



Chemical Compounds in Green Coffee and Impact on Quality

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SUNTORY



What determines the beverage quality of coffee ?



*Green beans
quality*



*Roasting
control*



*Extraction
control*

Green bean property may have major impact on beverage quality



Understand the relationship between green beans and cupping score



***Green beans
quality***

Cherry properties

Cultivar

Maturity

Location of the trees

Agronomic practice

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

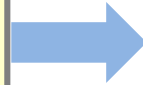


Growing condition



Fermentation Drying Threshing

Processing



Metabolite property



Green beans



Quality



Flavor & taste

Sample collection at HARC Kunia Field, Oahu, Hawaii



Harvesting and processing coffee cherry



Harvesting



Fermentation



Drying



Threshing

9 Cultivars **4 Maturity level**

1	Catimore 5175-1				
2	Red Catuai				
3	F1 Hybrid of Catimor and Tall Mokka (5175-1 xMA2-7)				
4	Maragogipe				
5	Tall Mokka MA 2-7				
6	SL28				
7	Typica				
8	Yellow Bourbon				
9	Yellow Catuai				

- *Green cherry*
- *Pink cherry*
- *Red cherry*
- *Dark Red cherry*

*** PLoS ONE 8(8):70098**

Strategy of Metabolic profiling

HARC, Kunia

Green beans

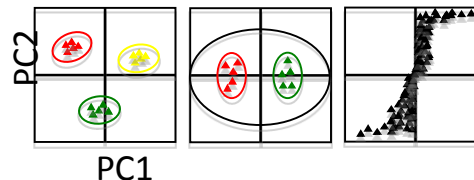
- 1) Grinding
- 2) Extraction by 70 % methanol



Labs at Suntory

Over 3,200 chemical signals

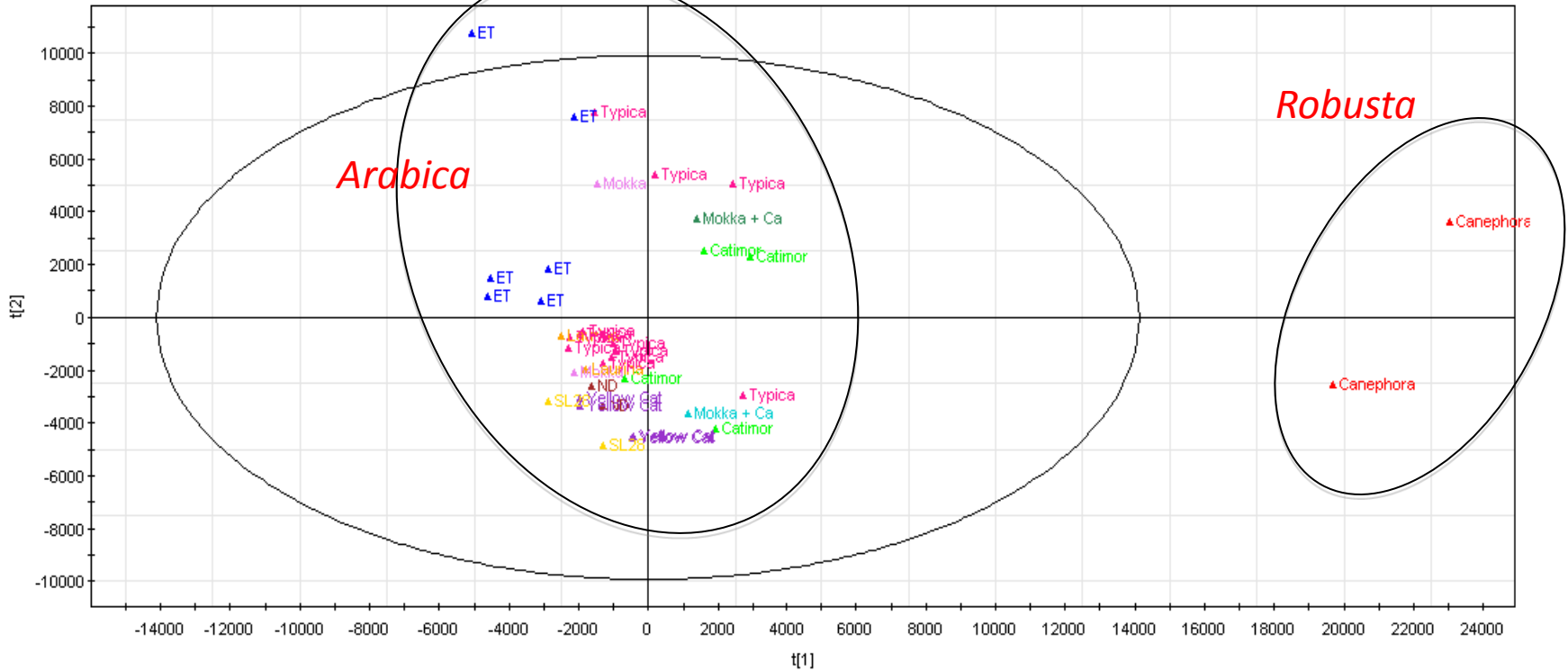
Multivariate analysis



**Data Processing
Multivariate analysis**

Arabica vs Robusta

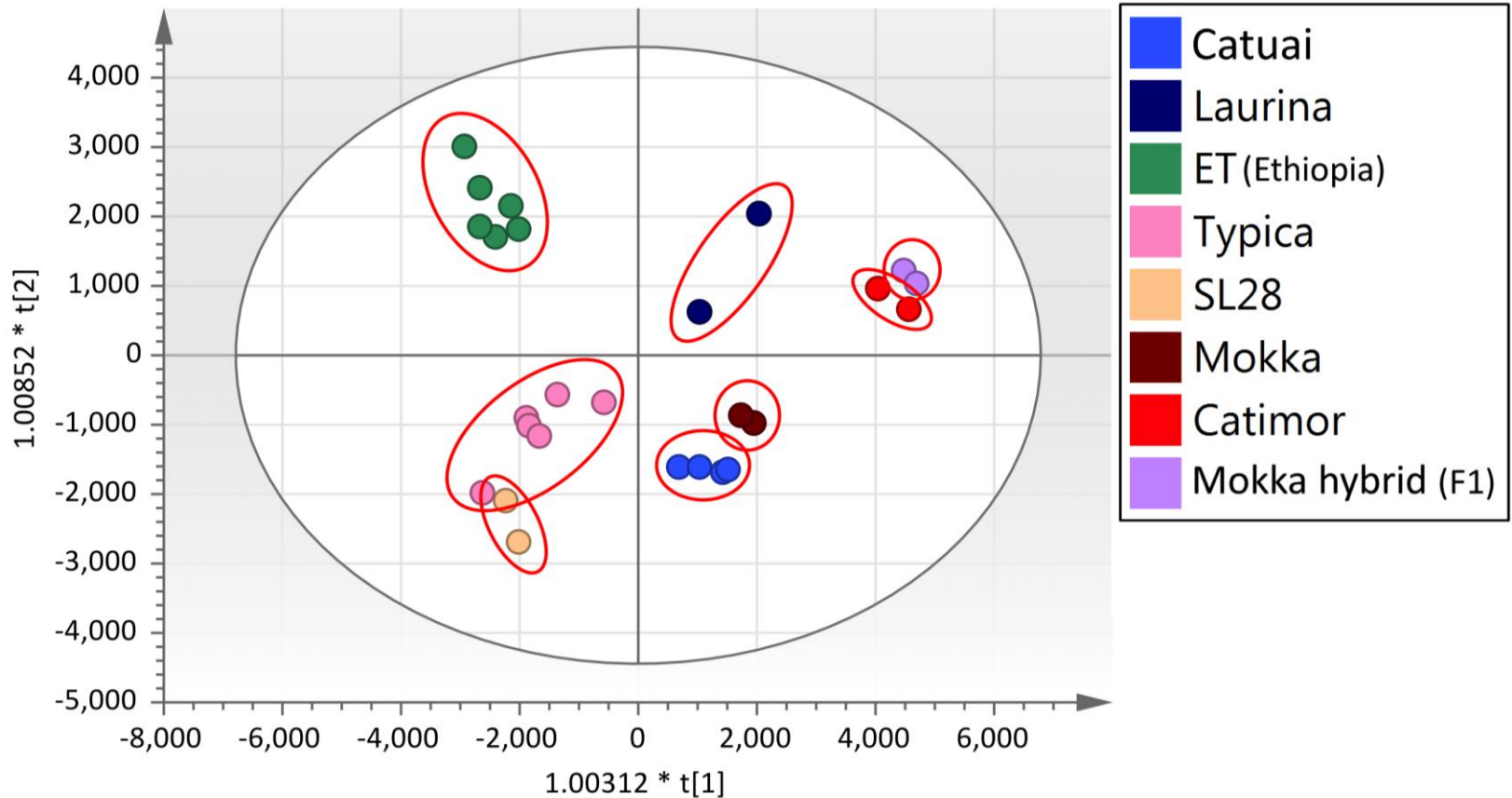
110110.M2 (PCA-X)
t[Comp. 1]/t[Comp. 2]
Colored according to Obs ID (Obs. Sec. ID:3)



R2X[1] = 0.308705 R2X[2] = 0.152184
Ellipse: Hotelling T2 (0.95)

Arabica cultivars

OPLS-DA Score Plot (Positive ionization mode)



$R^2X[1] = 0.223$

$R^2X[2] = 0.0955$

Ellipse: Hotelling's T^2 (95%)

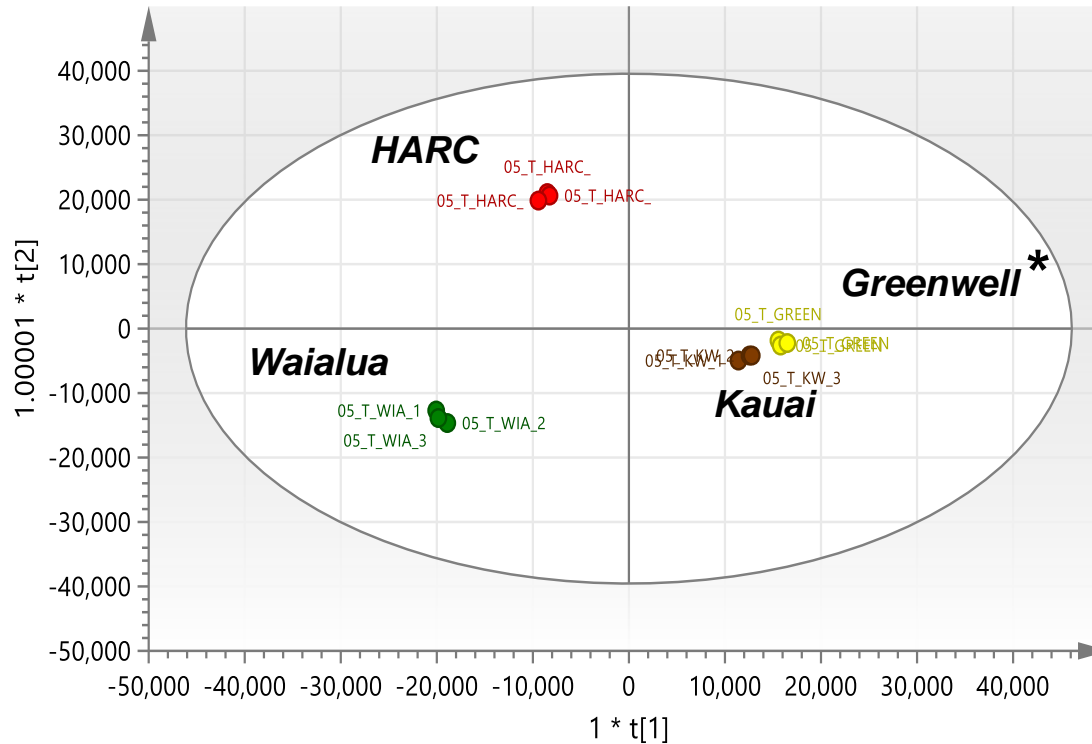
Typica from 4 growing areas on 3 islands

Location:	Fields	Harvest Dates
Waialua,	Waialua Estate Coffee & Chocolate	October 2012
Kunia,	HARC	October 2012
Kona,	Greenwell Farms	October 2012
Kauai,	Kauai Coffee	January 2013



Analysis of green beans from 4 fields - Cultivar : Typica

◆ OPLS-DA, Scatter Plot



= 0.376

R2X[2] = 0.276

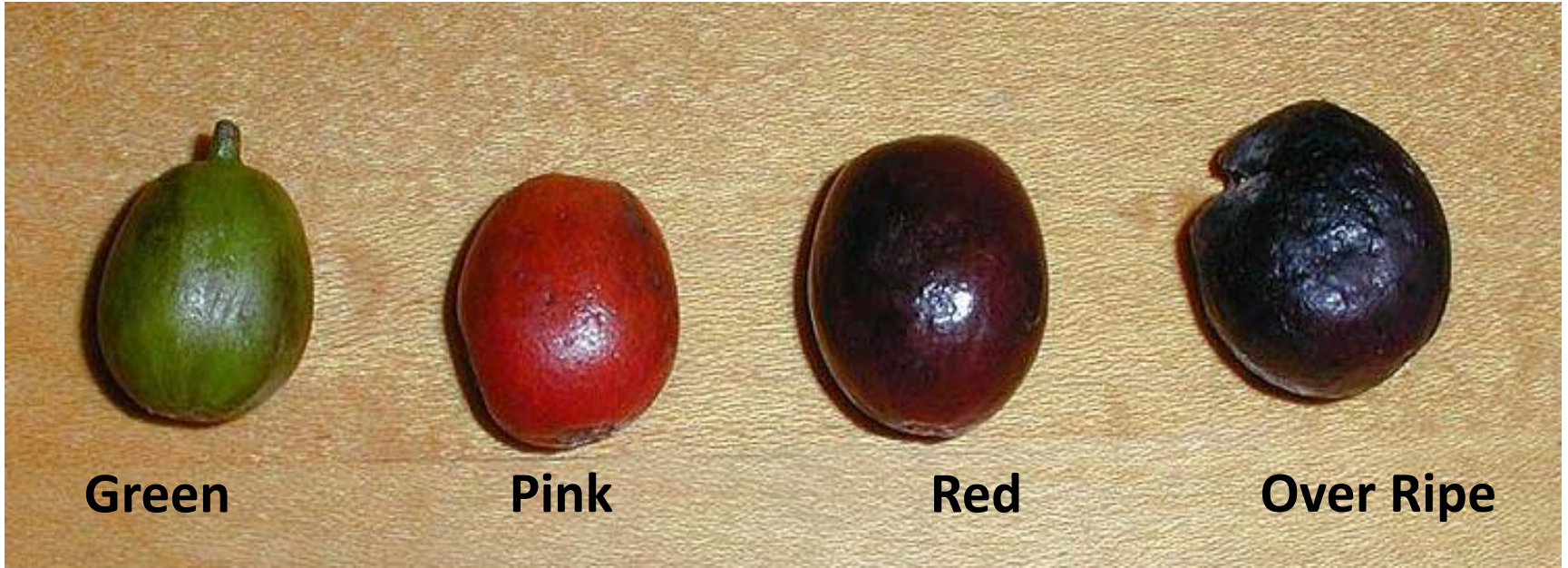
Ellipse: Hotelling's T2 (95%)

C:\MCA\120... 2012/07/12 13:48:54 (UTC+9)

* **Only Greenwell's beans are high density beans separated by gravity concentration.
The other beans are not separated.**

From the viewpoint of chemical components, the property of Kauai is similar to the property of Greenwell.

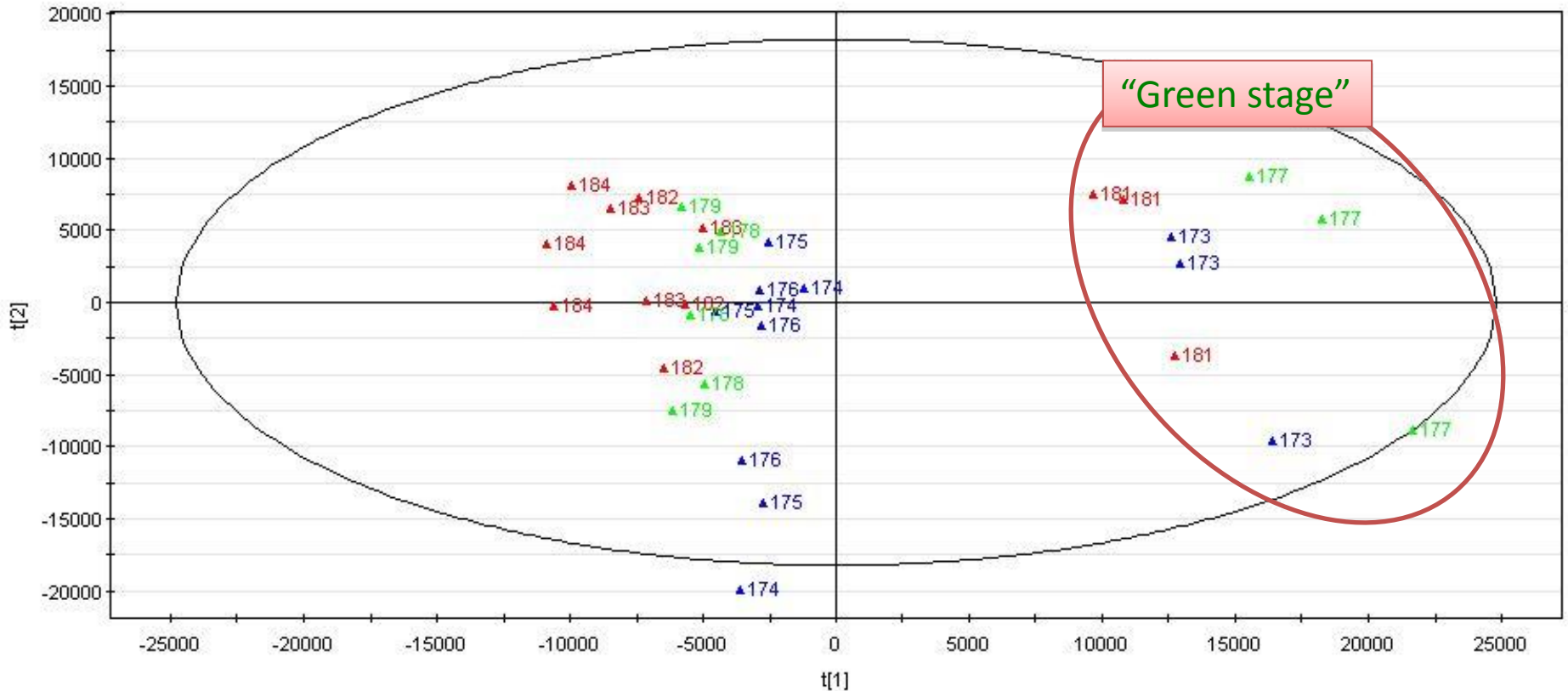
Maturity Levels of Cherries



PCA for Maturity Levels of 3 cultivars

110330_coffee_positive.M1 (PCA-X)
t[Comp. 1]/t[Comp. 2]
Colored according to Obs ID (Species)

▲ Catuai
▲ SL28
▲ Typica

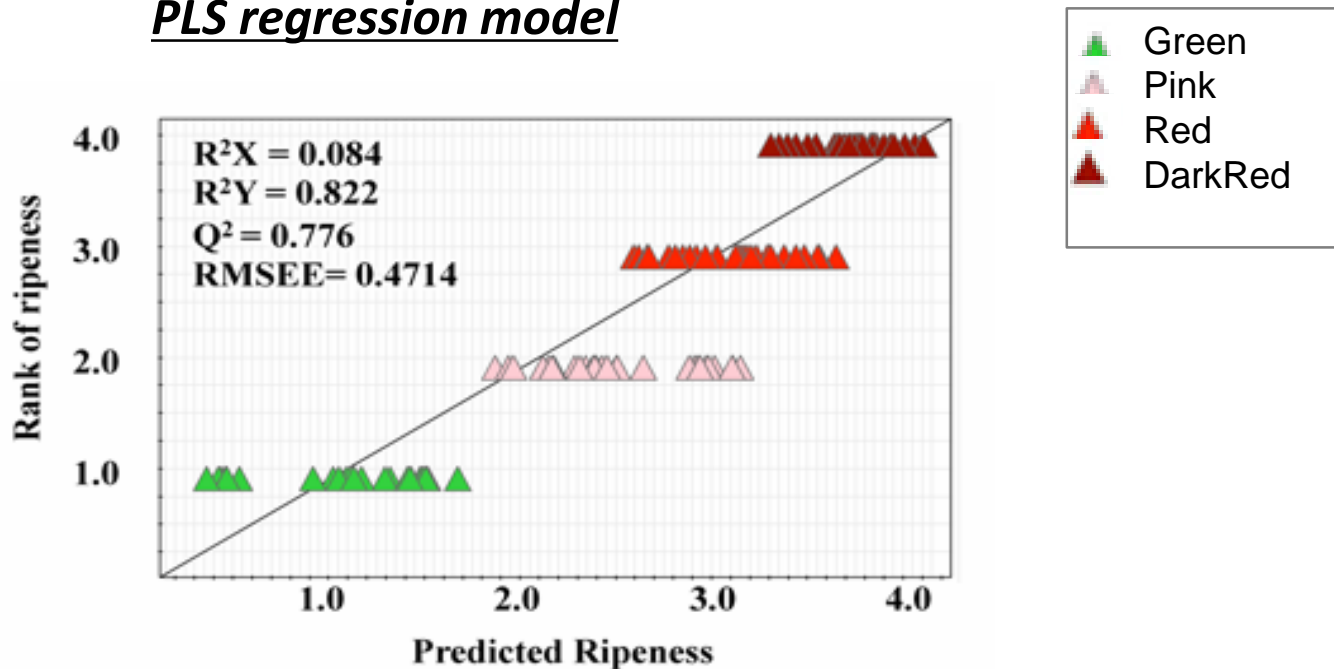


R2X[1] = 0.119303 R2X[2] = 0.0646472
Ellipse: Hotelling T2 (0.95)

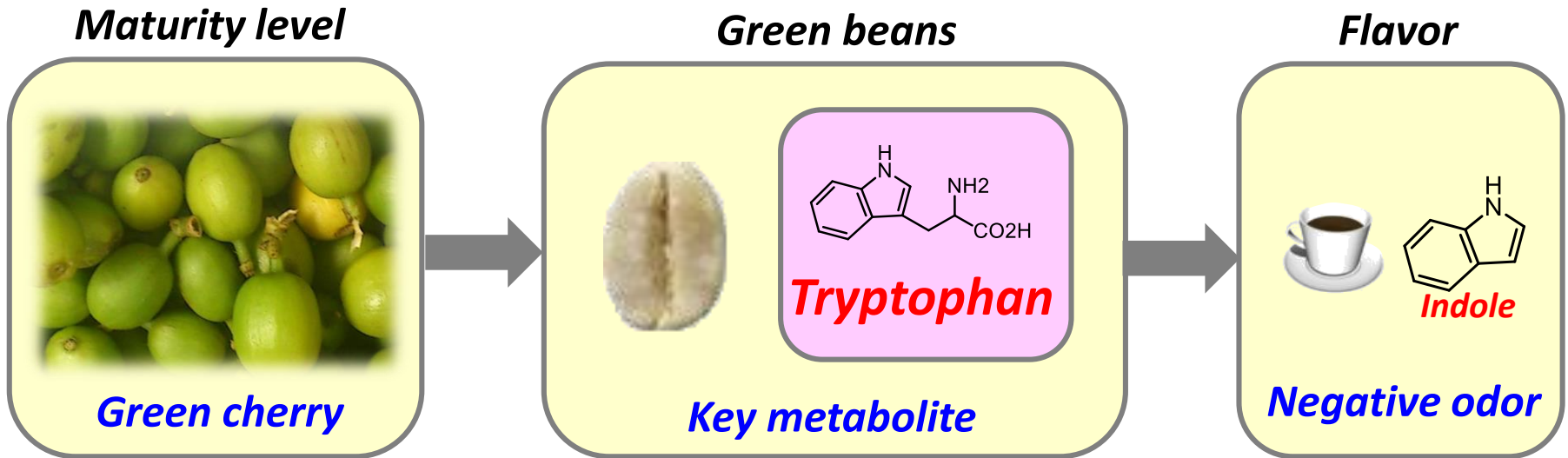
Prediction of Ripeness by Chemical profiling

Searching for “key metabolite” correlating to maturity level

PLS regression model



“key metabolite” correlating to maturity level



- 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.

<http://www.suntory.com/softdrink/news/pr/d/SBF0198.html>

Chemical compounds in green beans predict precisely the coffee cupping quality

Green coffee beans:

36 samples: various locations and producers in Guatemala



Powder,
Extraction



Roasting

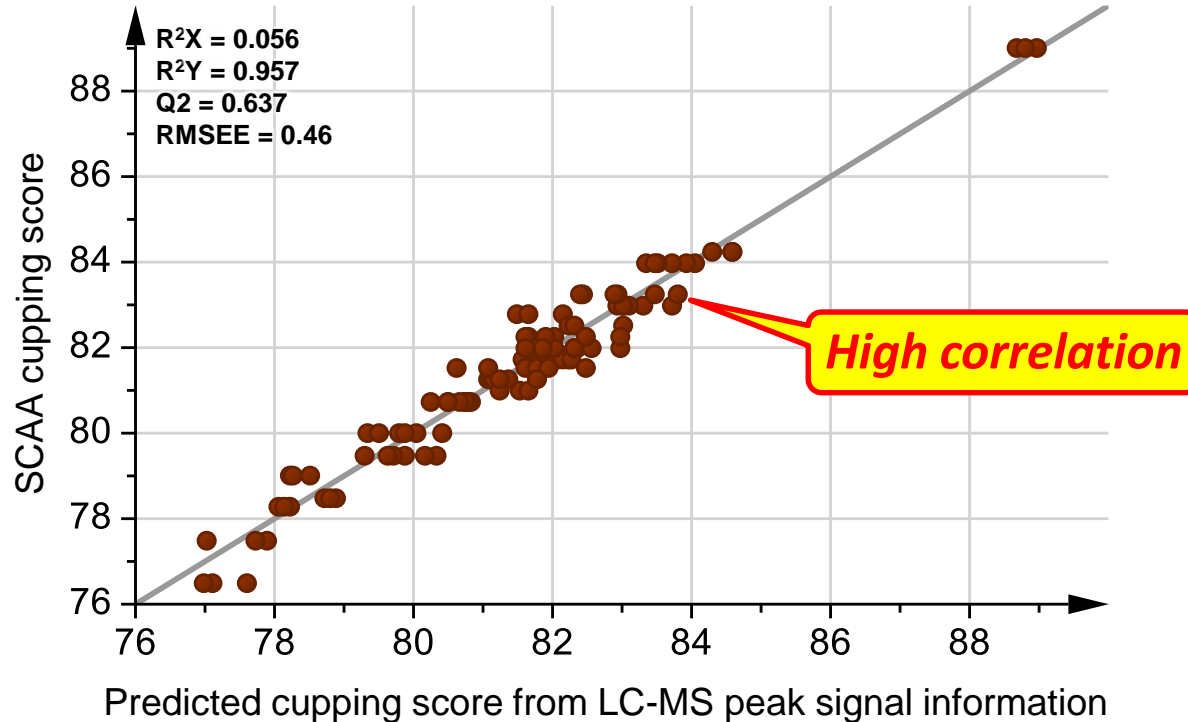
SCAA Cupping Score

SCAA cupping score (points)	
89	89.0
88	
87	
86	
85	
84	84.0, 84.0, 84.25
83	83.0, 83.0, 83.25, 83.25
82	82.0, 82.0, 82.0, 82.0, 82.0, 82.25, 82.25, 82.5, 82.75
81	81.0, 81.25, 81.25, 81.5, 81.5, 81.75, 81.75
80	80.0, 80.0, 80.75, 80.75, 80.75
79	79.0, 79.5, 79.5
78	78.25, 78.5
77	77.5
76	76.5

Chemical analysis by LC-MS

2,649 signals of metabolomic information

Prediction of beverage quality from green beans metabolites



Metabolomic information is a precise predictor of SCAA cupping score

Novel compounds in green beans

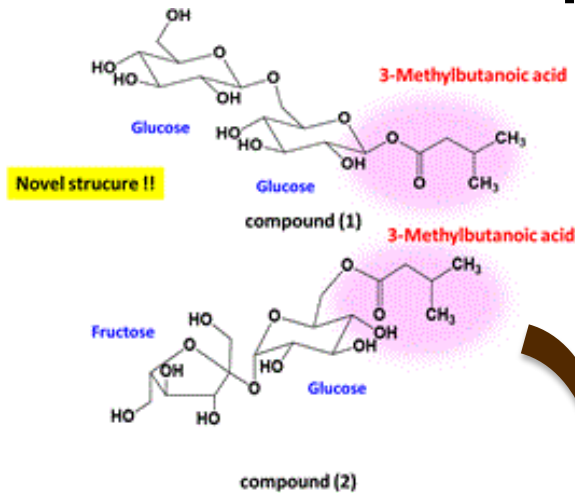
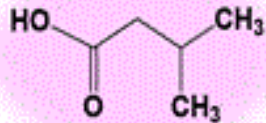


Figure 2. Two isomers of 3-methylbutanoyl glycosides in raw beans. These compound contents are higher in the raw beans with higher cupping score.

Roasting (230°C 10 min)

Thermal reaction product



3-Methylbutanoic acid

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

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

Cupping scores

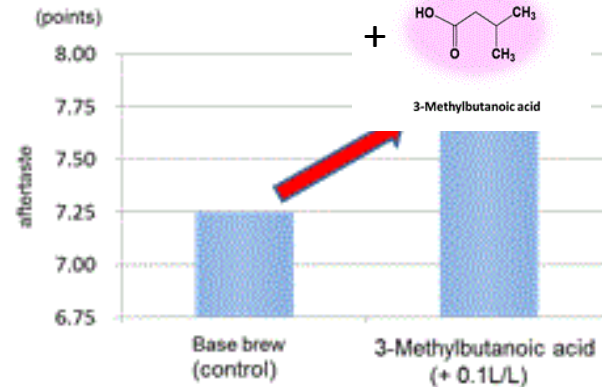


Figure 4. Sensory evaluation (cupping score of aftertaste)
The addition of 3-methylbutanoic acid improves the quality of coffee beverage.

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

References

Setoyama, D., K. Iwasa, H. Seta, H. Shimizu, Y. Fujimura, D. Miura, H. Wariishi, C. Nagai and K. Nakahara. High-throughput metabolic profiling of diverse green *Coffea arabica* beans identified tryptophan as a universal discrimination factor for immature beans. 2013. PLOS ONE 8(8): e70098. doi:10.1371/journal.pone.0070098

Iwasa, K., D. Setoyama, H. Shimizu, Y. Fujimura, D. Miura, H. Wariishi, C. Nagai and K. Nakahara. 2015. Identification of 3-Methylbutanol Glycosides in Green *Coffea Arabica* beans as causative determinants for the quality of coffee flavors. Journal of Food Chemistry, 63(14)3742-3751.

<http://www.suntory.com/softdrink/news/pr/d/SBF0198.html>

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

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