Visual Chemometrics – Interactive Software for Hyperspectral Image Exploration and Analysis

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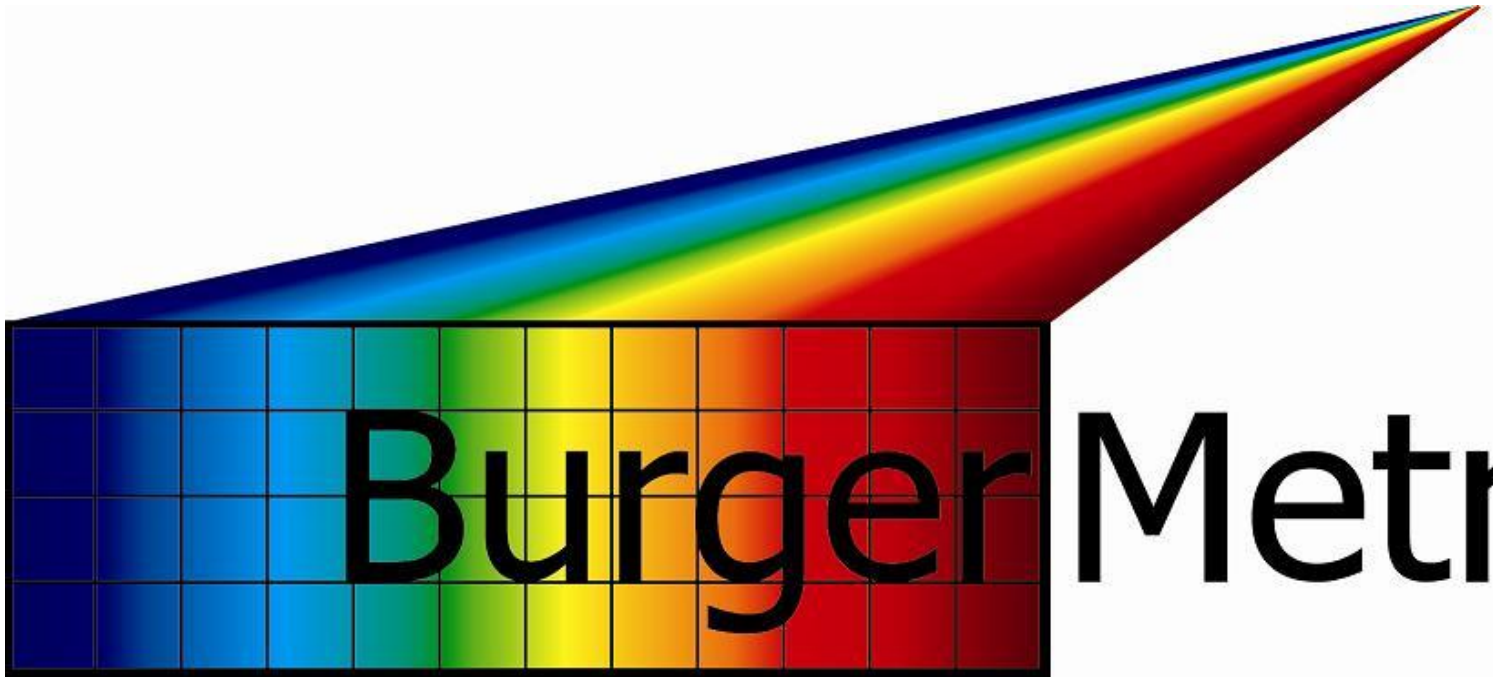


Inspiring Vision in Chemical Analysis


IASIM

What is a Hyperspectral Image?

‘RGB’ Digital Image

Color Image

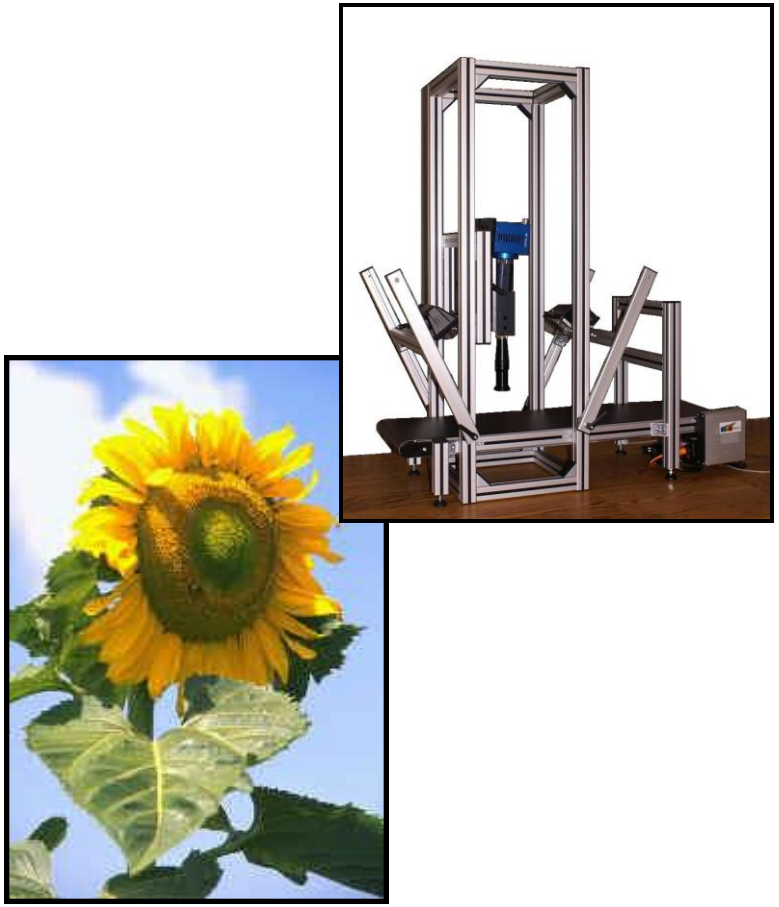
3 Gray Scale Images

Multi-Channel Image

Color Image

4 - 10 Gray Scale Images

Hyperspectral Image (HSI)

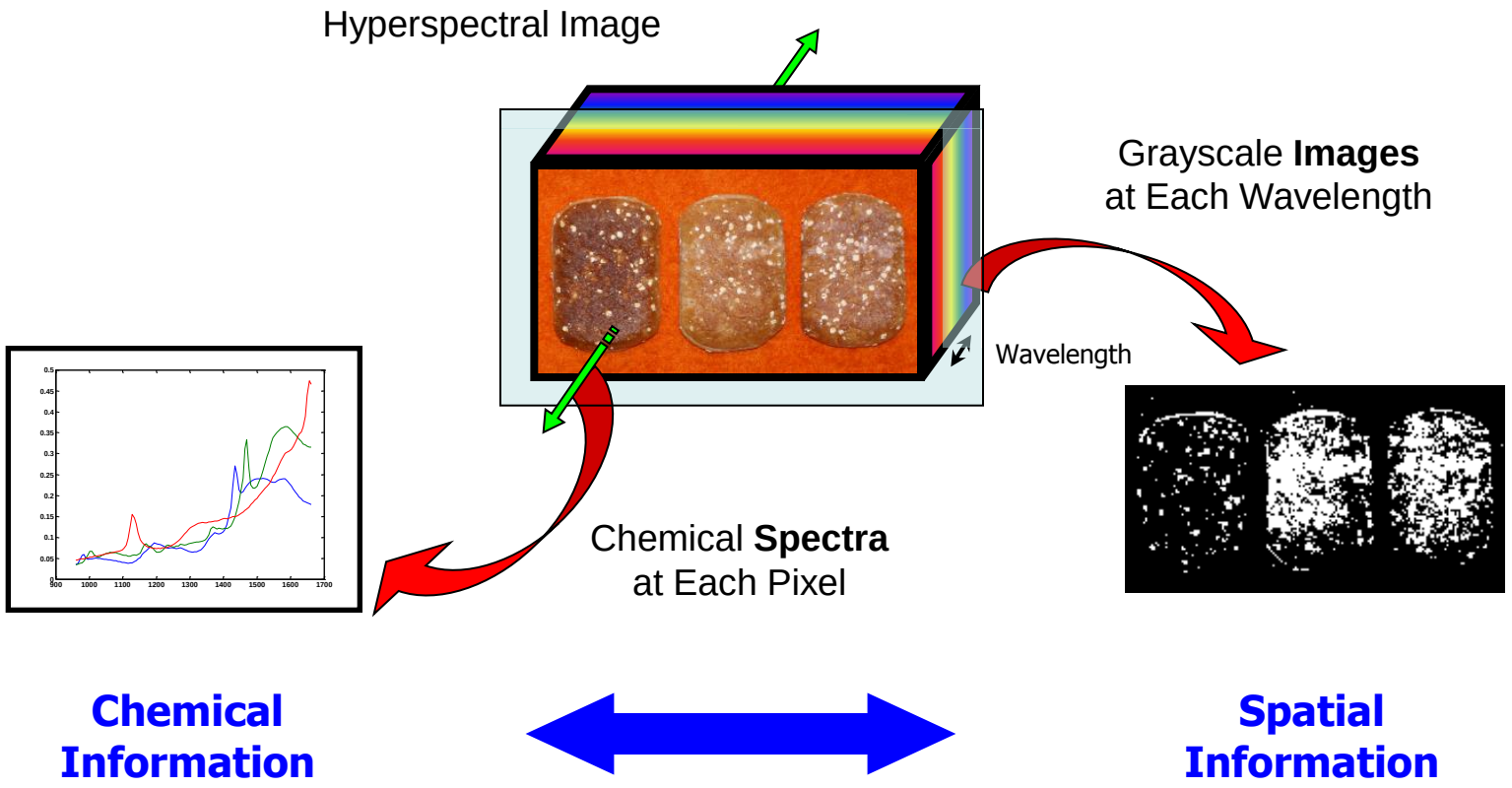


Color Image

100 + Gray Scale Images (Hypercube)

Hyperspectral Chemical Image (HCI)

Chemical + Spatial Information



What? / How much?

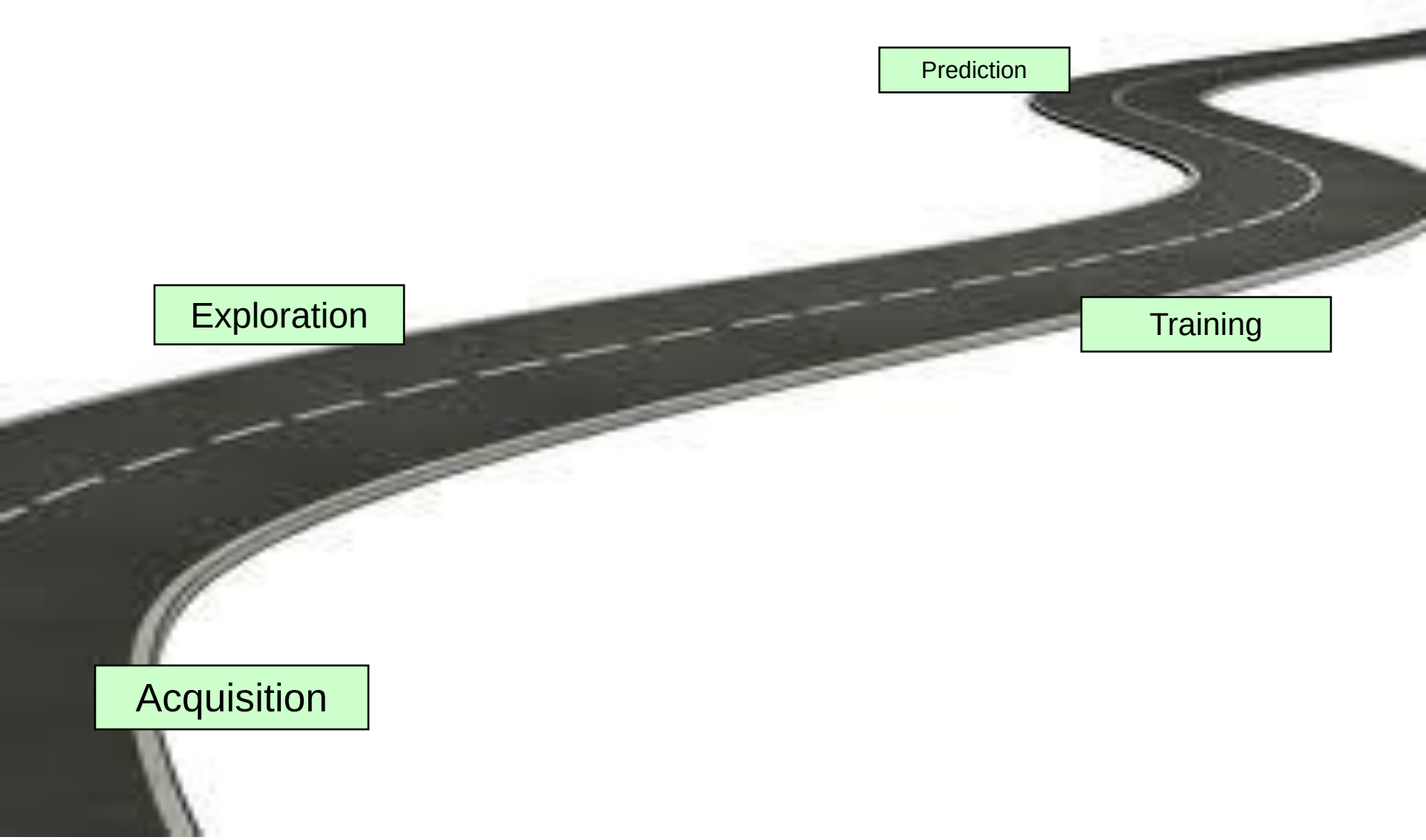
Where?

Complex Images + Complex Algorithms (Chemometrics)

Need Simple to Use Software

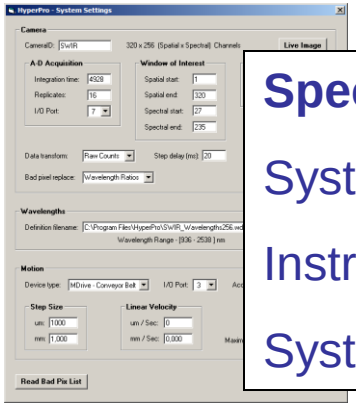
HyperPro HyperSee

The Hyperspectral Road



HCI Image Acquisition

Acquisition | Exploration | Training | Prediction



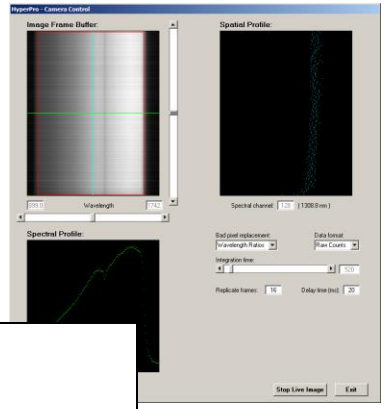
Camera Configuration

Spectroscopy:

System diagnostics

Instrument configuration

System calibration

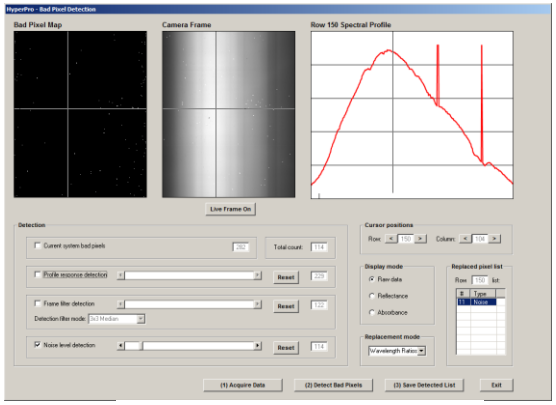


era Calibration

Hyperspectral:

Sample Motion Control

Bad Pixel Detection



Bad Pixel Detection

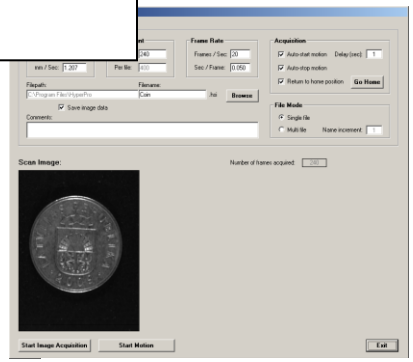
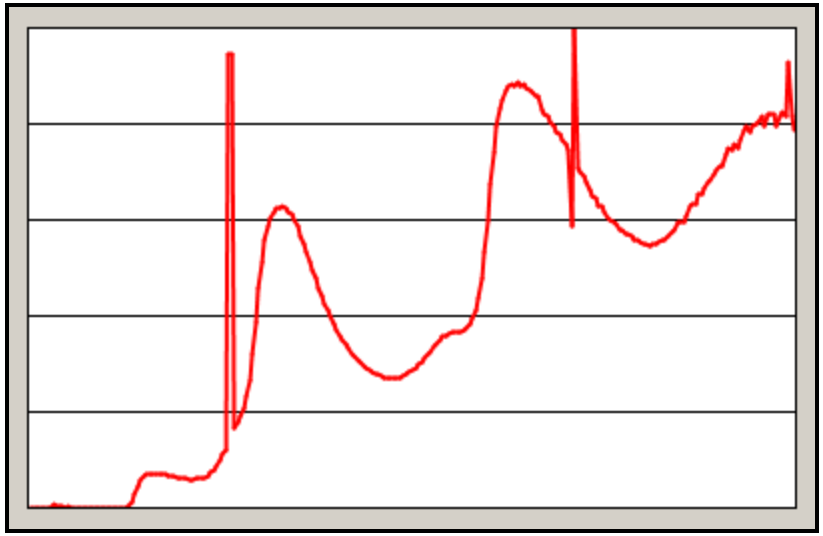


Image Acquisition

HCI Image Exploration

Acquisition | Exploration | Training | Prediction

Bad Pixels



Bad Pixels:

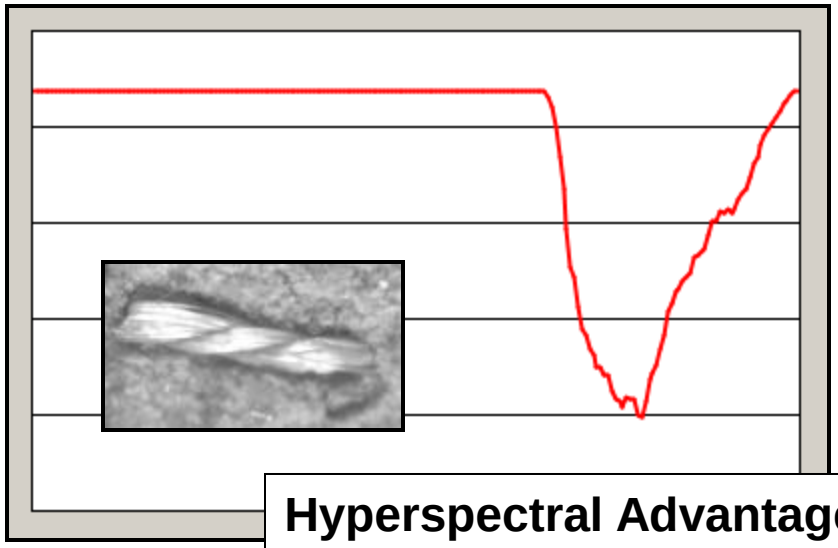
Linescan systems: Identify and replace

Staredown systems: Identify and throw out

HCI Image Exploration

Acquisition | **Exploration** | Training | Prediction

Pixel Saturation



Possible Causes

Specular reflection

Integration times

Reflectance calibration

Hyperspectral Advantage:

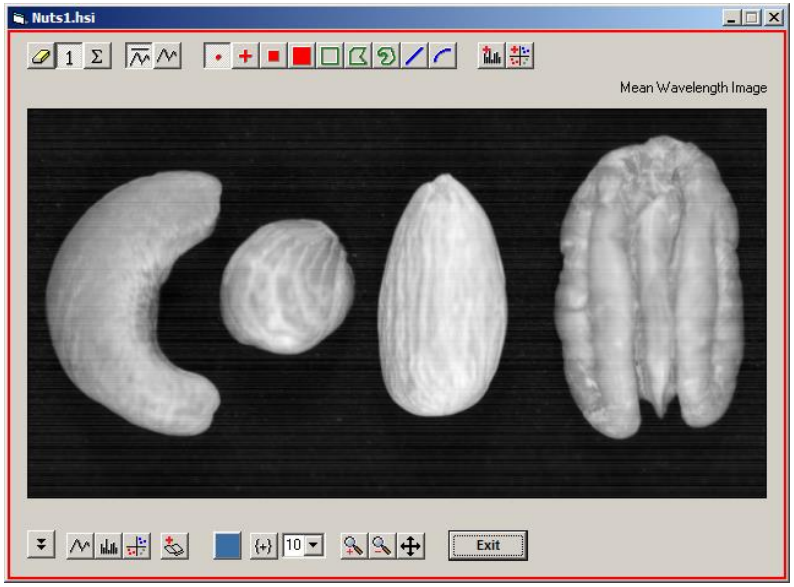
Identify problem data – throw it out! There is always plenty more to use.

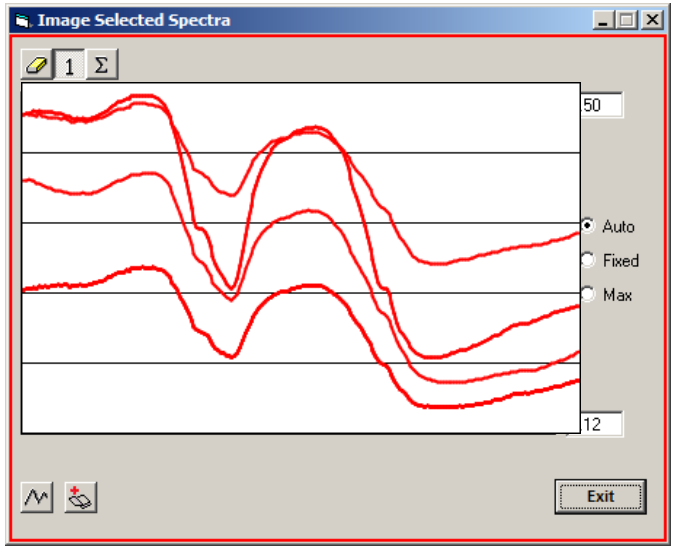
Large sample populations mean robust sample statistics.

HCI Image Exploration

Acquisition | **Exploration** | Training | Prediction

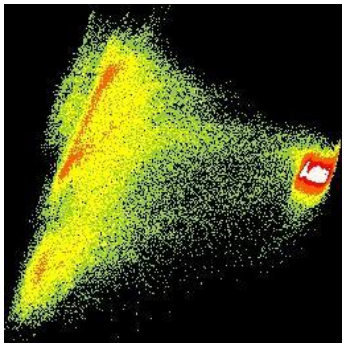
Mean Spectra – 4 Nut Types



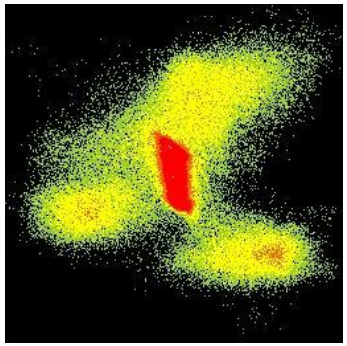


HCI Image Exploration

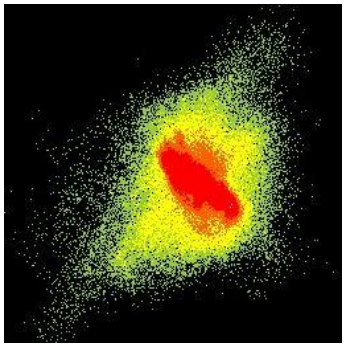
Acquisition | **Exploration** | Training | Prediction



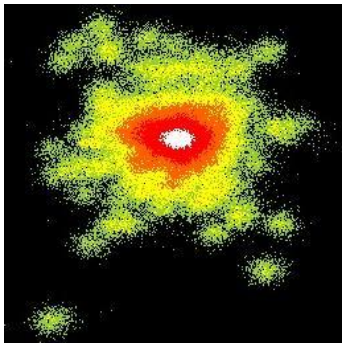
PC1 – PC2



PC2 – PC3



PC4 – PC5



PC8 – PC9

Score Plot Explorations:

Variance within class

Variance between classes

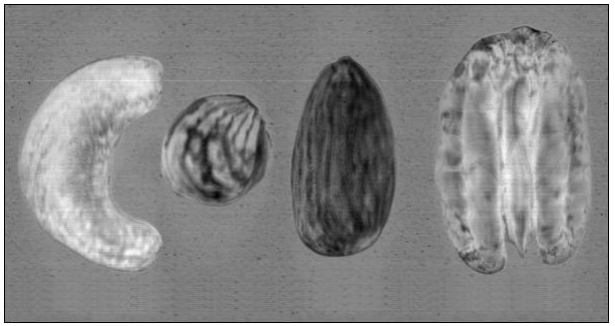
Number of dimensions (rank)

Chemical, physical, or instrument properties

HCI Image Exploration

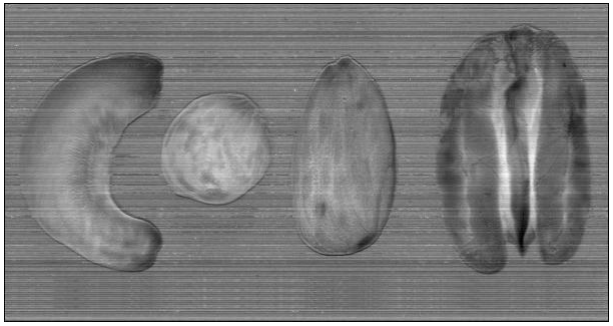
Acquisition | **Exploration** | Training | Prediction

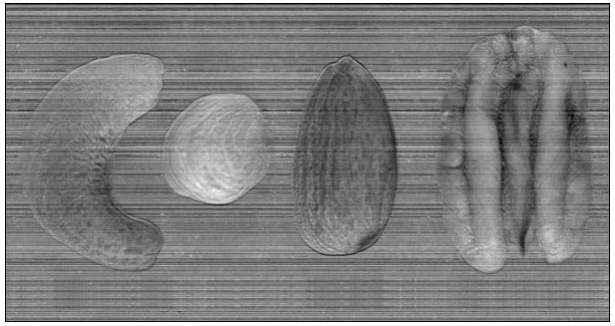
Mean Wavelength



PC2

PC5

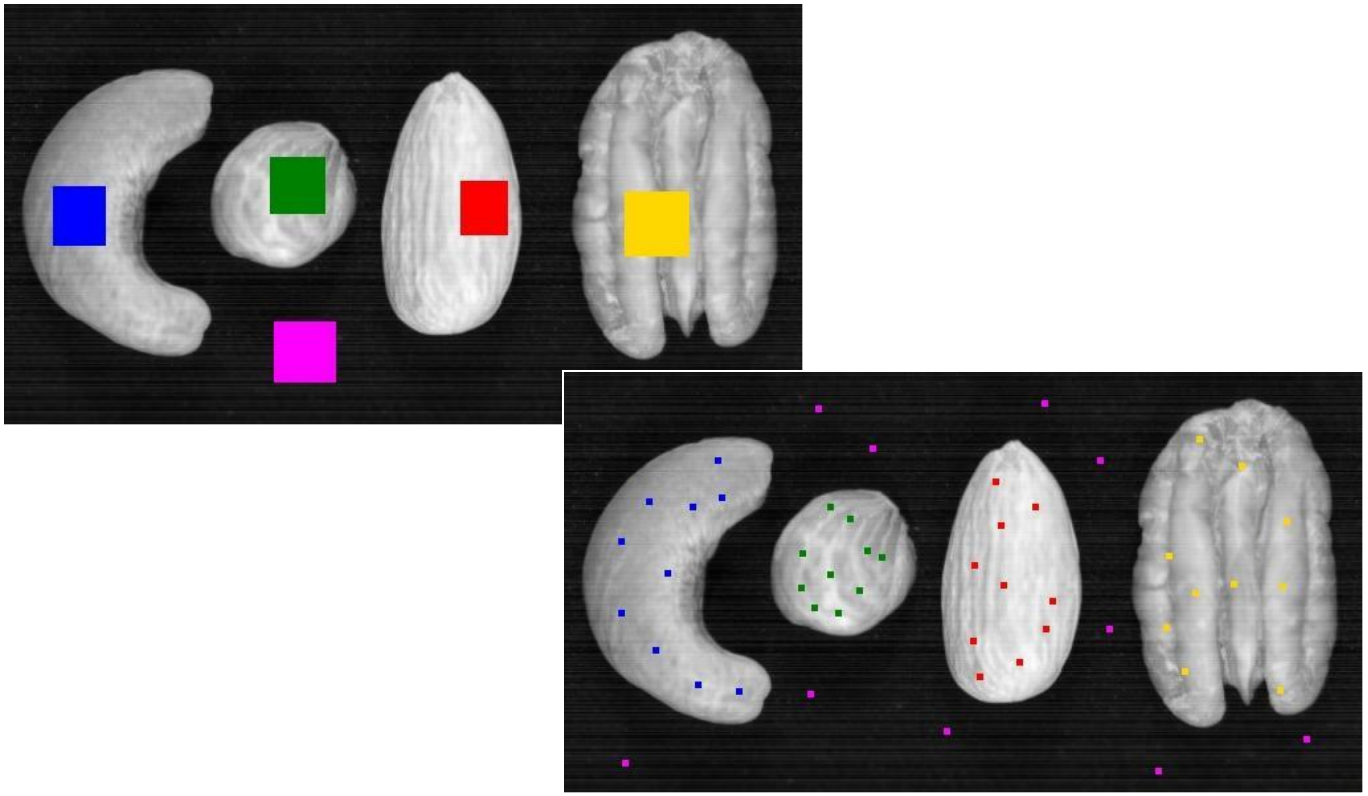




PC7

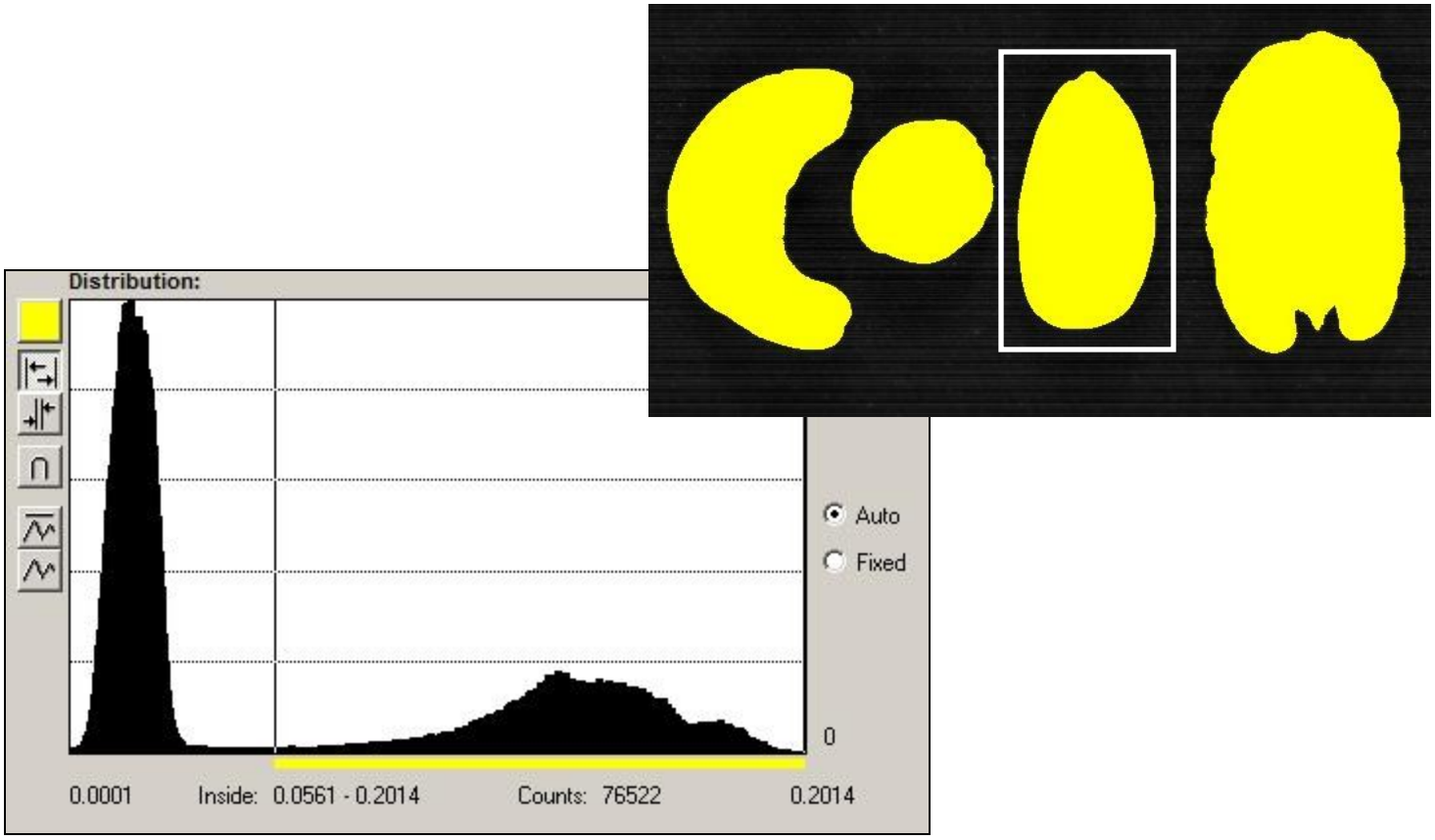
System Training

Acquisition | Exploration | **Training** | Prediction



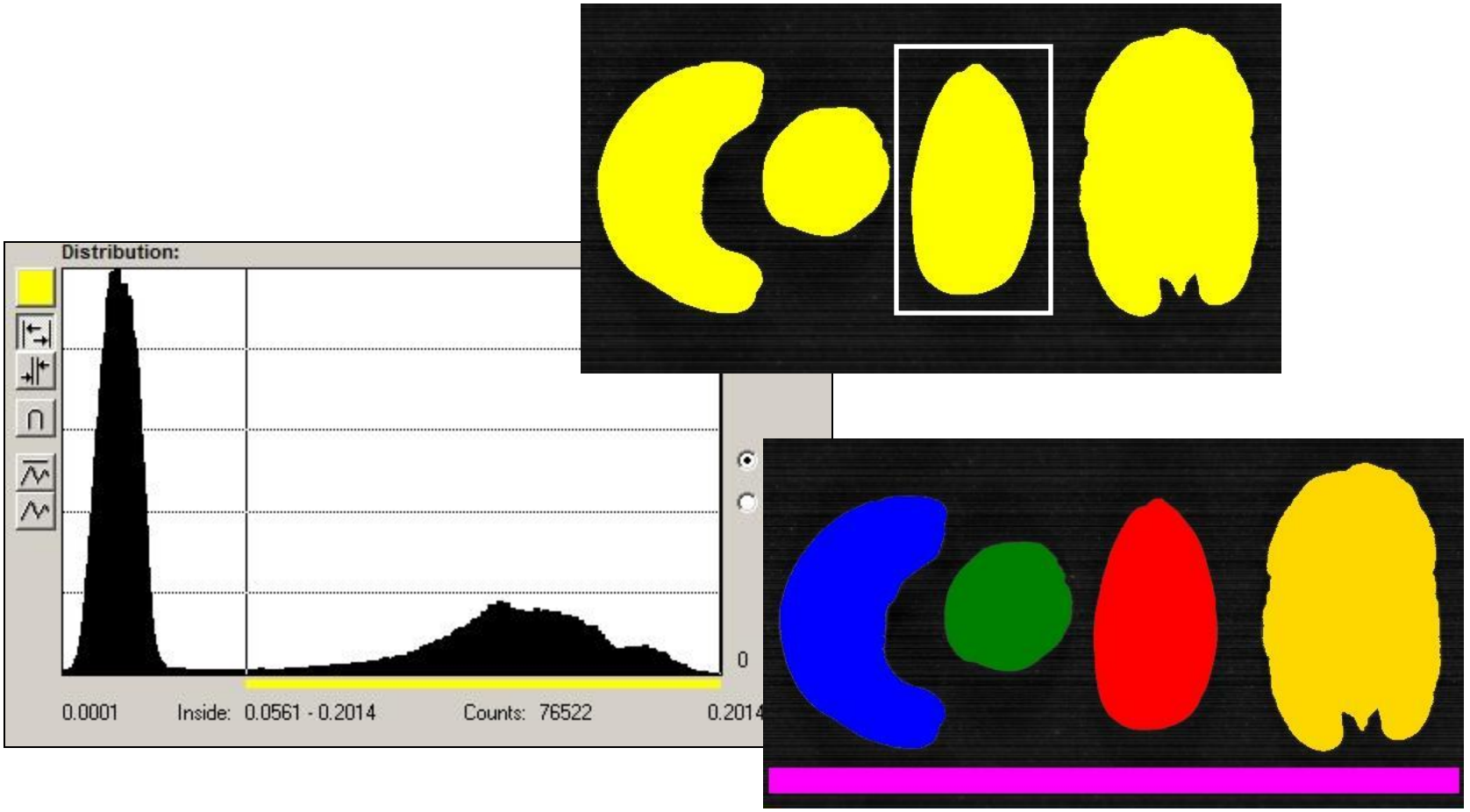
System Training

Acquisition | Exploration | Training | Prediction



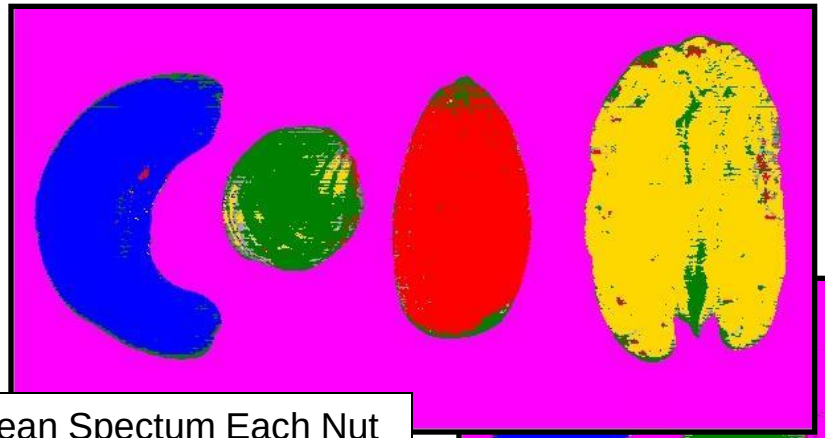
System Training

Acquisition | Exploration | Training | Prediction

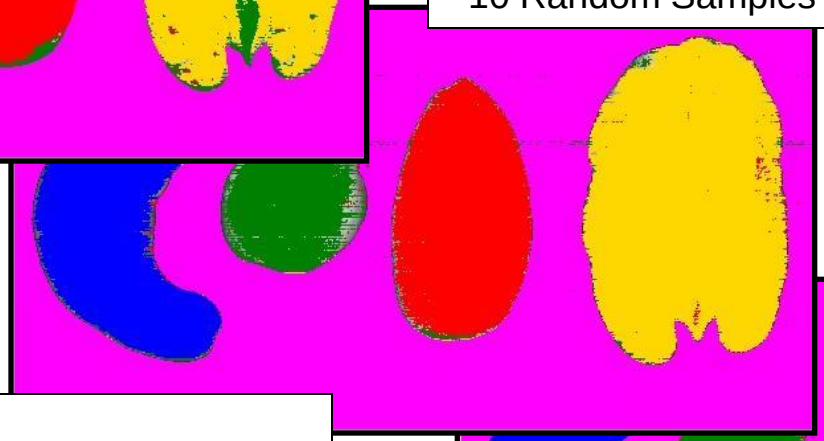


Model Predictions

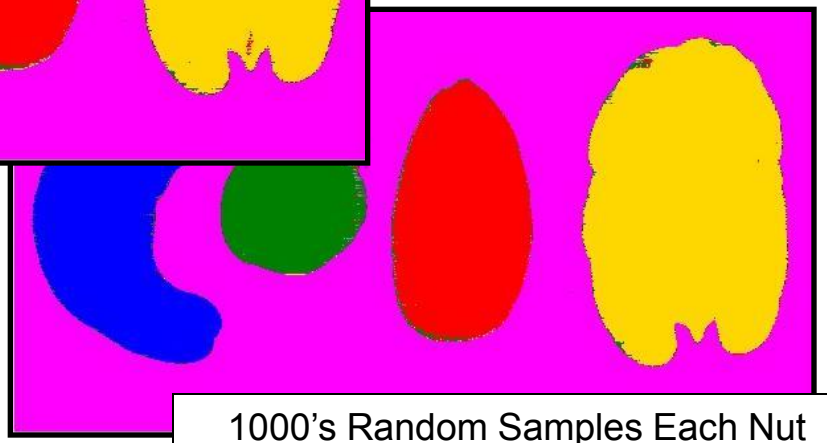
Acquisition | Exploration | Training | Prediction



Mean Spectum Each Nut



10 Random Samples Each Nut



1000’s Random Samples Each Nut

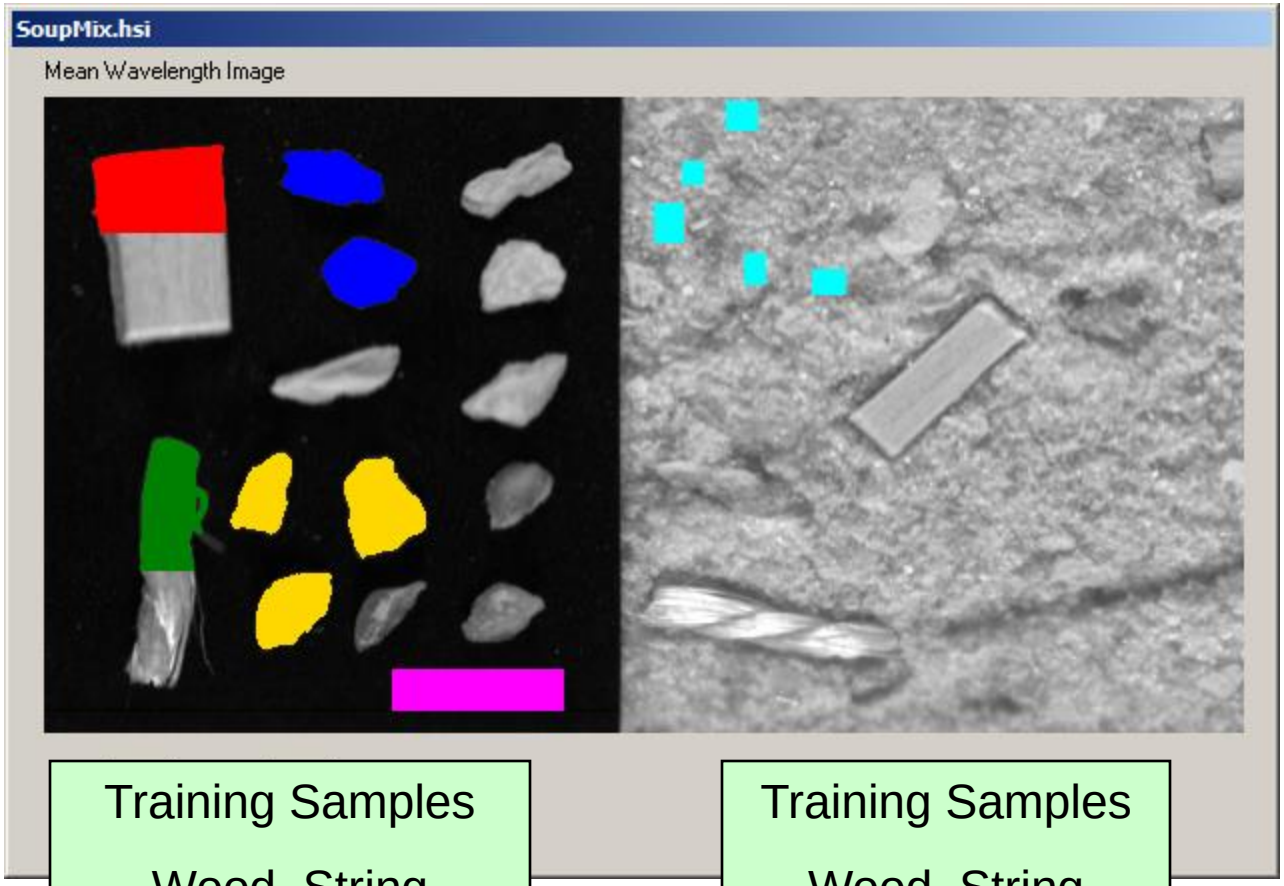
Model Performance:

Include sample variance in training

Validate by visual inspection

Food Contaminant Example

Dried Soup Mix



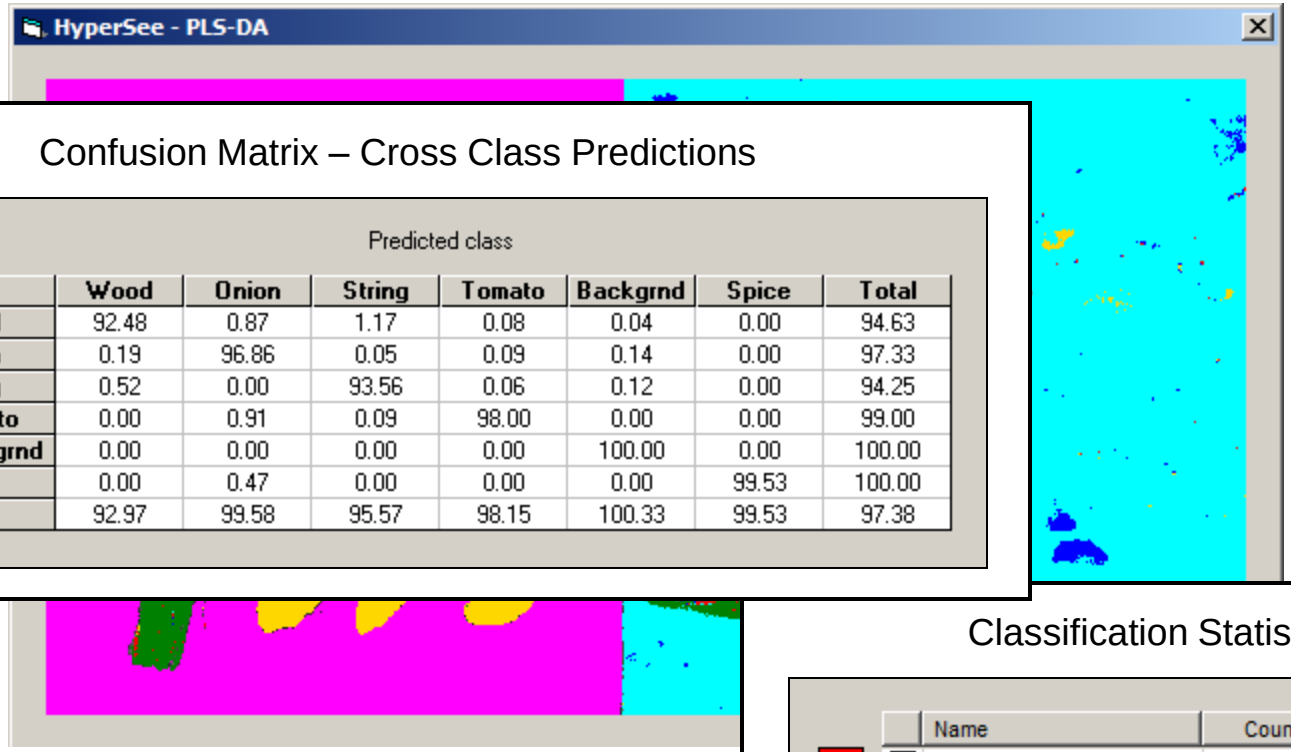
Training Samples

Wood, String
Onions, Tomatos

Training Samples

Wood, String
Spice Powder

Image Prediction



Confusion Matrix – Cross Class Predictions

Predicted class

Correct class	Wood	Onion	String	Tomato	Backgrnd	Spice	Total
Wood	92.48	0.87	1.17	0.08	0.04	0.00	94.63
Onion	0.19	96.86	0.05	0.09	0.14	0.00	97.33
String	0.52	0.00	93.56	0.06	0.12	0.00	94.25
Tomato	0.00	0.91	0.09	98.00	0.00	0.00	99.00
Backgrnd	0.00	0.00	0.00	0.00	100.00	0.00	100.00
Spice	0.00	0.47	0.00	0.00	0.00	99.53	100.00
Total	92.97	99.58	95.57	98.15	100.33	99.53	97.38

Classification Statistics

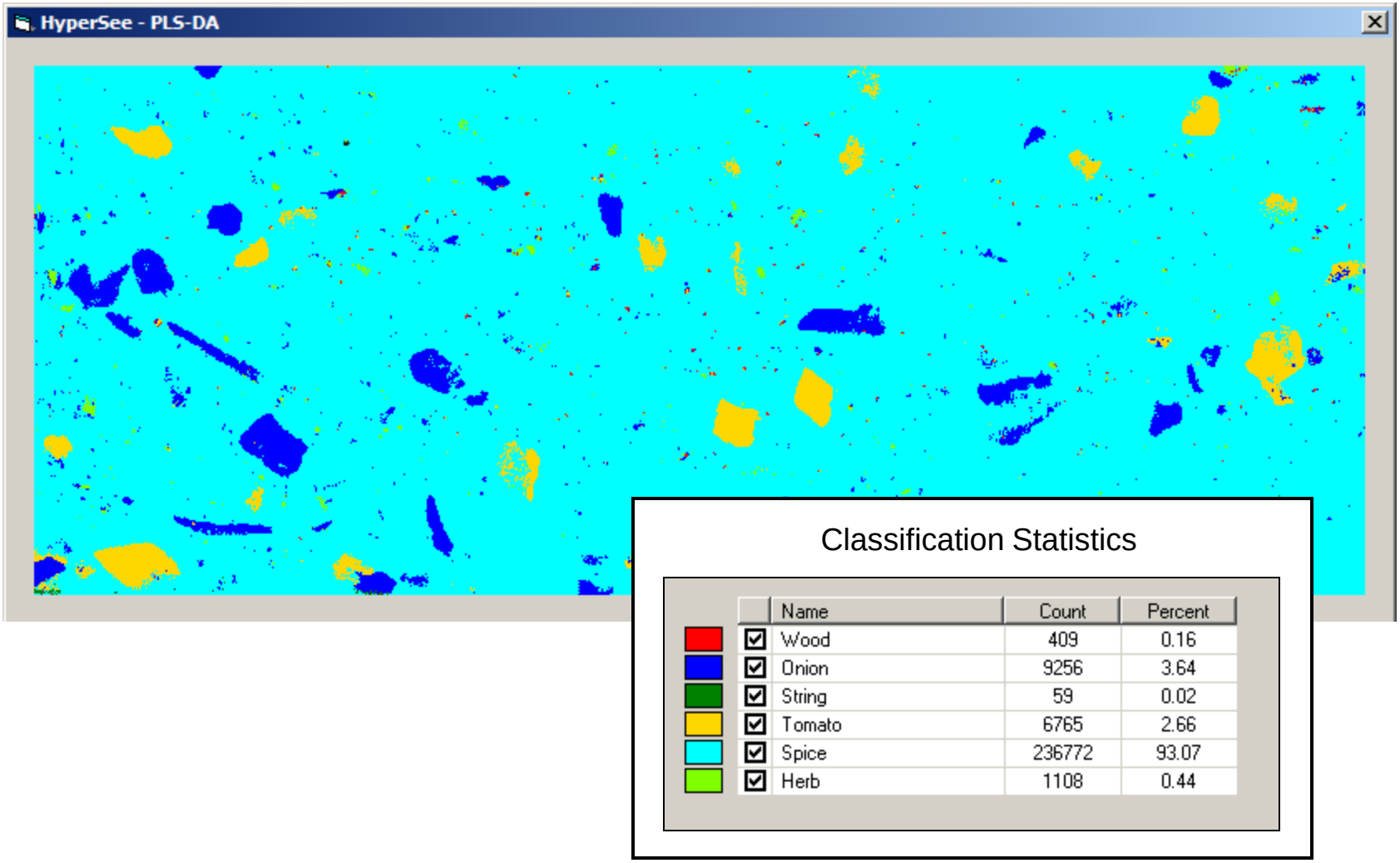
Name	Count	Percent
Wood	7909	4.15
Onion	8566	4.49
String	4758	2.49
Tomato	6438	3.37
Backgrnd	69392	36.37
Spice	92525	48.49

Test Image Predictions

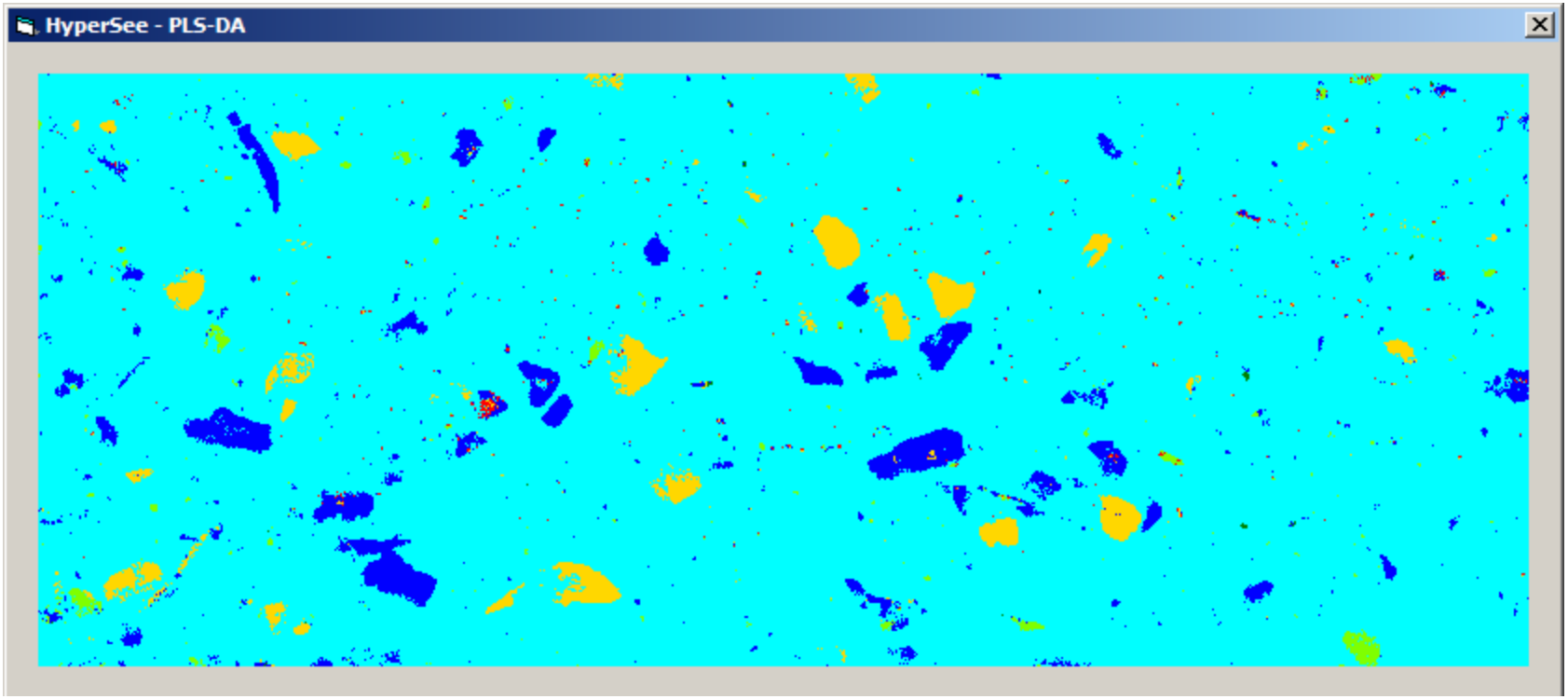
3 Independent Images / 600 lines

Classify and monitor production levels of ingredients

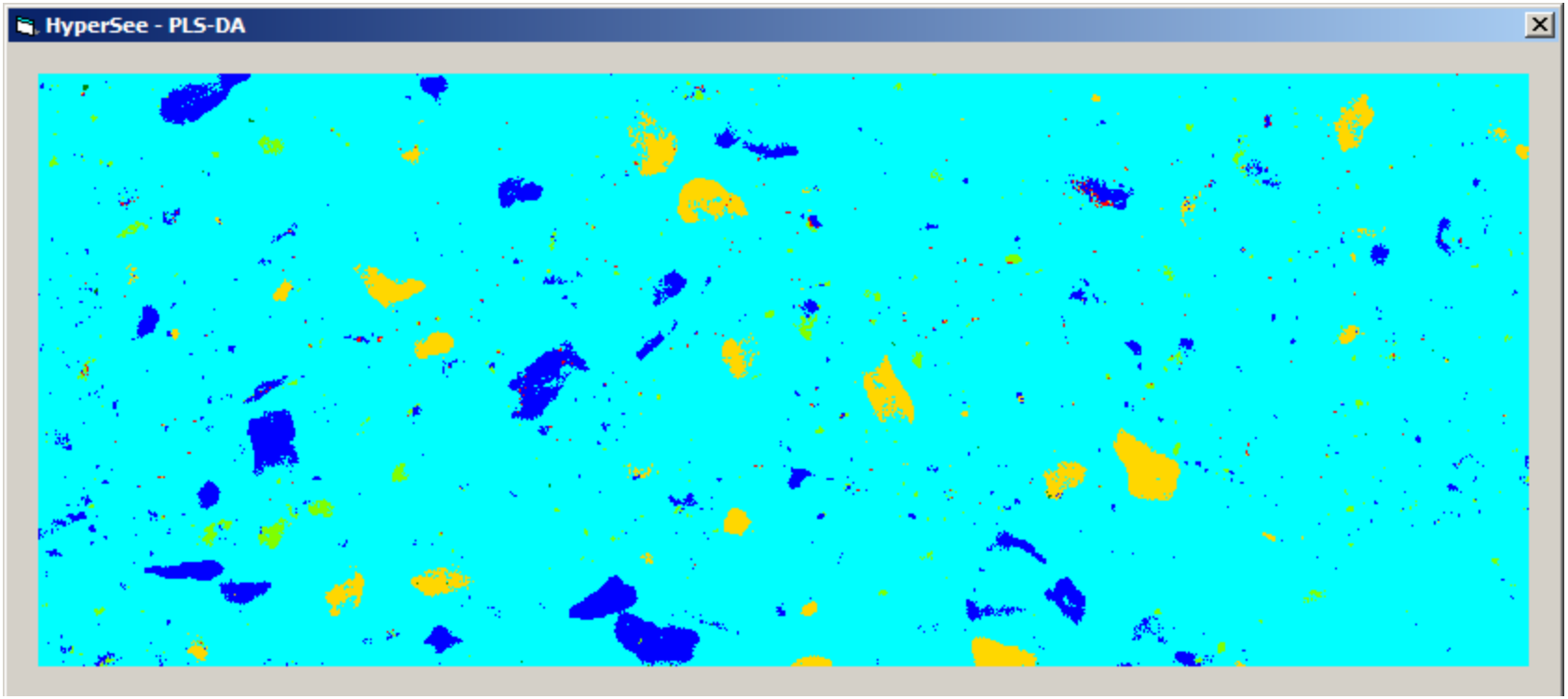
Process Control Images



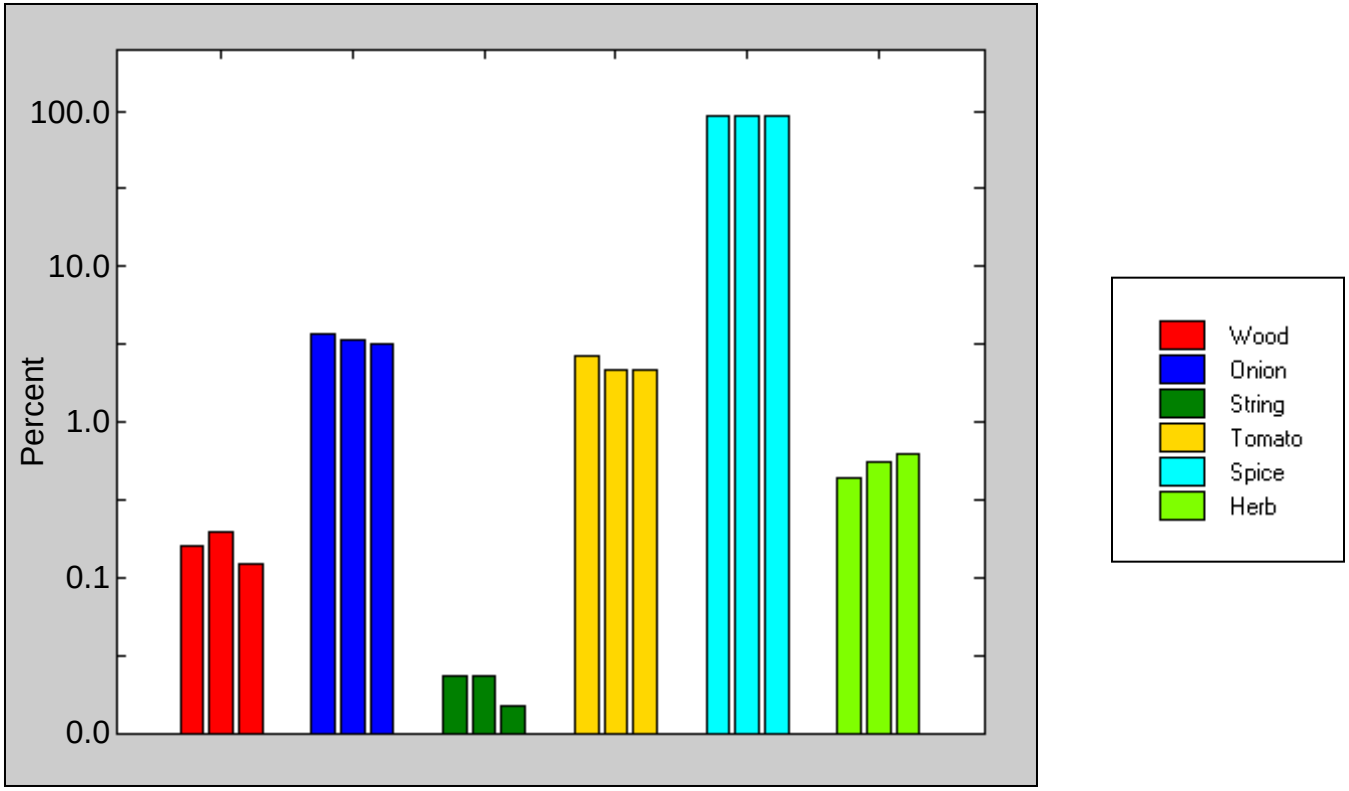
Process Control Images



Process Control Images

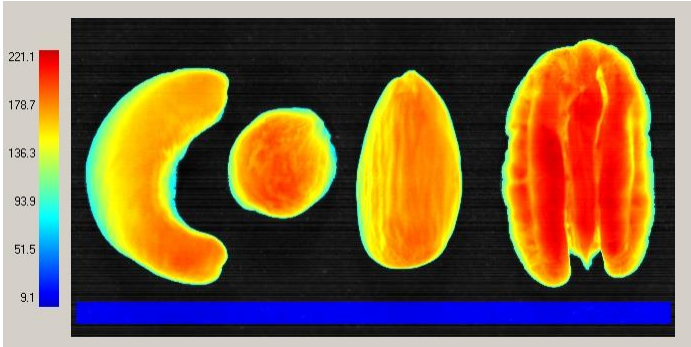


Predictions From Replicate Images

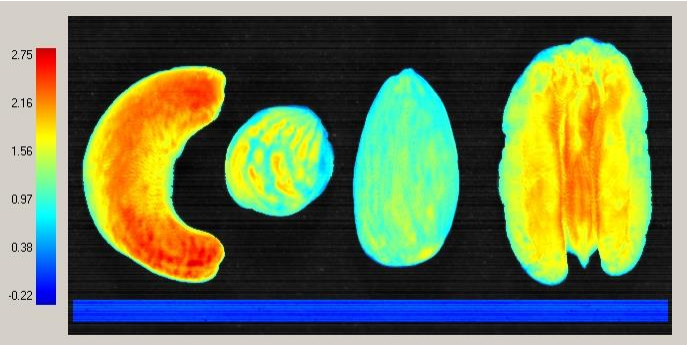


Quantitative Analysis

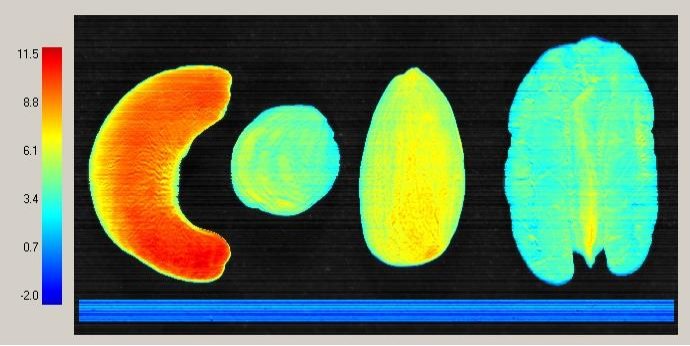
Quantitative Predictions



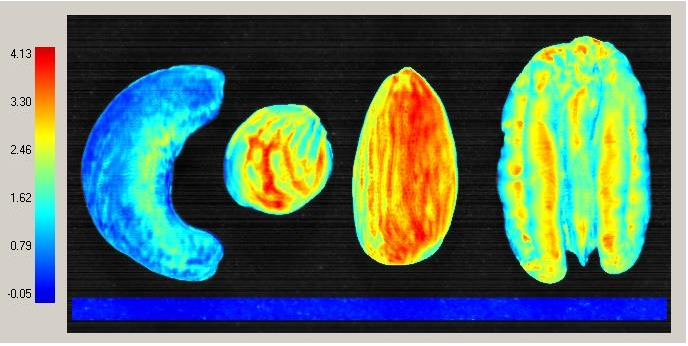
Total Calories



Saturated Fat



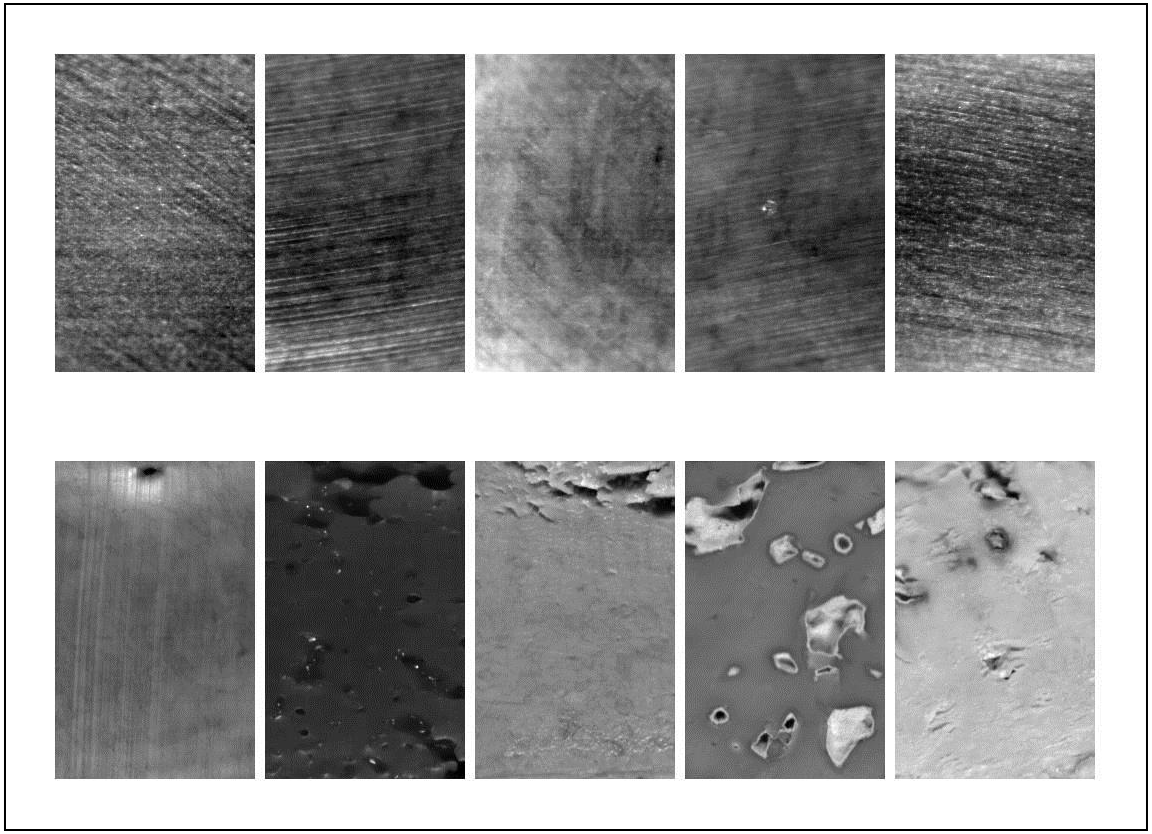
Total Carbohydrates



Fiber

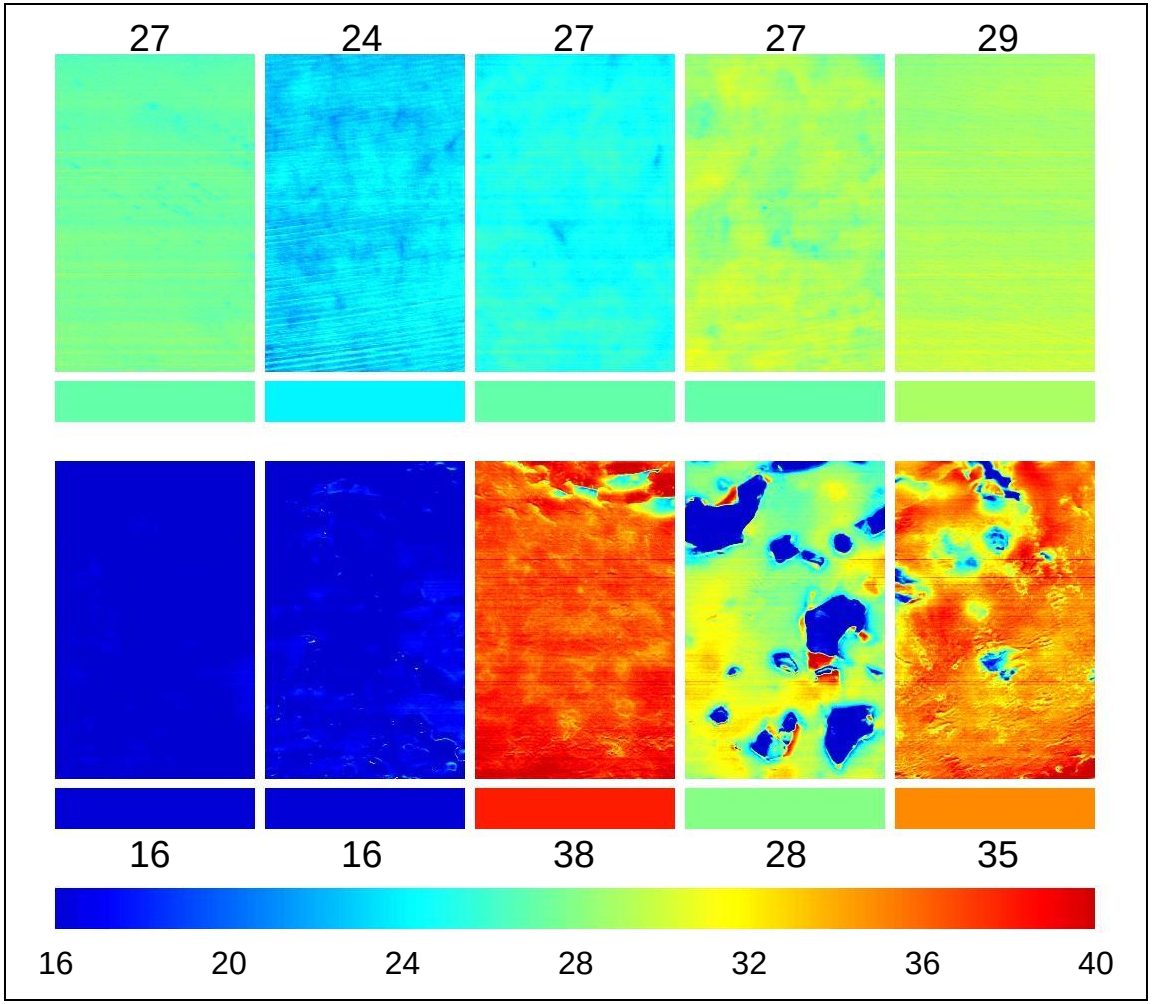
4 reference values with 4 samples = poor model

Cheese Fat Content



12 reference values with 12 samples = better model

Target Cheese Fat %

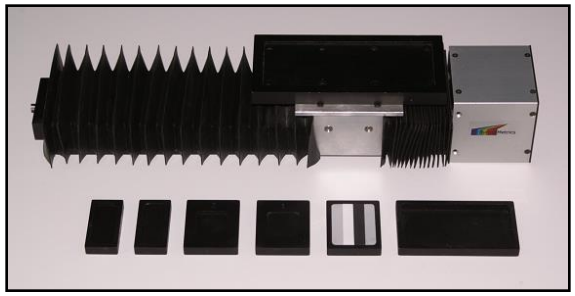


HyperPro

Customized Hyperspectral
Imaging Hardware Solutions

NIR System (960 – 1660 nm)

SWIR System (1100 – 2450 nm)



Linear Stage

Mini - Conveyor

Conclusions…

- Visual data (images) needs visual tools
- Massive amounts of data:
  - Need powerful interactive tools to explore and analyze
  - Selectively exclude data (saturation, bad pixels, background)
  - Include sample variance (many spectra) – more robust calibration models
- Spatial information
  - Uniformity of sample distributions
  - Particle sizes
- Increased sensitivity
- Unlimited scale of applications…
  - Almost any NIR application, plus spatial information!!!

THANK YOU !