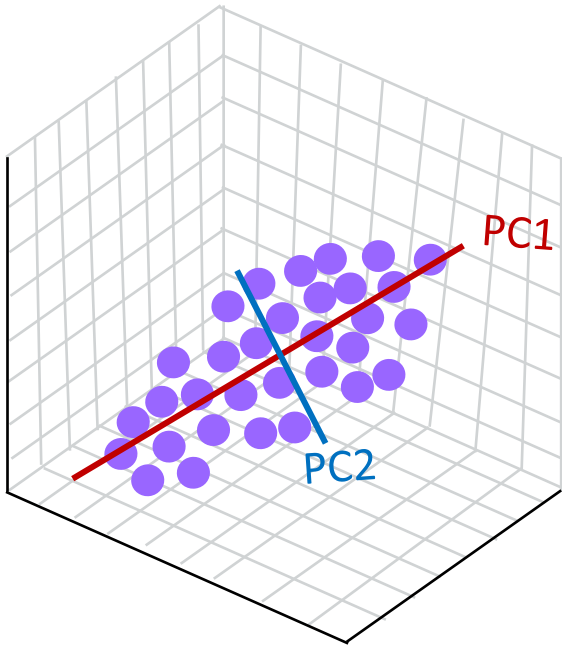
ChromaTOF	ChromaTOF Sync2D	R Statistical Software
Individual samples or quantitative/targeted datasets	Peak detection & deconvolution for developing an aligned peak table	Visualize multivariate data via complex statistical processing
Initial data processing	Generates a peak table for an entire data set	Software packages available for ease of use
Peak detection and deconvolution	Intended for identifying trends across a dataset	Customizable to meet the needs of individual experiments
Peak table compilation		

Dimensionality Reduction

Principal Component
Analysis (PCA)

Principal Coordinate
Analysis (PCoA)

Hierarchical Cluster
Analysis (HCA)



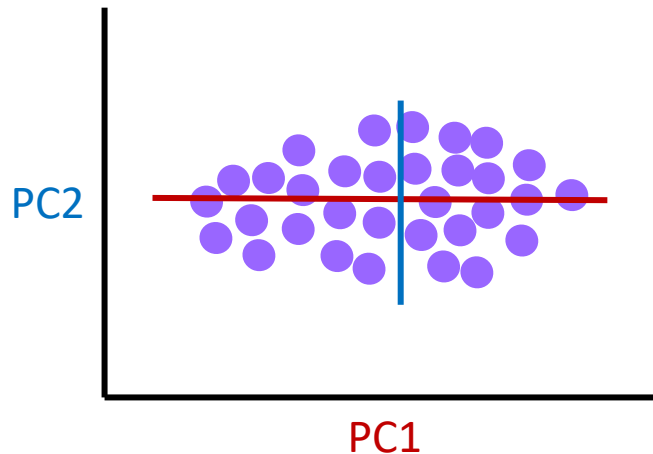
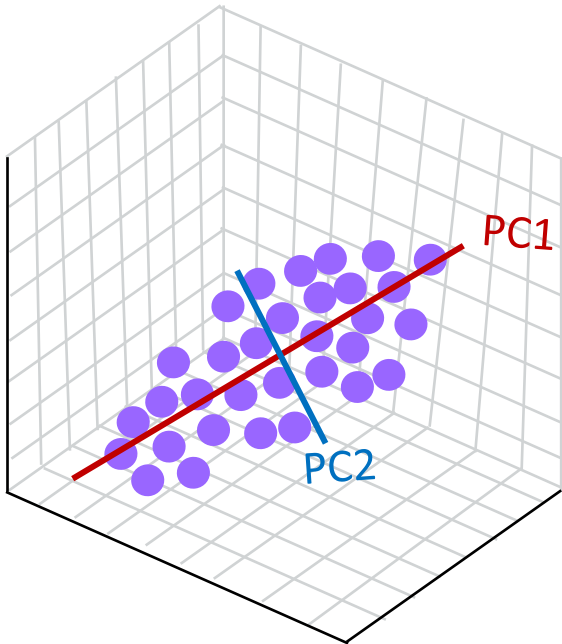
Dimensionality Reduction

Principal Component
Analysis (PCA)

Principal Coordinate
Analysis (PCoA)

Dissimilarity Matrix

PCA – Euclidean
PCoA – non-Euclidean



Basis of Clustering

PCA – shared analytes
PCoA – overall dissimilarity

Interpretation

PCA – analytes driving variance
PCoA – similarities/dissimilarities
in composition

Dimensionality Reduction

Principal Component
Analysis (PCA)

Dissimilarity Matrix
Euclidean or non-Euclidean

Principal Coordinate
Analysis (PCoA)

**Hierarchical Cluster
Analysis (HCA)**

Basis of Clustering

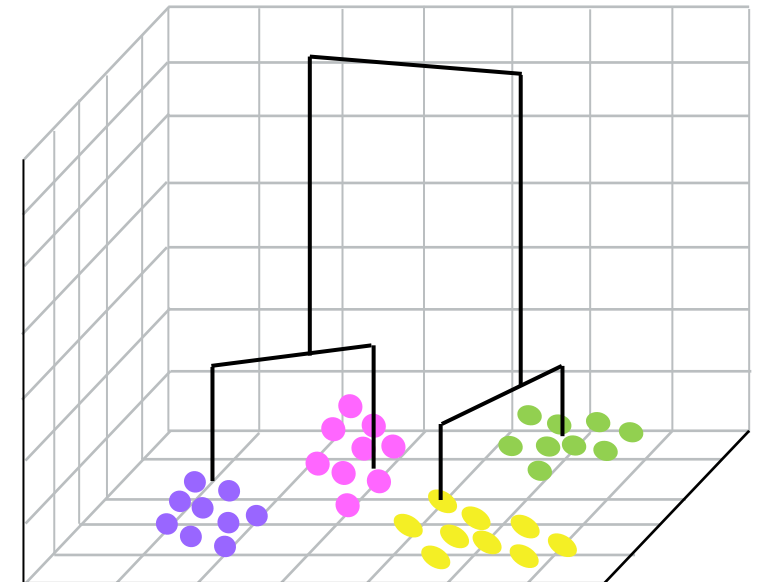
Presence, absence, and/or relative abundance of analytes

Interpretation

similarities/dissimilarities in composition

Shorter branches = more similar samples

Longer branches = more dissimilar samples

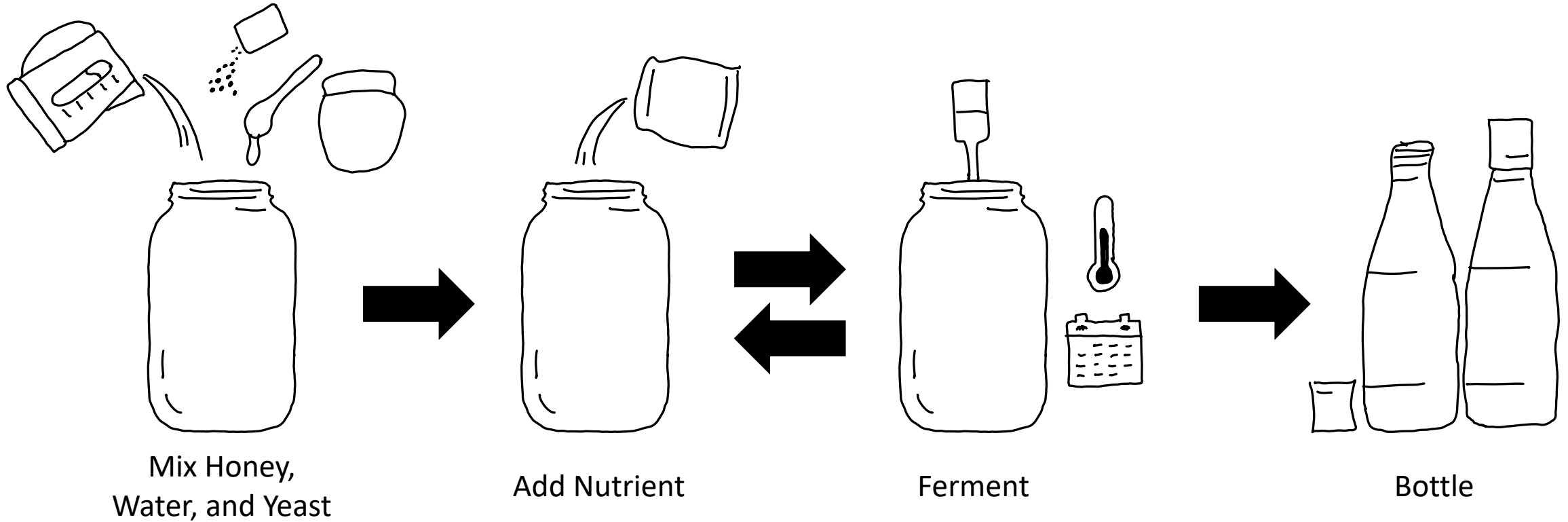


Goals

- Explore the application of GC×GC-TOFMS for the volatile analysis of mead
- Investigate the impact of yeast strains on the final aroma profile
 - Nontargeted data
 - Batch data (large # of samples, usually from different groups or treatments)
 - Extraction and comparison of features and classes to make meaningful conclusions



Mead Production



Products

Five Yeast Strains, 3 Honey Concentrations

Sample ID	Product	Code	Color
1	Kveik Voss 1.5 lbs	KV1M1	
2	Kveik Voss 3 lbs	KV2M2	
3	Kveik Voss 5 lbs	KV3M3	
4	Munich 1.5 lbs	M1M4	
5	Munich 3 lbs	M2M5	
6	Munich 5 lbs	M3M6	
7	EC-1118 1.5 lbs	EC1M7	
8	EC-1118 3 lbs	EC2M8	
9	EC-1118 5 lbs	EC2M9	
10	D47 1.5 lbs	D1M10	
11	D47 3 lbs	D2M11	
12	D47 5 lbs	D3M12	
13	Abbaye 1.5 lbs	A1M13	
14	Abbaye 3 lbs	A2M14	
15	Abbaye 5 lbs	A3M15	
16	Orange Blossom Honey	OBH16	
17	Filtered Water	FW17	

Yeast Strains:

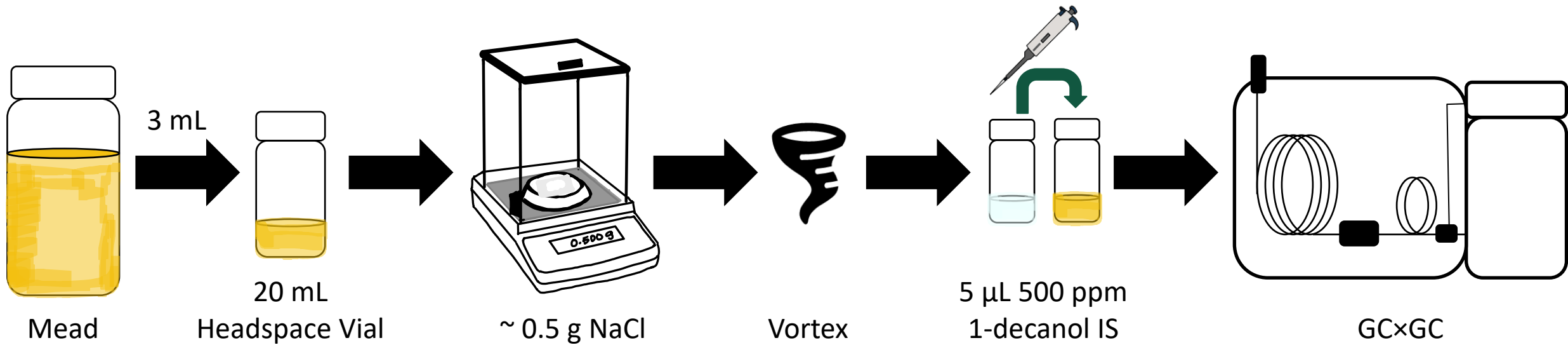
Kveik Voss
Munich
EC-1118
D47
Abbaye

Honey Amount:

1.5 lbs
3 lbs
5 lbs

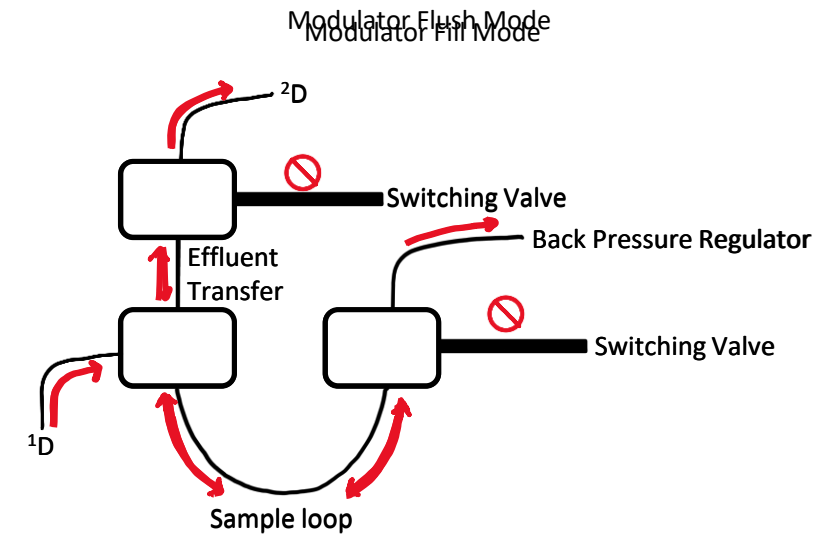
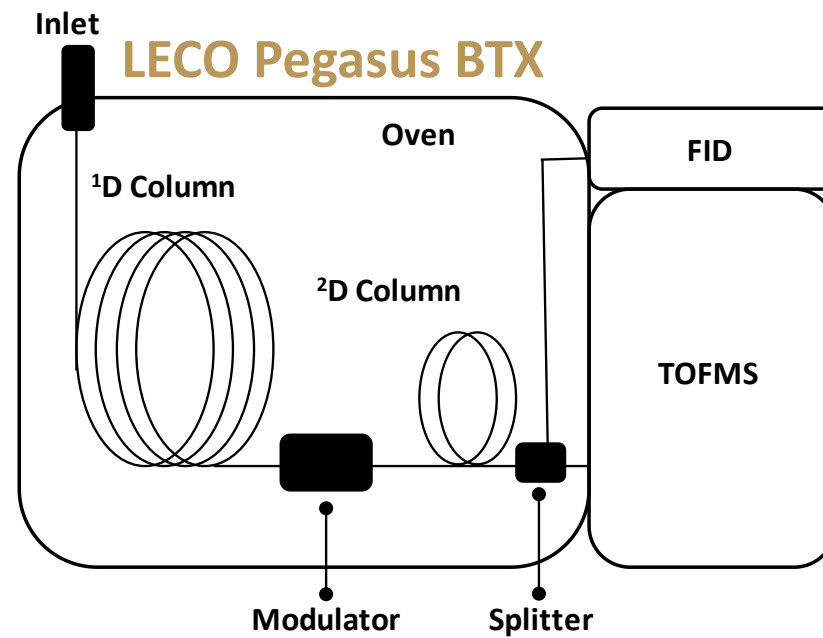
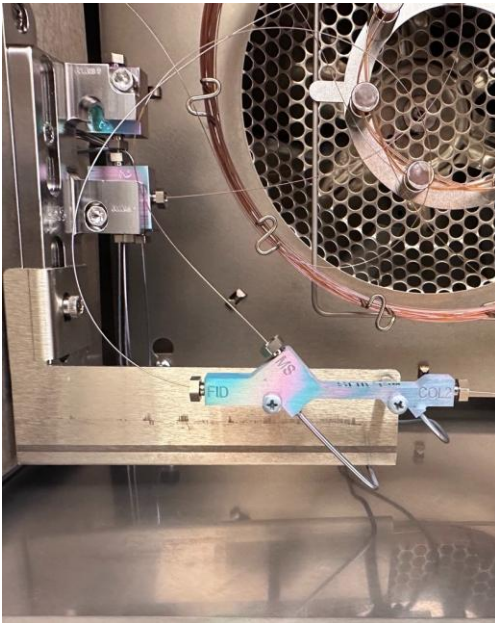


Experimental Design

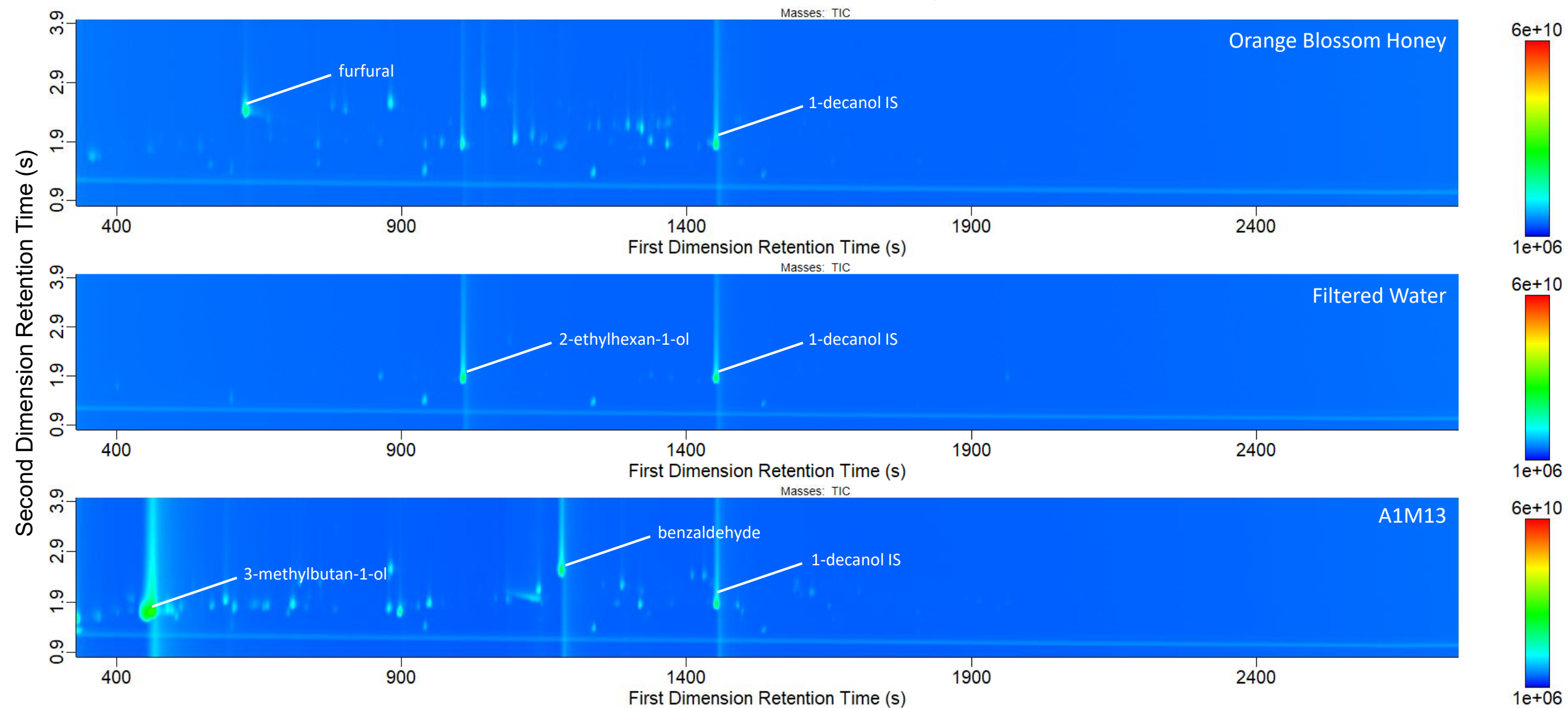


GC×GC-TOFMS

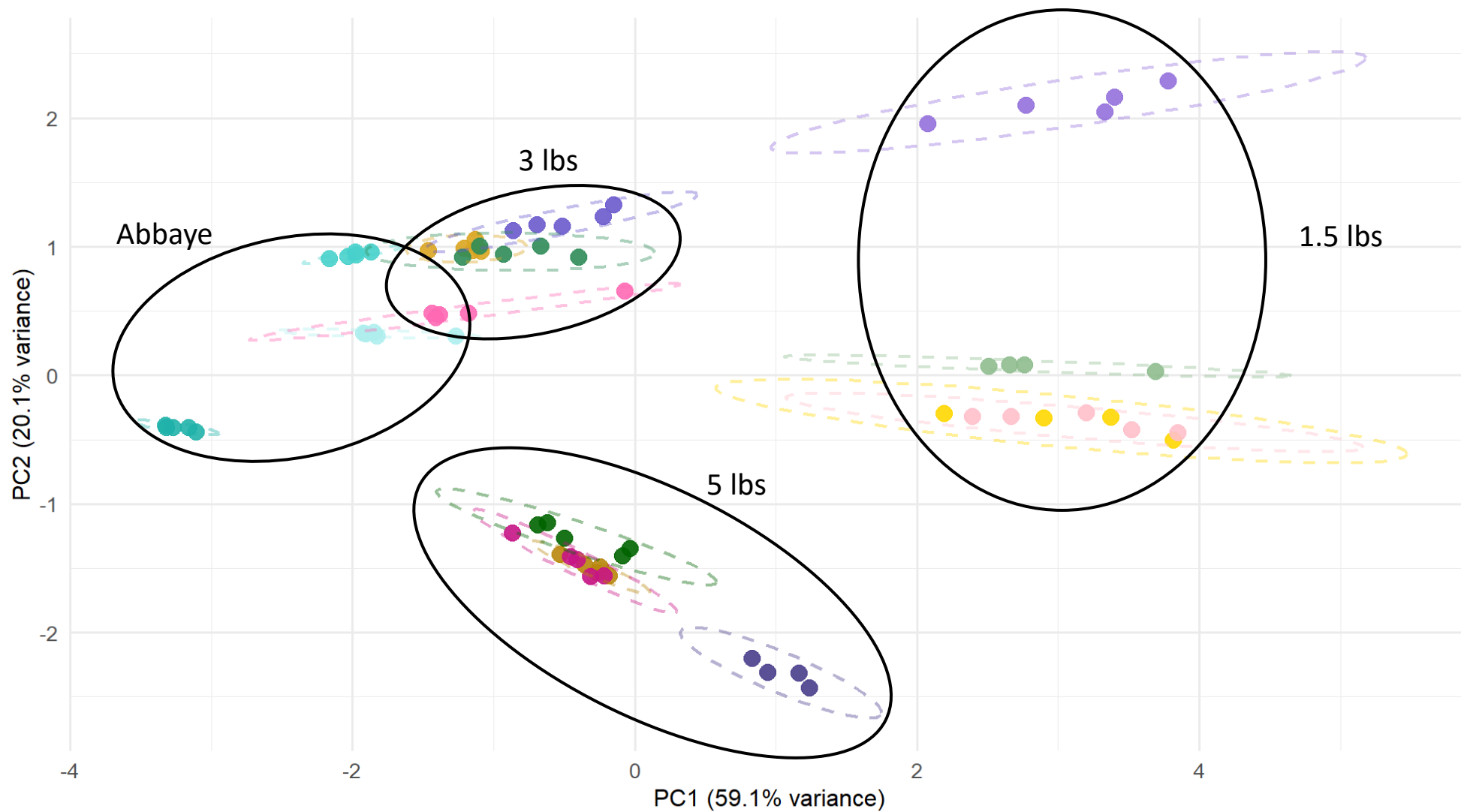
Paradigm Shift™ Reverse Fill-Flush (RFF) Flow Modulator



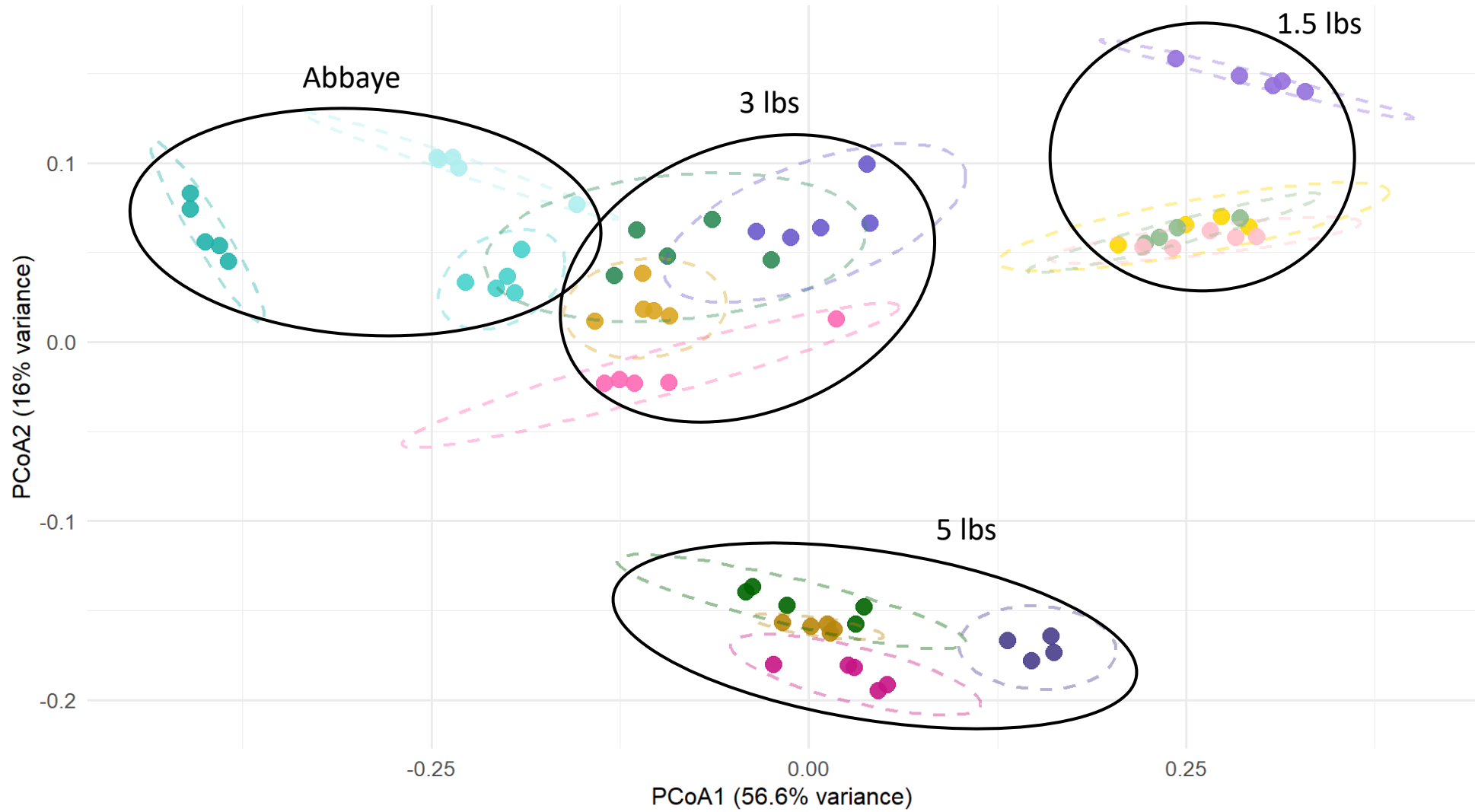
ChromaTOF Comparison



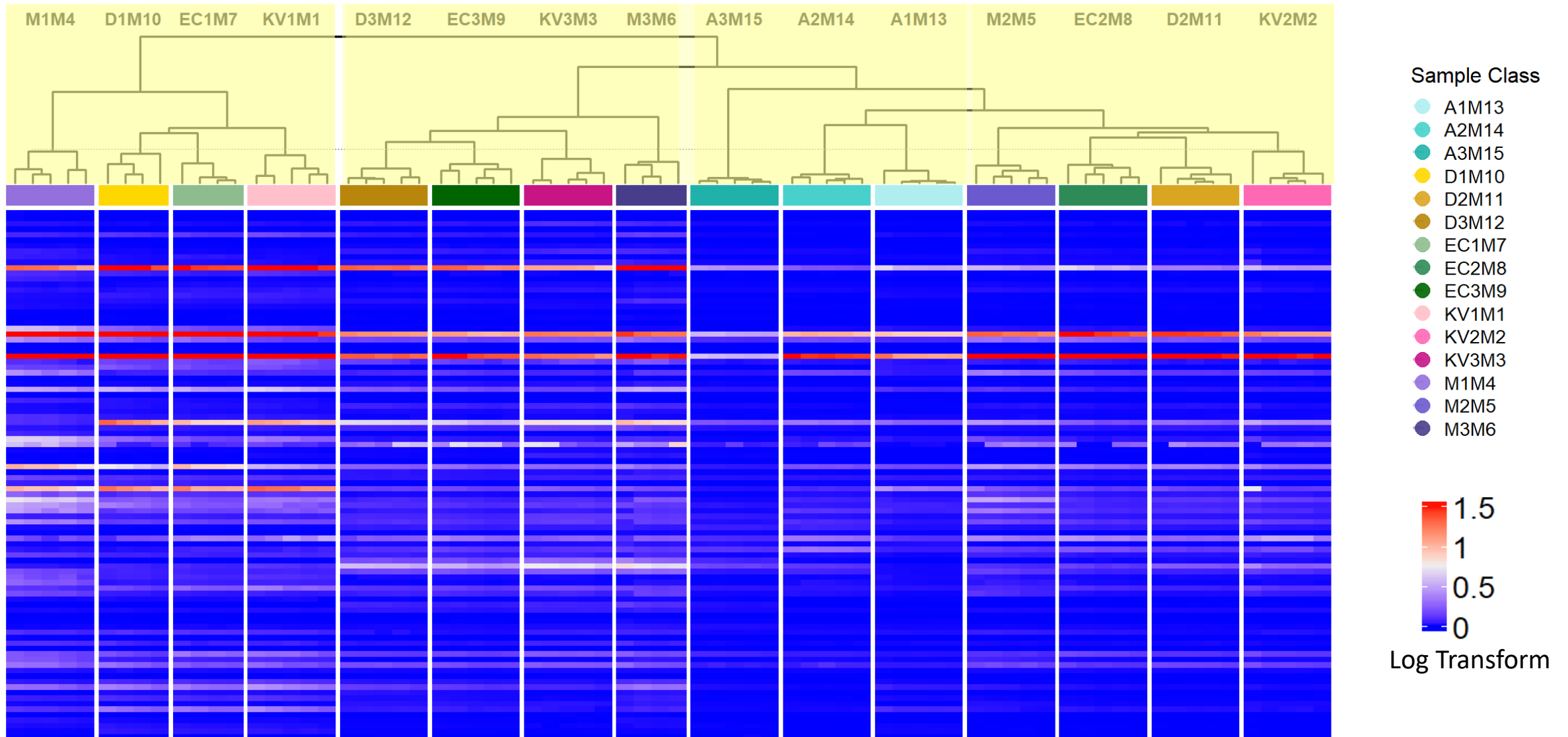
PCA Results



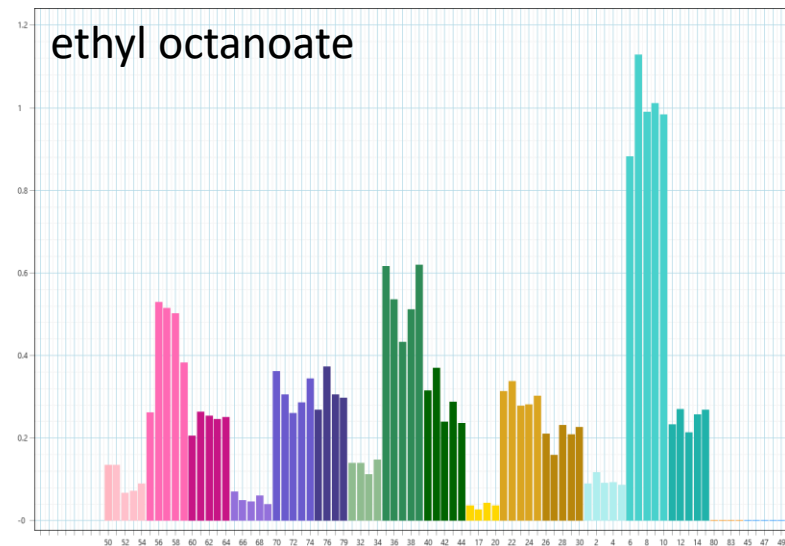
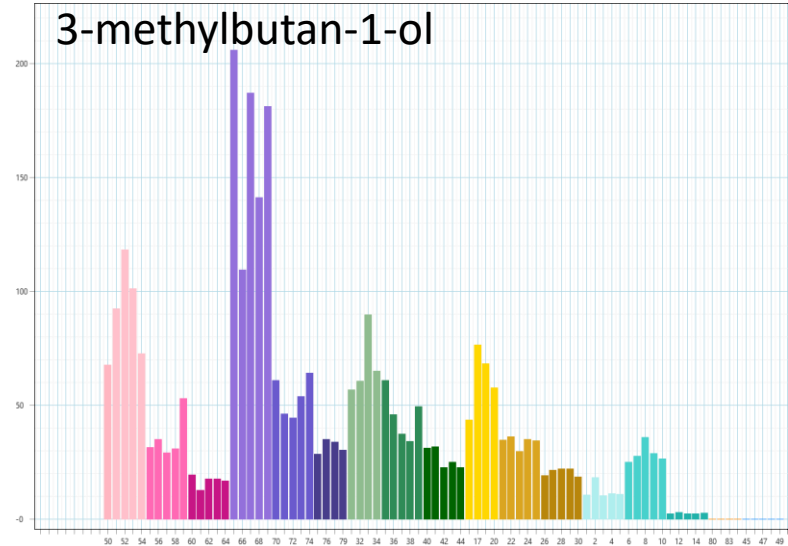
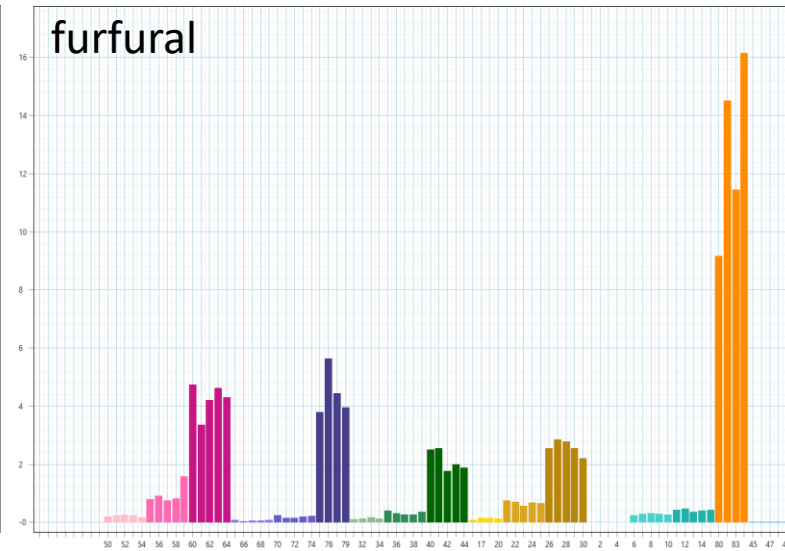
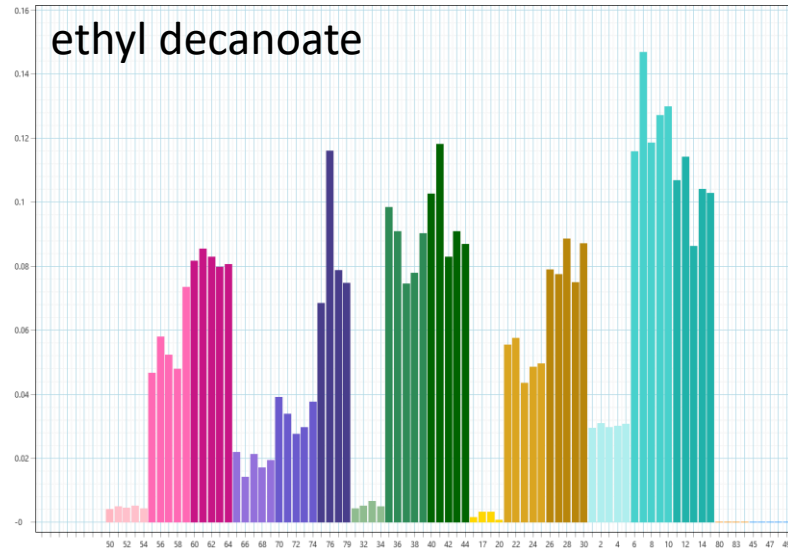
PCoA Results



HCA Results



VOC Patterns



Concluding Thoughts

- GC×GC-TOFMS was an effective strategy in the analysis of mead products
- Dimensionality reduction techniques can help highlight relationships between different sample classes
- More research is needed to explore the connection between microorganism kinetics and the volatile metabolites they produce

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