

Test Image Sample from Nestle-Purina

Testing Sandia's imageMCR

Howland Jones, 01/31/2012





Purpose

- **Greg Israelson from Nestle-Purina currently has a Test and Evaluation copy of imageMCR**
 - He would like to use this test image to convince his management that it would be valuable endeavor to have Sandia provide training and support for imageMCR.
 - Howland agreed to demonstrate imageMCR on his image



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



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)

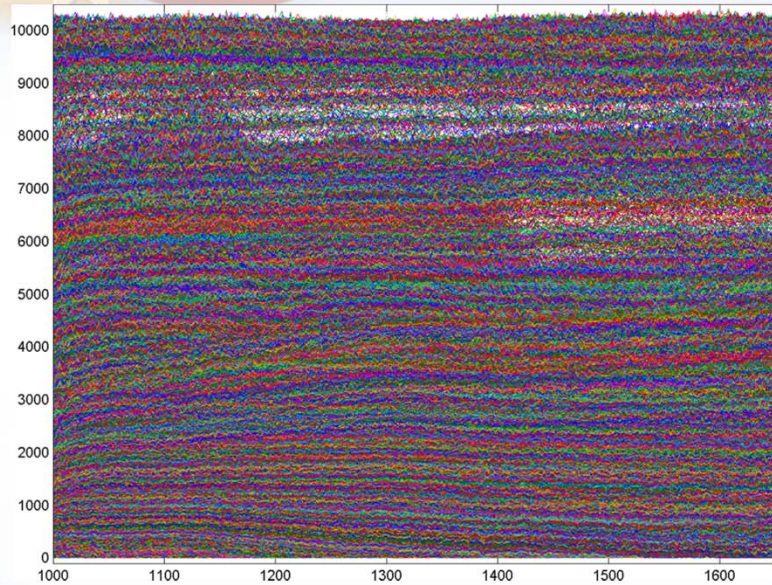
This sample showed a positive qualitative test for urea, indicating that it contained a significant amount of urea. A Chloroform flotation of the sample showed that, by weight, it contained approximately 86.8% organic material (meat/tissue, etc.) and 13.2% inorganic material (mineral/bone, etc.). If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

Beads

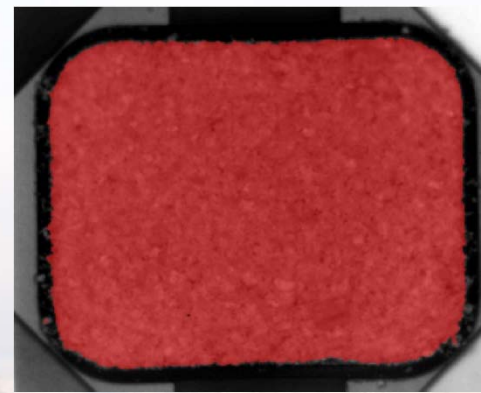
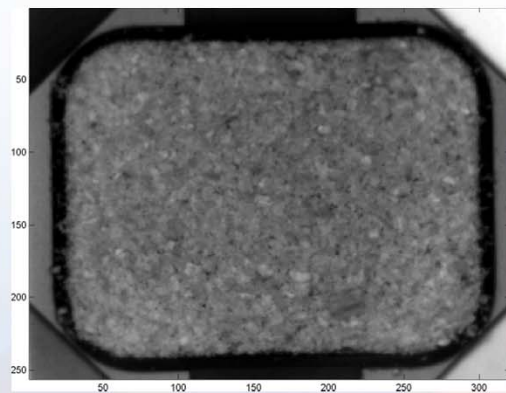
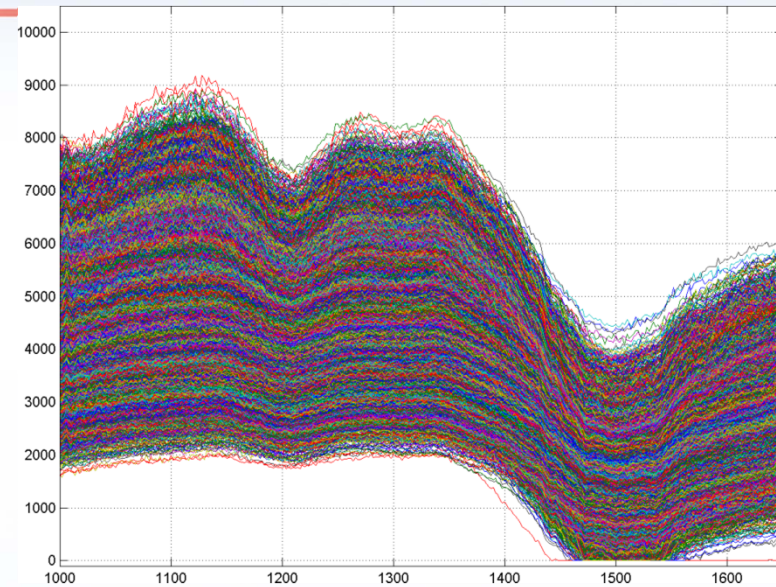


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Data from entire image



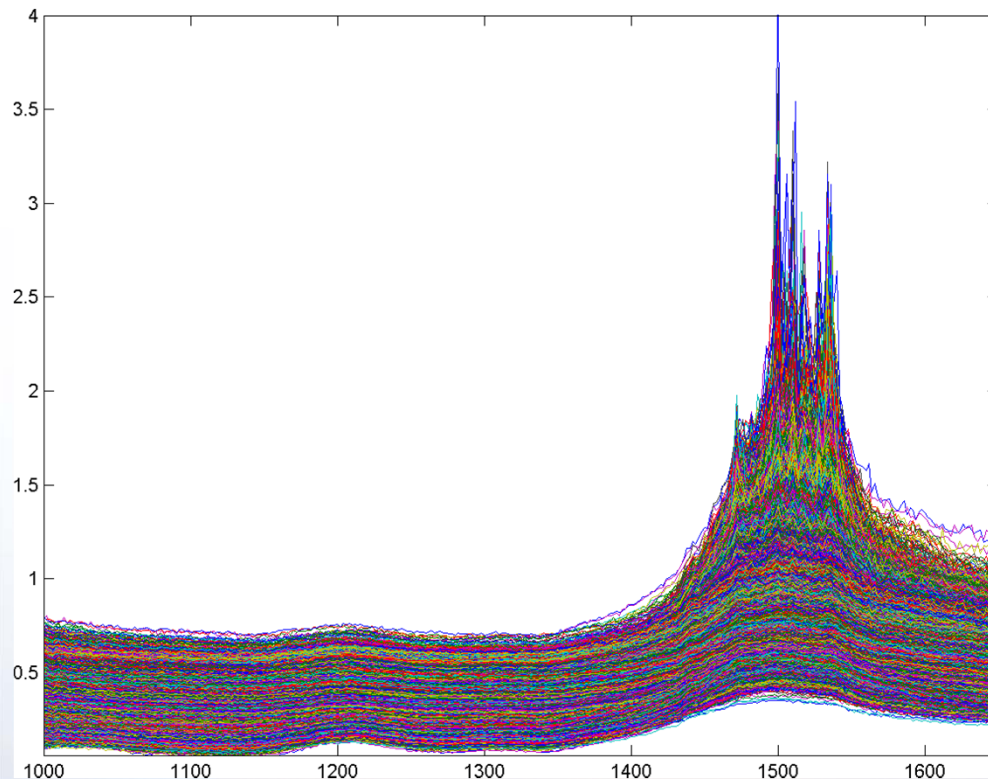
Data from only the sample region
(red shaded in image below)



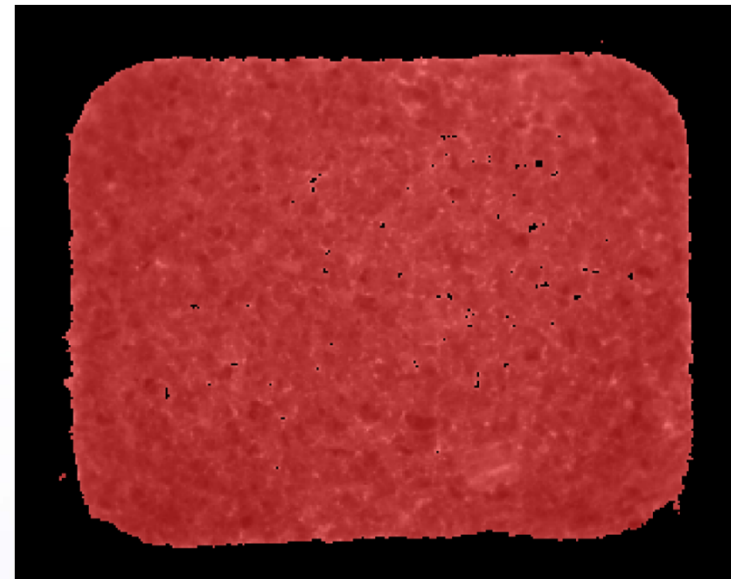
Notice that there are several spectra that bottom out at zero. I removed these from the analyses.



Log10(1/R) image data



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.



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



imageMCR Screenshot

imageMCR, Version 092711.1.0

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

Output Normalization Method: Max Peak

Analysis Summary

Preprocess

RCF

ExptDetails

Generate Xaxis

ROI Parameters

Mask: Spatial Mask

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

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

View

Pixel Selection

Initialization Values

Starting Pure Components: 7 stPCs

Starting Concentrations: No stConcs

Initialization Normalization Method: Unit Length

Make stPCs

Make stConcs

SandiaMCR Parameters

Change Default Settings

Required Inputs

Typical Inputs

Weighting Options

Defaults

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

Constraints

Spectral Equality: 7 Constraints

Concentration Equality: No Constraints

Spectral Non-Negativity: No Negative PCs

Concentration Non-Negativity: No Negative Concs

Spectral Unimodality: No Constraints

Concentration Unimodality: No Constraints

Constrain PCs

Constrain Concs

Unconstrain PCs

Unconstrain Concs

Constrain PCs

Constrain Concs

Plotting Parameters

Residuals: SandiaMCR Unweighted

Select Plots

Update Figures

FileNames

Plot Types

Line Plots

Rows

Columns

Plot Trace: NA

Auto Plot Trace

Rotate Images

Close Figures

Comments

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

Get Settings

Run Analysis

Run Batch

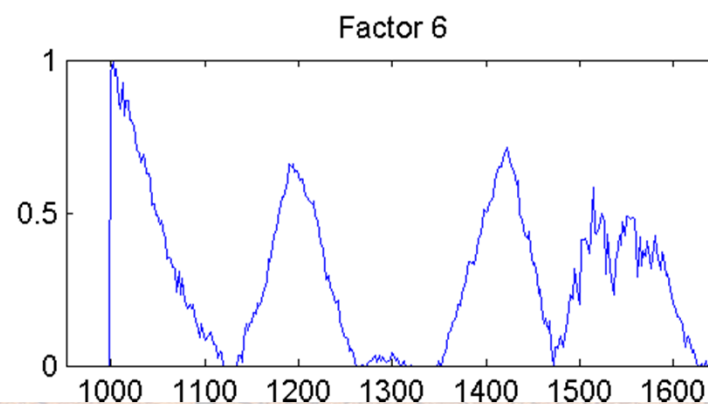
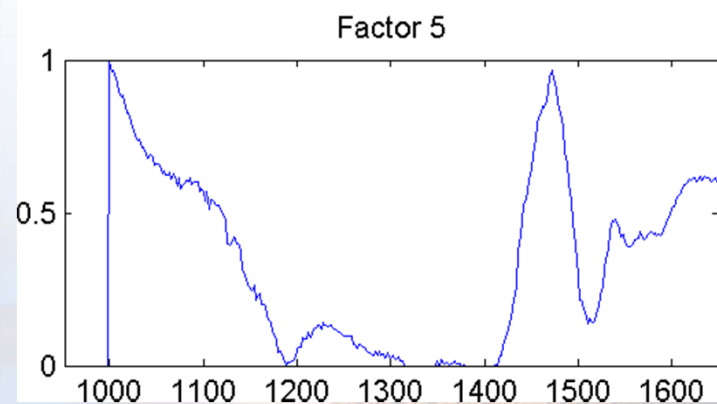
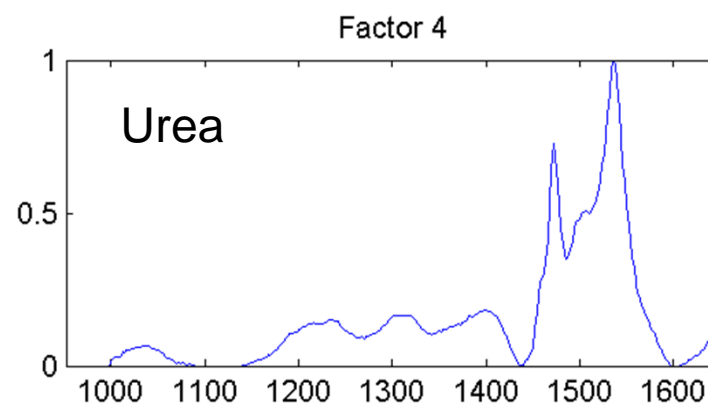
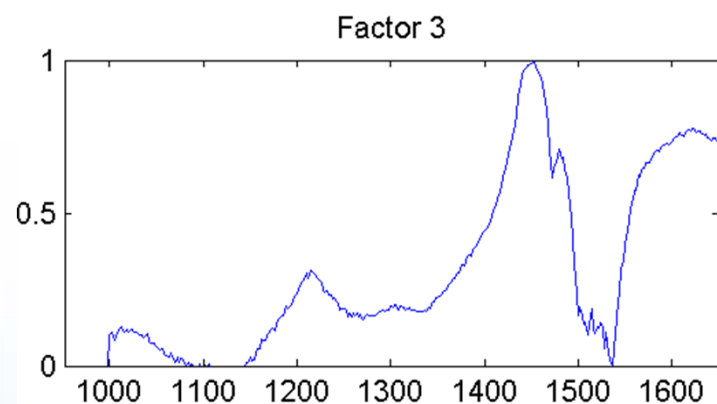
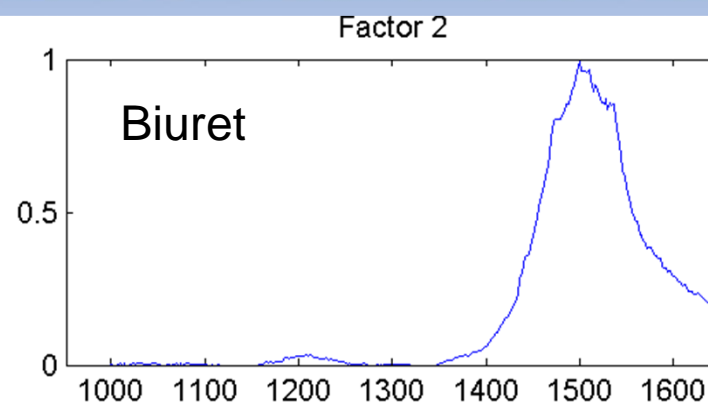
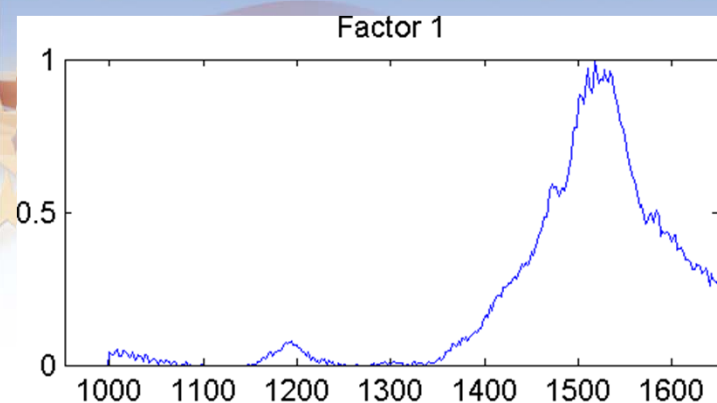
Save Settings

Plot Results

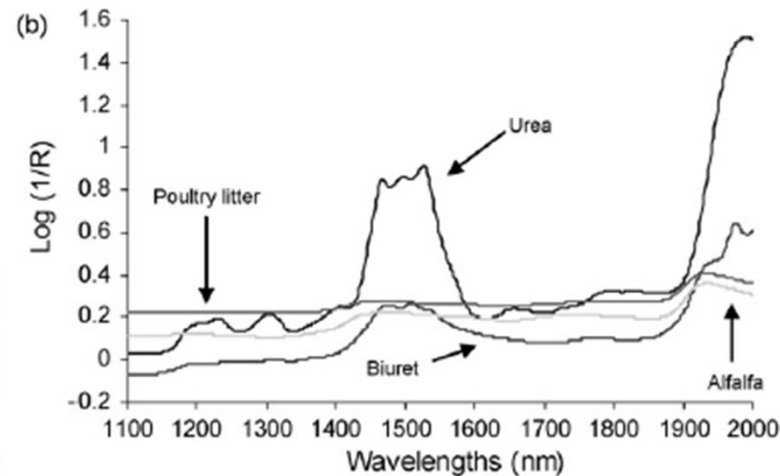
Exit



MCR Spectral Components



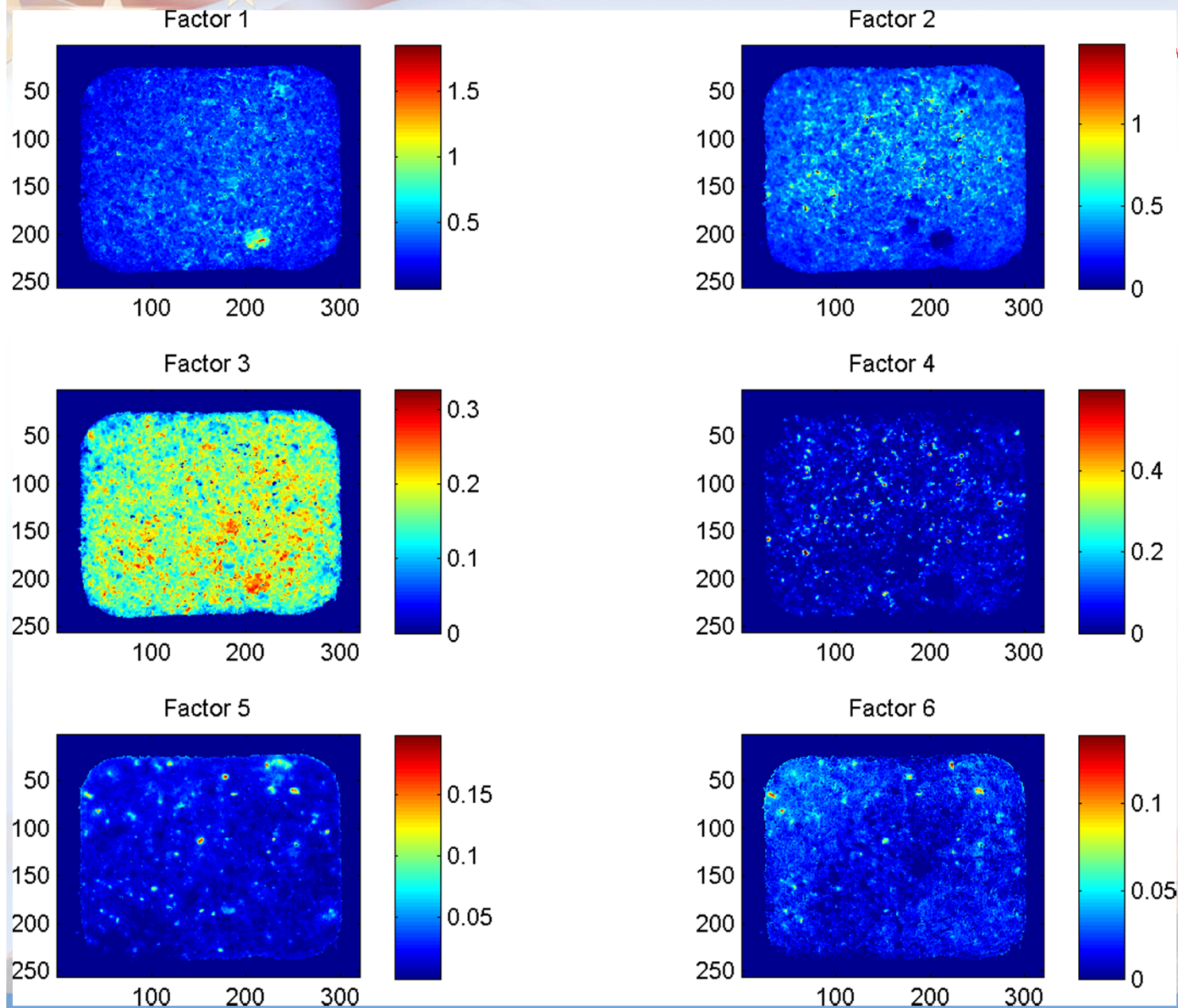
Did a search to see what the urea spectrum looks like and this is what I found, therefore I think factor 2 is biuret and factor 4 is urea. I can't identify the others.

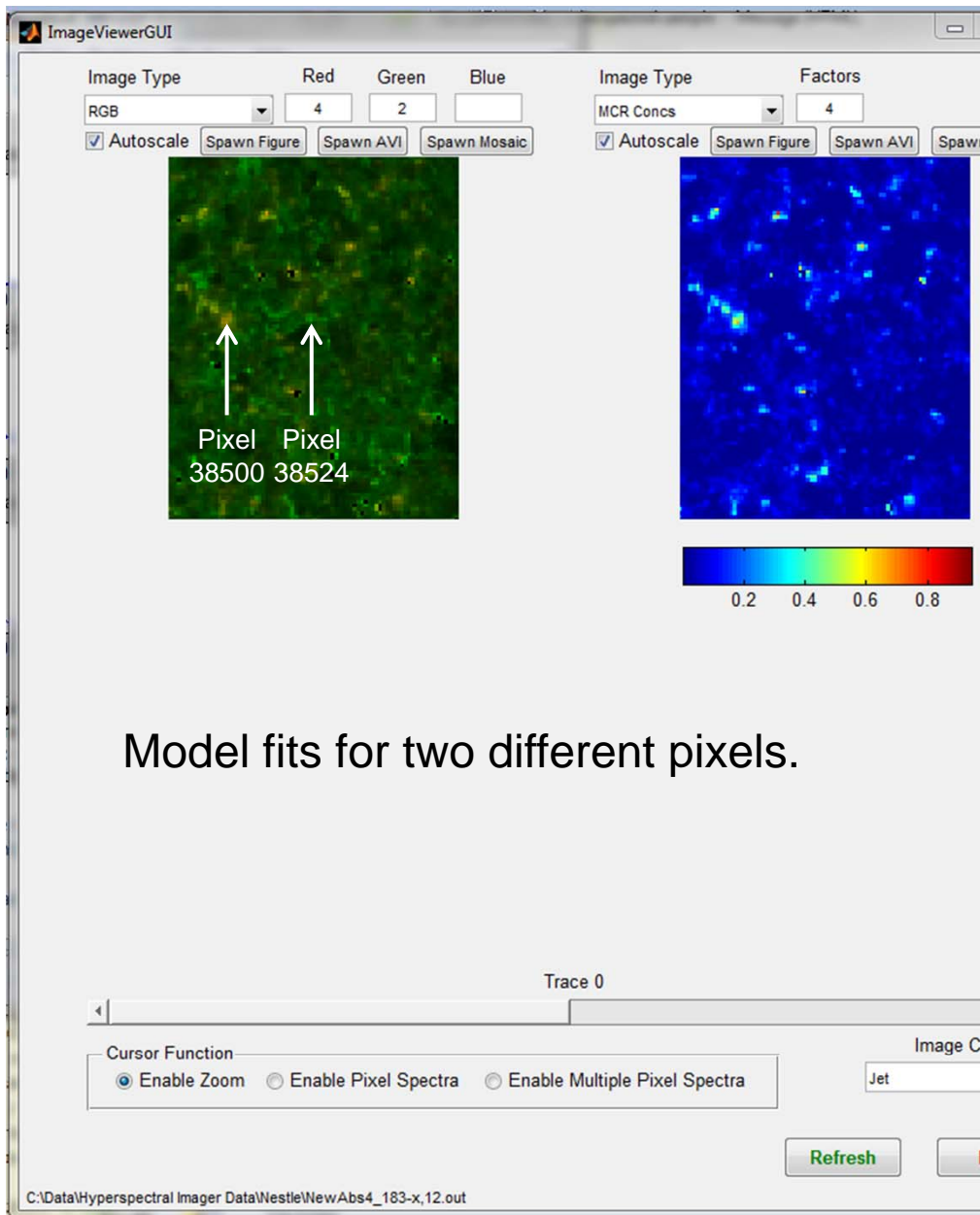


González-Martín, J.M. Hernández-Hierro,
Detection and quantification of additives
(urea, biuret and poultry litter) in alfalfas by
nir spectroscopy with fibre-optic probe,
Talanta, 76 (2008) 1130-1135.



MCR Concentration Maps





Model fits for two different pixels.

