Visualization of Two-way, Three-way and Higher Order Data Sets

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Data Order

- Data Order defined by the number of dimensions in which it is logically arranged
- Two-way: conventional data tables
  - *Samples* by *variables*
- Three-way: data cubes
  - EEM: *Samples* by *excitation* by *emission*
  - GC-MS: *Samples* by *retention* by *mass number*
  - Hyperspectral: *x* by *y* by *spectra*
- Four-way: series of data cubes
  - SIMS depth profiling: *x* by *y* by *z* by *spectra*
- Five-way: array of data cubes
  - EEM images: *sample* by *x* by *y* by *excitation* by *emission*
- Etc.

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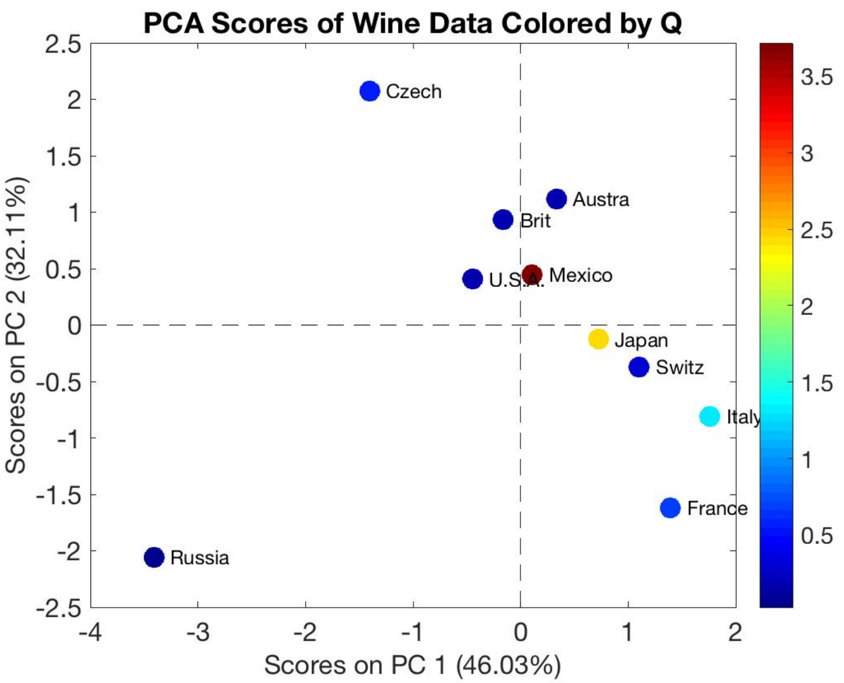
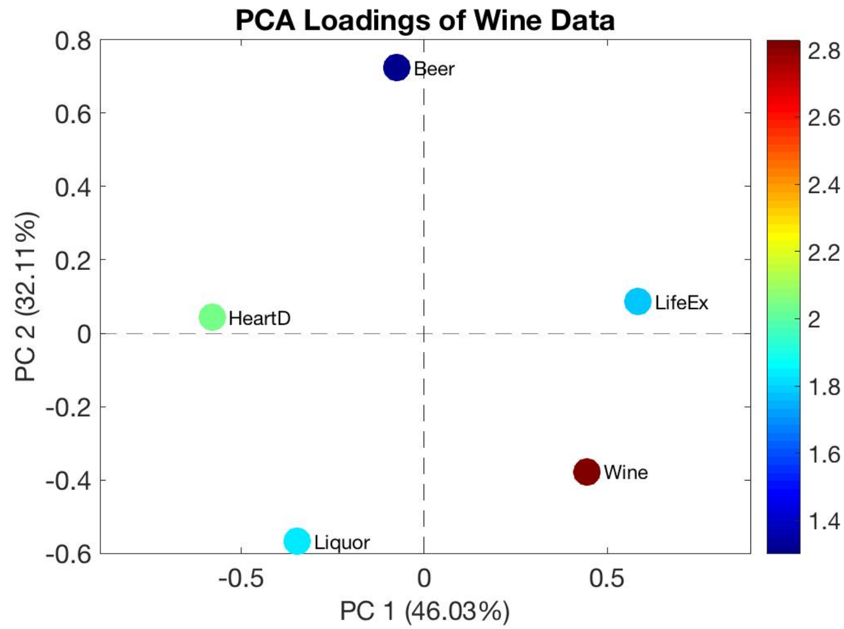
Visualization Progress





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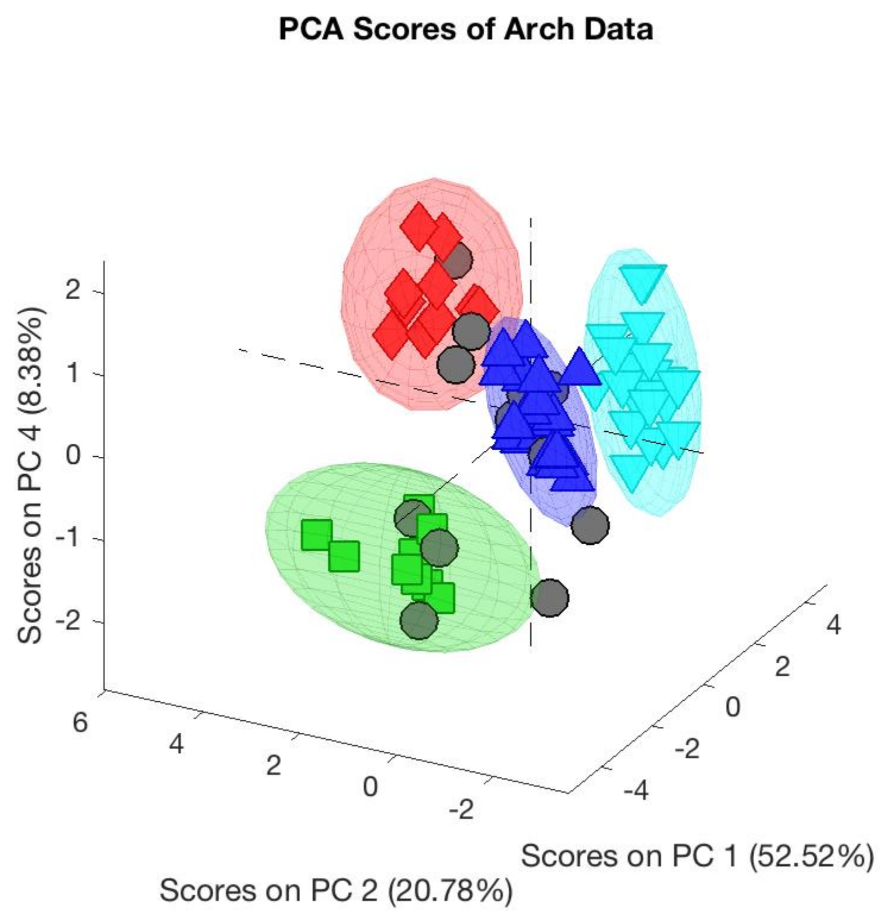
Continued Refinement



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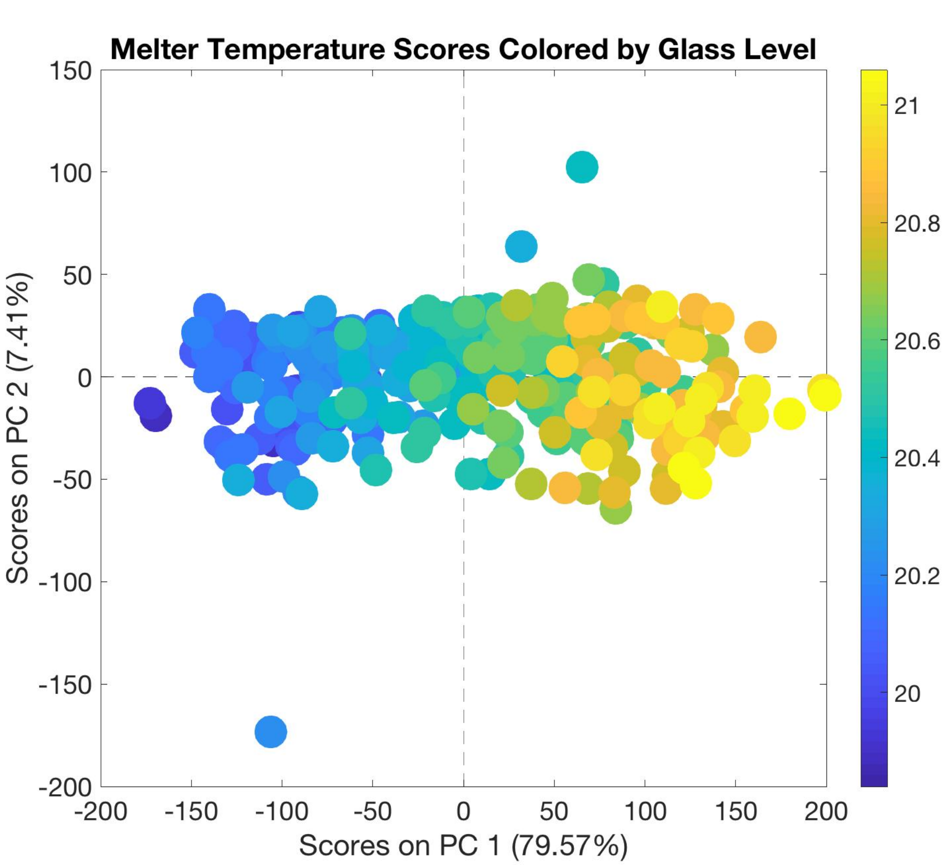
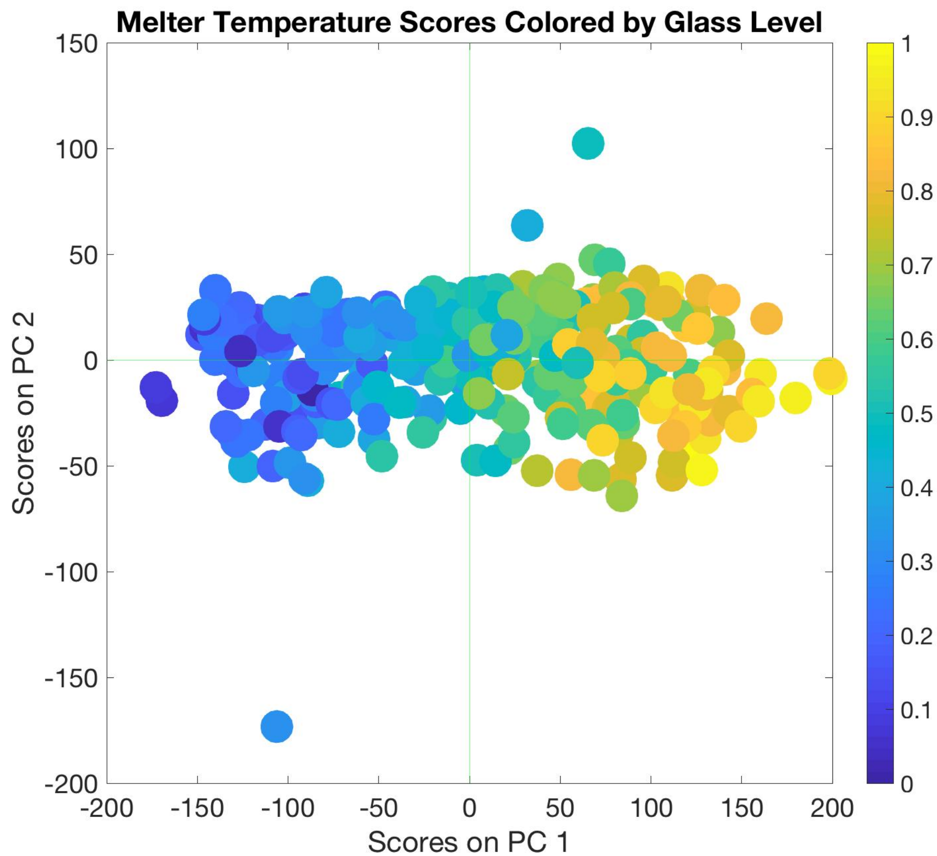
Issues With Larger Data Sets



Colorby Layered



Colorby Unsorted

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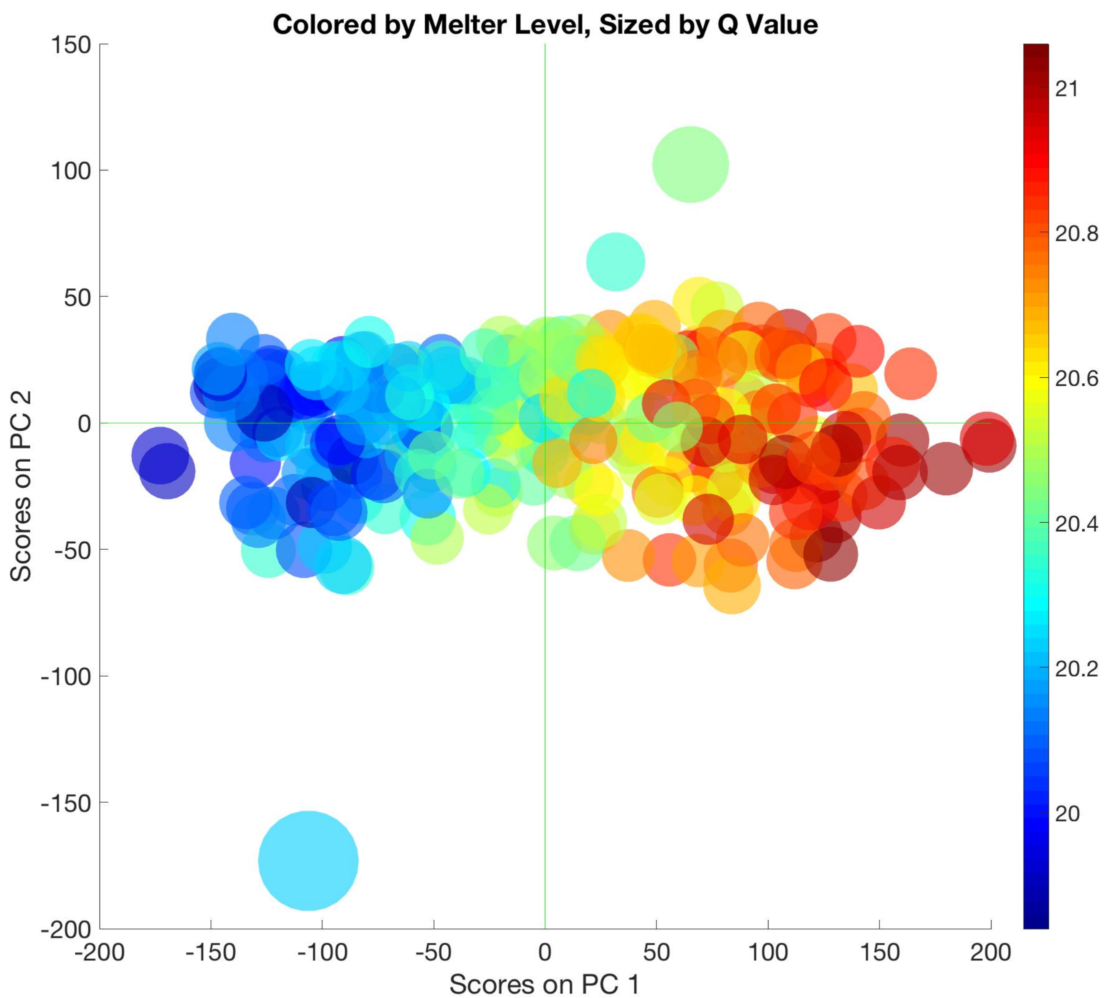
Translucent Data Points? Size?



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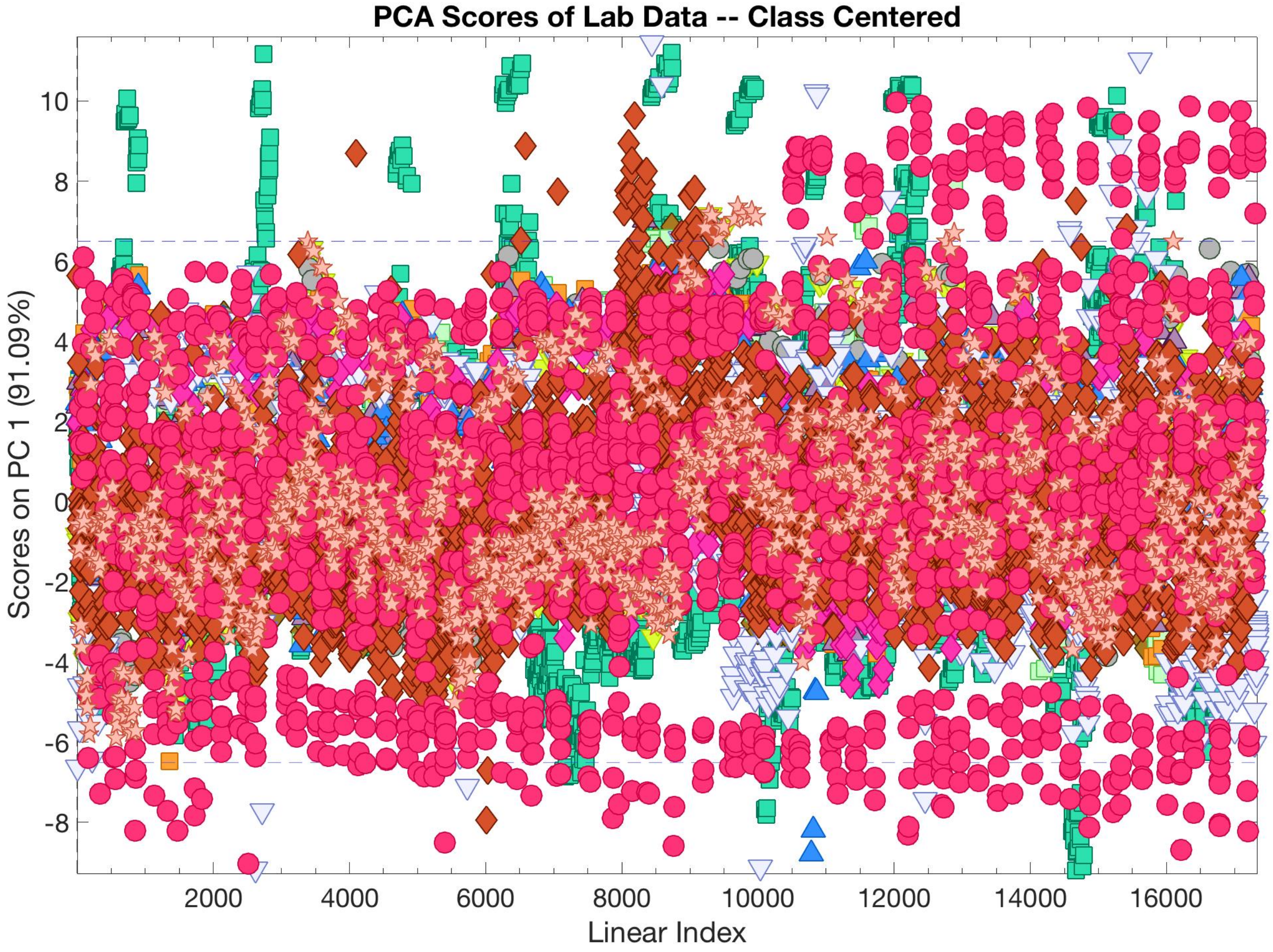
And There Are Limits



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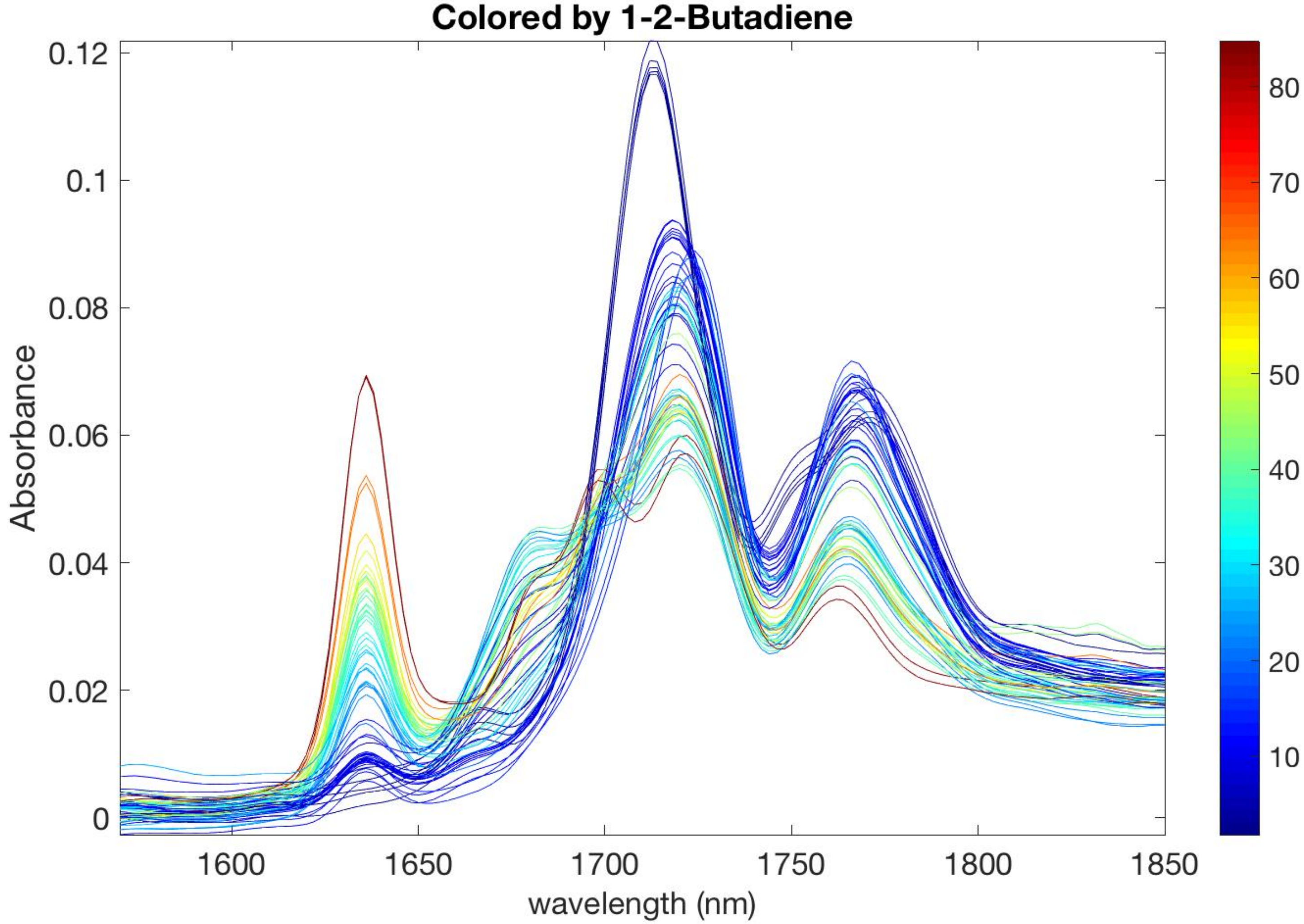
Visualizing Raw Data



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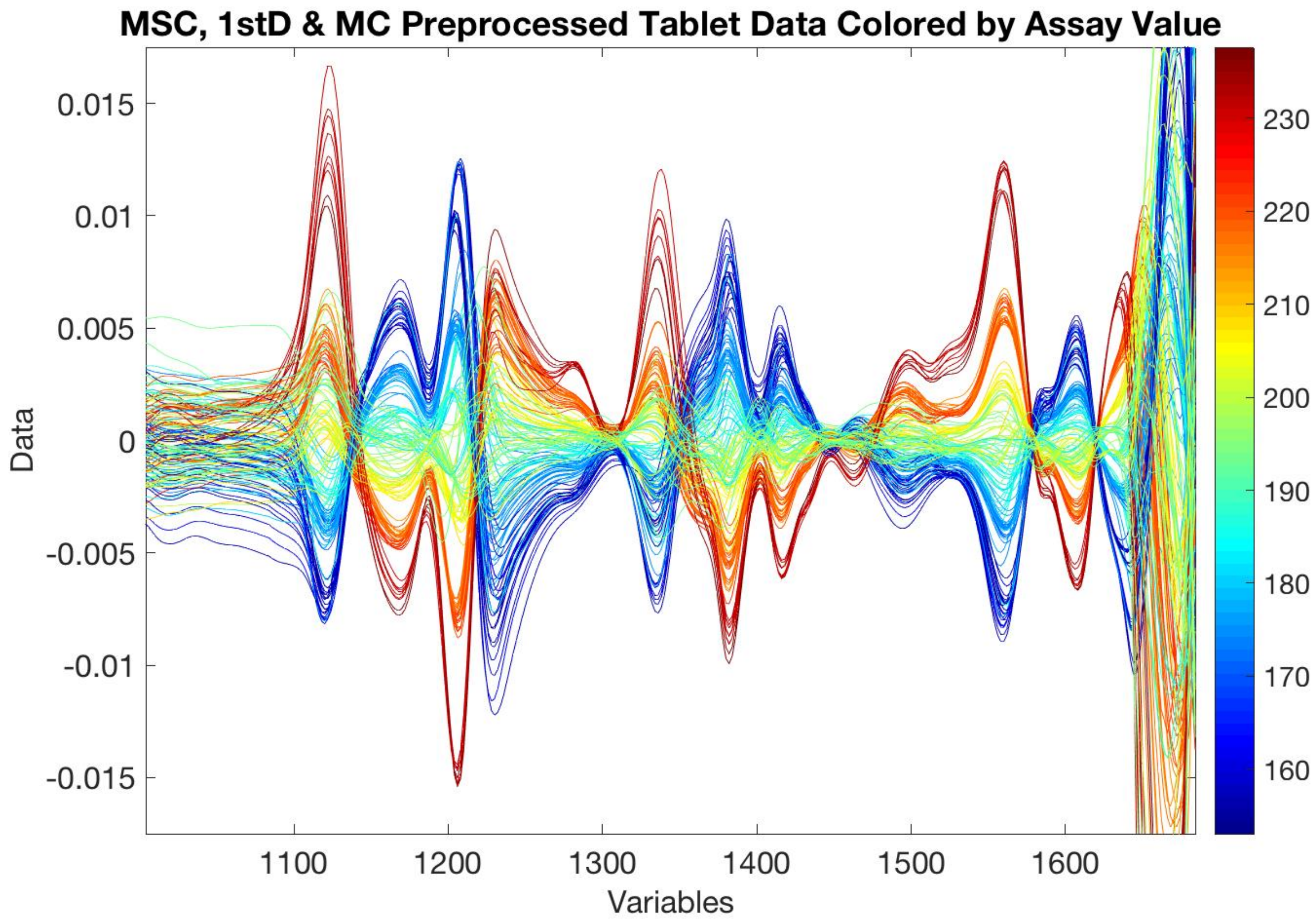
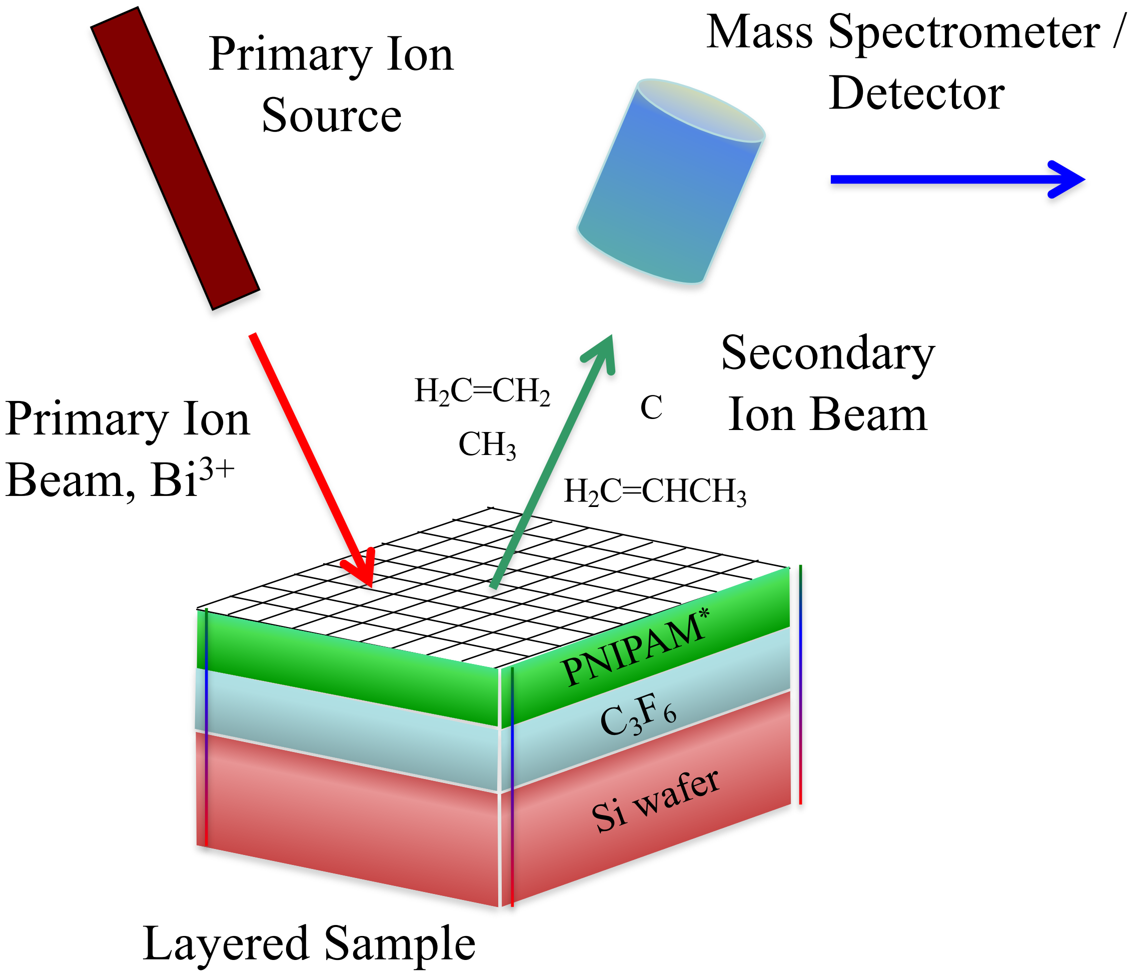
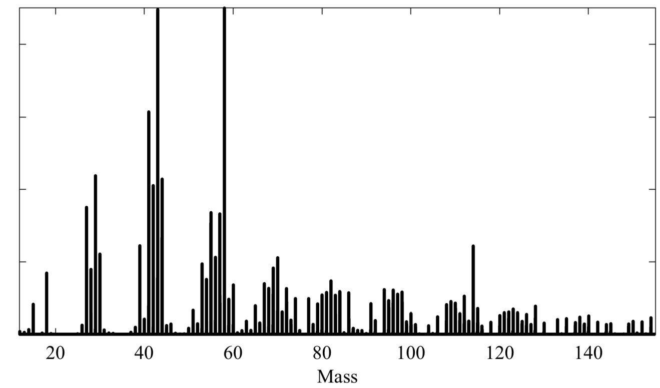
Visualizing Preprocessing



Secondary Ion Mass Spectrometry (SIMS)



*Poly(N-iopropylacrylamide)



The primary ion source is moved over the sample surface in a pseudo-random pattern to obtain a hyperspectral image.

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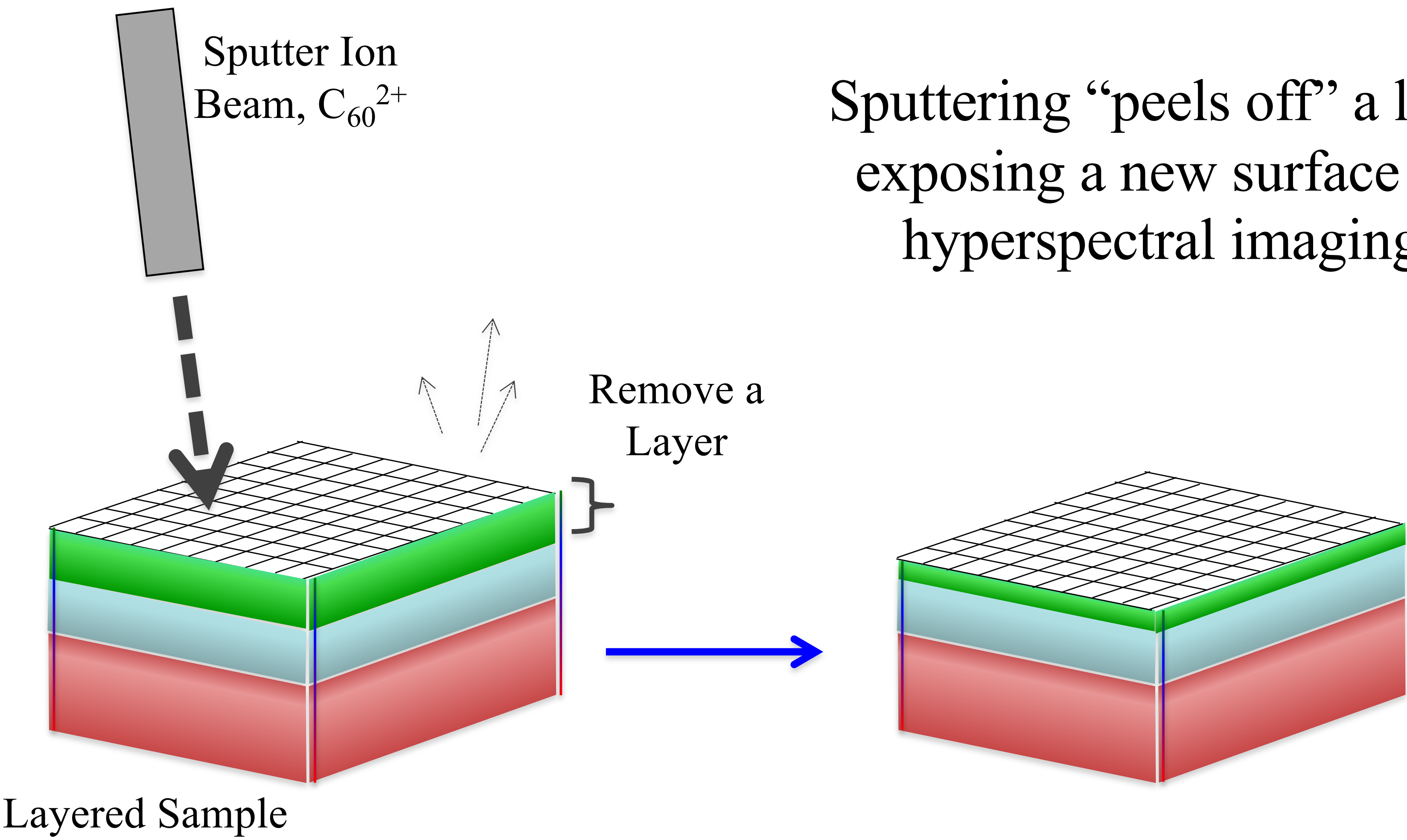
Sputtering → Depth Profiling



Sputtering "peels off" a layer exposing a new surface for hyperspectral imaging.

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ToF-SIMS Imaging & Depth Profiling

- The primary beam is scanned over the surface
  - mass channel spectrum (time of flight) at each pixel
  - 256x256 hyperspectral image of the surface
- Depth profiling is achieved by sputtering
  - multiple hyperspectral images at 50 different depths (~200 nm depth profile)
- 256x256x406+x50 reduced to 85x85x300x50
  - use mean of 3x3 windows, remove edge pixels, remove highest mass channels

+406 peaks were selected and integrated across all mass spectr

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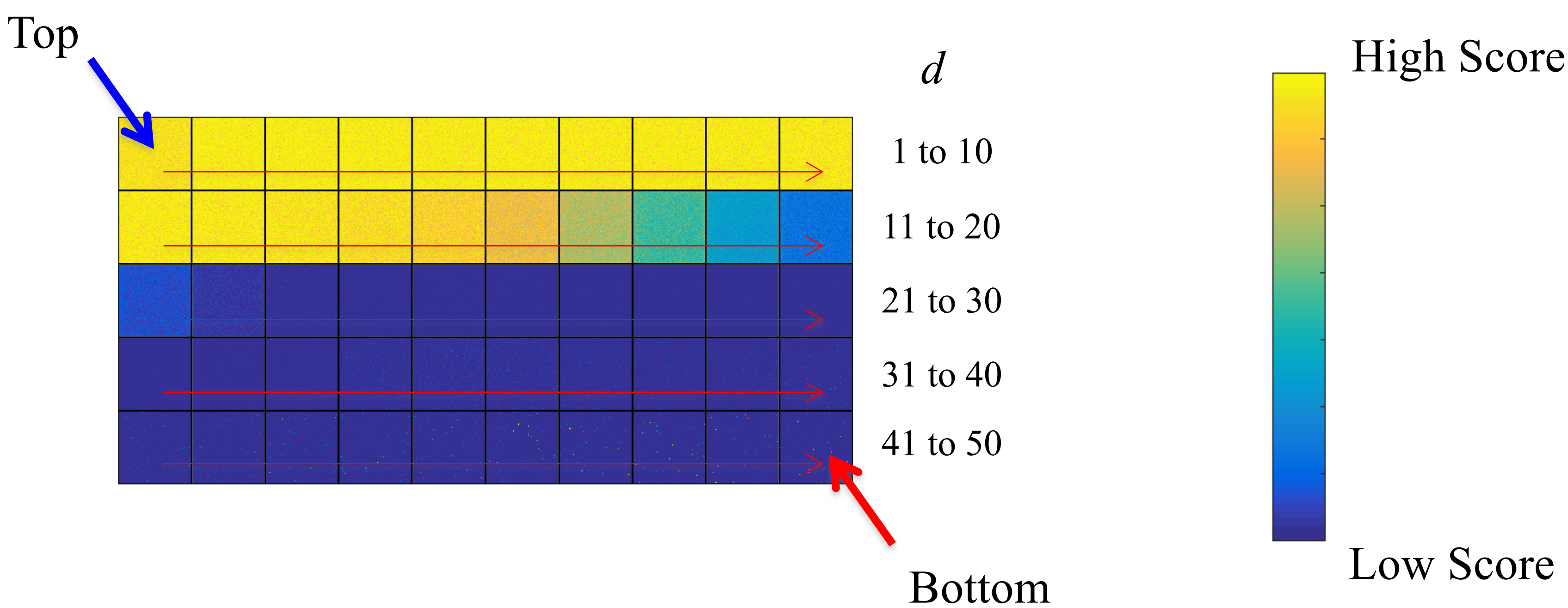
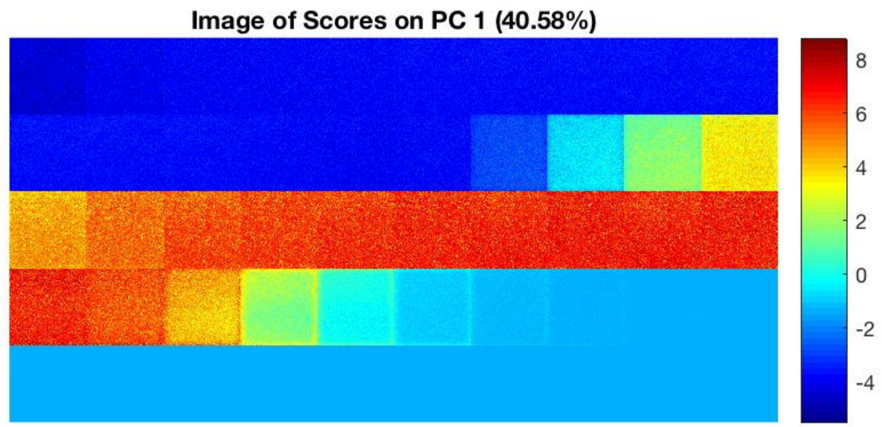
Data Analysis

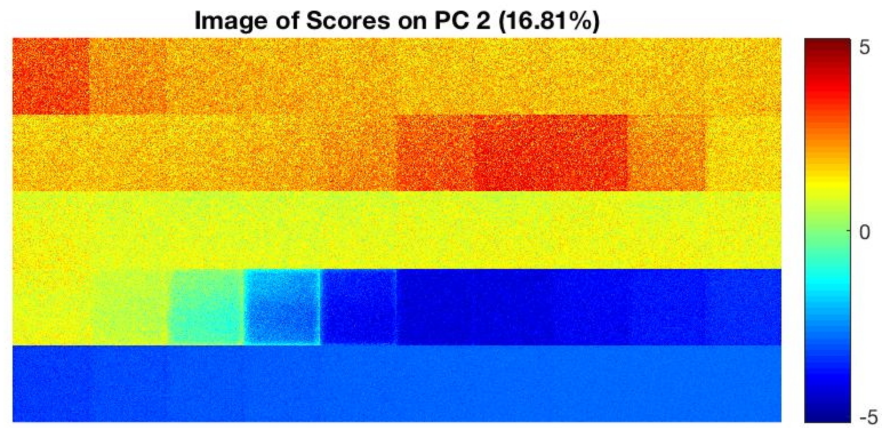
- Principal Components Analysis (PCA)
  - orthogonal scores / loadings
- Multivariate Curve Resolution (MCR)
  - attempt to obtain pure component, non-negative scores and factors that are more physically interpretable
- Use Poisson scaling
  - allows lower signal (higher mass channels) to influence the model
- Parallel Factor Analysis (PARAFAC)

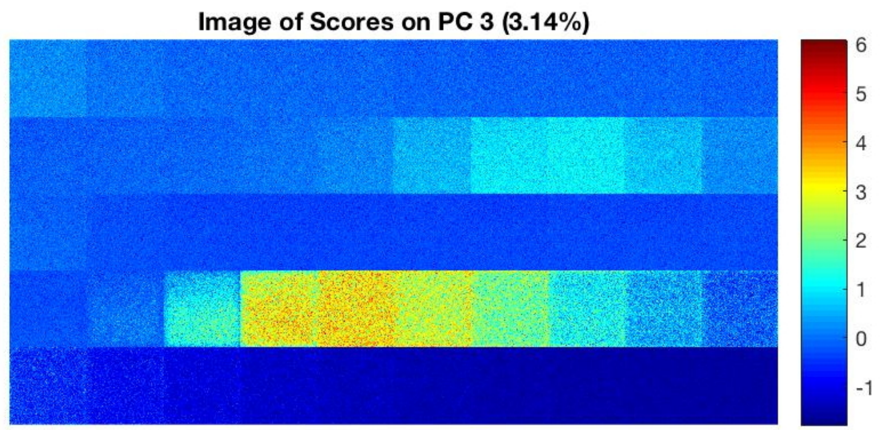
Example Image

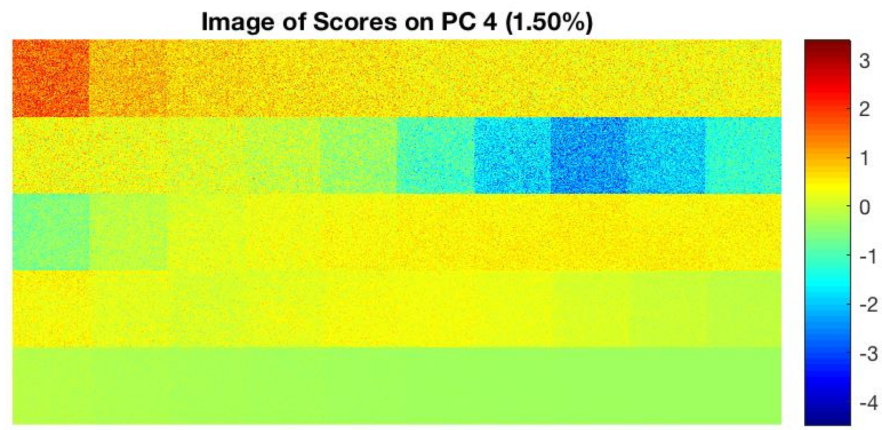


PCA Results Tiled Scores

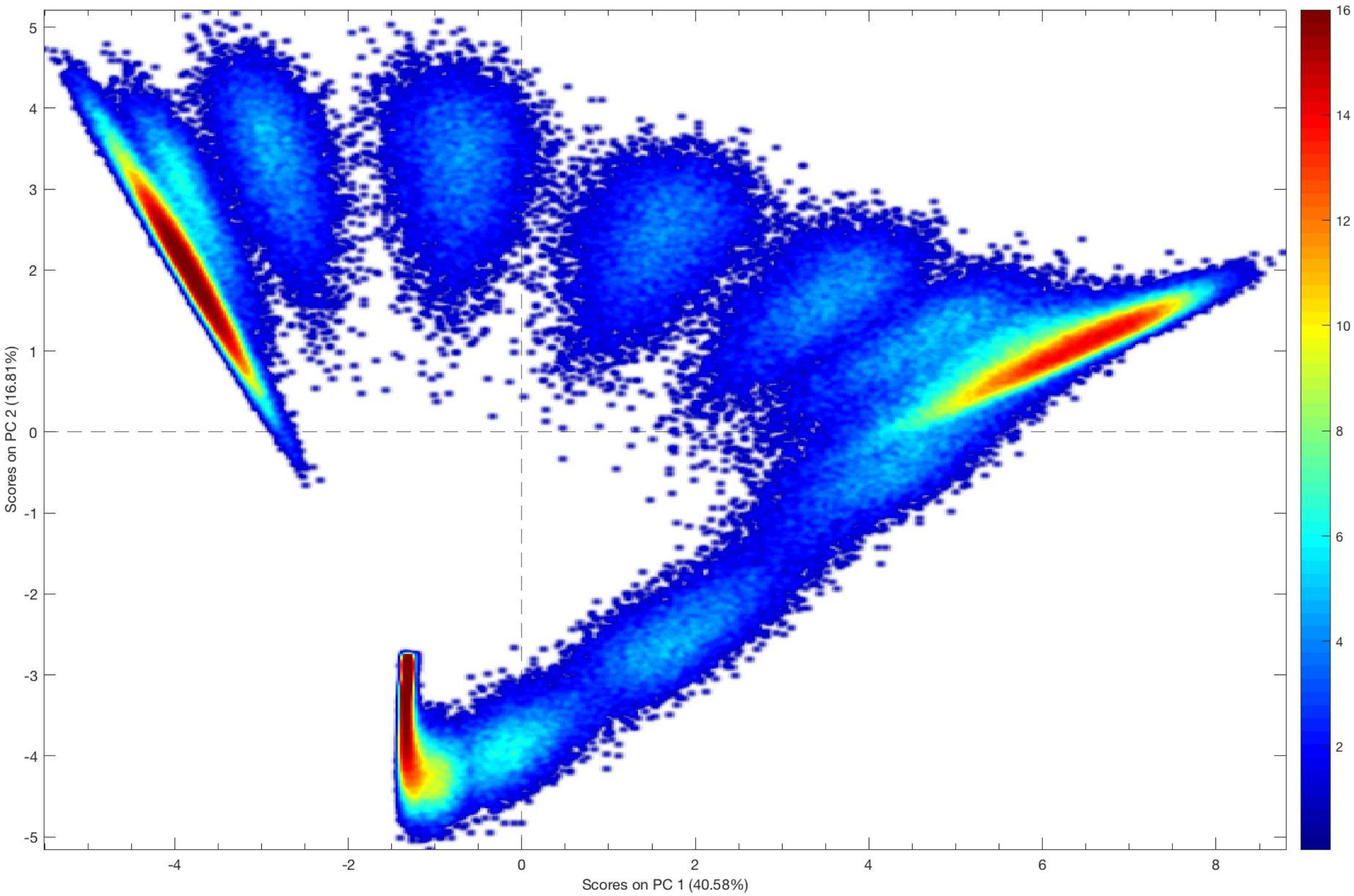




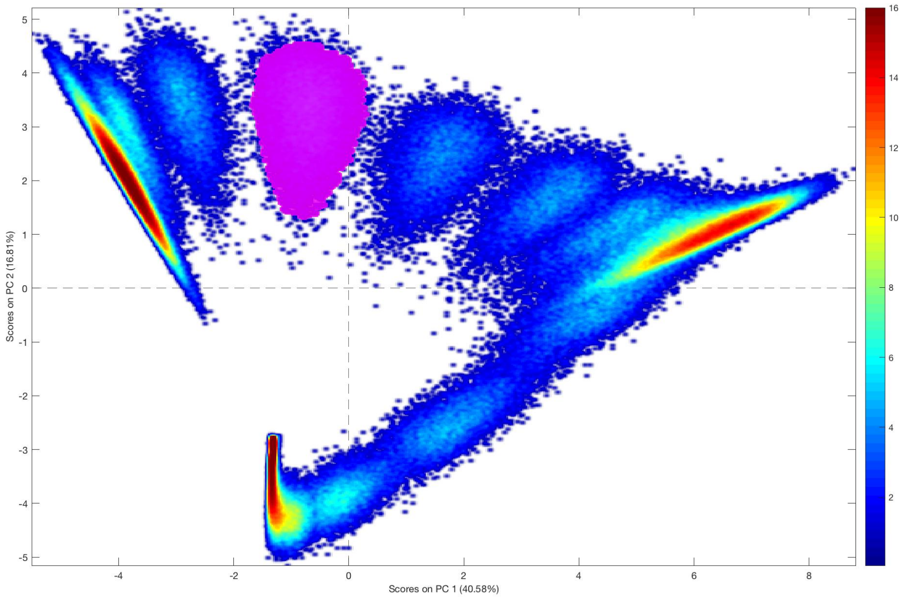


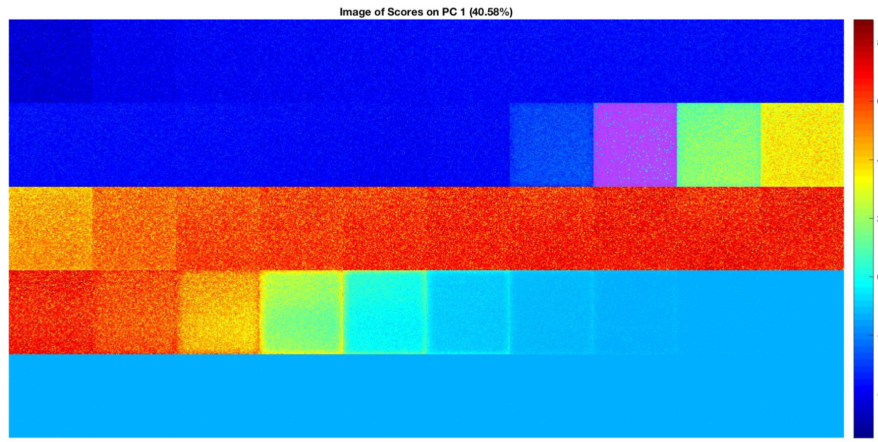


Score-Score Plots



Linking





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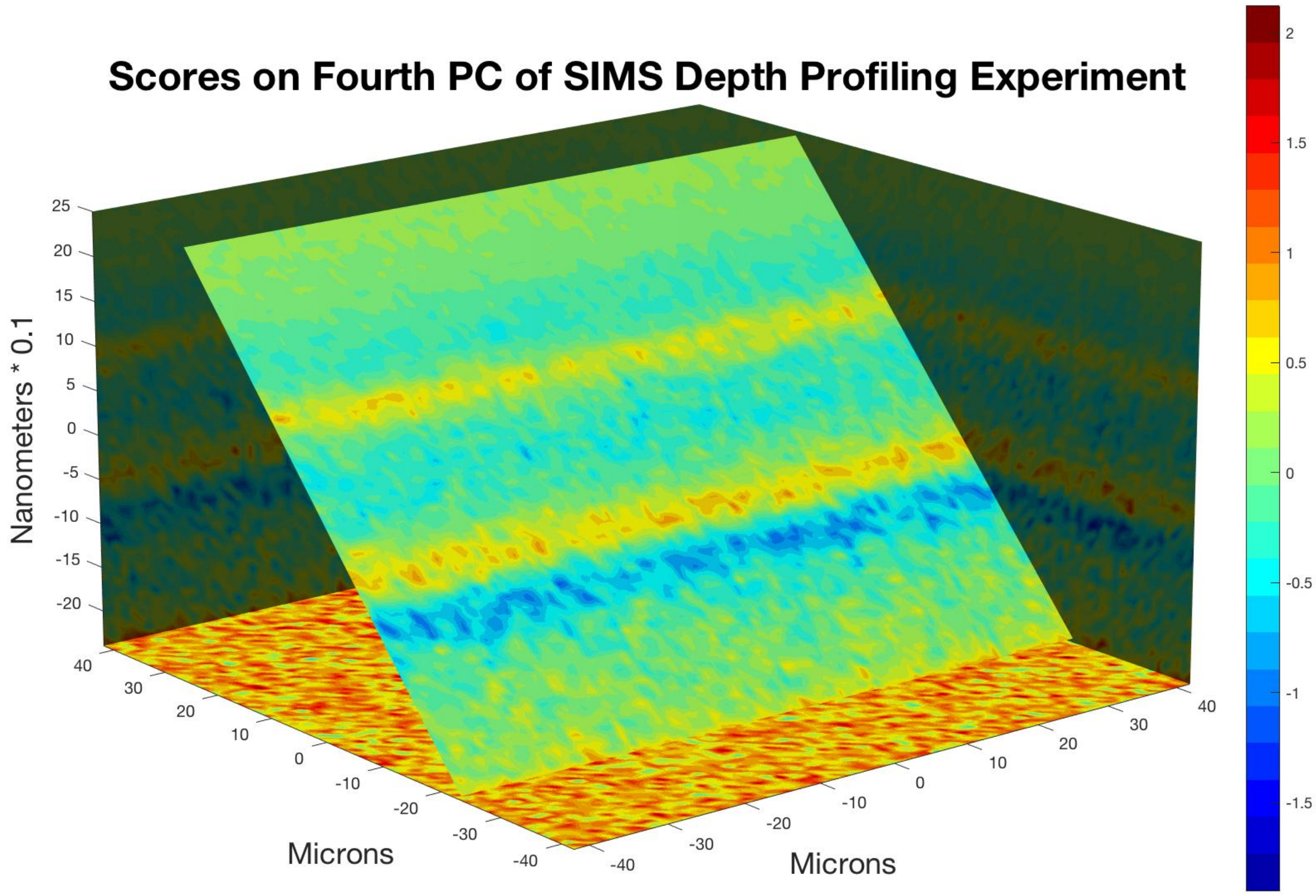
Visualizing 3-D Volume



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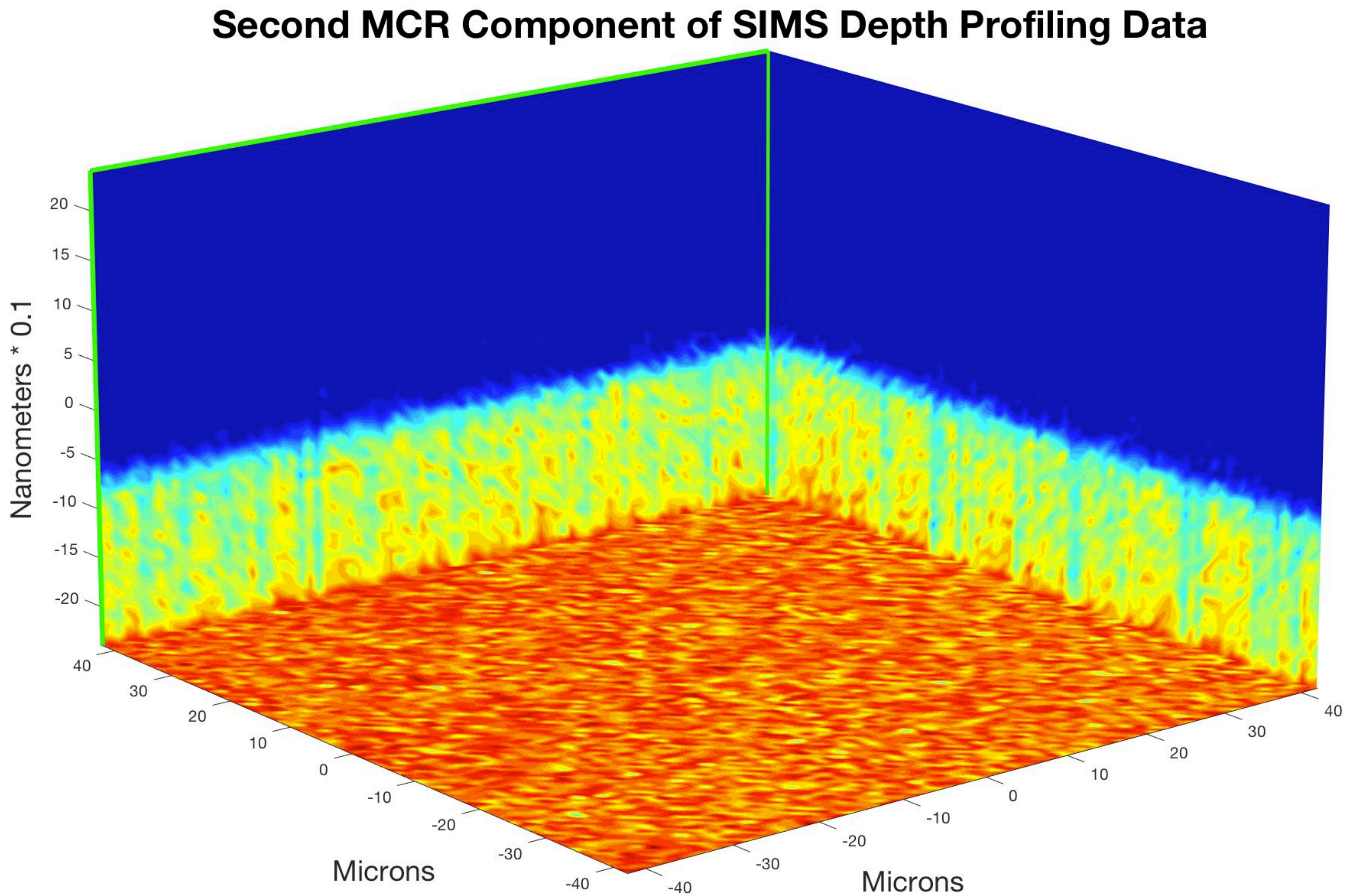
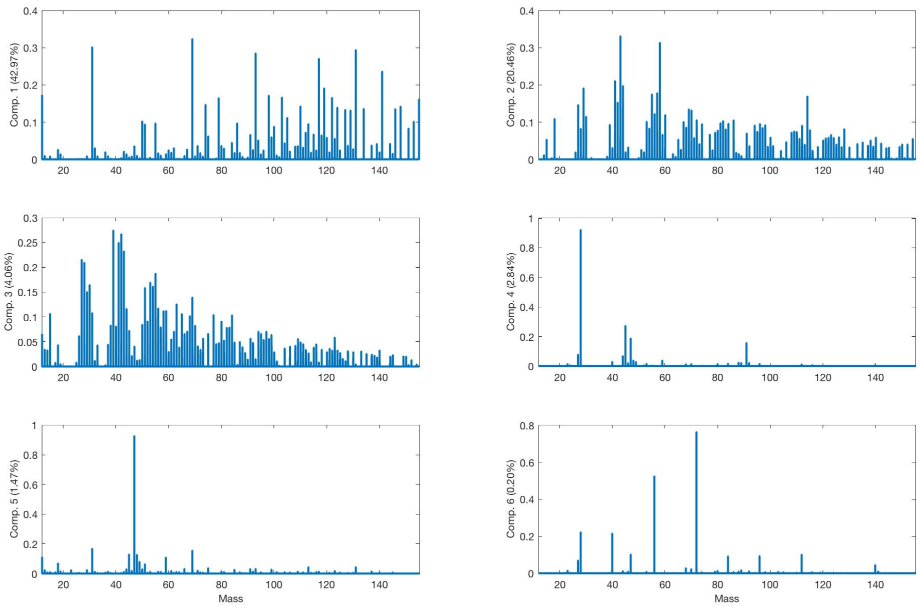
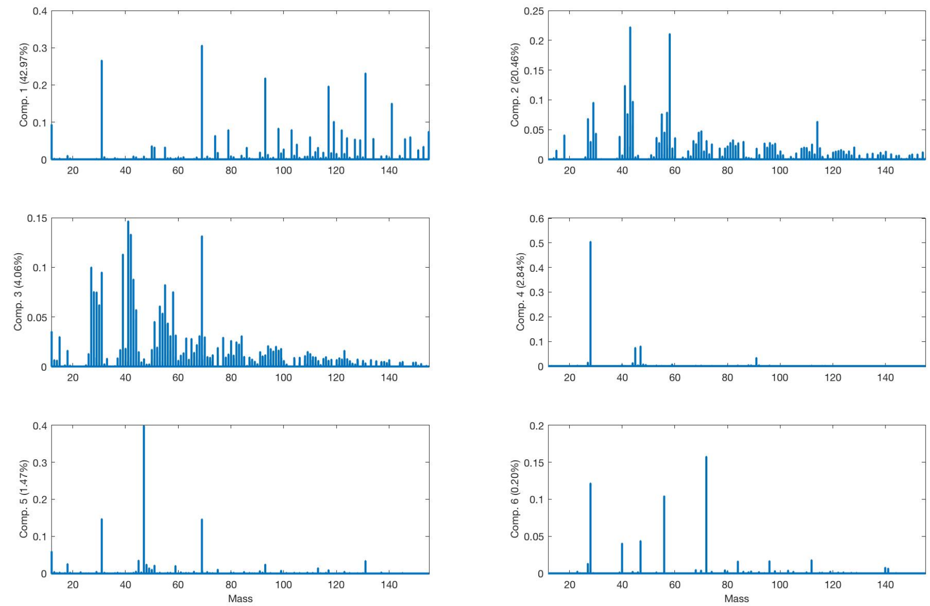

Second MCR Component of SIMS Depth Profiling Data
Nanometers * 0.1
20
15
10
5
0
-5
-10
-15
-20
Microns
40
30
20
10
0
-10
-20
-30
-40
Microns
-40
-30
-20
-10
0
10
20
30
40

Undo Preprocessing





As recovered

Preprocessing undone

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Another take: PARAFAC

- Unfold 4-way data array in pixel (x-y) modes
  - 7225 pixels by 300 mass channels by 50 layers
- Use Parallel Factor Analysis to model data as outer product of the three modes
- Fold pixel mode back up to make images
- Used non-negativity constraint

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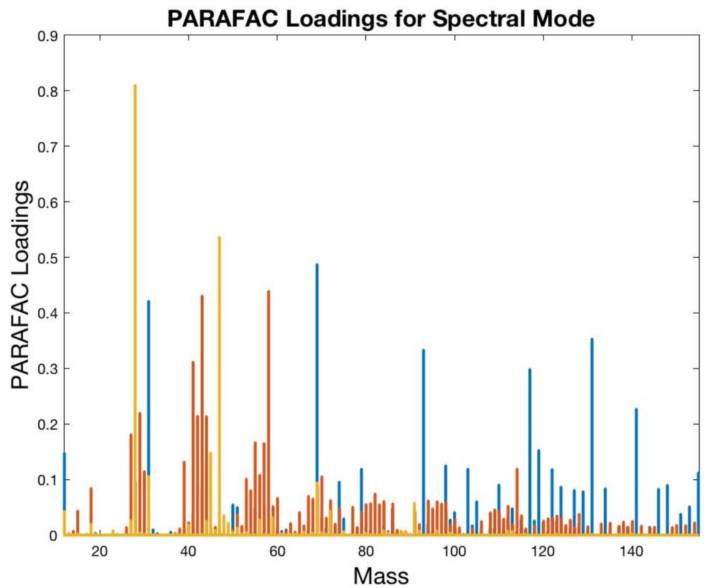
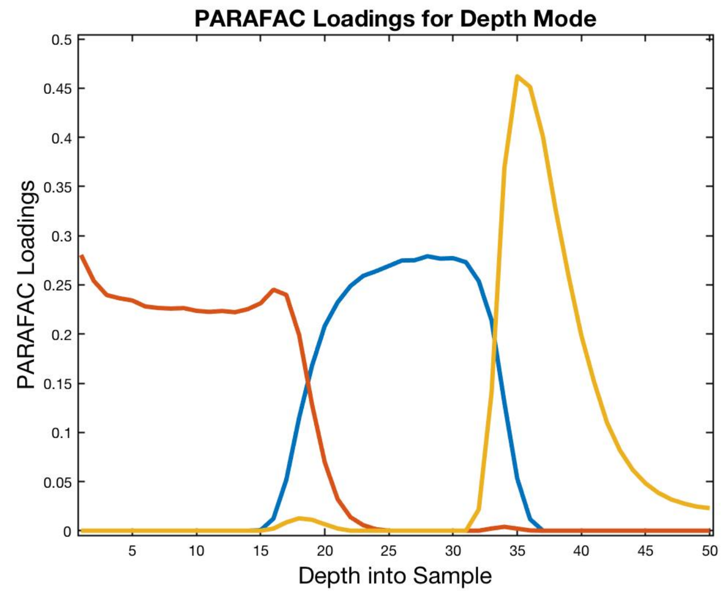
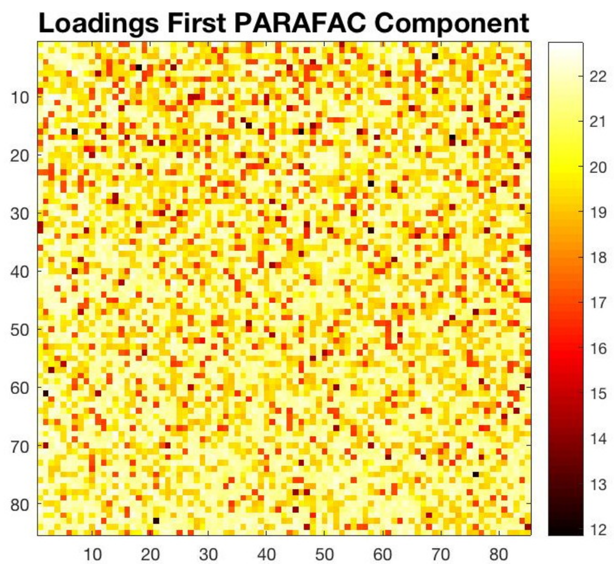
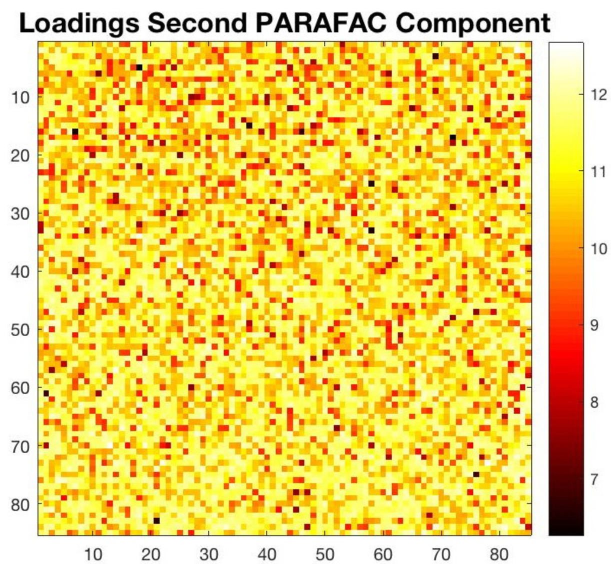
PARAFAC Model

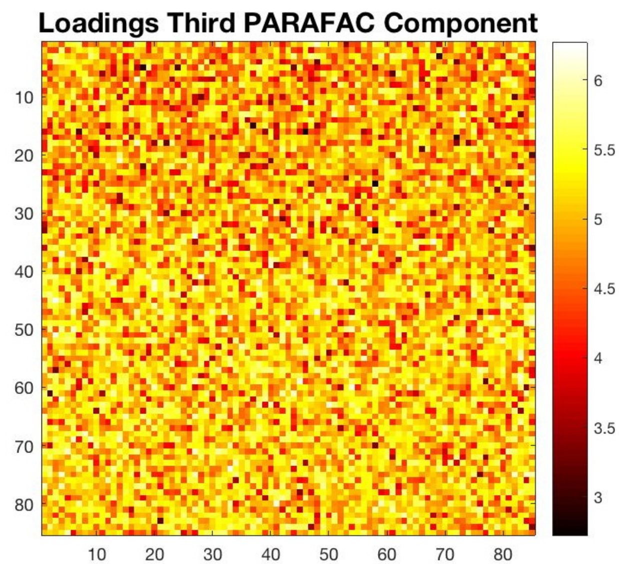
88.1% Variance Captured!



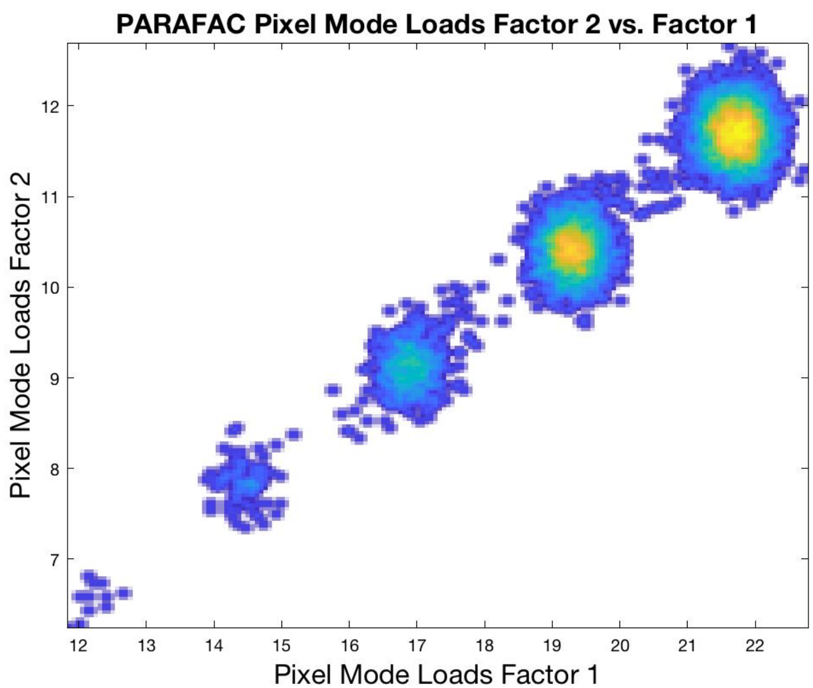


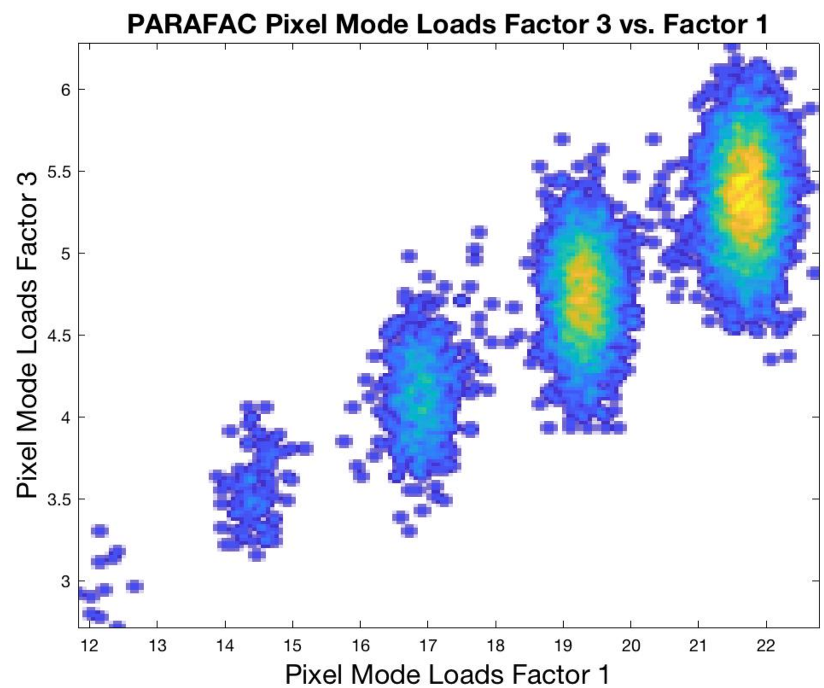






Pixel Factors Correlated!





- Variations in signal strength at each pixel persist as depth is profiled
- Seems to be 5 discrete signal strength levels
- Sampling problem??

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Software

- MATLAB®
- PLS_Toolbox
- MIA_Toolbox

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Conclusions

- Many ways to look at data!
- "Color-by" especially useful on raw data or for adding info to other plots
- Factor based methods (PCA, MCR, PARAFAC, etc.) can condense data down to lower dimensions while retaining info
- Slicing and adding motion can reveal things previously un-noticed

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