Chemical Compounds in Green Coffee and Impact on Quality

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What determines the beverage quality of coffee?

Green bean property may have major impact on beverage quality.

Understand the relationship between green beans and cupping score.
Cherry properties

- Cultivar
- Maturity
- Location of the trees
- Agronomic practice

Green beans quality
Background and Need of the Project

1. No universal standard to assess the quality of coffee green beans in the coffee market

2. Grading criteria for green beans:
   - Number of defective beans
   - Screen size of beans
   - Elevation of the growing areas

4. Factors affecting green bean and cupping quality:
   - Cultivar
   - Environment (soil, temperature, sunlight, rainfall/irrigation, fertilizer etc)
   - Bean maturity

5. Tools to evaluate green beans for cupping quality:
   - Cupping scores by qualified cuppers
   - Limited chemical analysis
Goals of the Collaborative Research

• Develop a new tool to select green beans which produce high quality coffee beverages.

• Understand the relationship between chemical components of green beans and cupping scores.
The strategy

- Green beans: Known cultivars,
  In the same field at HARC Kunia
  Harvested within 2-3 days
  Same processing method

- Chemical Analysis = **Metabolomics**
  Systematic study of metabolites.
  Metabolites are chemical products produced in living organisms
Green beans metabolites determine the beverage quality

Green beans property

Quality of Coffee beverage
What is the key metabolites for quality?

Factors
- Cultivar
- Maturity level
- Growing condition
- Processing

Metabolite property
- Green beans
- Metabolites

Quality
- Flavor & taste
Sample collection at HARC Kunia Field, Oahu, Hawaii
Harvesting and processing coffee cherry

<table>
<thead>
<tr>
<th>9 Cultivars</th>
<th>4 Maturity level</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Catimore 5175-1</td>
<td>Green cherry</td>
</tr>
<tr>
<td>2 Red Catuai</td>
<td>Pink cherry</td>
</tr>
<tr>
<td>3 F1 Hybrid of Catimore and Tall Mokka (5175-1 xMA2-7)</td>
<td>Red cherry</td>
</tr>
<tr>
<td>4 Maragogipe</td>
<td>Dark Red cherry</td>
</tr>
<tr>
<td>5 Tall Mokka MA 2-7</td>
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<tr>
<td>6 SL28</td>
<td></td>
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<tr>
<td>7 Typica</td>
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<td>8 Yellow Bourbon</td>
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<tr>
<td>9 Yellow Catuai</td>
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* PLoS ONE 8(8):70098

Harvesting  >  Fermentation  >  Drying  >  Threshing
Strategy of Metabolic profiling

Green beans

1) Grinding
2) Extraction by 70% methanol

LCMS data of green bean extracts

Over 3,200 chemical signals

Multivariate analysis

Data Processing
Multivariate analysis

HARC, Kunia

Labs at Suntory
Arabica cultivars

OPLS-DA Score Plot  (Positive ionization mode)

- Catuai
- Laurina
- ET (Ethiopia)
- Typica
- SL28
- Mokka
- Catimor
- Mokka hybrid (F1)

$R^2[1] = 0.223$
$R^2[2] = 0.0955$

Ellipse: Hotellina’s T2 (95%)
Typica from 4 growing areas on 3 islands

<table>
<thead>
<tr>
<th>Location</th>
<th>Fields</th>
<th>Harvest Dates</th>
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<tbody>
<tr>
<td>Waialua, Waialua Estate Coffee &amp; Chocolate</td>
<td>October 2012</td>
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<td>Kunia, HARC</td>
<td>October 2012</td>
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<td>Kona, Greenwell Farms</td>
<td>October 2012</td>
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<td>Kauai, Kauai Coffee</td>
<td>January 2013</td>
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</table>
From the viewpoint of chemical components, the property of Kauai is similar to the property of Greenwell.

*Only Greenwell’s beans are high density beans separated by gravity concentration. The other beans are not separated.*
Maturity Levels of Cherries

Green  Pink  Red  Over Ripe
PCA for Maturity Levels of 3 cultivars

11033D_coffee_positive.M1 (PCA-X)
t[Comp. 1]/t[Comp. 2]
Colored according to Obs ID (Species)

“Green stage”

R²X[1] = 0.119303  R²X[2] = 0.0646472
Ellipse: Hotelling T² (0.95)
Prediction of Ripeness by Chemical profiling
Searching for “key metabolite” correlating to maturity level

**PLS regression model**

Iwasa et al. 2013
- Tryptophan is a specific marker of immature green beans.
- Tryptophan is the cause of indole and methyl indole by roasting.
- Indole and methyl indole give coffee beverage the negative odor.

Chemical compounds in green beans predict precisely the coffee cupping quality

Green coffee beans: 36 samples: various locations and producers in Guatemala

Chemical analysis by LC-MS 2,649 signals of metabolomic information

<table>
<thead>
<tr>
<th>SCAA Cupping Score</th>
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<tbody>
<tr>
<td>SCAA cupping score (points)</td>
</tr>
<tr>
<td>89</td>
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<td>87</td>
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<td>76</td>
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Iwasa et al 2015
Prediction of beverage quality from green beans metabolites

Metabolites to Cupping score

Prediction

\[ R^2_X = 0.056 \]
\[ R^2_Y = 0.957 \]
\[ Q^2 = 0.637 \]
\[ RMSEE = 0.46 \]

Predicted cupping score from LC-MS peak signal information

High correlation

Metabolomic information is a precise predictor of SCAA cupping score
Novel compounds in green beans

3-Methylbutanol disaccharides (3MDs) are 2 key compounds in green beans.

Figure 2. Two isomers of 3-methylbutanoyl glycosides in raw beans. These compound contents are higher in the raw beans with higher cupping score.

Roasting (230°C 10 min)

Thermal reaction product

3-Methylbutanoic acid

Figure 3. 3-Methylbutanoic acid in roasted beans. This compound is generated by the thermal reaction of 3-methylbutanoyl glycosides.

Cupping scores

Figure 4. Sensory evaluation (cupping score of aftertaste). The addition of 3-methylbutanoic acid improves the quality of coffee beverage.
Conclusion

By using chemical information of green beans, we were able to discriminate cultivars, maturity levels and cupping scores.

In future

We are going to focus on:

- Agronomical practices: Irrigation/Fertilization
- Processing methods: Wet process, Natural
- Correlation between metabolites and gene expression


www.Suntory.com/softdrink/news/pr/d
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