



# ***NIR-based Determination of differences in green coffee chemical composition due to geographical origin***

**Adrian Haiduc, Charlotte Gancel, Valerie Leloup**  
**Nestle**



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## ***Introduction***

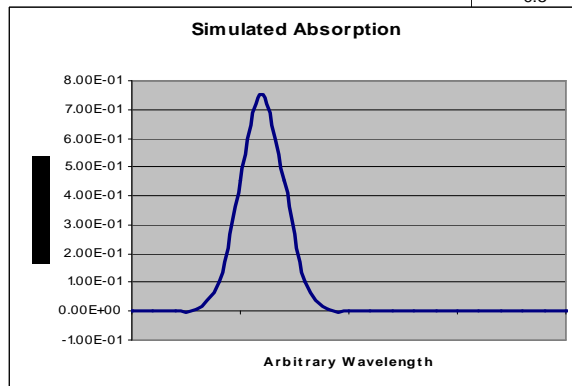
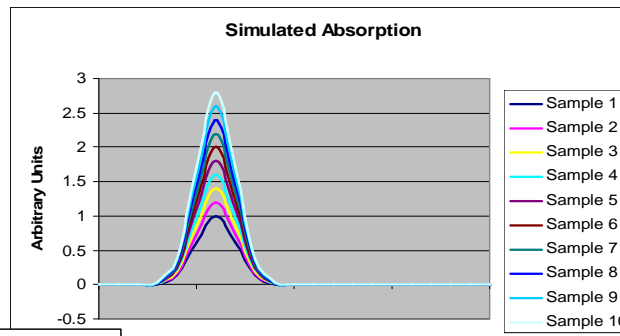
- **Relatively easy to determine external ingredients: chicory, cereals, etc**
- **Well established analytical method to confirm a coffee's appellation of origin is lacking**
  
- **Isotope ratios-Global scale**
- **NIR-Regional Scale**



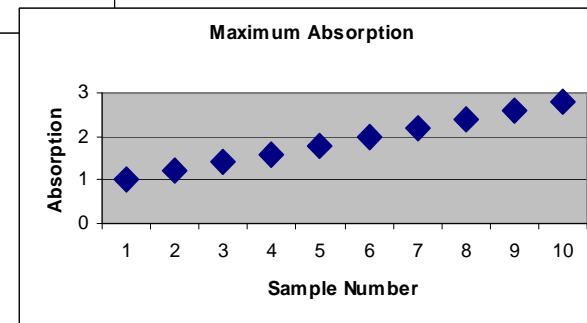
# NIR Calibrations: Introduction

- What is PCA, PLS, PLS-DA.....

NIR Absorption



Loading



Scores



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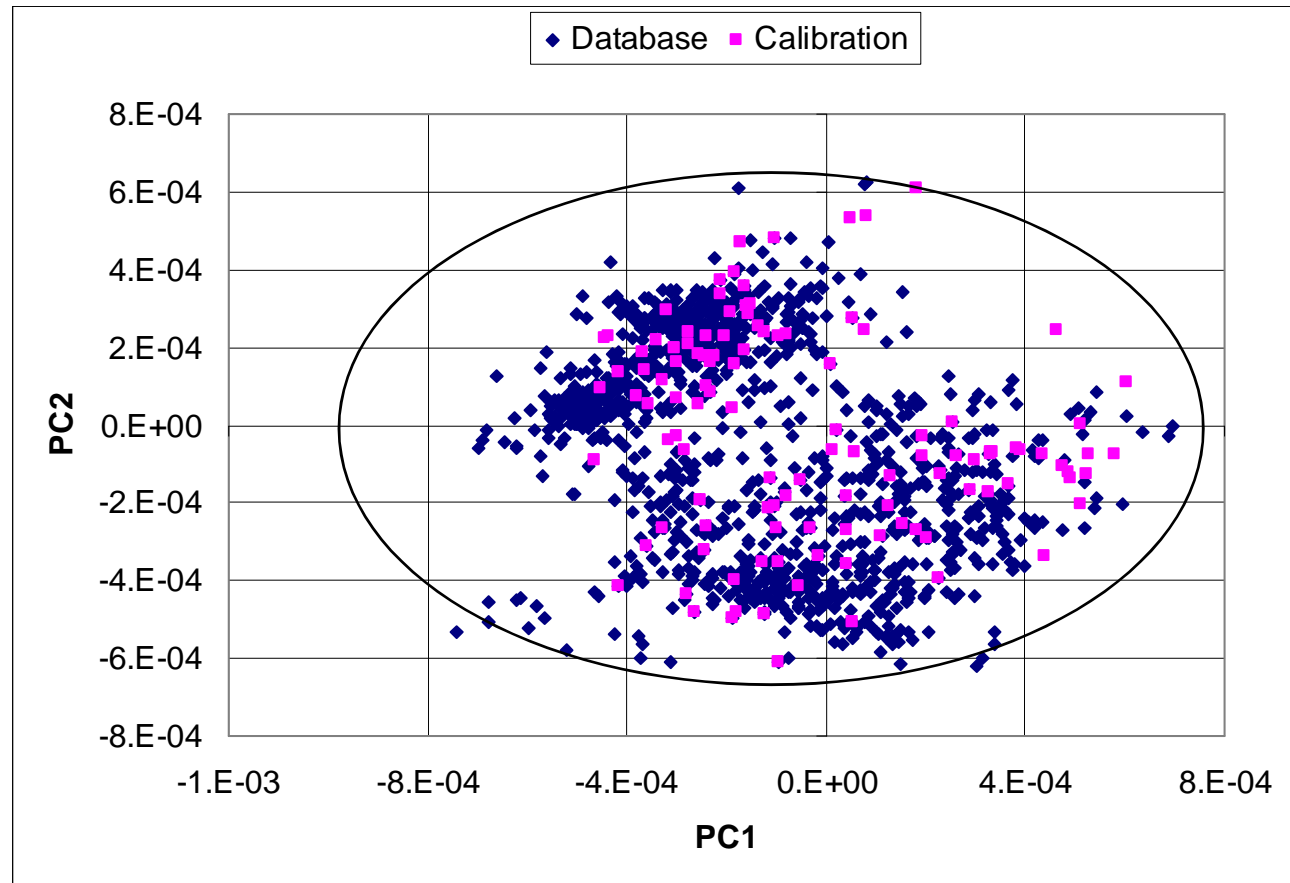
## ***NIR Calibration***

- **Calibration : 120 Samples**
- **Parameters: Moisture, Lipids, Caffeine, Trigonelline, Chlorogenic Acids, Organic Acids, Sucrose, Protein**
- **Determine composition of 1200 samples: Arabica and Robusta, Africa and South America.**



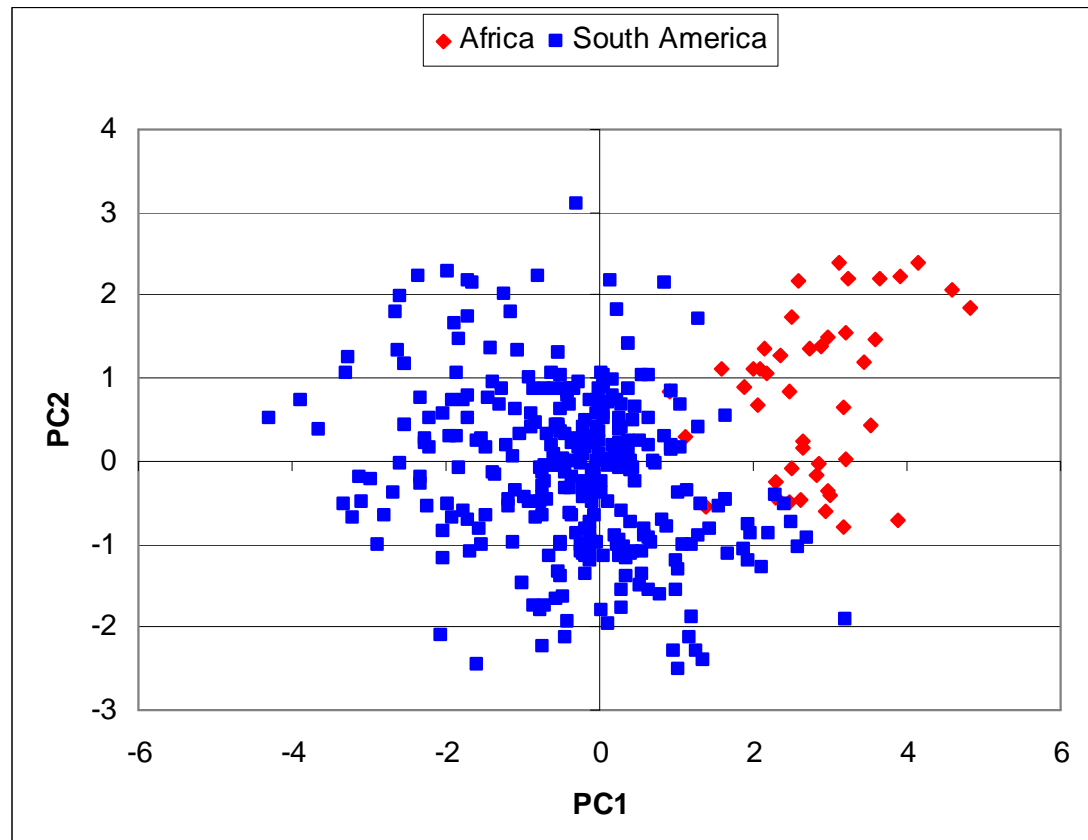
# NIR Calibration

- Calibration Space



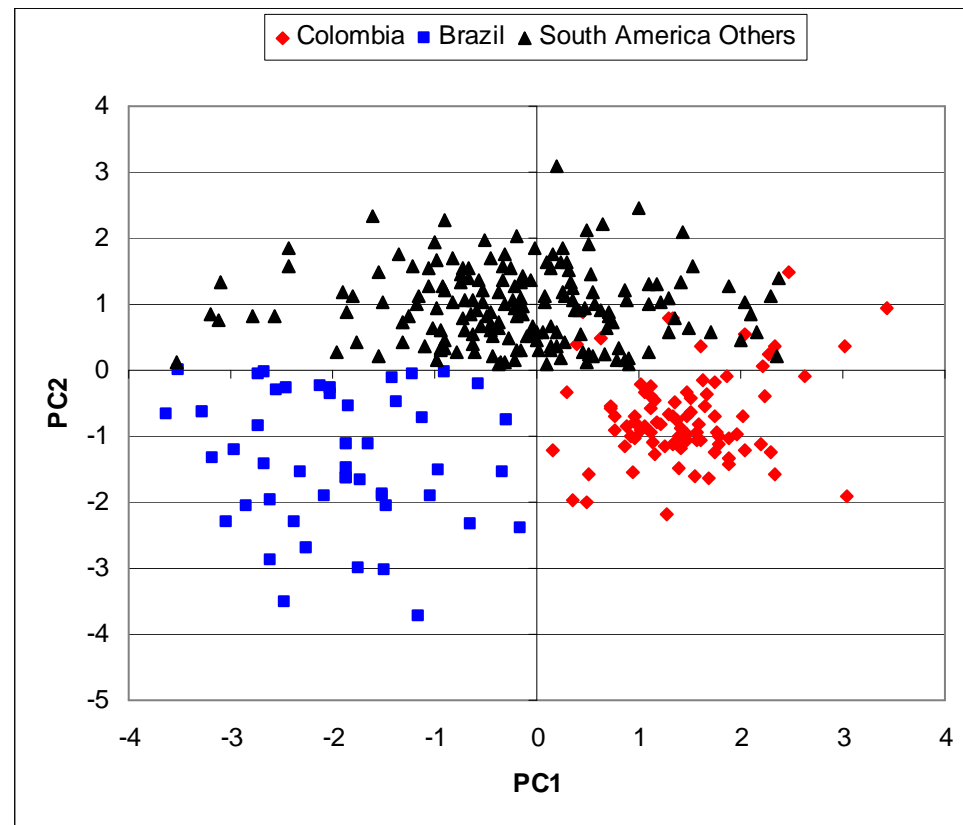
## *First Class Africa-South America*

- **Classification based on Composition**



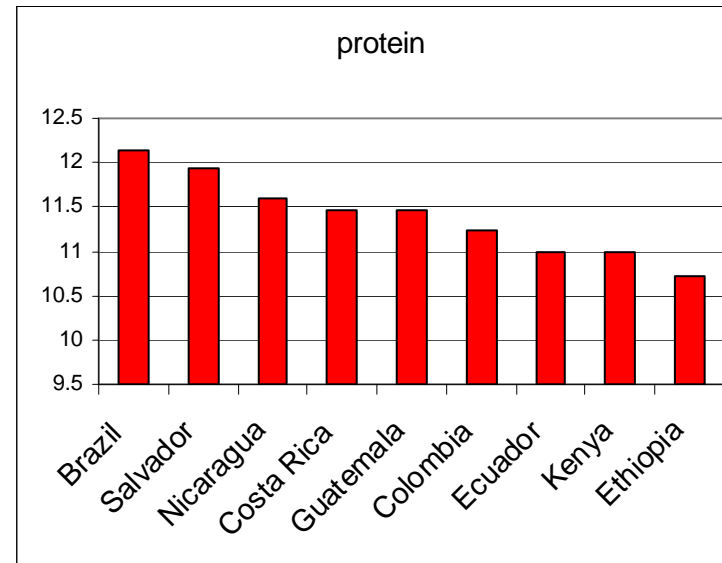
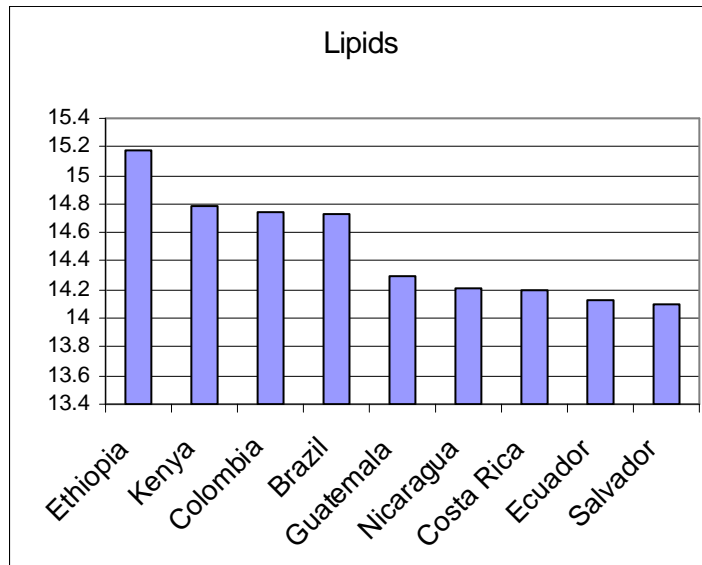
# Classification South America

- **Classification based on Composition**



# Compositional Differences

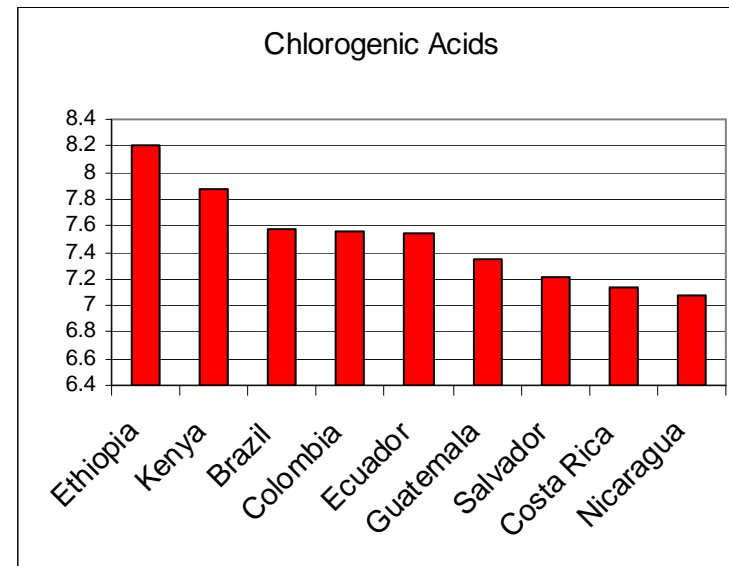
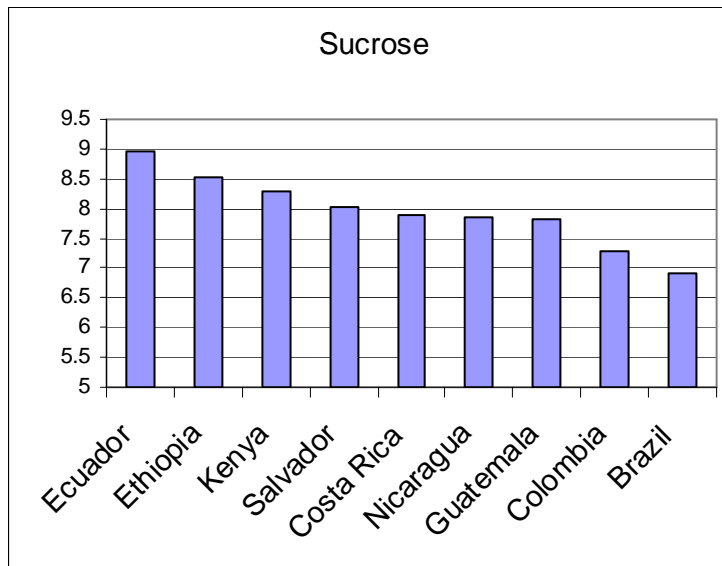
	Dry Matter	Lipids	Caffeine	Trigonelline	Chlorogenic Acids	Organic Acids	Sucrose	protein
Costa Rica	90.57	14.2	1.25	0.82	7.14	2.28	7.89	11.47
Guatemala	90.13	14.3	1.25	0.81	7.35	2.24	7.81	11.47
Salvador	90.68	14.1	1.22	0.83	7.21	2.34	8.02	11.93
Ecuador	91.64	14.13	1.36	0.72	7.54	2.32	8.95	10.99
Brazil	90.6	14.73	1.3	0.9	7.58	2.33	6.93	12.15
Colombia	89	14.74	1.31	0.81	7.56	2.23	7.28	11.24
Nicaragua	89.39	14.21	1.26	0.79	7.08	2.27	7.87	11.59
Ethiopia	91.26	15.17	1.26	0.84	8.21	2.22	8.54	10.71
Kenya	90.78	14.79	1.19	0.82	7.88	2.24	8.28	10.98





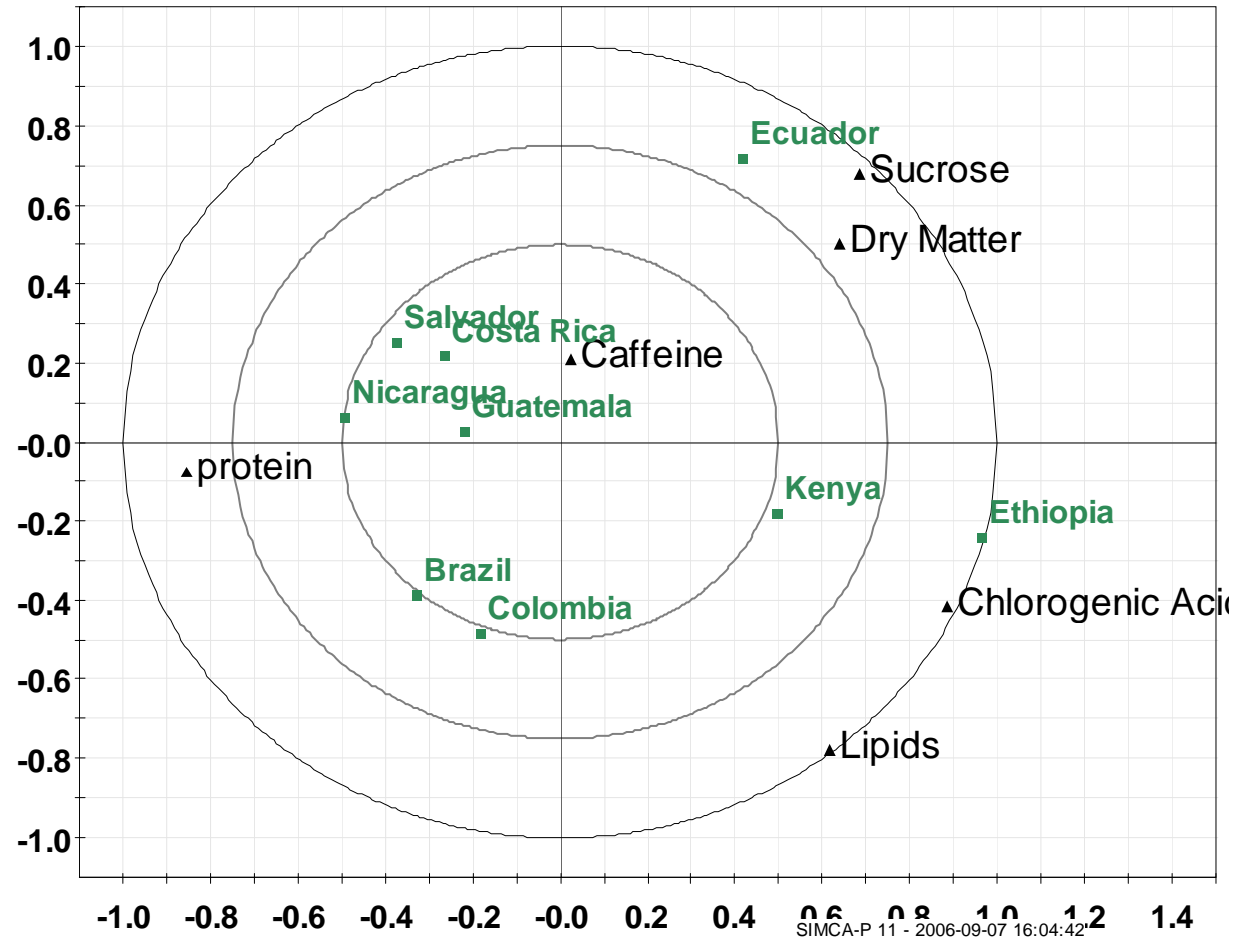
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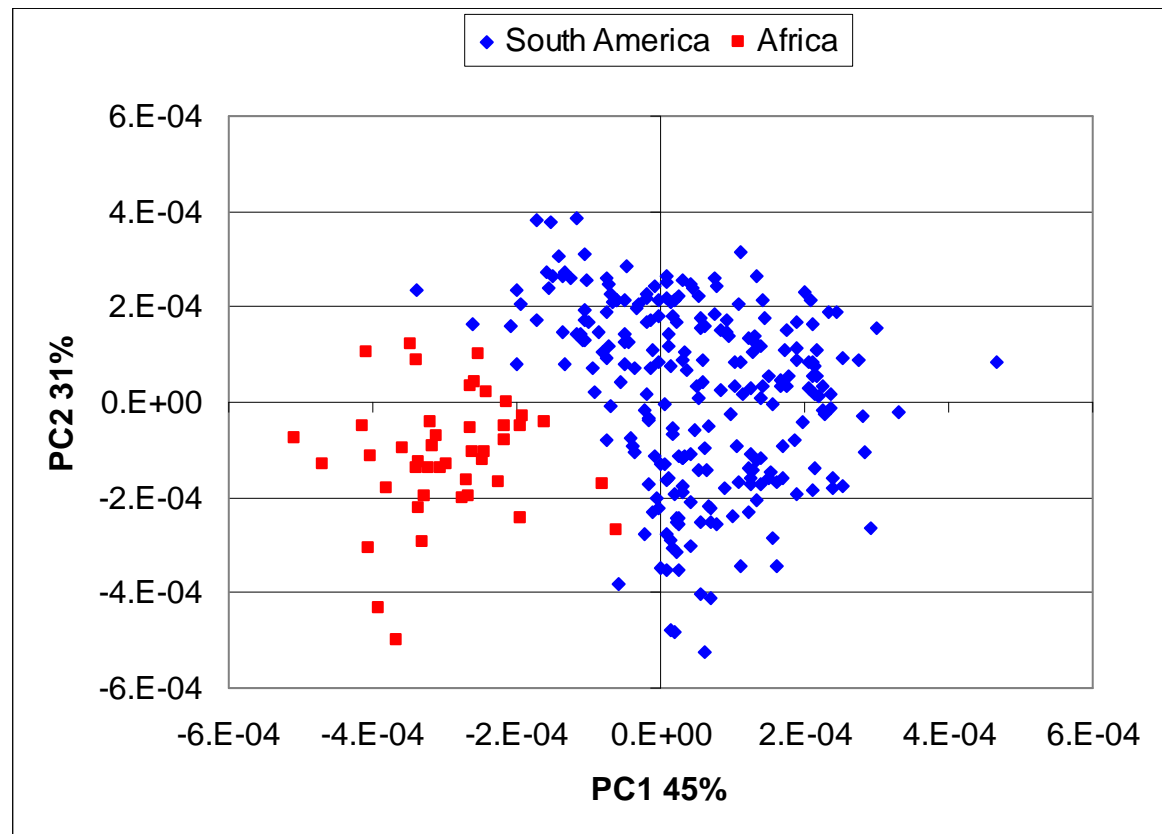


# Compositional PCA



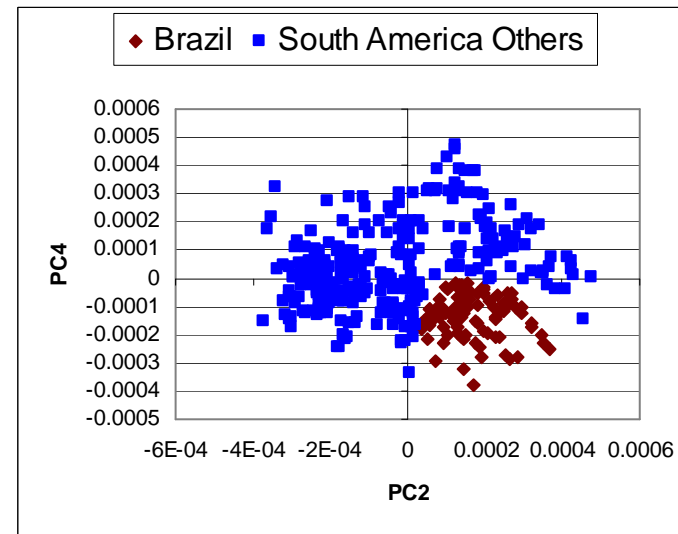
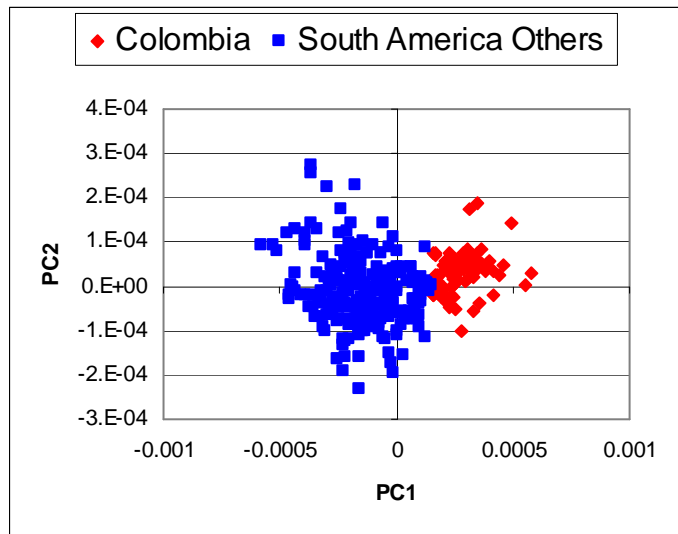
## *NIR full spectra: Africa America*

- For use as a predictive model
- Loadings: Lipids



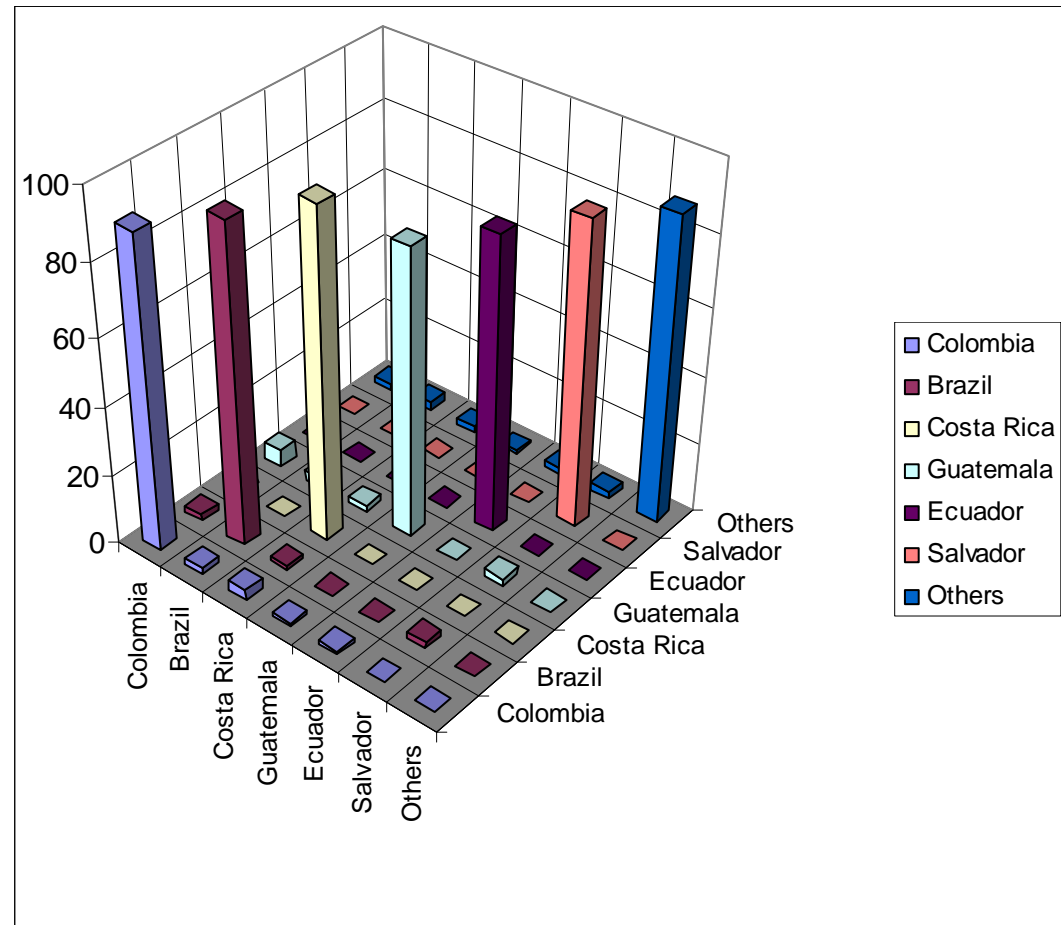
## *NIR full spectra: South America*

- **Good Separation: Brazil, Colombia, Costa-Rica, Guatemala, Ecuador, Salvador**
- **One Group: Mexico, Honduras, Nicaragua**
- **Loadings: Lipids and Protein**



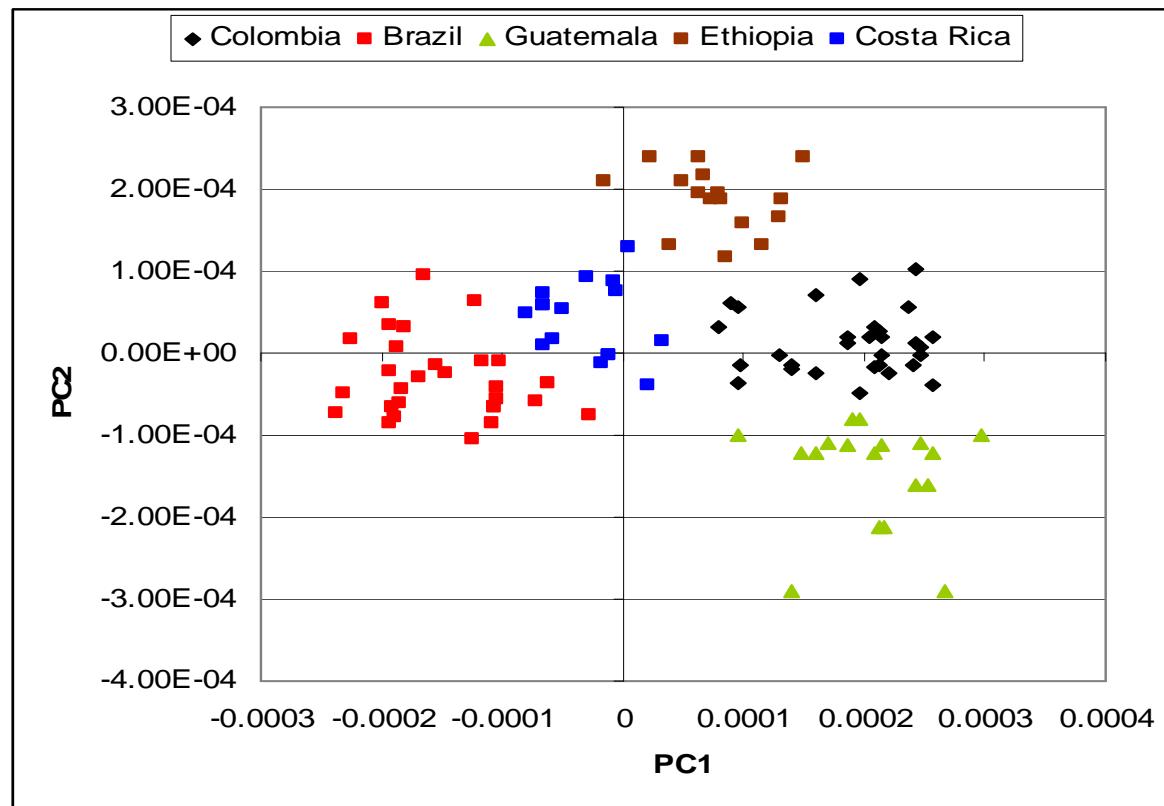
## PLS-DA Validation 2002-2004

- 2/3 Model Development
- 1/3 Model Validation
- 90 % of the validation samples are correctly classified



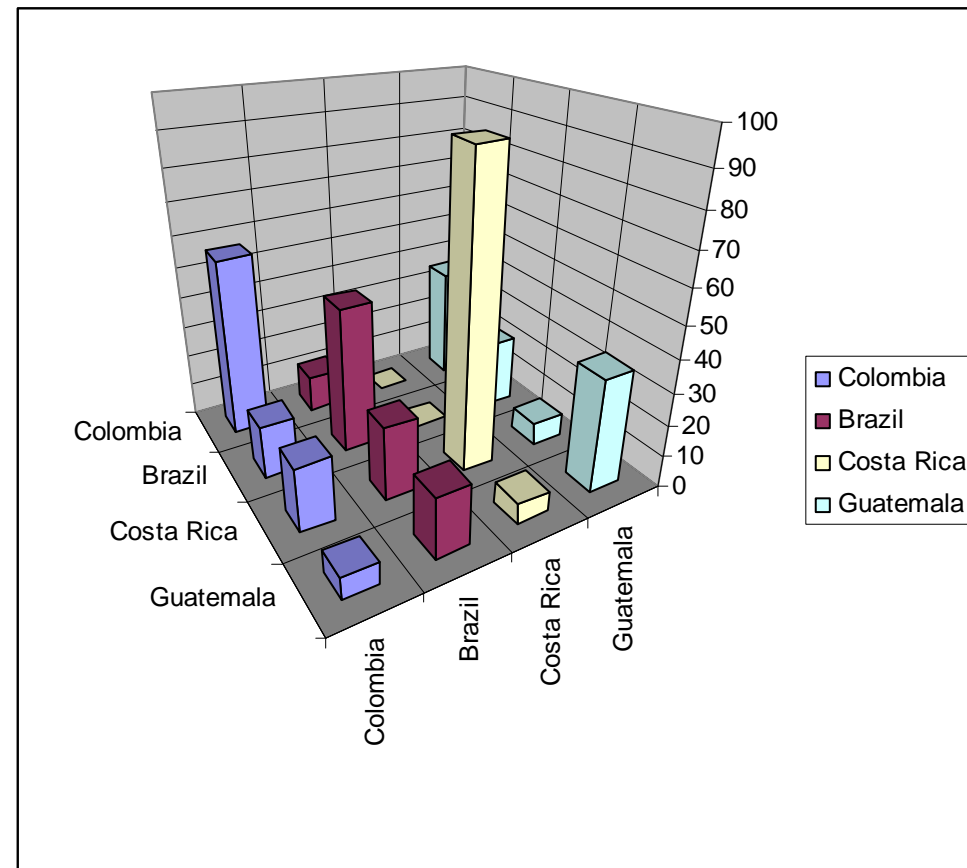
## PLS-DA 2005

- Clustering based on origin is again feasible

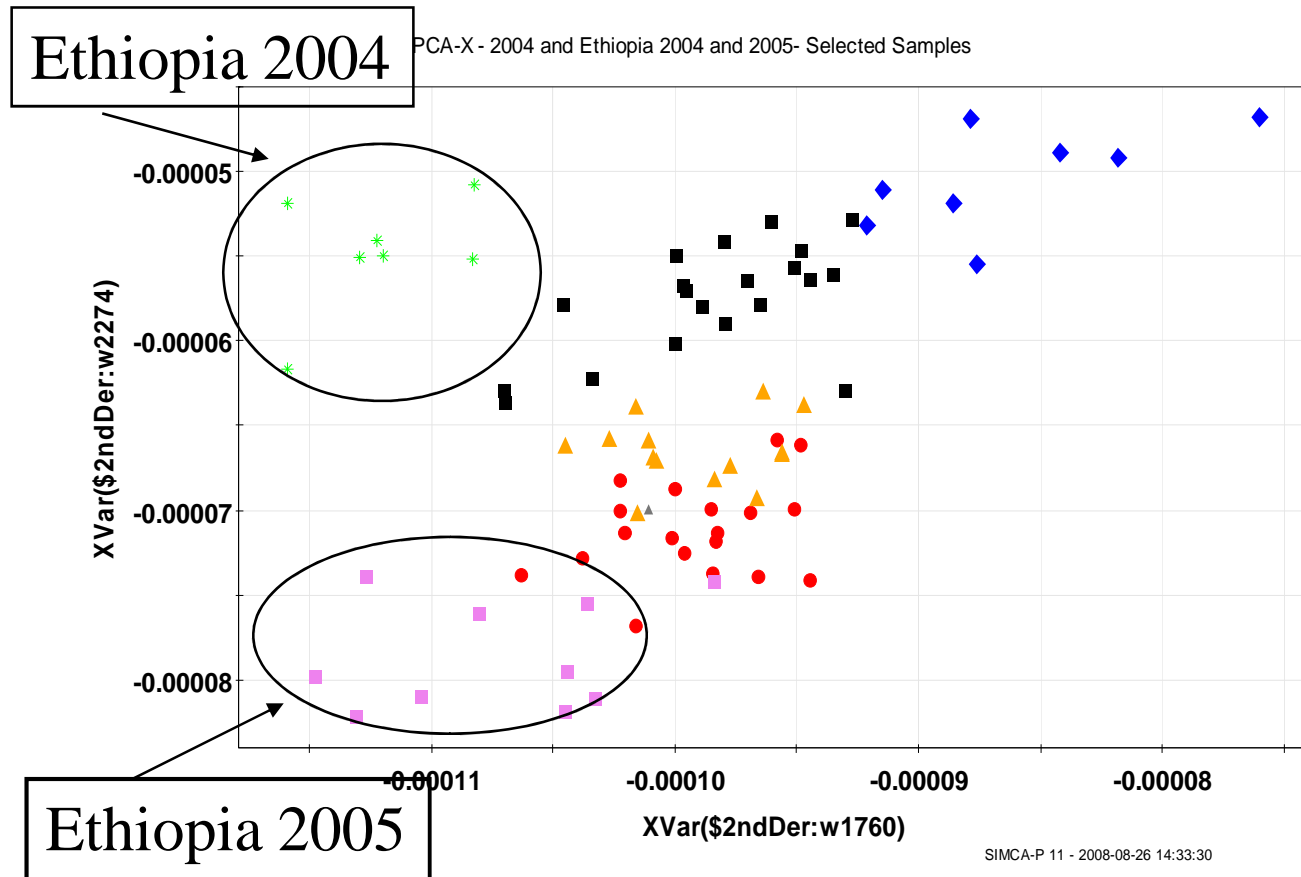


## Validation 2005 on 2002-2004

- Best validation is performed with Independent samples
- Failure rate:
- **50 %**



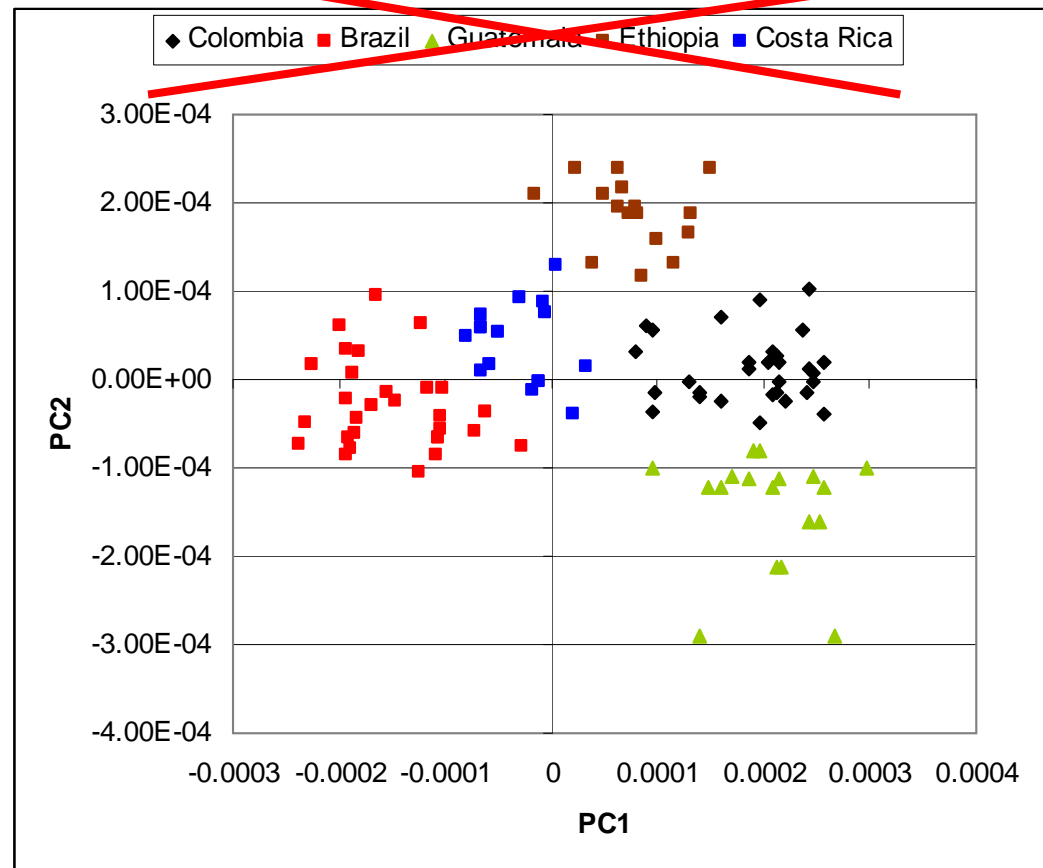
# Samples from same region show high differences between crop years





# Predictive versus Functional

- Predictive: Indirect
- Functional: Direct
- Real Grouping:
  - environmental factors
  - agricultural practices





## ***Conclusion***

- **NIR Calibration of composition has good portability**
- **Global Discriminant models can be established**
- **Global Discriminant models are not portable over different crop years**



*Thank You*

Questions?



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