

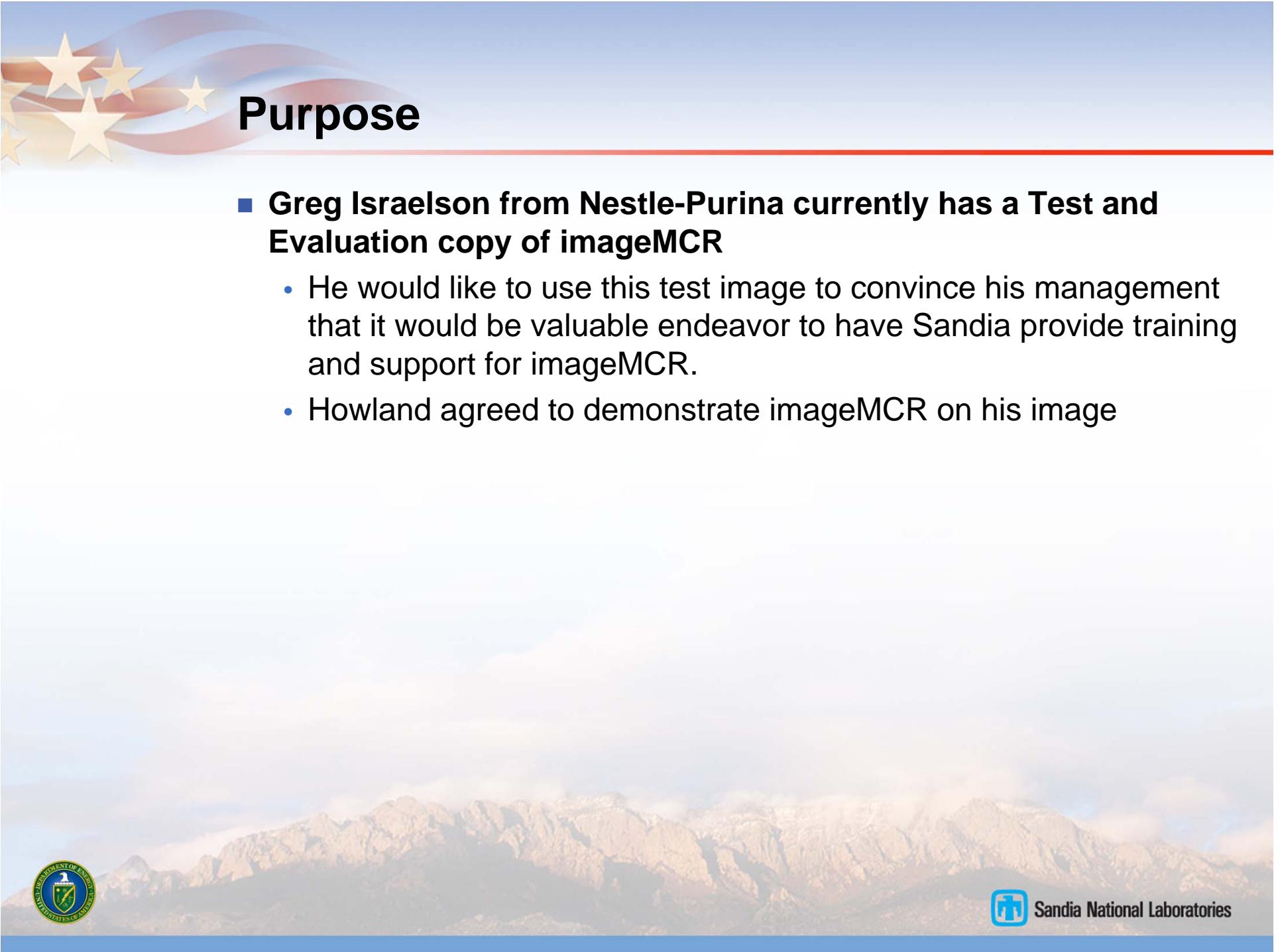
# **Test Image Sample from Nestle-Purina**

**Testing Sandia's imageMCR**

**Howland Jones, 01/31/2012**



**Sandia National Laboratories**



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# A single unknown test image is not ideal

- I get this request frequently and I enjoy the challenge, but this is not the preferred route for analyzing hyperspectral images
  - Although MCR, in general, does not require *a-priori* information about the spectral data, it does help
  - The MCR algorithms are generally helped by the following:
    - Initiating the MCR analysis with spectral components that are suspected to be in the hyperspectral image
      - **Experimentally obtain pure spectral components of suspected components**
      - **Spectral libraries**
        - Build upon your library each time you identify a new component
        - Use the library for future analyses
    - Understanding your instrument noise and spectral artifacts
      - **Recognizing the noise and artifacts will prevent confusion whether or not the spectral component is truly in the sample**
    - Increasing the number of images to analyze (imageMCR can analyze multiple images at a time)
      - **Helpful for completely unknown sample images**
      - **MCR requires that the spectral components be linearly independent**
      - **The more looks at a particular sample will increase your odds that the spectral components vary independently (e.g., different samplings of the same lot of material)**
- With all of that said, here are my results



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# Information about sample image from Greg

Analysis: As received at the laboratory, this sample was identified as "Poultry Meal 183". A visual examination showed the sample had a medium grayish brown color and a very off odor which may indicate that the original raw material was badly decomposed.

A further microscopic examination of the sample showed that it contained:

- 1) Significant number of rounded clear and some black irregularly shaped beads of unidentified material
- 2) Significant number of unidentified clear irregularly shaped crystals
- 3) A number of charred/burned particles of what appear to be pieces of muscle tissue
- 4) Low trace amount of sunflower seed hulls
- 5) Wheat midds and other unidentified extraneous plant material
- 6) A small number of unidentified animal hairs (identification of origin would require further investigation)

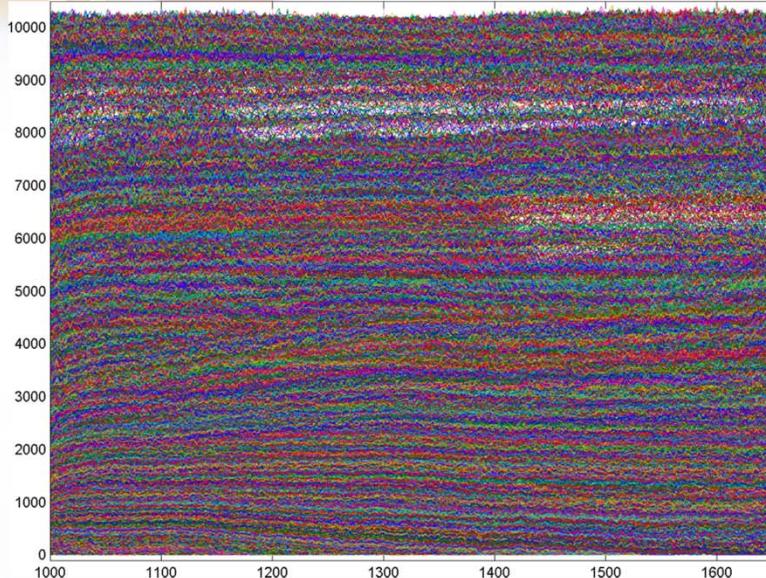
This sample showed a positive qualitative test for urea, indicating that it contained a significant amount of urea. A Chloroform flotation of the sample showed that, by weight, it contained approximately 86.8% organic material (meat/tissue, etc.) and 13.2% inorganic material (mineral/bone, etc.). If this sample is, in fact, poultry meal, than it is of very poor quality.

Beads

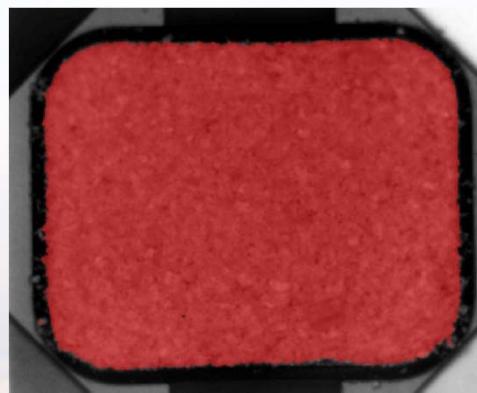
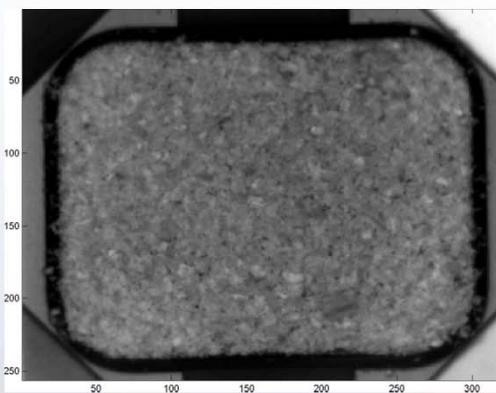
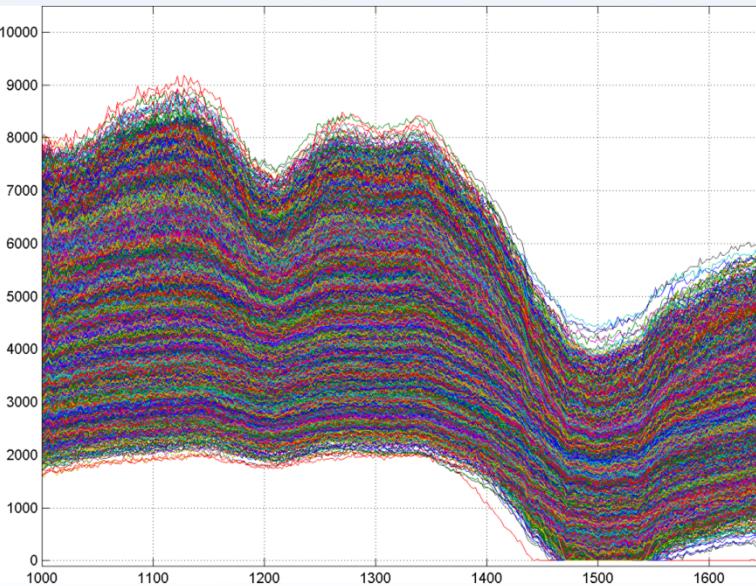


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Data from entire image



Data from only the sample region  
(red shaded in image below)

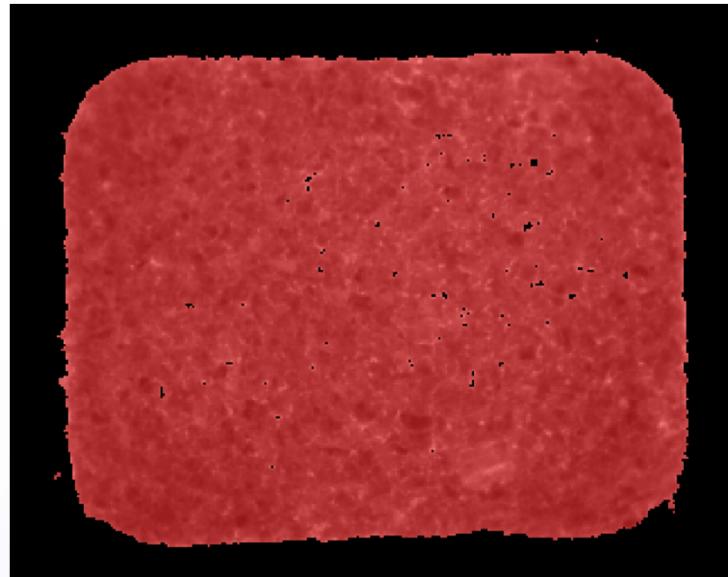
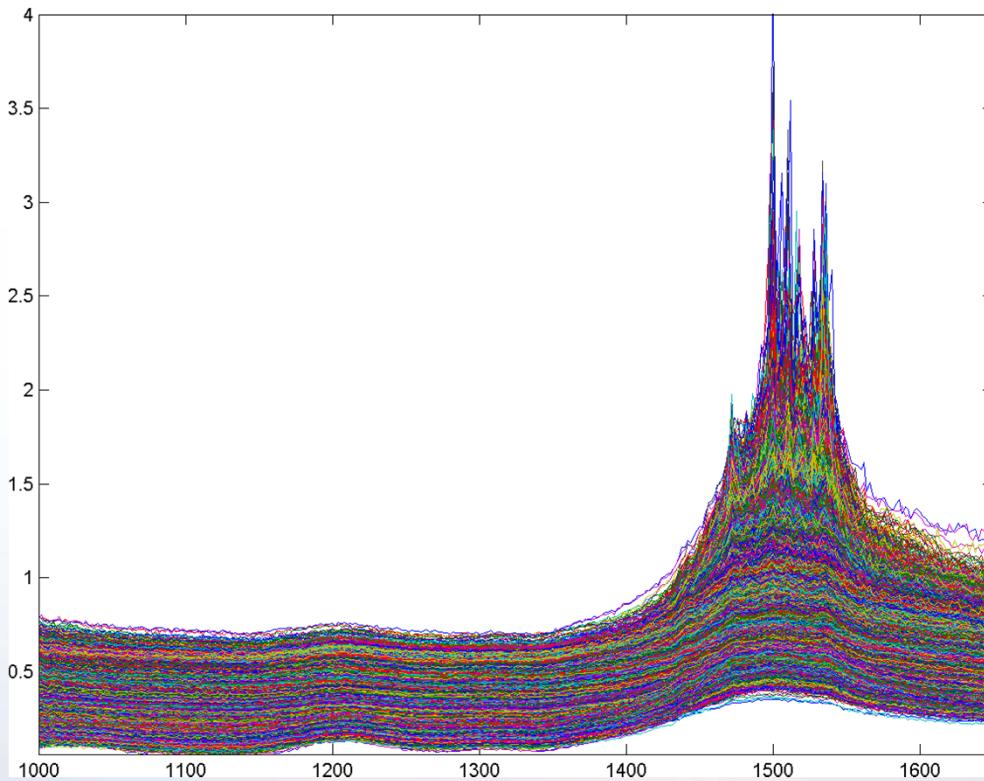


Notice that there  
are several  
spectra that  
bottom out at  
zero. I removed  
these from the  
analyses.



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# Log10(1/R) image data



Notice the several spectra that I removed (black specks amongst the red mask).

Initially I also removed the highly absorbing spectra above 1.5 to get less noisy spectral components. Applied these spectral components to the entire data set.



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# imageMCR Screenshot

imageMCR, Version092711,1.0

**File Management**

File Path to Save Results: C:\Data\Hyperspectral Imager Data\Nestle\

Data Filename: NewAbs4\_183-x.s3d

Output Filename: NewAbs4\_183-x,12.out

Xaxis Filename: 183\_newxaxis.mat

Increment Output Filename

Analysis Summary, Preprocess, RCF, ExptDetails, Generate Xaxis, Output Normalization Method (Max Peak)

**ROI Parameters**

Mask: Spatial Mask, View, Pixel Selection

Rows: [1:256], Trace(s): [0]

Columns: [1:320], Channels: [1:350]

**Initialization Values**

Starting Pure Components: 7 stPCs, Make stPCs

Starting Concentrations: No stConcs, Make stConcs

Initialization Normalization Method: Unit Length

**SandiaMCR Parameters**

1) Analysis Type: 33

2) Channels Compression Factor: 1

3) Columns Compression Factor: 1

4) Depths Compression Factor: 1

5) Rows Compression Factor: 1

6) Upsampling: 0

7) Weighting: 0

8) Baseline Correction: 0

9) Use Double Precision Binary Combinations: 0

10) Convergence Criteria: 0

11) Number of Factors to use for Data: 64

12) End MCR: 1

13) Normalize Spectral Equality Constraints: 0

14) Final Scale: 0

15) First Channel: 1

16) Initial Values: 3

17) Last Channel: 350

18) Maximum Iterations: 50

19) Maximum Eigenvalues Calculated: 64

20) Starting Point For Auto Npures: 0

21) Non-negativity Concentrations: 1

22) Non-negativity Spectra: 1

23) Number of Pures: 7

24) Use Compressed File: 0

25) Multiplier for Concentration Bias Correction: 0

26) Multiplier for Spectral Bias Correction: 0

27) Number Of Residual Factors: 6

28) Weighted Residuals: 0

29) Output Scores and Loads: 1

30) Sort by Significance: 0

Change Default Settings, Weighting Options, Required Inputs, Typical Inputs, Defaults

**Constraints**

Spectral Equality: 7 Constraints, Constrain PCs

Concentration Equality: No Constraints, Constrain Concs

Spectral Non-Negativity: No Negative PCs, Unconstrain PCs

Concentration Non-Negativity: No Negative Concs, Unconstrain Concs

Spectral Unimodality: No Constraints, Constrain PCs

Concentration Unimodality: No Constraints, Constrain Concs

**Plotting Parameters**

Residuals: SandiaMCR Unweighted, Select Plots, Update Figures

Filenames, Plot Types

Line Plots, Plot Trace: NA, Rotate Images, Auto Plot Trace, Close Figures

**Comments**

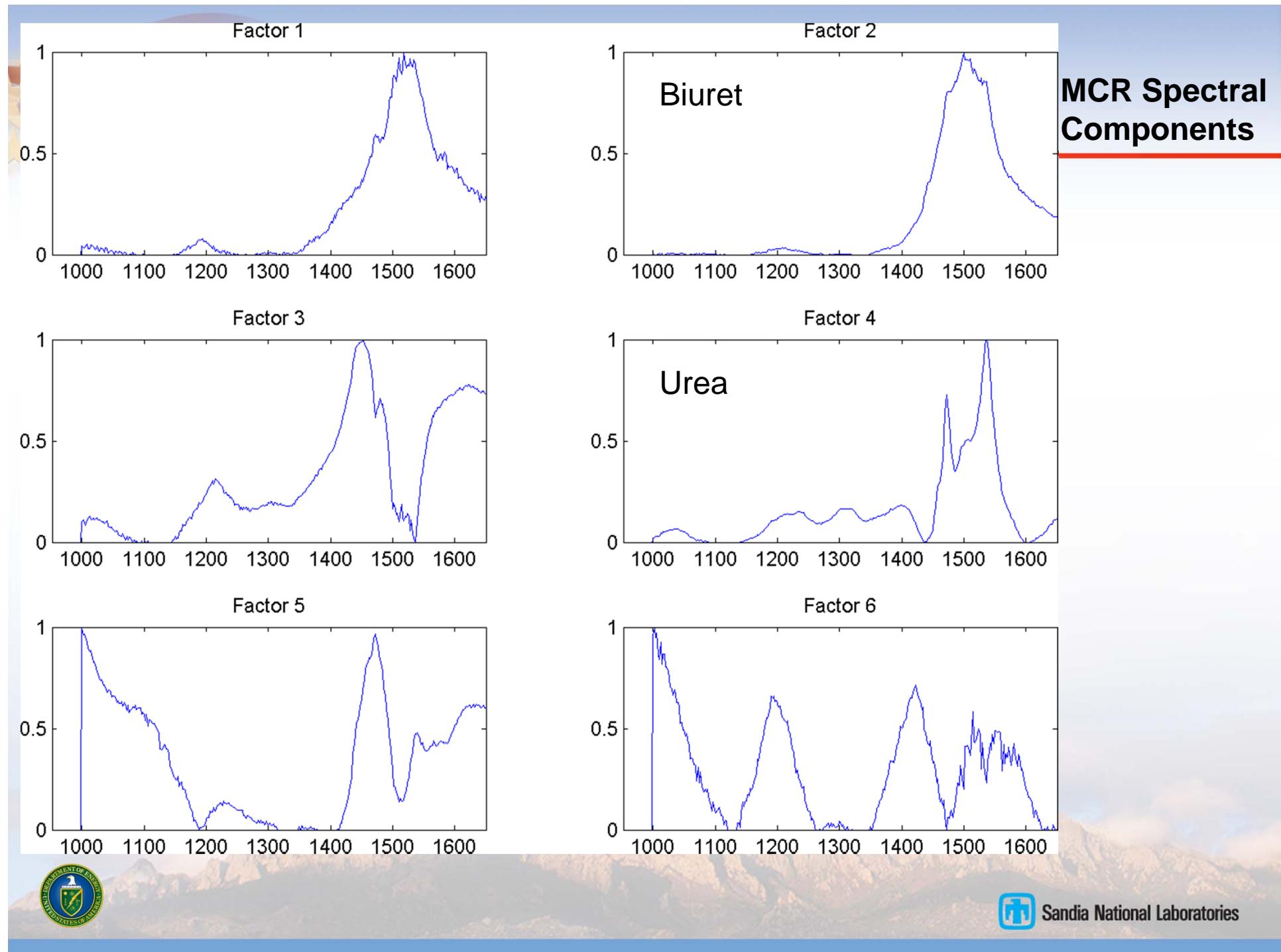
Spectral components applied to entire image (minus the spectra that bottom out to zero)

**Buttons**

Get Settings, Run Analysis, Run Batch, Save Settings, Plot Results, Exit

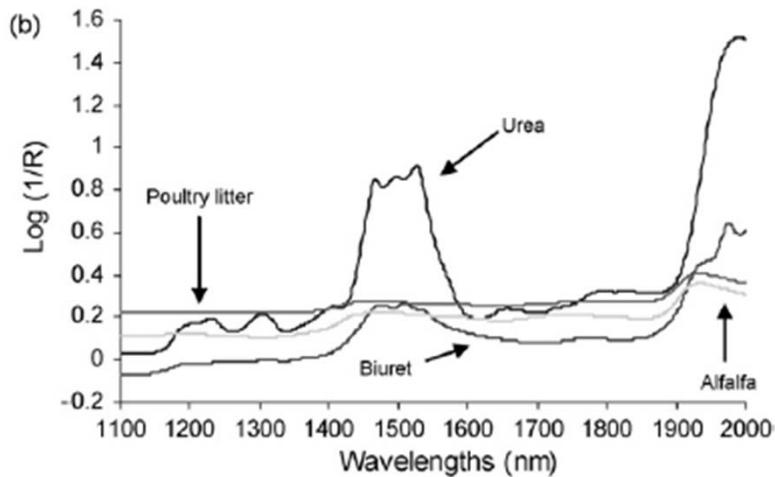


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Did a search to see what the urea spectrum looks like and this is what I found, therefore I think factor 2 is biuret and factor 4 is urea. I can't identify the others.

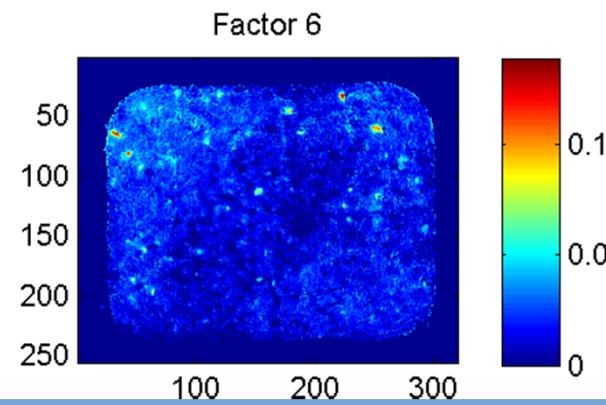
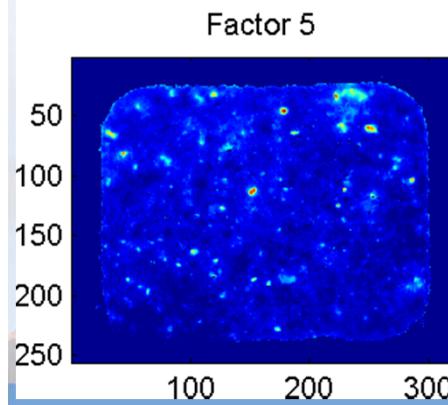
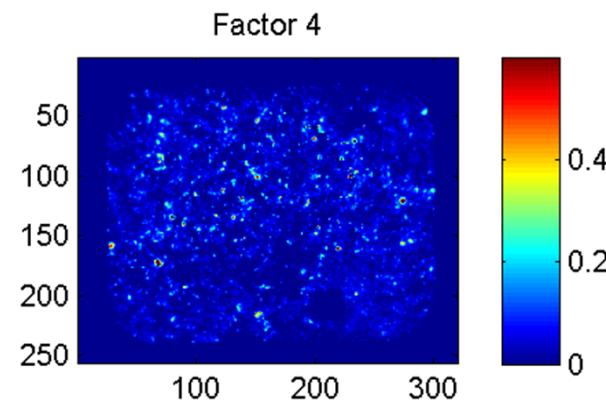
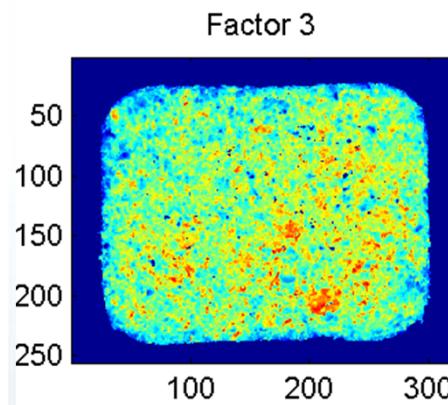
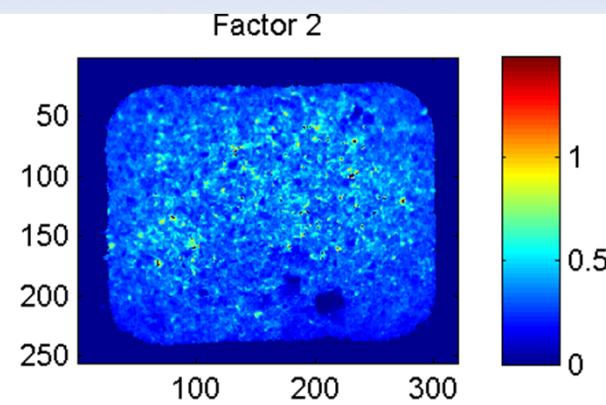
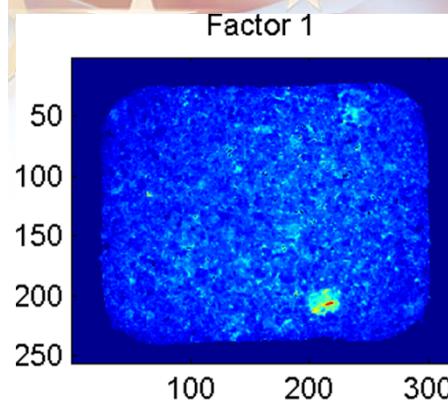


González-Martín, J.M. Hernández-Hierro,  
Detection and quantification of additives  
(urea, biuret and poultry litter) in alfalfas by  
nir spectroscopy with fibre-optic probe,  
Talanta, 76 (2008) 1130-1135.



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# MCR Concentration Maps



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