



Molecular Biomarkers of Wines Contaminated by Wildfire Smoke

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Background

Wildfires have increasingly threatened wine production in the Western U.S. and other fire-prone wine-growing regions. Grapevines exposed to wildfire smoke absorb and metabolize smoke-related volatile compounds. These volatiles bind to sugars in grape berries, forming glycosidic-bound compounds. They introduce a flavor profile often compared to ashtrays or cigar butts—not at all like the toasty, smoky notes associated with oak-aged wines. Wines can be treated to remove free volatiles prior to aging, but bound volatiles continue to be released in extended storage producing harsh, acrid aromas and flavors.

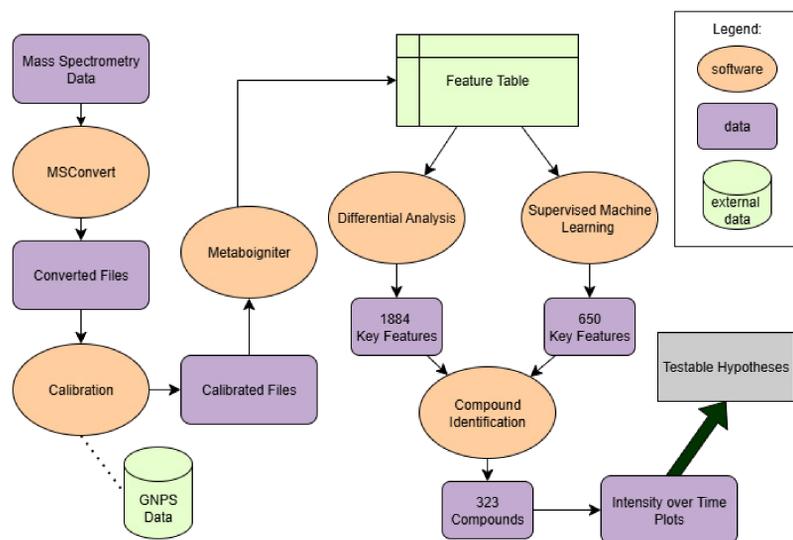
Research Objectives

1. Identify biomarkers indicative of smoke taint in wine before it is placed in long-term storage that will continue to release smoke taint in the wine.
2. Use metabolomic profiling of smoke-exposed wine to explore which volatiles are released during storage and what metabolic processes are altered by smoke taint



(Photo Credit: Eric Risberg)

Workflow



Methods

Sample Preparation

- Cabernet Sauvignon samples from 2019 wildfire-exposed & control vineyards
- Treated with hydrochloric acid at 80°C for up to 4 hours to rapidly simulate long-term storage
- Collected at 6 timepoints: 30, 60, 90, 120, 180, and 240 minutes



Photo credit: Palle/ZUMA Wire/REX/Shutterstock, The Guardian (2017)

Chemical Analysis

- Ionized and analyzed via LC-QTOF mass spectrometry
- Masses calibrated using known smoke and wine compounds
- MS data processed in Metaboigniter, outputting a feature table with:
- Sample, m/z, retention time, intensity, quality

Feature Selection

- Differential analysis
 - Aggregated feature intensities by mean per time point
 - Compared treated vs. control using T-tests for normal distribution and PCA to assess batch effects
 - Identified 1884 significant features, annotated with fold change, p-value, and adjusted p-value
- Supervised machine learning
 - Supervised ML model using 80/20 train-test split
 - 650 features selected via Boruta importance ranking

Feature identification

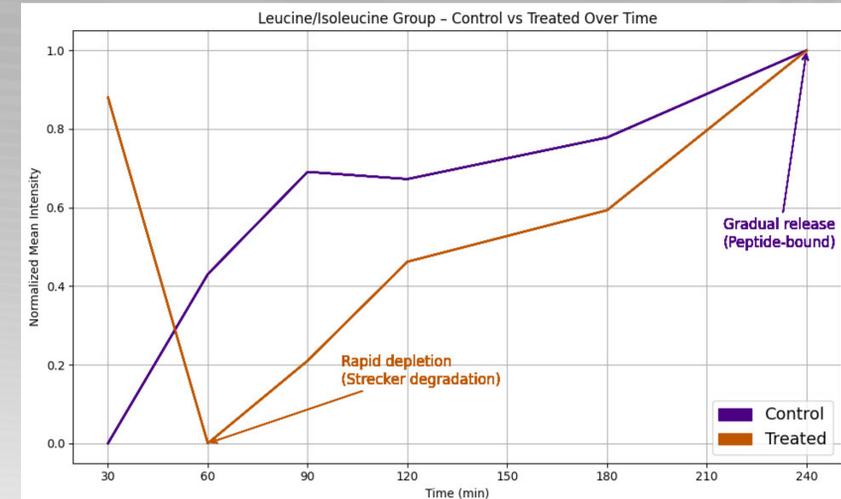
- Features were matched using the smoke taint and known wine metabolite lists
 - Differential: 392/1884 matched
 - Random Forest: 141/650 matched
 - 323 features were shared across both methods

Visualization

- 28 compound groups created based on chemical similarity
- For each compound:
 - Intensity plotted over time across treatment groups
 - Color-coded by control vs. smoke exposure
- Highlighted features with distinct time-based trends and treatment-specific behavior

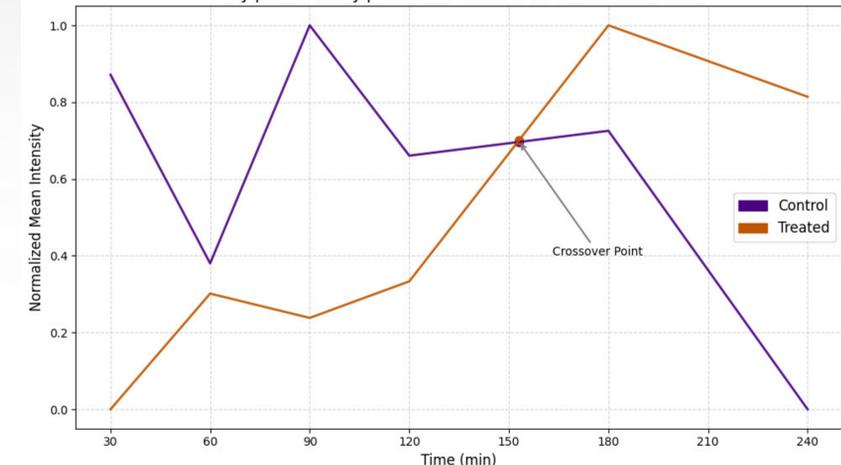
Results

Identifying Biomarkers of Smoke Taint



- Leucine and isoleucine are both amino acids and serve as precursors to Strecker aldehydes, volatile compounds linked to harsh, ashy off-aromas
- Their rapid depletion in treated samples suggest altered metabolism in smoked wines and may act as early biomarkers of smoke taint

Ethylphenol Acetylpenoside - Control vs Treated Over Time



- Ethylphenol acetylpenoside decreases over time in control samples, but increases in smoked samples
- The increase indicates ongoing release of volatile phenols, responsible for the 'barnyard' and 'medicinal' flavors of tainted wine

Data Driven Hypotheses

Amino Acid Pools: In leucines, smoke-treated wines begin with higher free levels, implying protein degradation or preexisting metabolic stress

Hypothesis: Smoke exposure accelerates peptide degradation or disrupts amino acid regulation in grapes

Delayed Release of Polyphenols: Compounds like resveratrol, syringol, and rutin release later in smoked samples, indicating stronger glycosidic bonding

Hypothesis: Smoke changes glycosylation or storage of phenolic compounds in grape tissue

Conclusion

This study identifies potential biomarkers of smoke taint in wine and reveals metabolic processes altered by smoke exposure, providing a data-driven foundation for generating testable hypotheses to better understand and mitigate smoke-induced changes in wine chemistry.

References

- GNPS: Global Natural Products Social Molecular Networking (Wang et al., 2016)
 ScienceDirect. Strecker degradation. Retrieved July 28, 2025, from <https://www.sciencedirect.com/topics/chemistry/strecker-degradation>