Advanced predictive analytical-sensory correlation: Towards a better understanding of the perception of coffee flavor

Baggenstoss, J., Poisson, L., Glabasnia, A., Moser, M., Rytz, A., Thomas, E., Blank, I., Kerler, J.
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The flavor of coffee can be compared to a symphony played by an orchestra.
The flavor of coffee can be compared to a symphony played by an orchestra.
The key impact odorants of coffee were identified with the aroma value approach.

I. Screening of potent odorants with AEDA
II. Identification of potent odorants
III. Quantification and odor-activity values
IV. Sensory comparison of model vs. coffee
V. Omission experiments

>800 volatiles
50 important aroma cpds
23-26 key odorants

Outline and objective of the study

Objectives

- establish predictive model based on quantitative analysis of flavor compounds
- identify well correlated marker compounds for sensory descriptors
- take a step forward in the understanding of analytical-sensory correlation
54 aroma and taste compounds were analyzed for the present study.

<table>
<thead>
<tr>
<th></th>
<th>substance</th>
<th>flavor quality</th>
<th></th>
<th>substance</th>
<th>flavor quality</th>
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<tbody>
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<td>methanethiol</td>
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<td>2-acetylthiazole</td>
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<td>2</td>
<td>dimethyl sulfide</td>
<td>cabbage, sulfur</td>
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<td>furfural</td>
<td>grass, almond</td>
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<td>cyclo-Val-Pro</td>
<td>bitter</td>
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<td>cyclo-Phe-Pro</td>
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<td>2-acetylpyridine</td>
<td>popcorn</td>
<td>54</td>
<td>caffeine</td>
<td>bitter</td>
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</tbody>
</table>
Absolute in-cup quantification was carried out with different methods

**Quantitative analysis of**

- 42 aroma compounds (quantification with isotope dilution assay)
  a. SPME-GC-MS
  b. SPME-GCxGC-TOF MS
  c. SPE-GC-MS

- 12 taste compounds (external quantification)
  a. HPLC-DAD
  b. LC-MS/MS
Comprehensive GCxGC-TOF MS is the emerging technique in coffee aroma analysis.

Analysis of methional

Methional peak hidden behind other peaks

Resolved by deconvolution and 2-dimensional techniques
Sensory profiling was carried out with an expert panel (n=12)

The basic attributes...
- roasty
- bitter
- acid

...describe the basic properties of an Espresso coffee

The 'subtle' aroma descriptors...
- fruity-floral
  red fruits, lemon, jasmine
- green-vegetal
  herbs, fresh vegetables
- dry-vegetal
  wood, malt, cereal
- vegetal-humus
  earthy, mushroom
- cacao
  roasted, cacao, dark chocolate
- sweet
  vanilla, caramel, honey

...describe the signature aroma of an Espresso coffee

...are grouped based on olfactory similarity
Based on the sensory data, a PCA plot is established and defines the sensory space of the Nespresso coffees.

- PCA performed on the sensory attributes
- The variables “Intensity” (computed on the analytical data) and “CTn” are projected
- Coffees are mainly separated by intensity / dilution
Based on the sensory data, a PCA plot is established and defines the sensory space of the Nespresso coffees.

- Flavor compounds are inter-correlated and correlated to intensity.
- The intensity should be subtracted from this representation.

Flavor compounds include:
- Green-vegetal
- Fruity-flowery
- Sweet
- Roasty
- Bitter
- Cocoa
- Dry-vegetal
- Vegetal-humus
The sensory and analytical datasets need to be transformed and standardized for correlation.

Fechner’s law: perception \( \sim k \log (\text{concentration}) \)

**Sensory data**
- Normalize

**Instrumental Data**
- Subtract (instrumental) intensity
- Take logarithm
- Normalize

**Correlation of the two datasets**
\[ X'' = Y'' + P \]

C. Lindinger et al., Anal. Chem. 2008
After subtraction of the intensity, a new PCA plot is generated.

- Separation by flavor descriptors (not intensity)
- The more 'subtle' correlations become visible
The projections of flavor compounds on the PCA are now well spread on the sensory space.

- The analytical data is projected on the PCA.
- Correlated arrows are close to each other.
- The longer an arrow, the better its representation in the sensory space.
Around 30 compounds exhibit strong correlation to the sensory descriptors:

- **Sweet**: fufuryl acetate, phenylacetaldehyde
- **Roasty**: 3-methyl-2-butene-thiol, N-methylpyrrole
- **Dry**: furaneol
- **Vegetal**: acetaldehyde, methanethiol, 2,3-butanedione, 2,3-pentanedione, dimethyl sulfide, sotolon, furaneol, methional, furfural, 2-methylbutanal
- **Acid**: vanilline, 2-acetylthiazole, hexanal, 2-isobutyl-3-methoxypyrazine, 2-methylpropanal
- **Cocoa**: 2,3,5-trimethylpyrazine, 2-furfurylthiol
- **Bitter**: 2-acetylpyridine, pyridine, furfuryl thiol, N-methylpyrrole, 2-isopropyl-3-methoxy-pyrazine, 2-methyl-3-furathiol
- **Fruity-Flowery**: 2,3-methylpyrazine, ethylguaiacol, guaiacol, vinylguaiacol, dimethyl trisulfide, 2,3,5-trimethylpyrazine, 2-furfurylthiol
- **Vegetal-Humus**: p-cresol, 4-ethylguaiacol, guaiacol, 4-vinylguaiacol, dimethyl trisulfide, 2,3-diethyl-5-methylpyrazine
- **Green-Vegetal**: 2,3-butanedione, 2,3-pentanedione, dimethyl sulfide, sotolon, furaneol, methional, furfural, 2-methylbutanal
- **Acid**: vanilline, 2-acetylthiazole, hexanal, 2-isobutyl-3-methoxypyrazine, 2-methylpropanal

**Notes:**
- **Vegetal**: Green and vegetal notes.
- **Fruity-Flowery**: Fruity and flowery notes.
- **Sweet**: Sweet notes.
- **Roasty**: Roasty notes.
- **Dry**: Dry notes.
- **Vegetal-Humus**: Humus and vegetal notes.
The statistical model gives a good prediction of the sensory profile.
Conclusion

1. Identification of new quality markers with good correlation to sensory descriptors
Conclusion

1. Identification of new quality markers with good correlation to sensory descriptors

2. A step forward to molecular-sensory guided development of coffee blends