Flavor and Aroma of a Modern IPA:
Correlations Between Sensory and Chemical Analysis

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Overview

- Project Objectives
- Brewing, Sensory and Compound Classes
- Chemical Analysis Method – Beer
- Data Sets; Deconvolution and Scaling
- Results
- Discussion / Questions

Project Objectives

- Evaluate untargeted chemical analysis tools for predicting flavor/aroma in beer.
- Test dependence of statistical models on data processing and quantitative vs non-quantitative data.

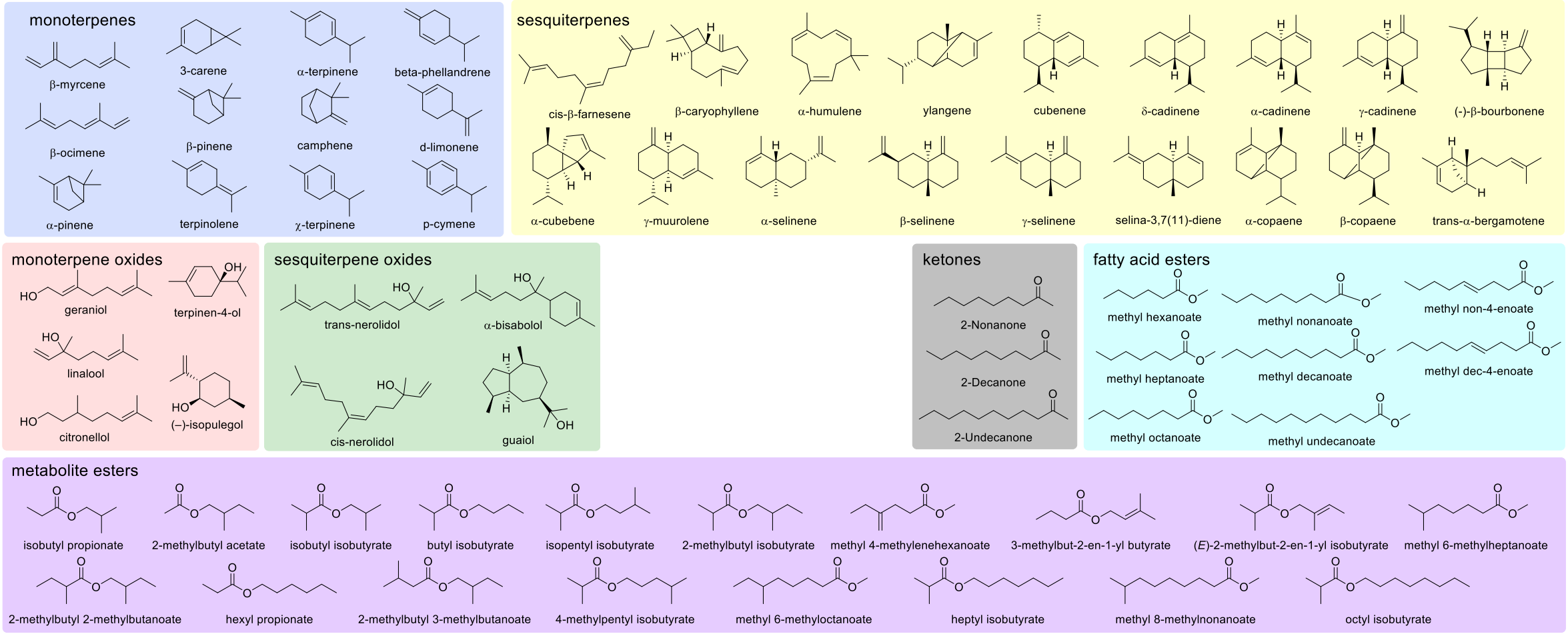
Brewing

- Beers were produced at the John I Haas Nanobrewery.
- 10 single hop beers for the evaluation of experimental HBC hops (2018 CY).
- Same grains, yeast, bittering and dry hop additions with whirlpool additions based on alpha acid content.

Sensory

- Beers were evaluated by the Haas sensory panel
  - 12-attribute Hopsessed lexicon, as well as aromatic impact and hedonic liking (Drexler, 2017).
- Evaluations were performed in duplicate
  - Utilizing quantitative descriptive analysis (QDA) and check-all-that-applies (CATA)
  - QDA sensory data was analyzed by Analysis of Variance (ANOVA) and LS means to normalize results across replicates and sessions.

Compound Classes

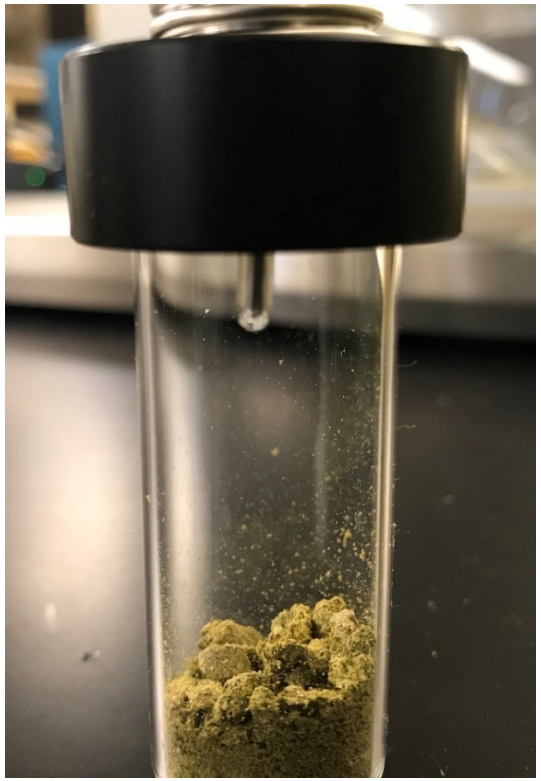


Extraction and Analysis of Beers

Analytical Method

Solid Phase Micro Extraction (SBSE/SPME)

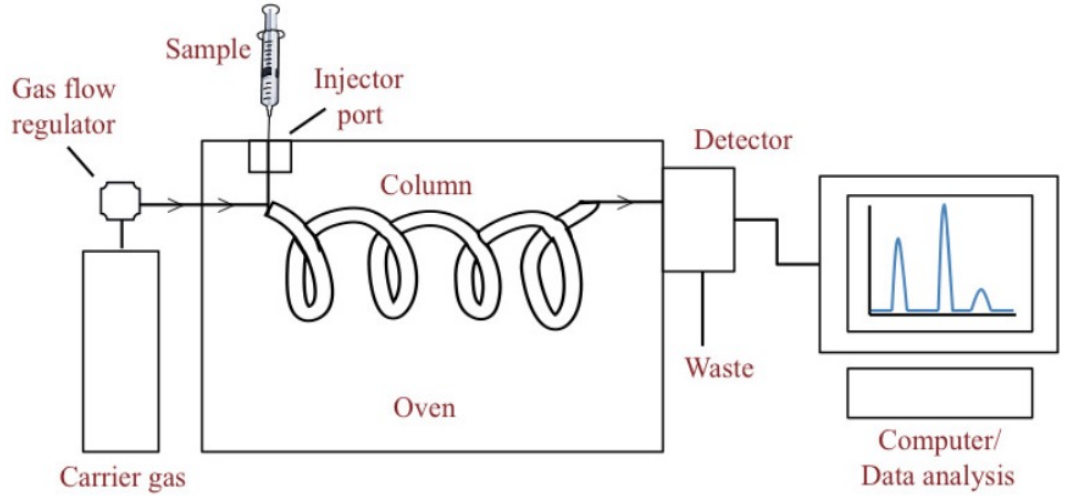
Hops

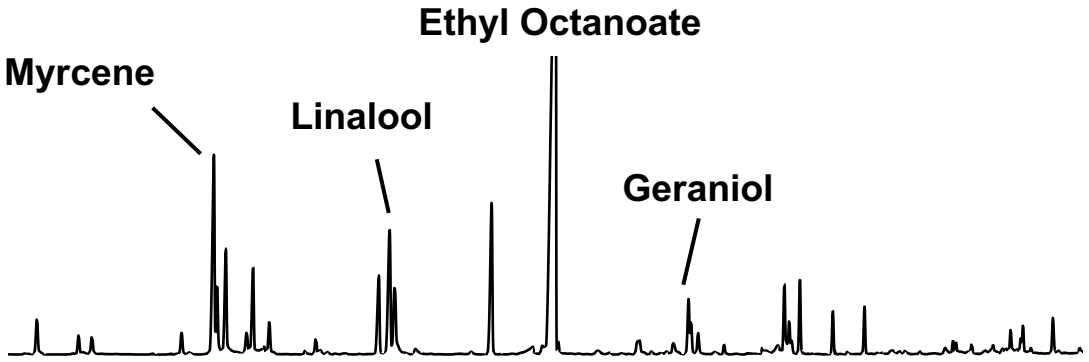


Beer

Analytical Method

Gas Chromatography - Mass Spectrometry





Data and Scaling

Data Sets and Correction Factors

- Data Set 1:
  - Data was minimally deconvoluted
  - Different integration types and parameters were evaluated
  - The Agile integrator from Agilent's Mass Hunter program was used throughout

Data Sets and Correction Factors

- Data Set 2:
  - Deconvolution of peak areas for overlapping retention times was accomplished through extracted ion chromatograms (EICs) and peak area “reconstruction” using NIST mass spectra.

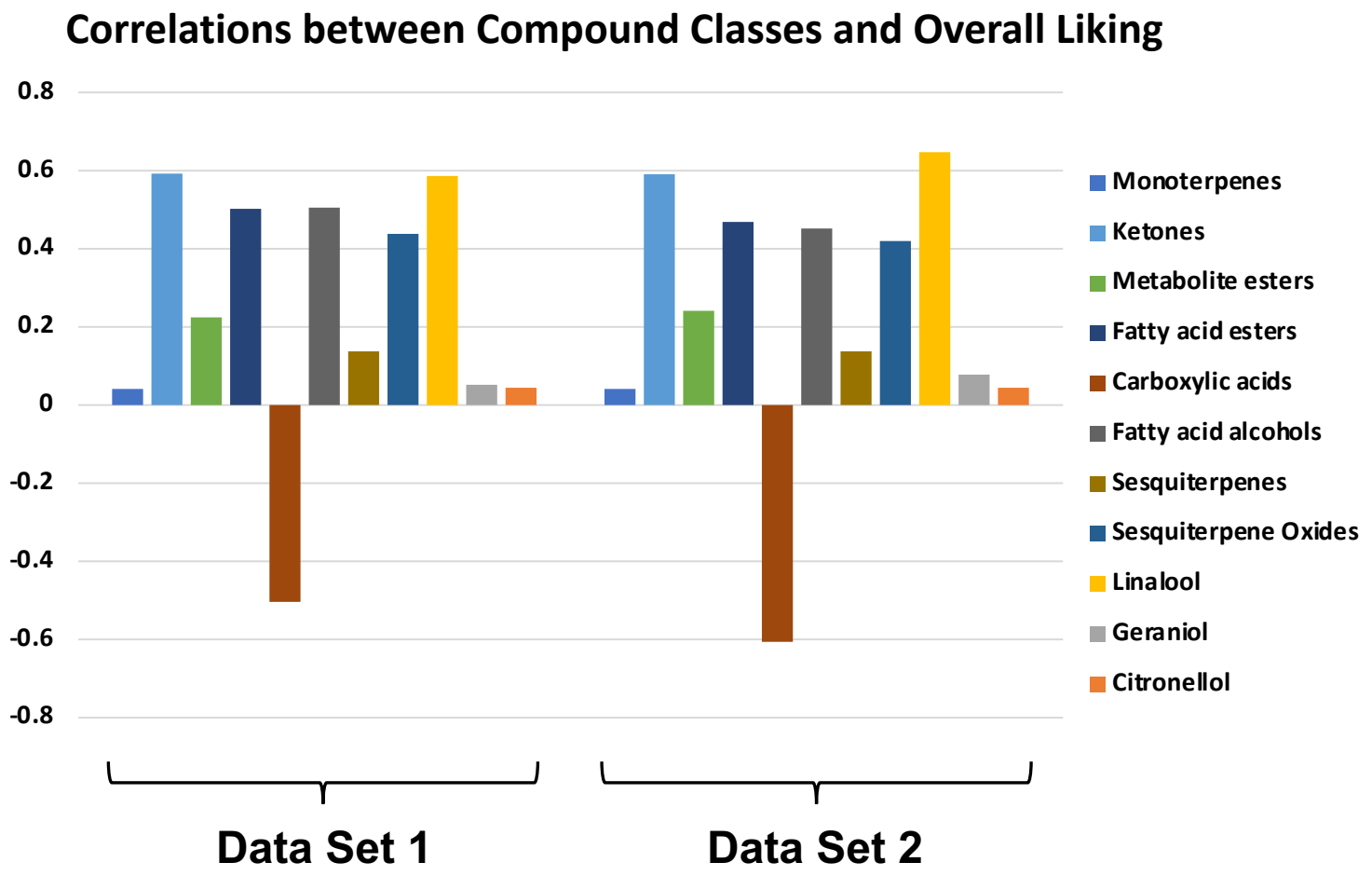
Data Sets and Correction Factors

- Data Set 3:
  - The deconvoluted peak areas were scaled using water/octanol partition coefficients and the Twister Calculator.
  - Additionally, peak areas were normalized by the identified compounds' molecular weight.

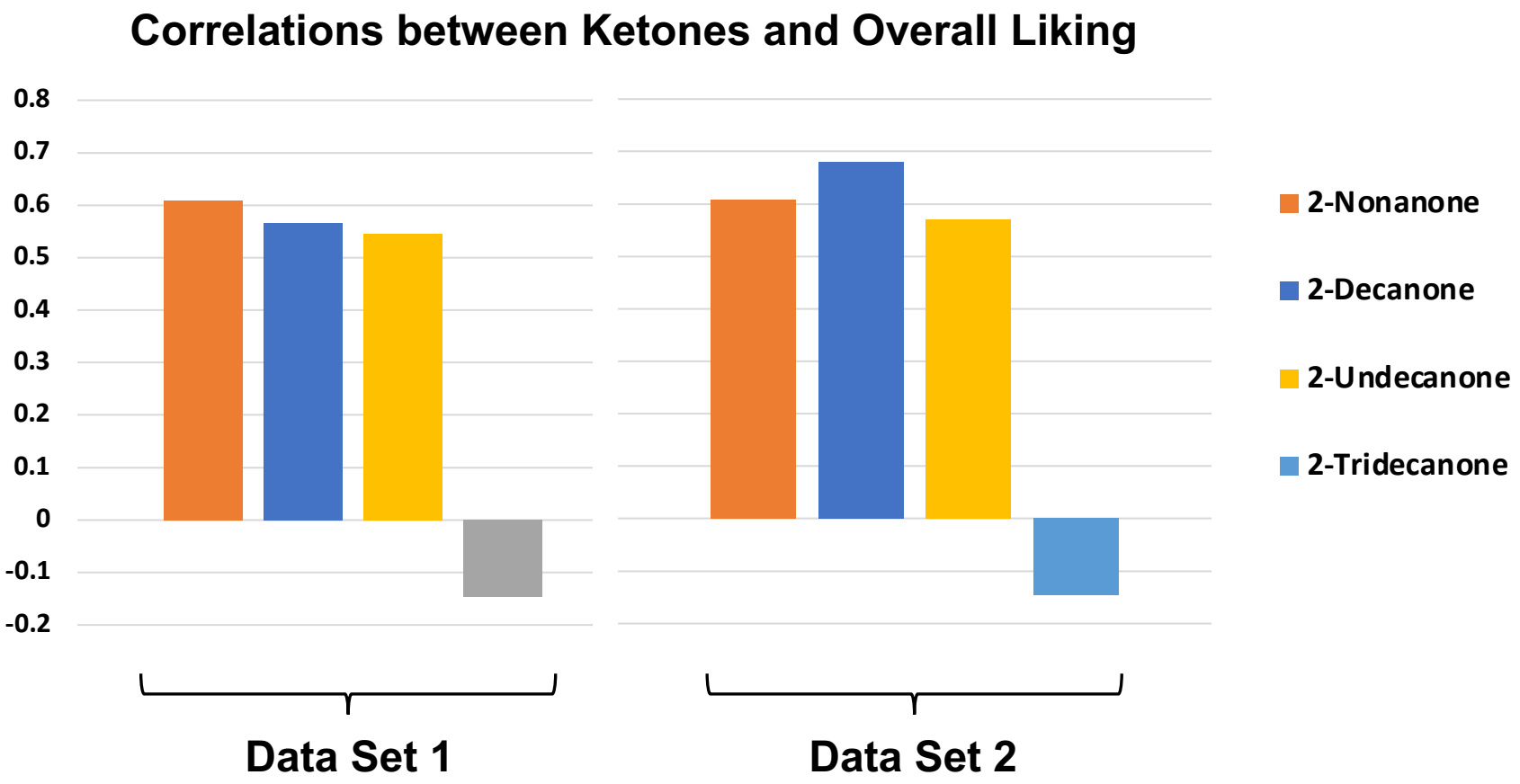
Statistics

- Calculations were performed with JMP 14:
  - Bivariate correlations were tested on compound classes and individual compounds against sensory categories.
  - Partial Least Squares (PLS) models were evaluated against individual sensory categories and groups of categories.

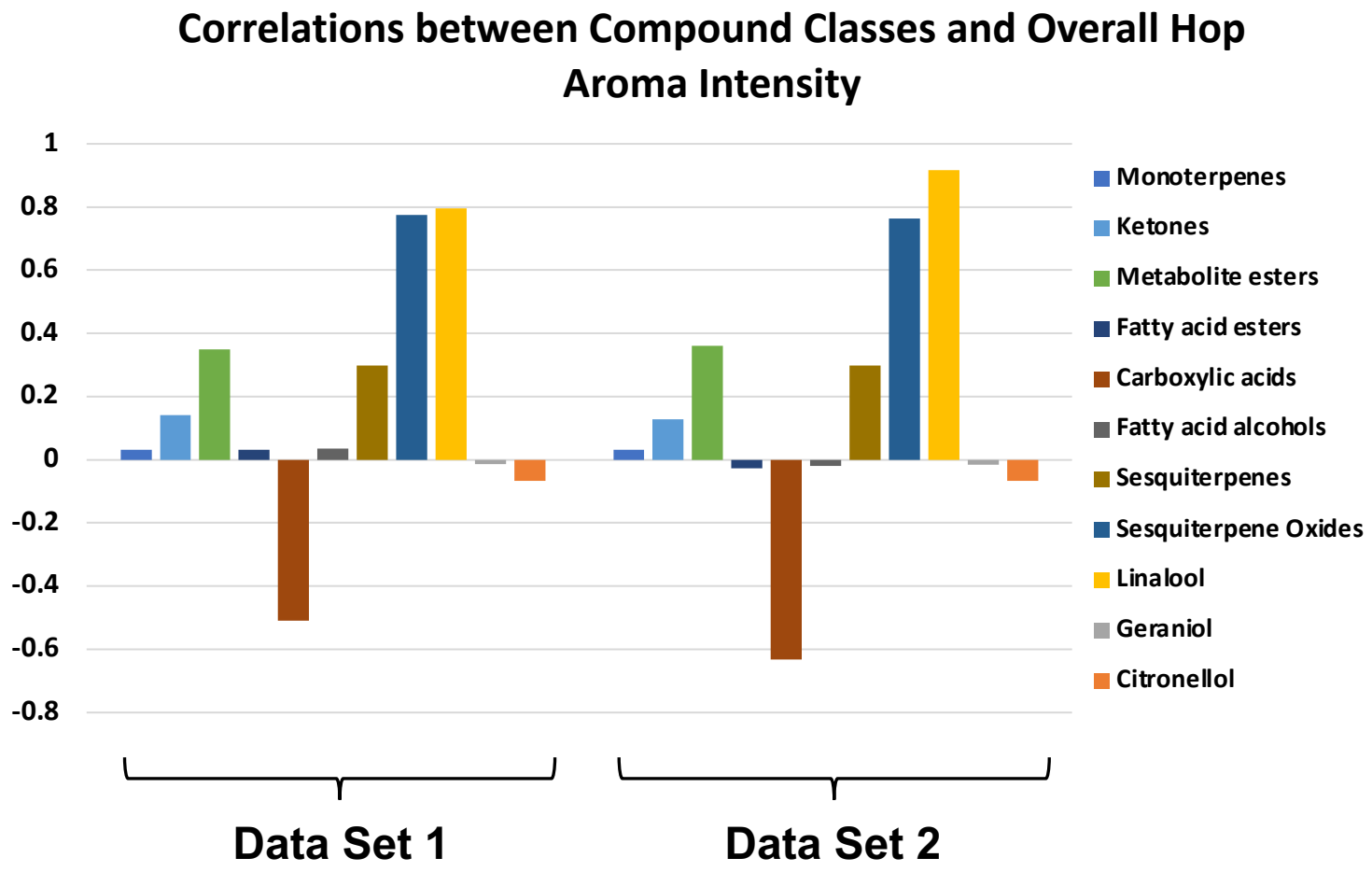
Bi-Variate Correlations with Overall Liking



Bi-Variate Correlations with Overall Liking



Bi-Variate Correlations with Overall Hop Aroma Intensity

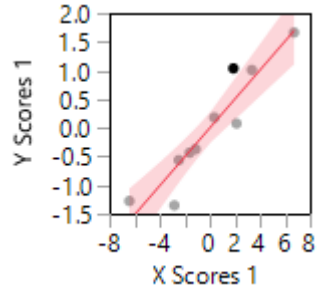


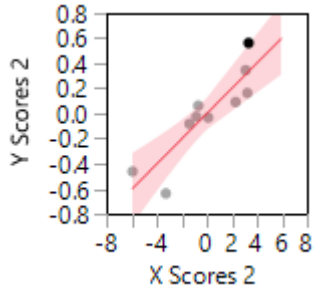
Partial Least Squares (PLS) Modeling

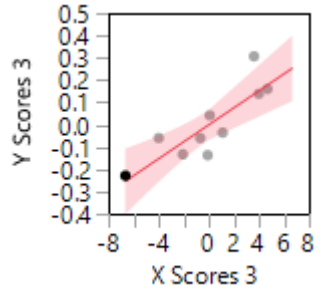
Partial Least Squares Model of Overall Liking

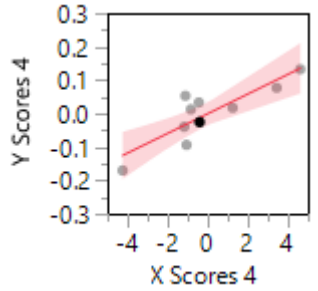
- 70 compounds were used
- Model was minimized with 5 factors
  - 69% of the variation in the 70 components is explained in 5 factors
  - 99.9% of the variation in Overall Liking explained

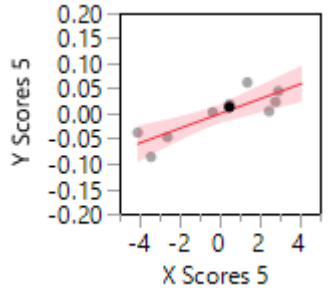
Partial Least Squares Model of Overall Liking

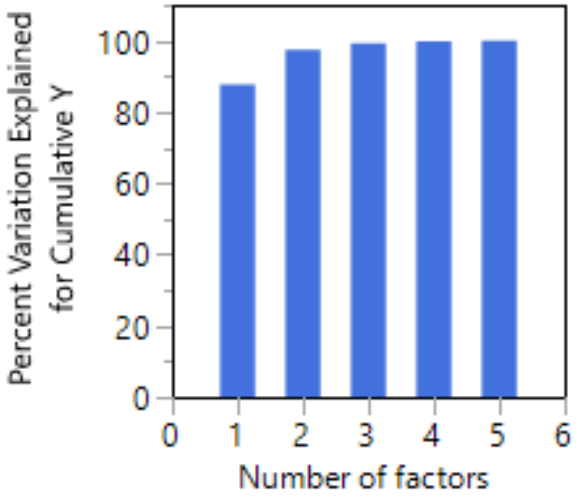


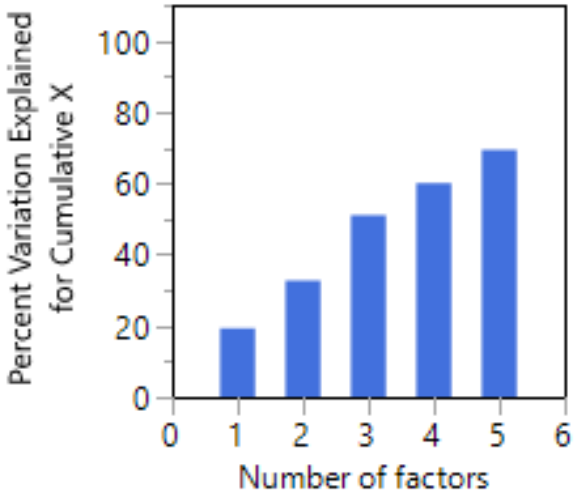




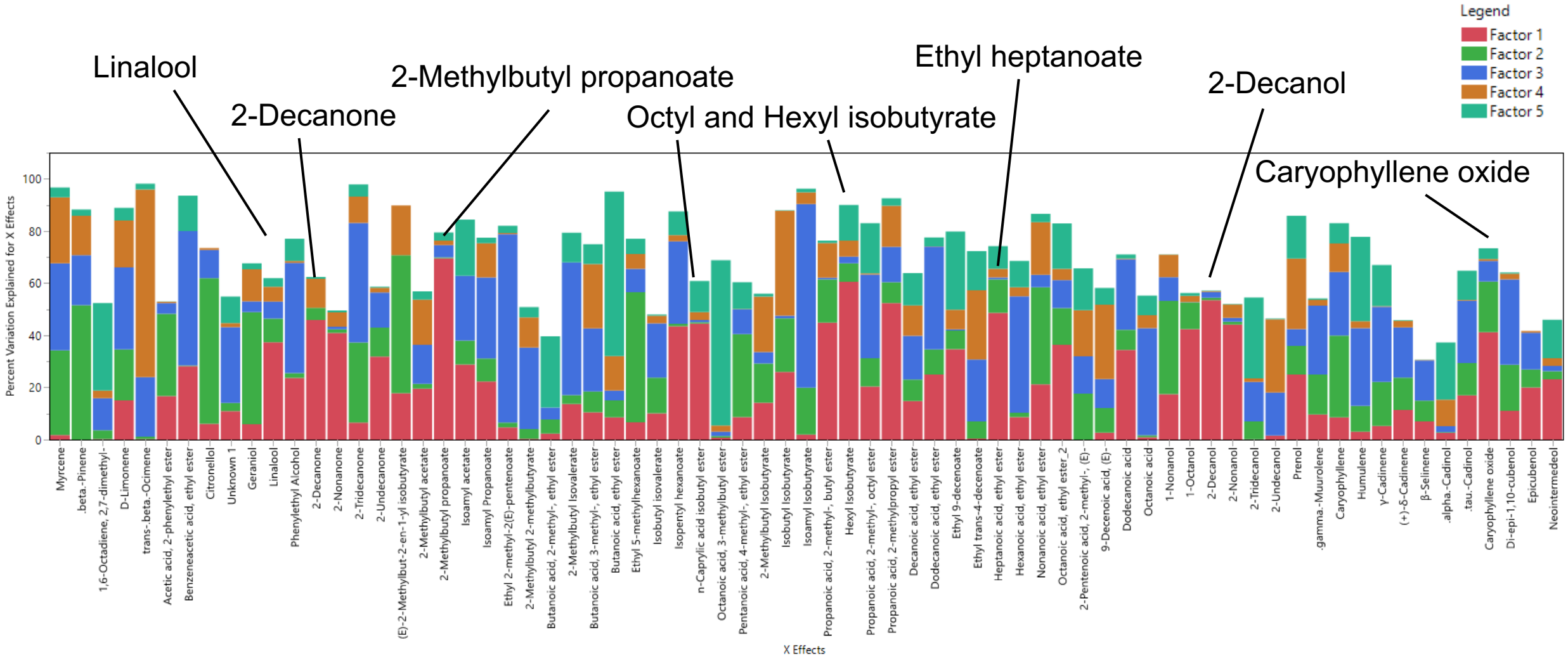




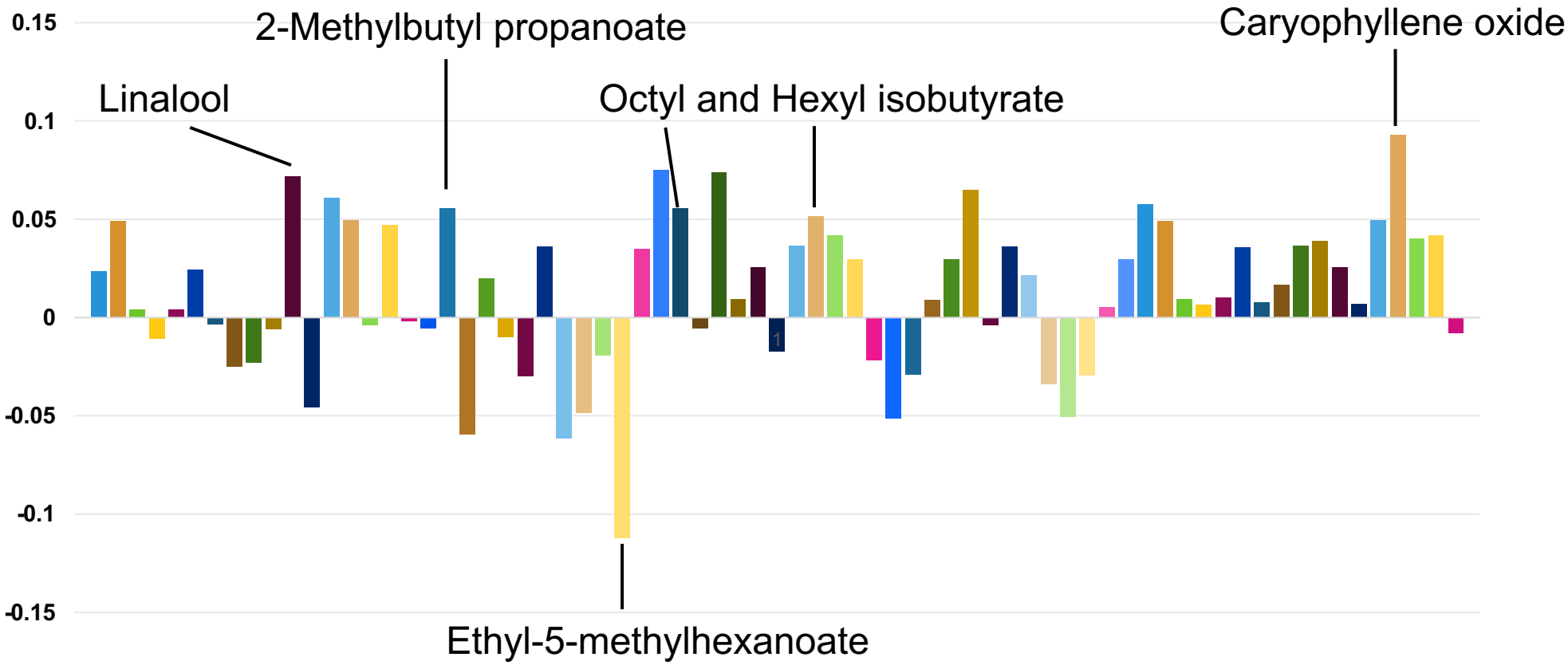




Partial Least Squares: % Variation Explained



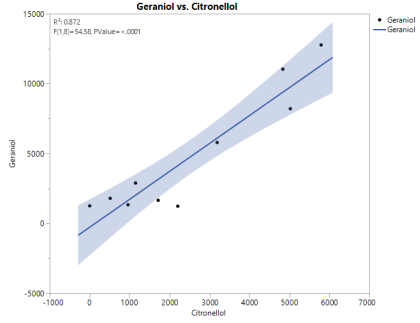
Partial Least Squares: Model Coefficients



Results

- Deconvolution and scaling did not change the qualitative information at the compound class level, but it refined the models and confidence in results.

- Surprisingly good bi-variate correlations observed;
  - Linalool and Sesquiterpene oxides *vs* Hop Aroma Intensity
  - Ketones, Linalool, 2-methylbutyl propanoate *vs* Overall Liking
  - Observed some biotransformation processes
    - Geraniol *vs* Citronellol



Next Steps

- Continue to build out and refine the PLS models
  - Add more single hop beers
- Dosing individual and groups of compounds to confirm direct or indirect correlations with sensory.

Acknowledgements

- Innovations team at John I Haas
- Sensory panel at John I Haas
- Dr. Luke Chadwick

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