Application of Py-MBMS & Multivariate Analysis to Characterize Oil Shales & Heavy Oils

***Eun-Jae Shin*[1], *Robert J. Evans*[1], *Andrew M. Herring*[1], *and Michael Batzle*[2]**

[1]Department of Chemical Engineering, Colorado School of Mines, Golden, CO 80401, USA
[2]Department of Geophysics, Colorado School of Mines, Golden, CO 80401, USA

CERI 26th Oil Shale Symposium
Golden, CO, Oct. 16th-18th, 2006

Need of Alternative HC Resources

- **Huge Oil Shale Reserves**
  - **Western Colorado, Utah and Wyoming: 500 billion to 1 trillion barrels of recoverable oil**
- **Huge Heavy Oil Reserves**
  - **>500 billion barrels in Venezuela, Canada, Alaska, …**
- **Technical and Environmental Challenges**
  - **Water & Energy Consumption, Environmental Restoration**
  - **Disposal of Waste Rock (mining), Water Contamination (in-situ)**

Understand Chemistry

- To Facilitate Extraction and/or Conversion Processes
- To Develop Predicting Capabilities for End Products of Various HCs Resources

Objective

- **Correlate Geophysical Characterization of Oil Shales with Chemical Information**
  - **Establish seminal knowledge on the chemical composition of pyrolysis products from different oil shales & heavy oils**

Experimental

- **Batch experiments in Tubular Reactors**
  - **30~200mg sample, T=550°C, R.T. < 0.1s**
- **Molecular Beam Mass Spectrometry**
  - **Rapid and Near-Universal Analysis of Products from Realistic Environments**
- **Data Analysis: Multivariate Analysis**
  - **Identify and Quantify Trends**
  - **Predicting Capability**

HC Samples Used

- 2 Oil Shale
- 1 Gilsonite
- 1 Asphaltine Block
- 16 Heavy Oil

Total: 20 samples, 2 replicates

Outcrop Sample
Colorado Oil Shale

Heavy Oil Outcrop (Asphalt Ridge, Utah)

SEM Image of Kerogen in Rock

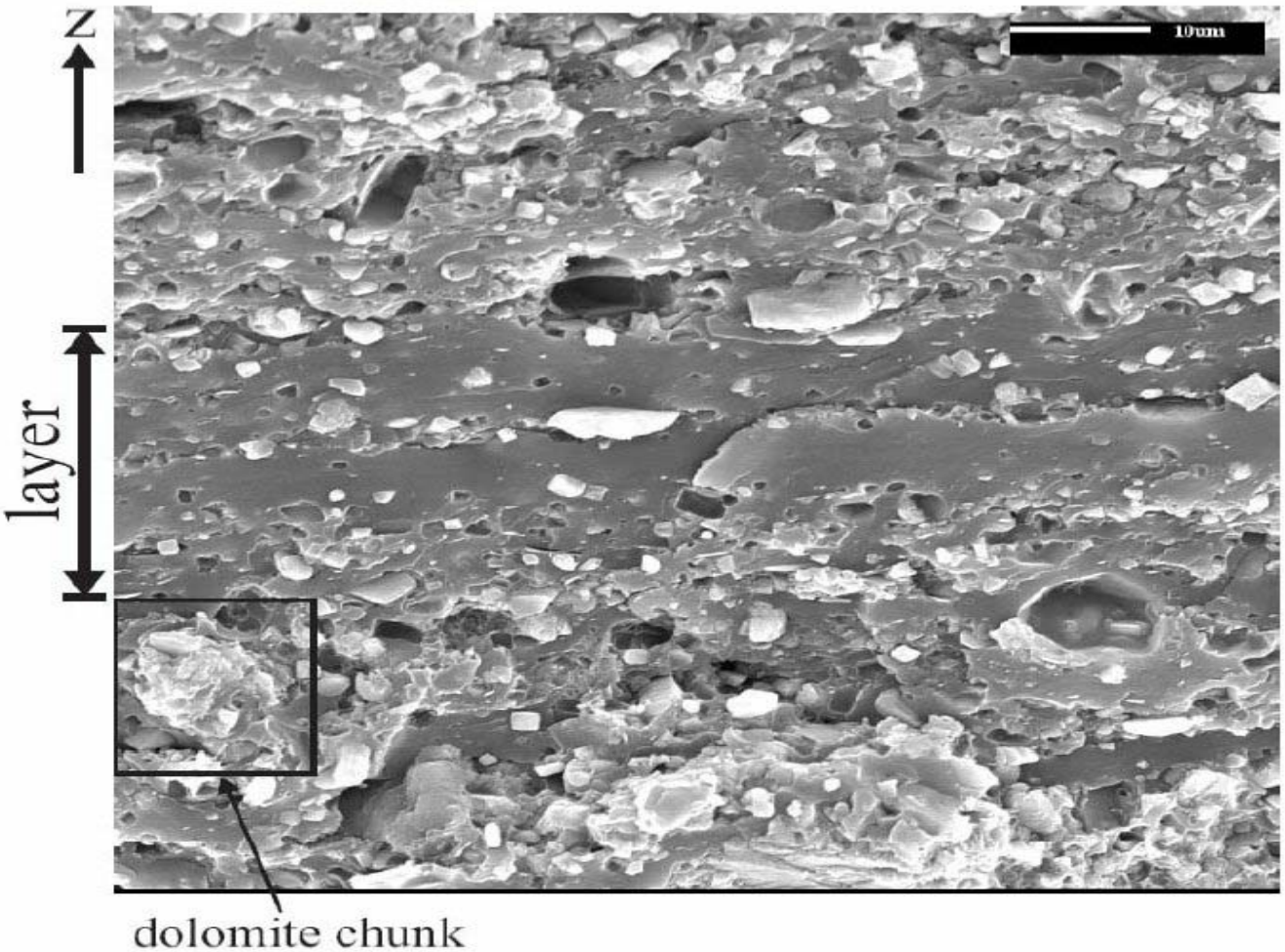
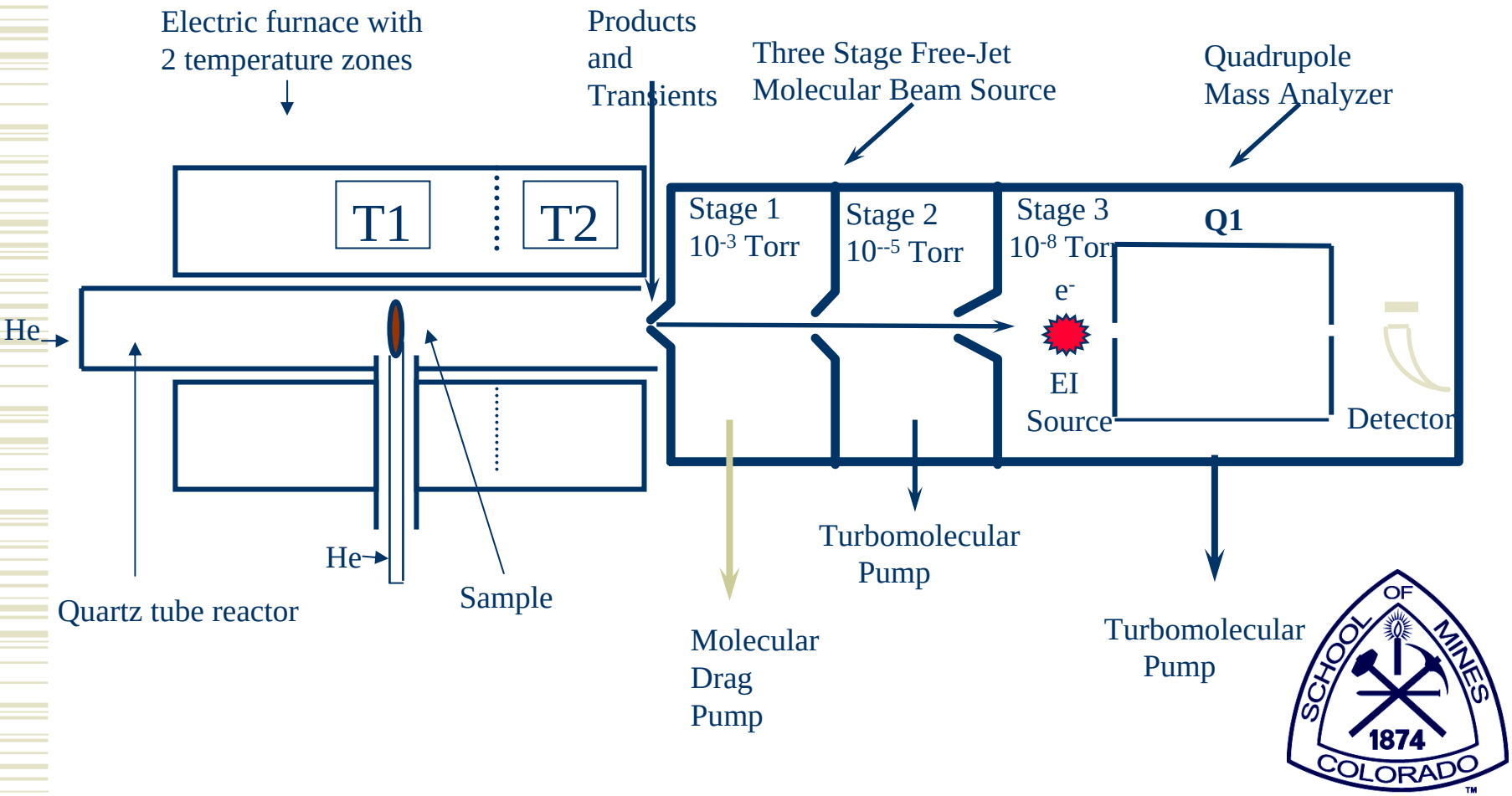


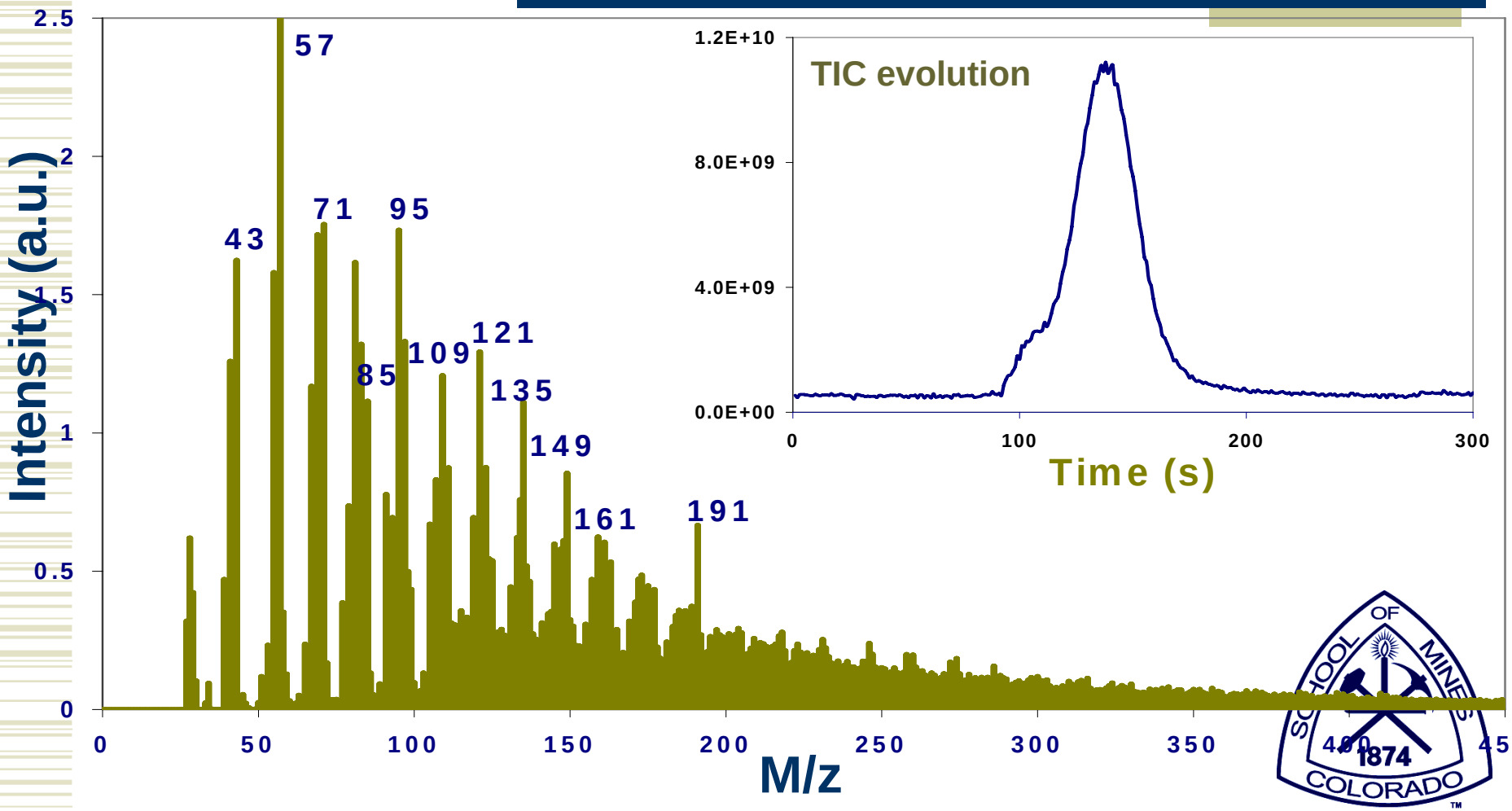
Figure 6. Scanning electron microphoto of a portion of oil shale. Individual mineral grains can be seen, as well as the amorphous kerogen material. Layering is obvious (from Mah, 2005). Note 10 μm scale in upper right corner.

Mah, Ph.D. thesis 2005

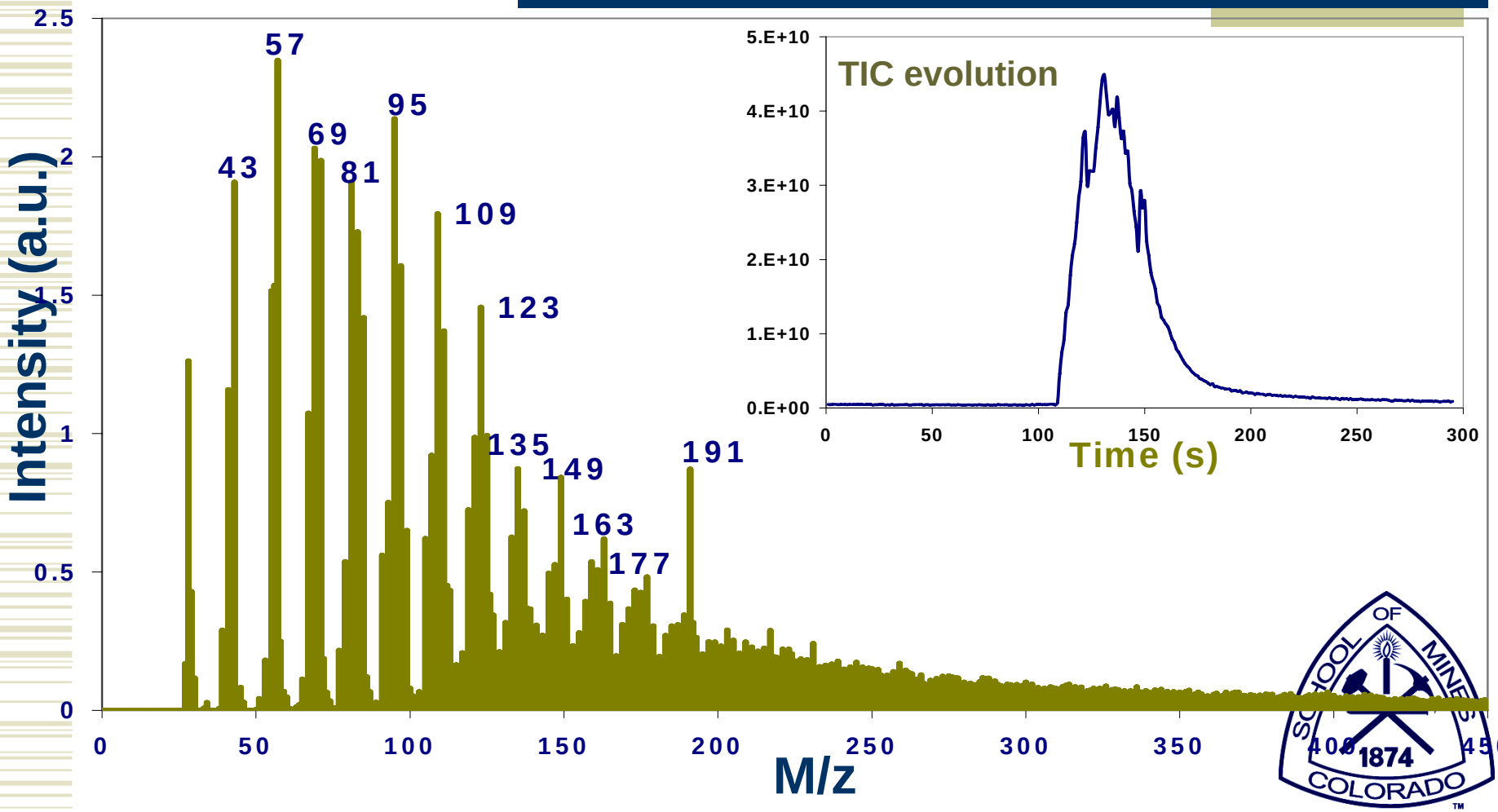
Schematic of Pyrolysis Reactor & MBMS Sampling System



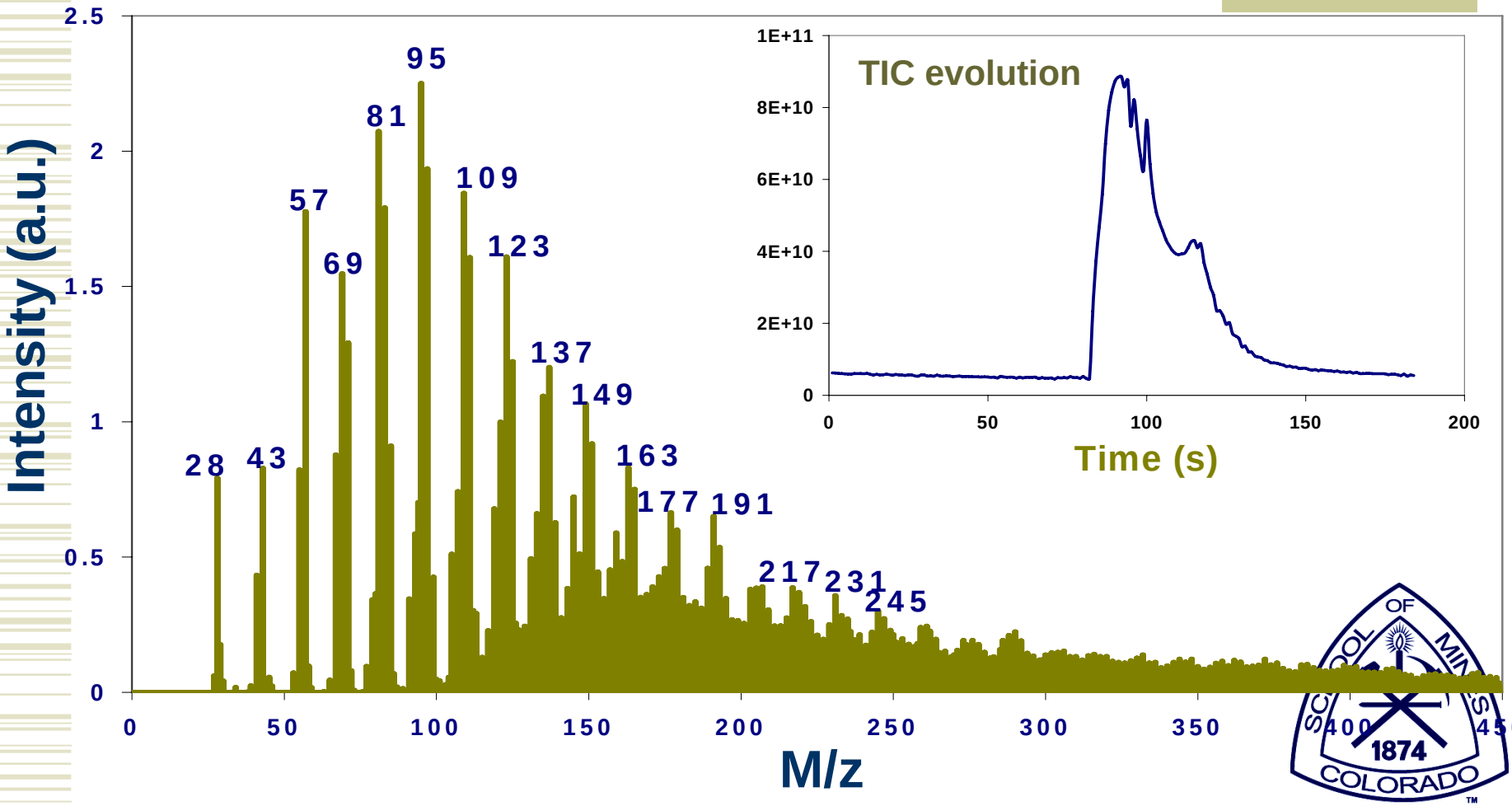
Raw Spectra-Oil Shale



Raw Spectra-Gilsonite



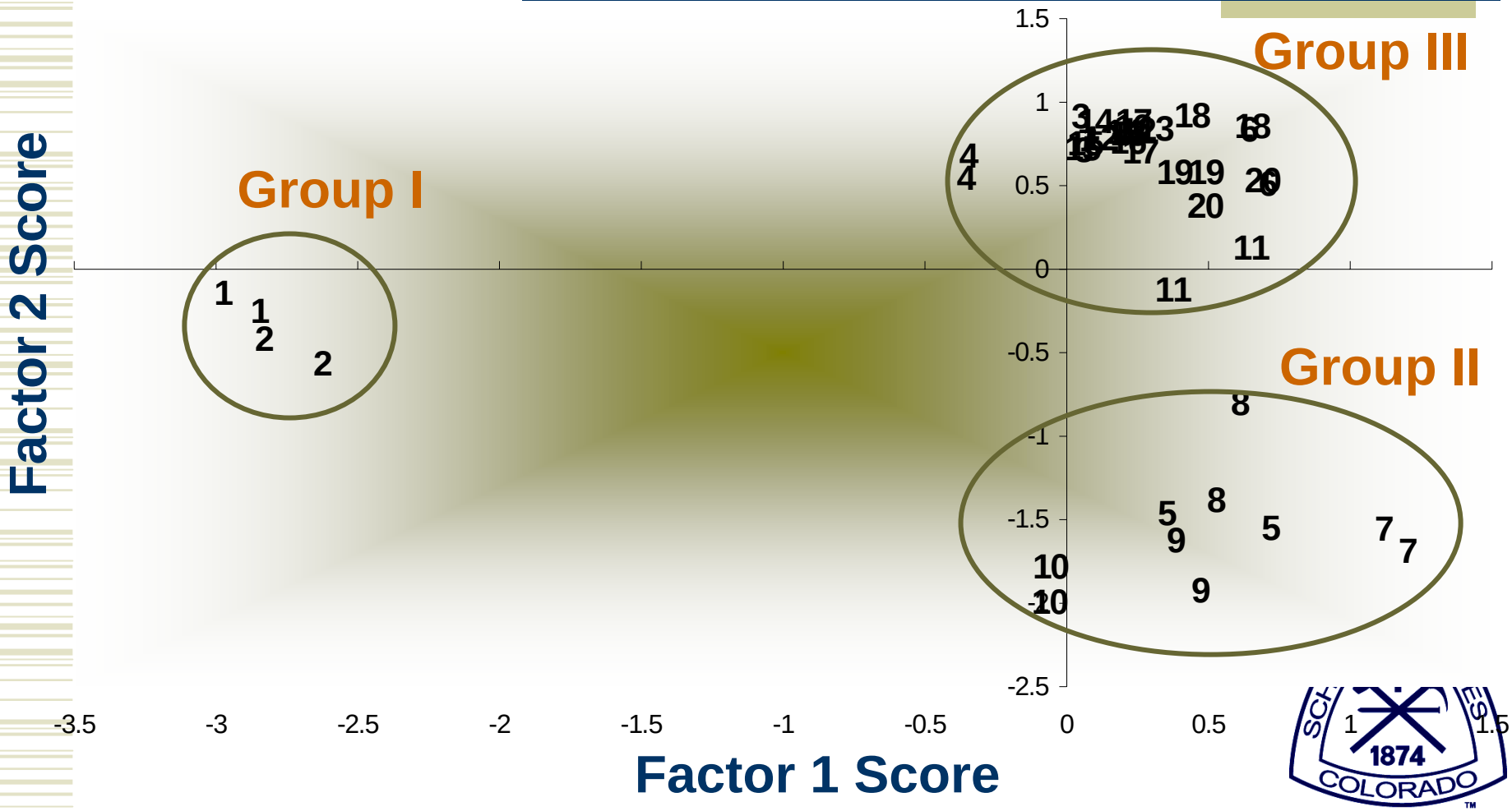
Raw Spectra-Heavy Oil



Multivariate Analysis

- ***Data Reduction:*** **Reduce the number of variables by finding correlated behavior**
  - **e.g., 5 Factors can contain 80% of information in original 300 masses**
- ***Noise Reduction:*** **Factor extracted in order of importance (maximum variance)**
- ***Pattern Recognition:*** **Correlated masses indicate underlying chemical processes**

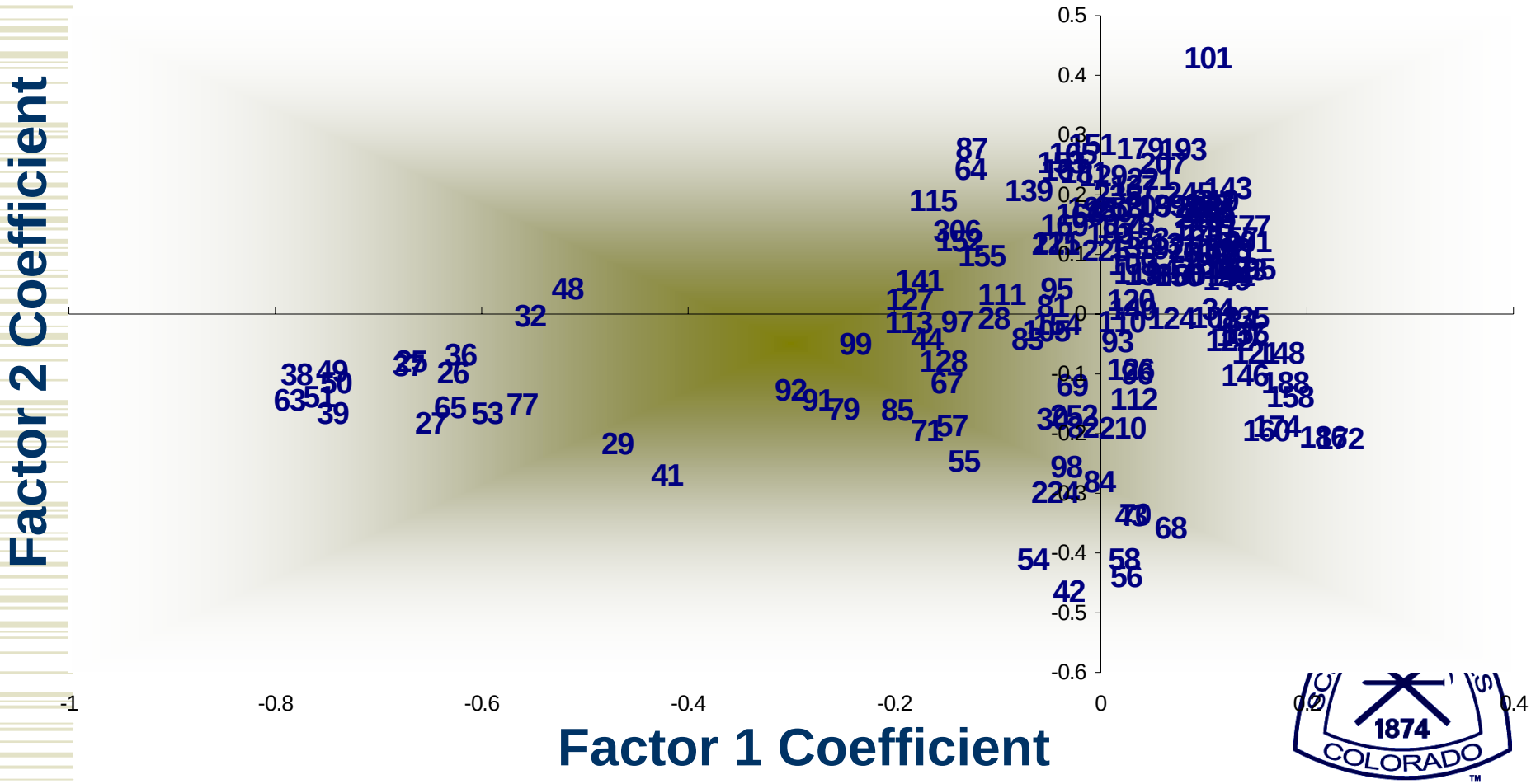
Differences vs. Similarities



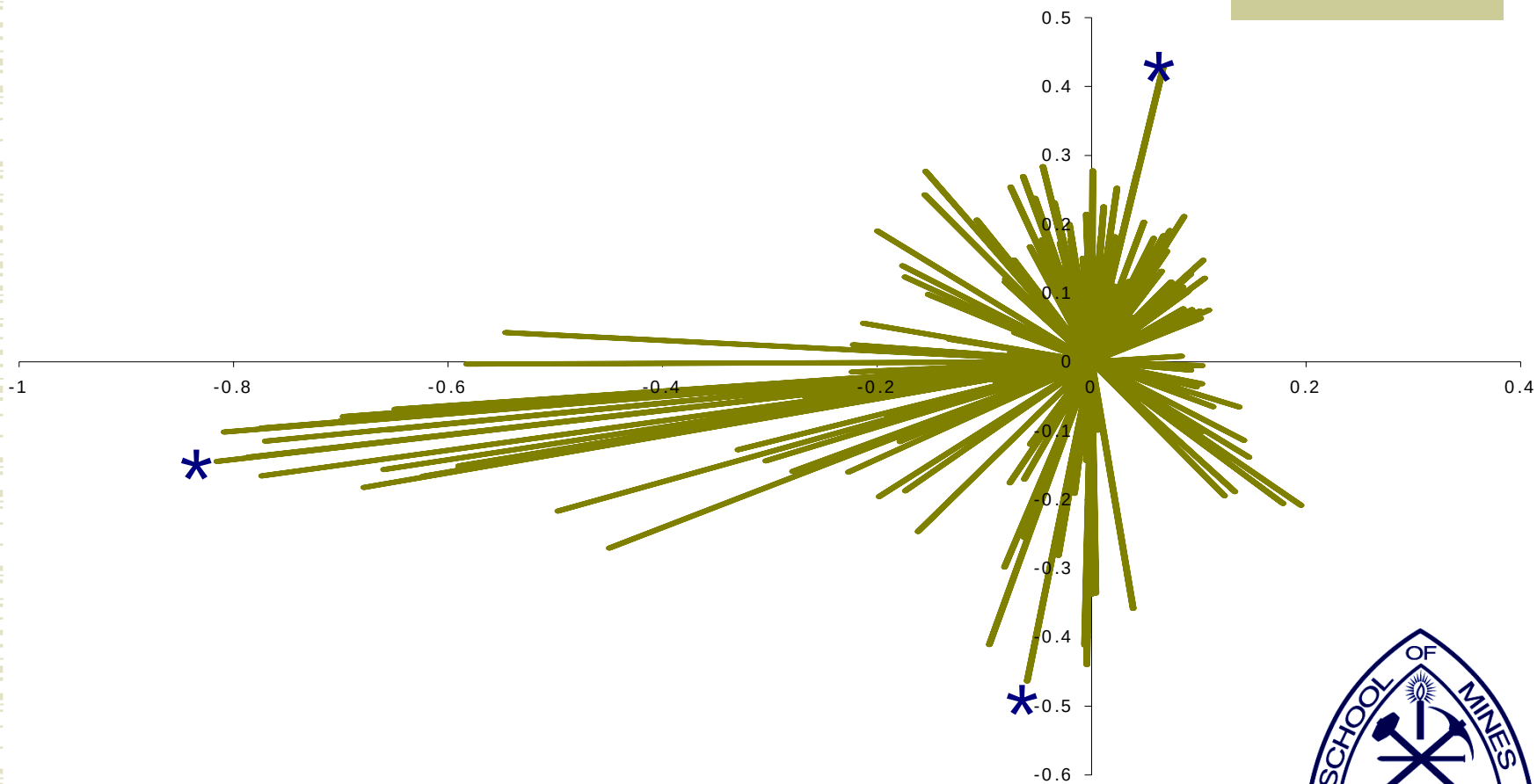
Classification

- **Group I**
  - **Heavy Oils (4500ft depth)**
- **Group II**
  - **Oil Shales**
  - **Gilsonite**
  - **Asphaltine Block**
- **Group III**
  - **Heavy Oils (near surface)**

Mass Loading Distribution



Mass Loading as Vectors

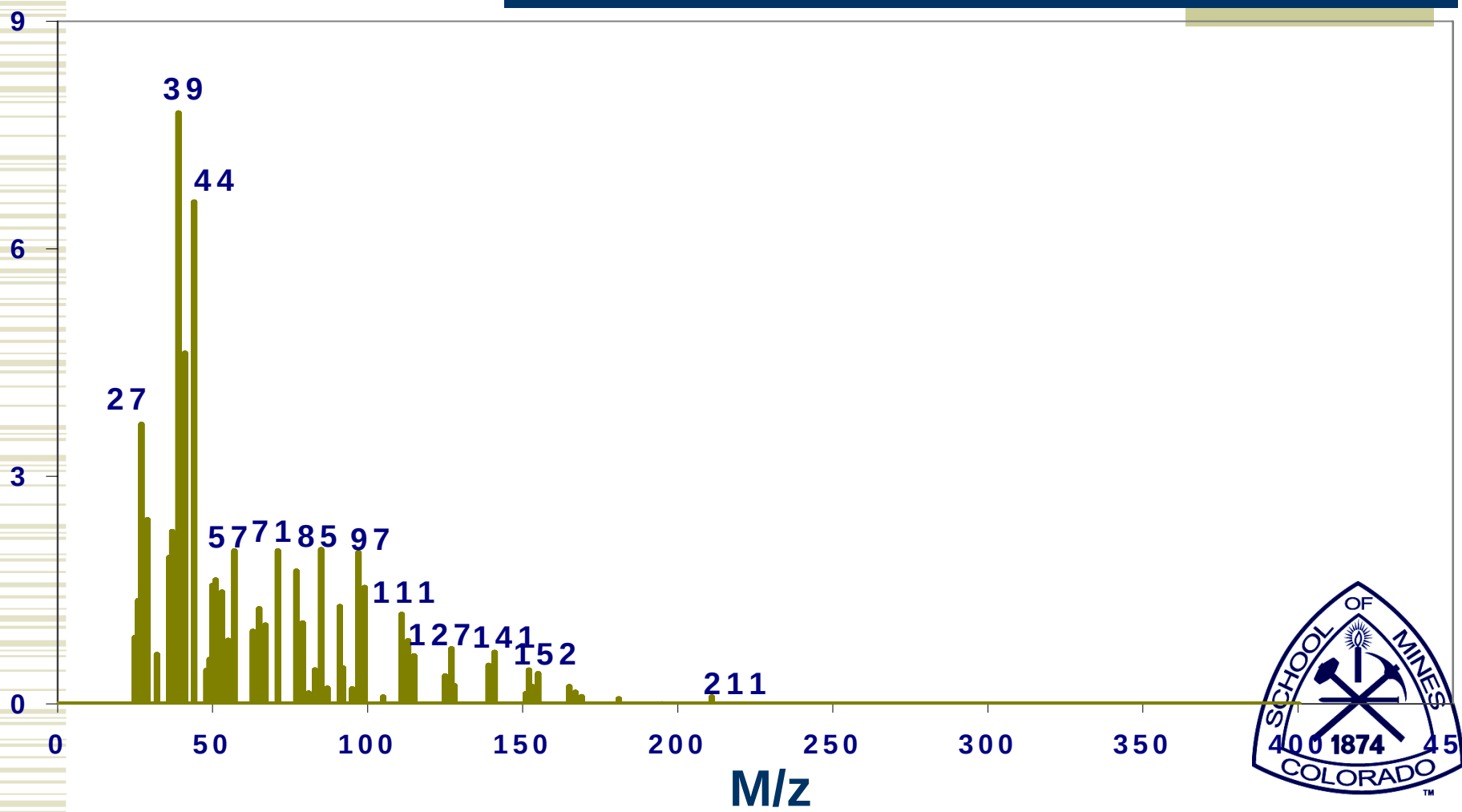


Factor 2 Coefficient

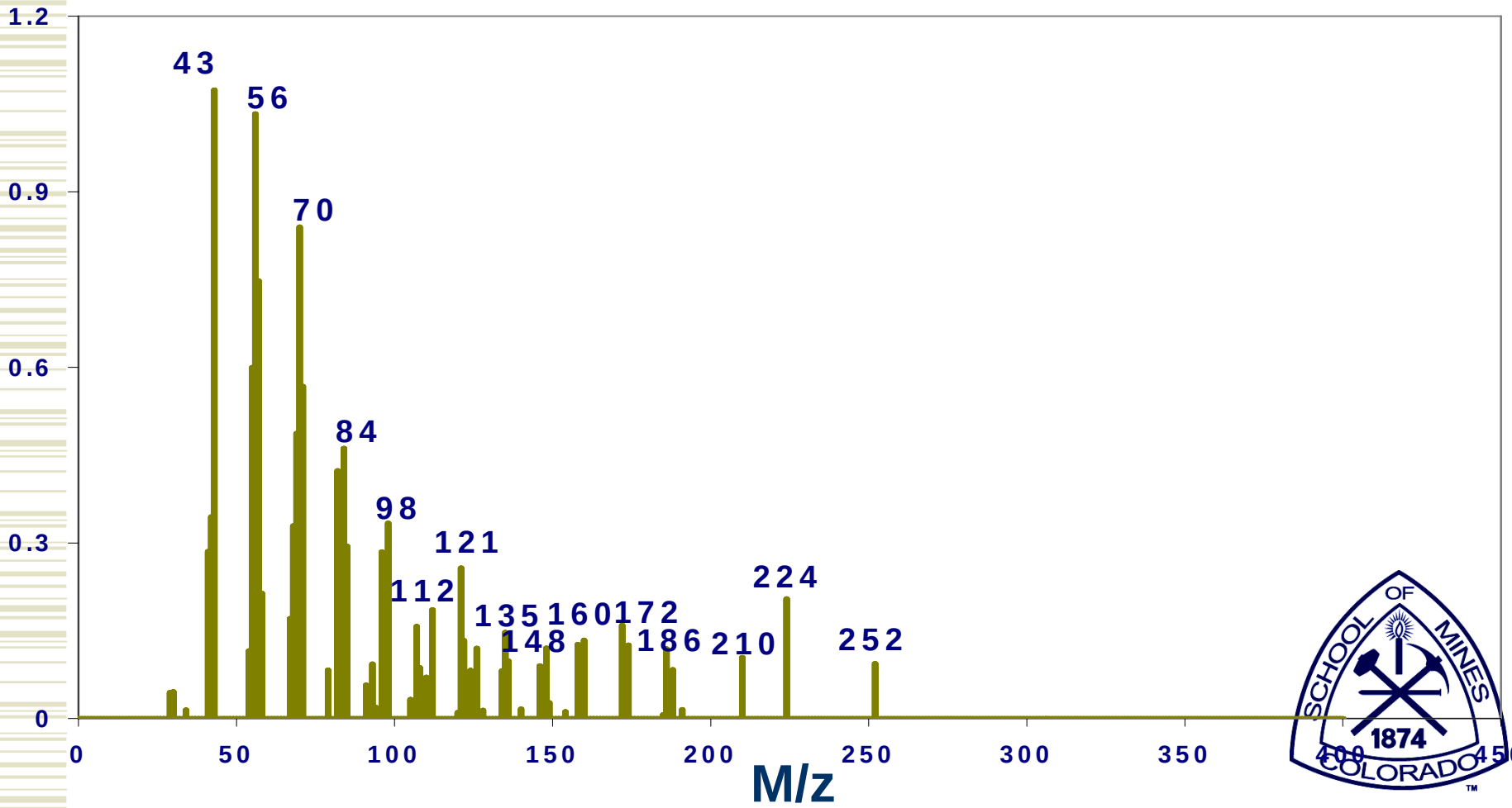
Factor 1 Coefficient

SCHOOL OF MINES 1874 COLORADO

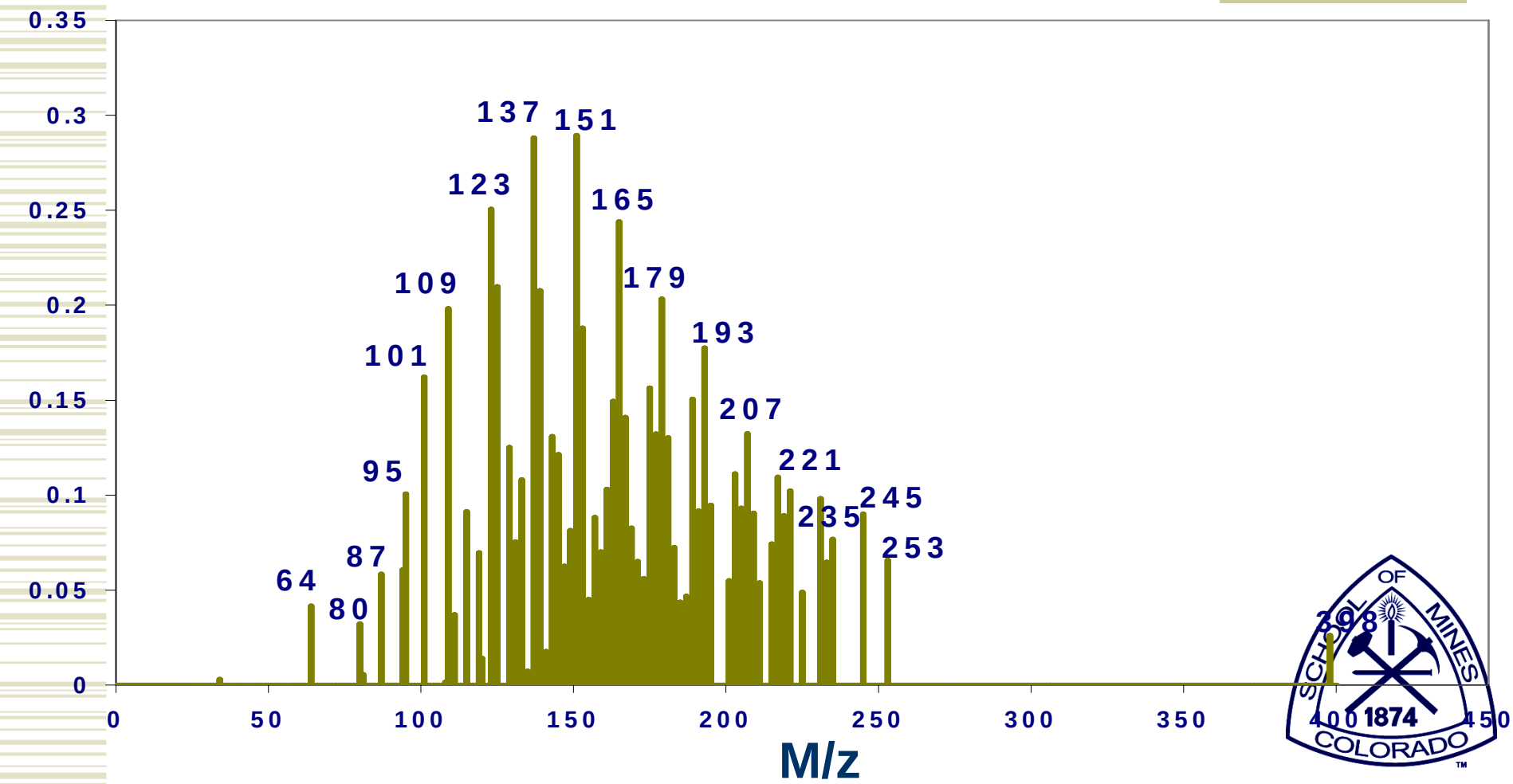
Characteristic Mass – Group I



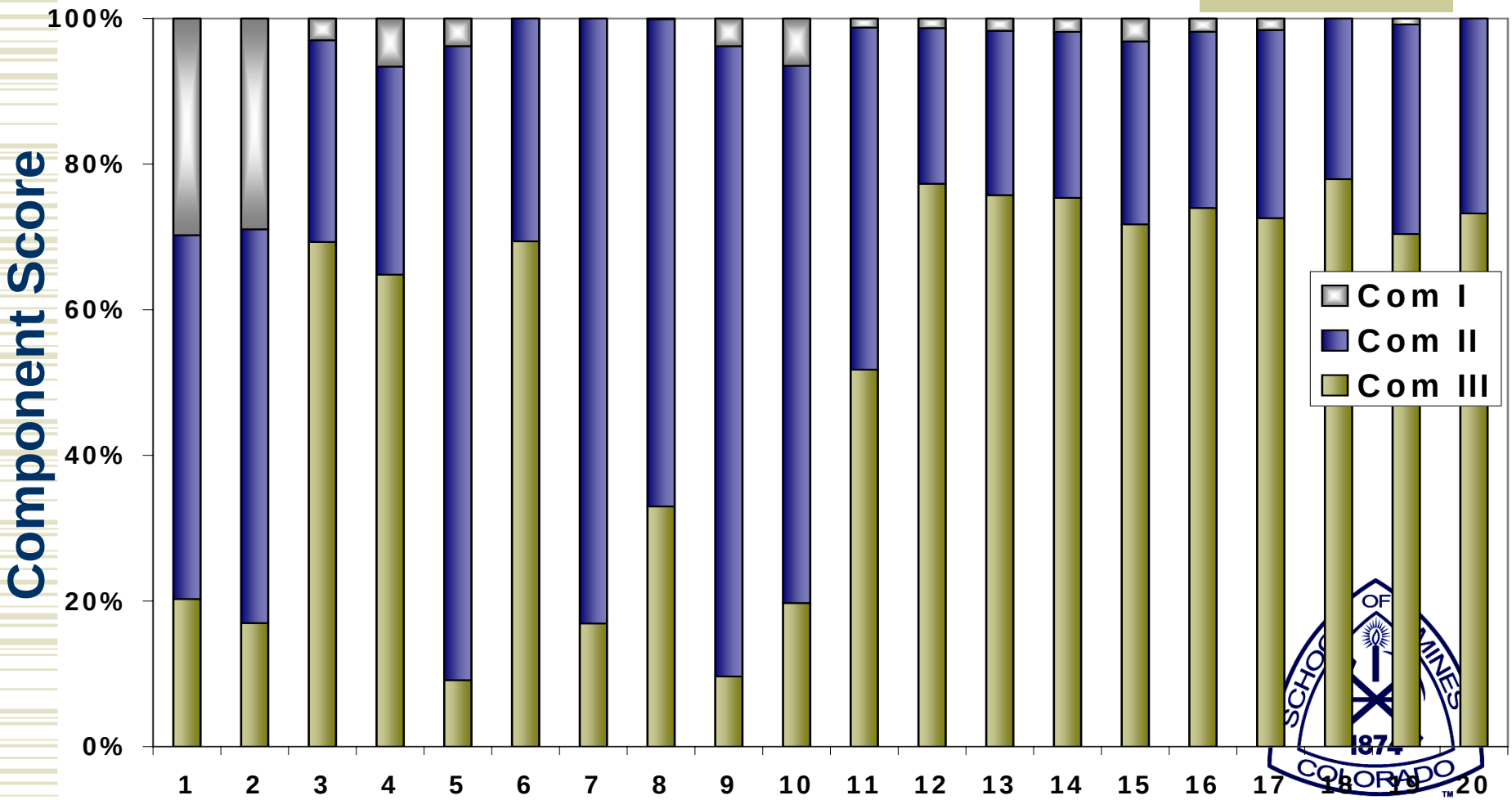
Characteristic Mass – Group II



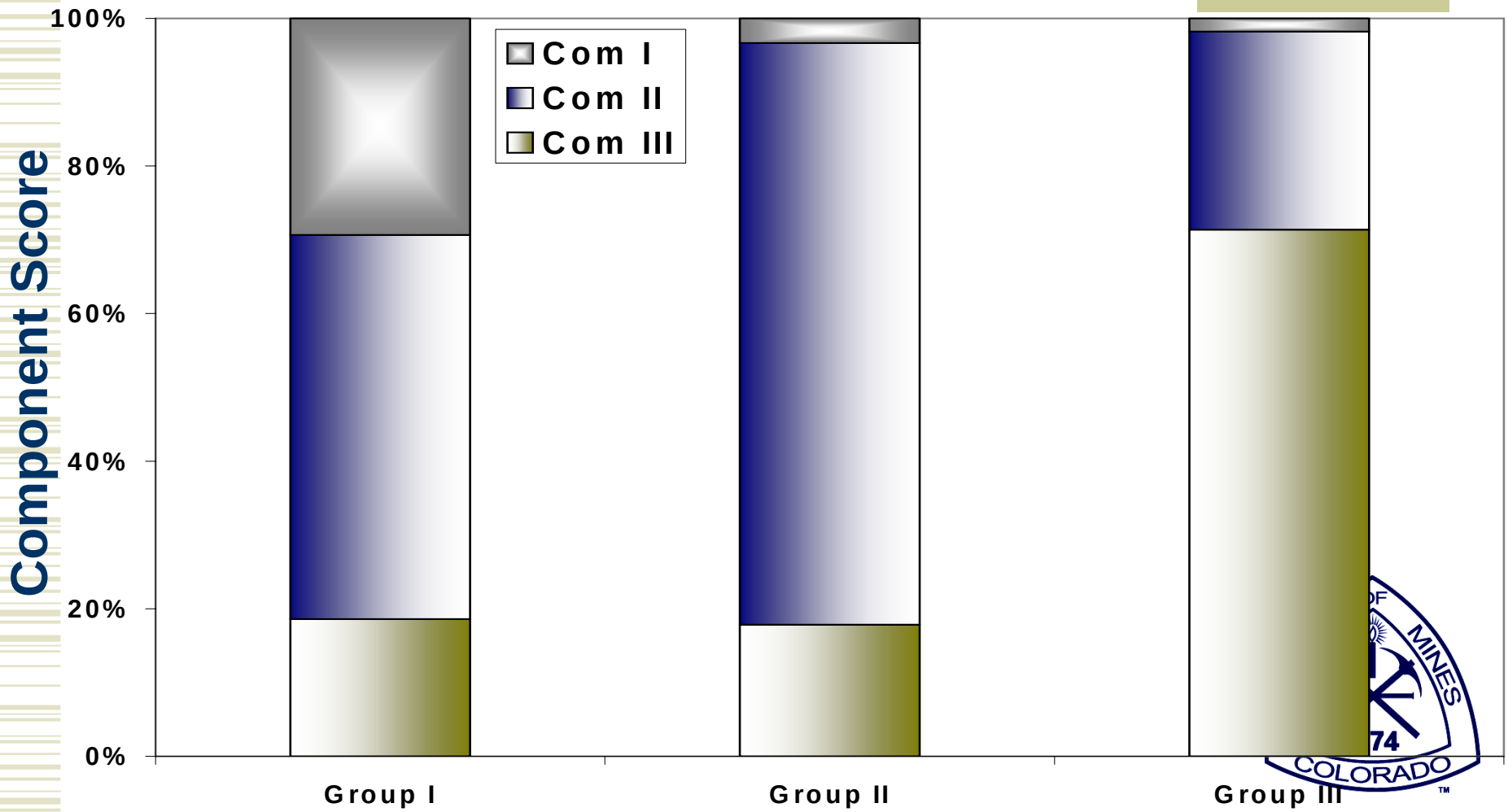
Characteristic Mass – Group III



Component Score



Component Score

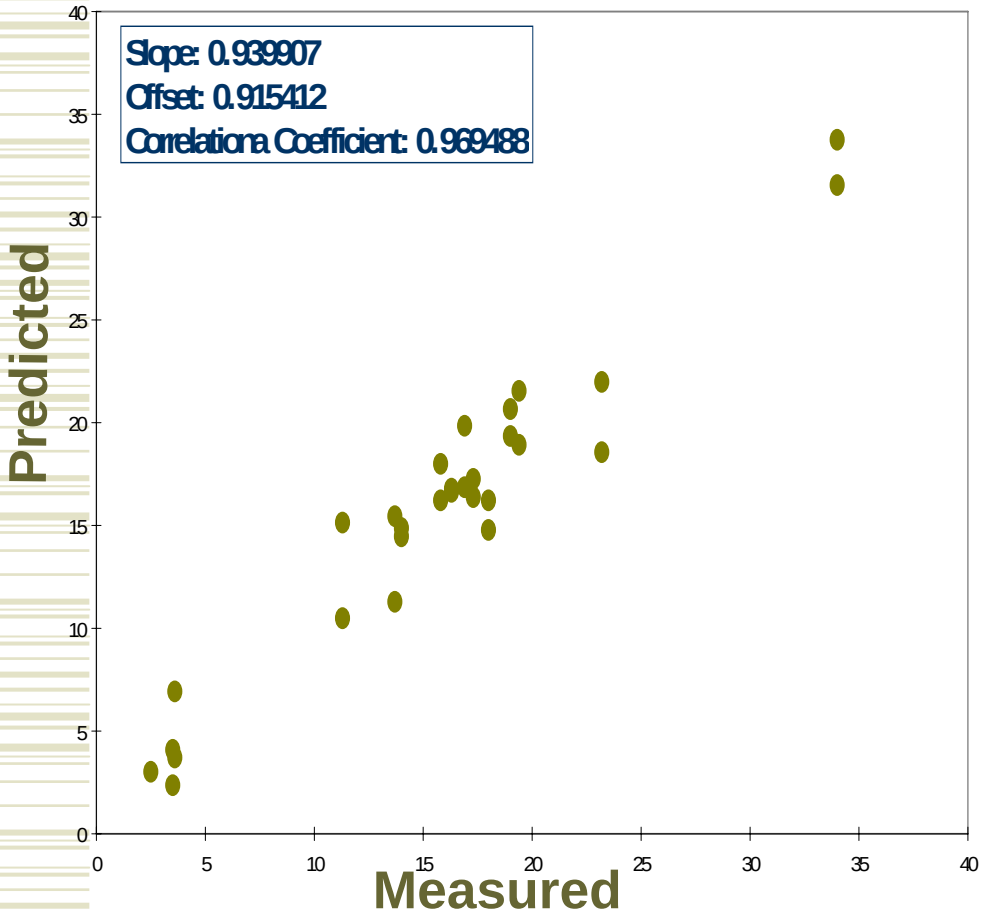


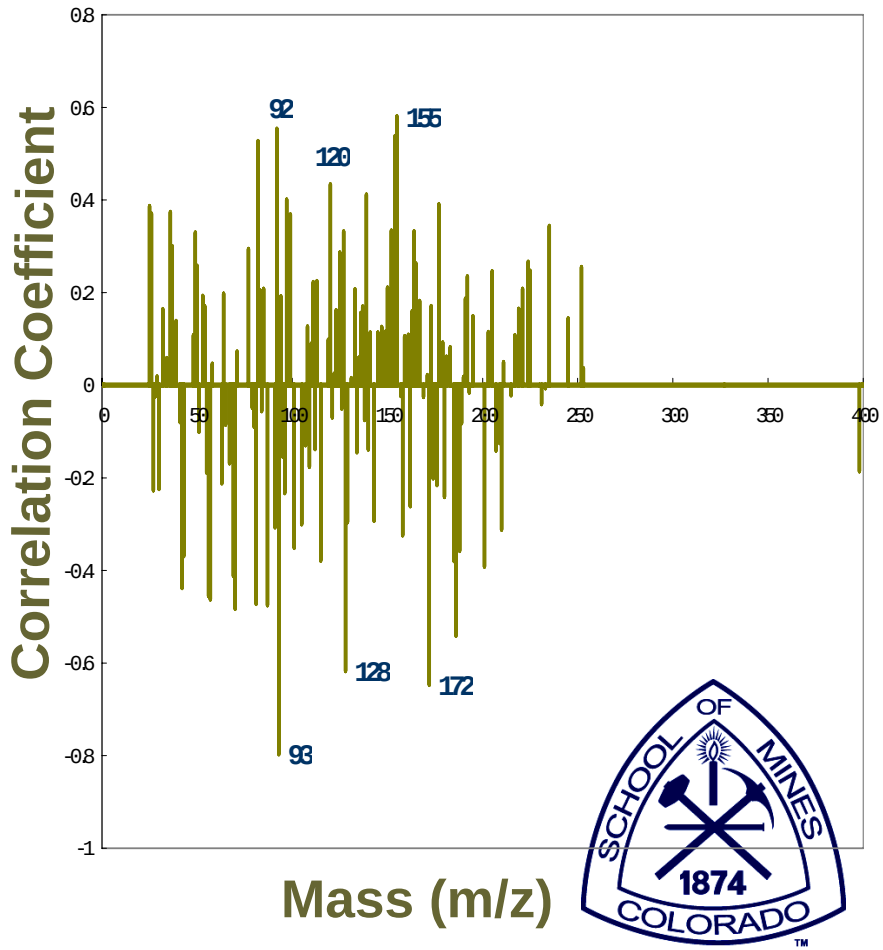
Solvent Extraction and L.C. Results: Heavy Oils

		Saturate	Aromatic	Resin	Asphaltene	Sulfur
I	1	34.0	17.6	27.6	19.6	3.02
	2	11.3	12.2	13.7	62.5	1.44
II	9	2.5	1.3	12.1	83.8	0.69
	10	13.7	8.1	12.9	52.0	6.11
III	19	19.0	31.9	29.0	18.3	3.68
	20	23.2	22.1	35.1	18.3	1.54

* Humble Geochemical Service Division

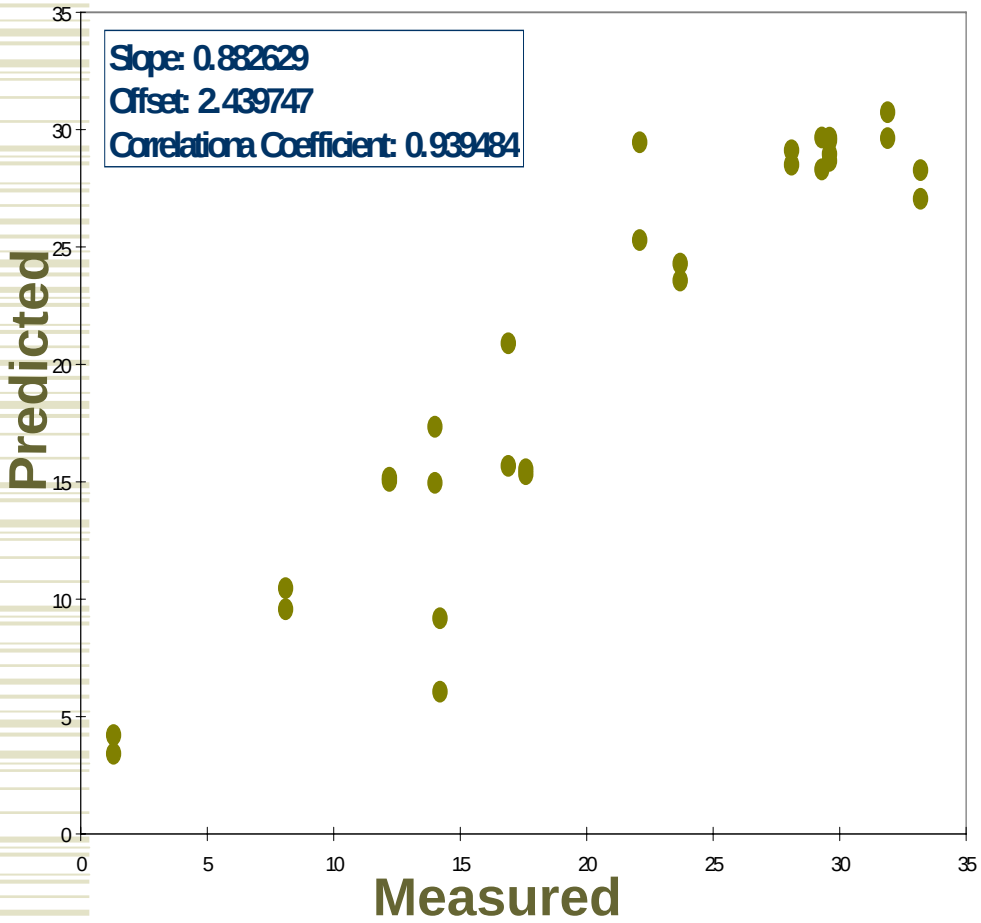
PLS Regression Analysis: Saturates

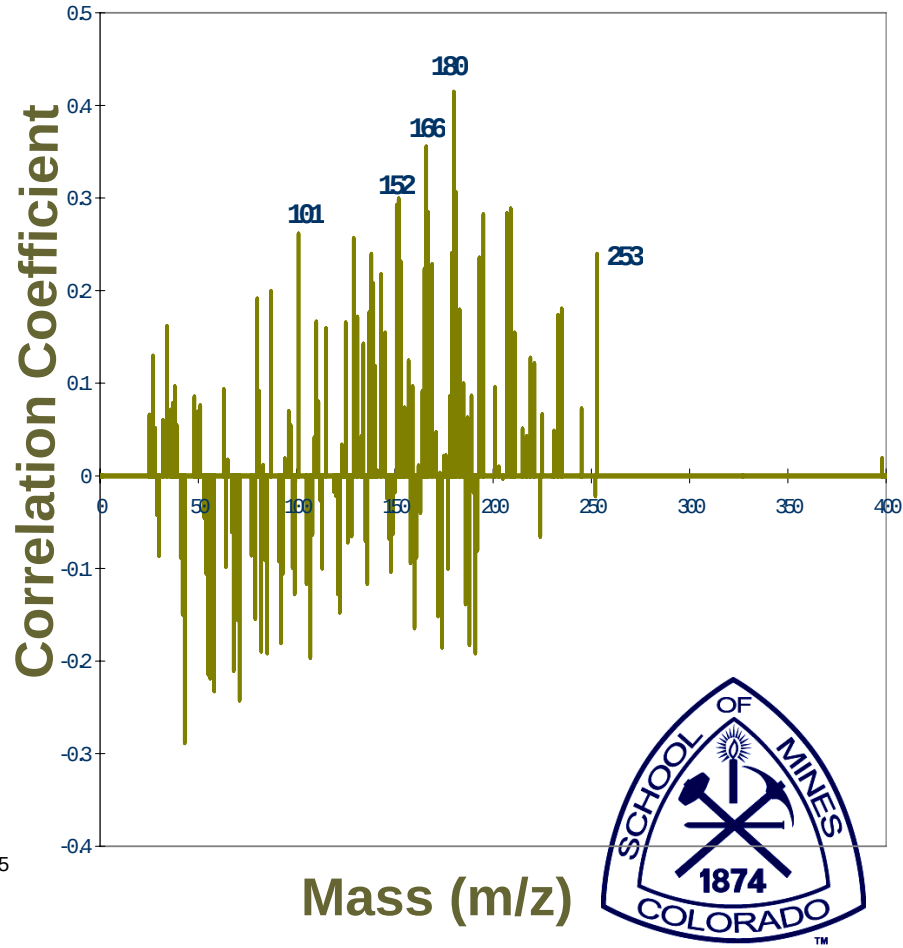




SCHOOL OF MINES 1874 COLORADO

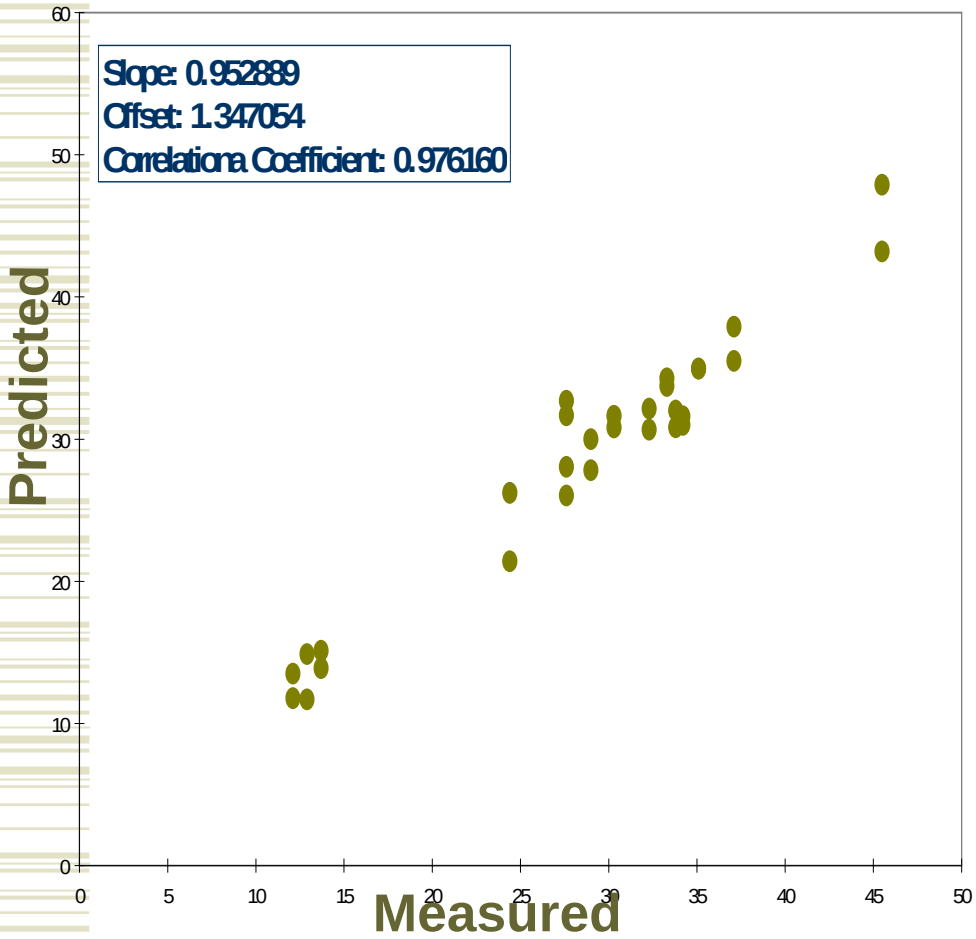
PLS Regression Analysis: Aromatics

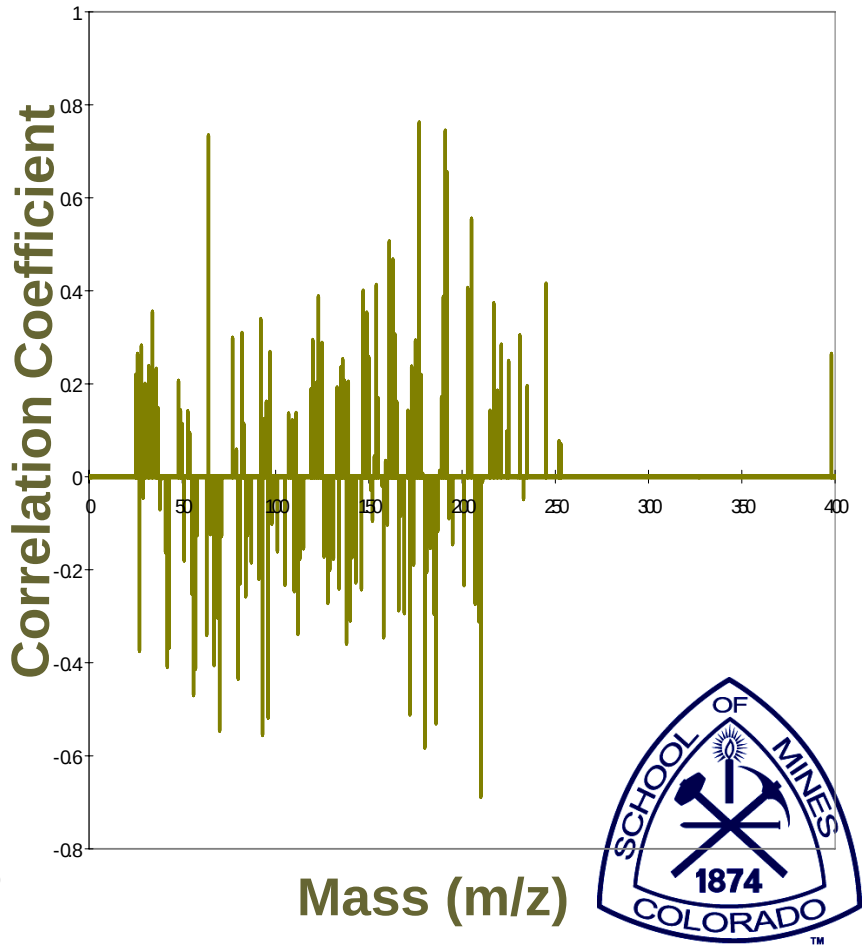




SCHOOL OF MINES 1874 COLORADO

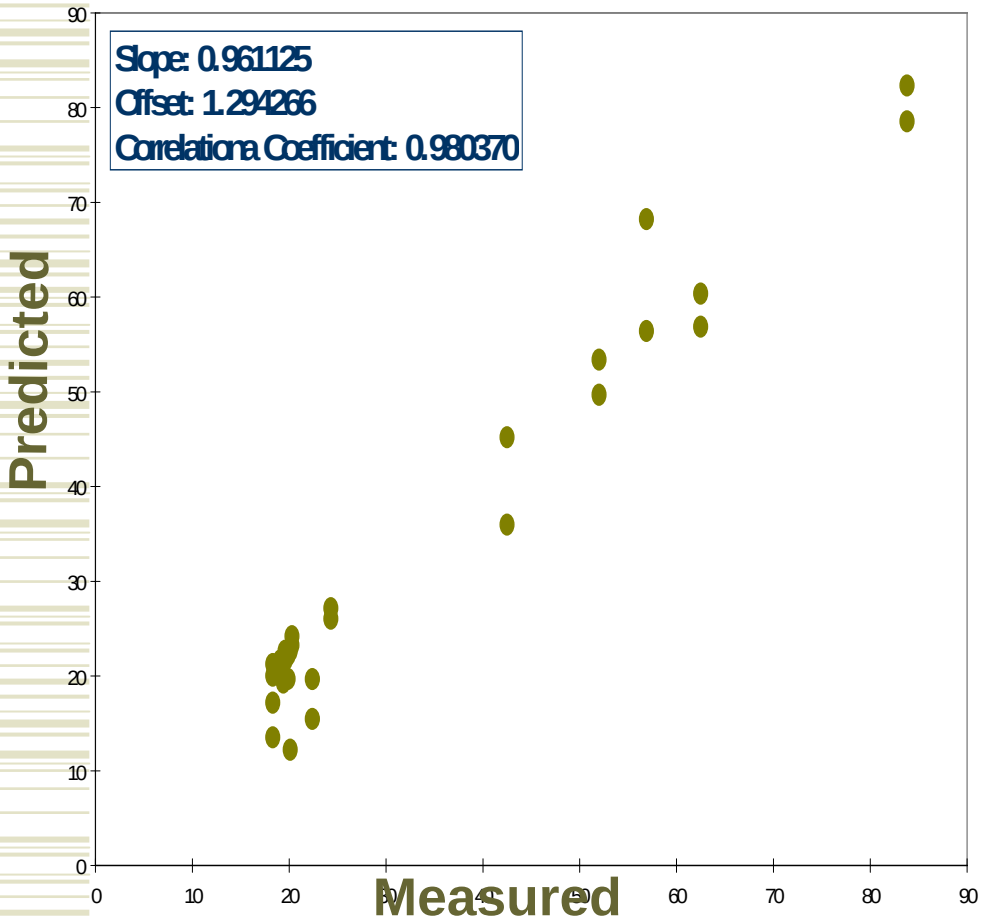
PLS Regression Analysis: Resins

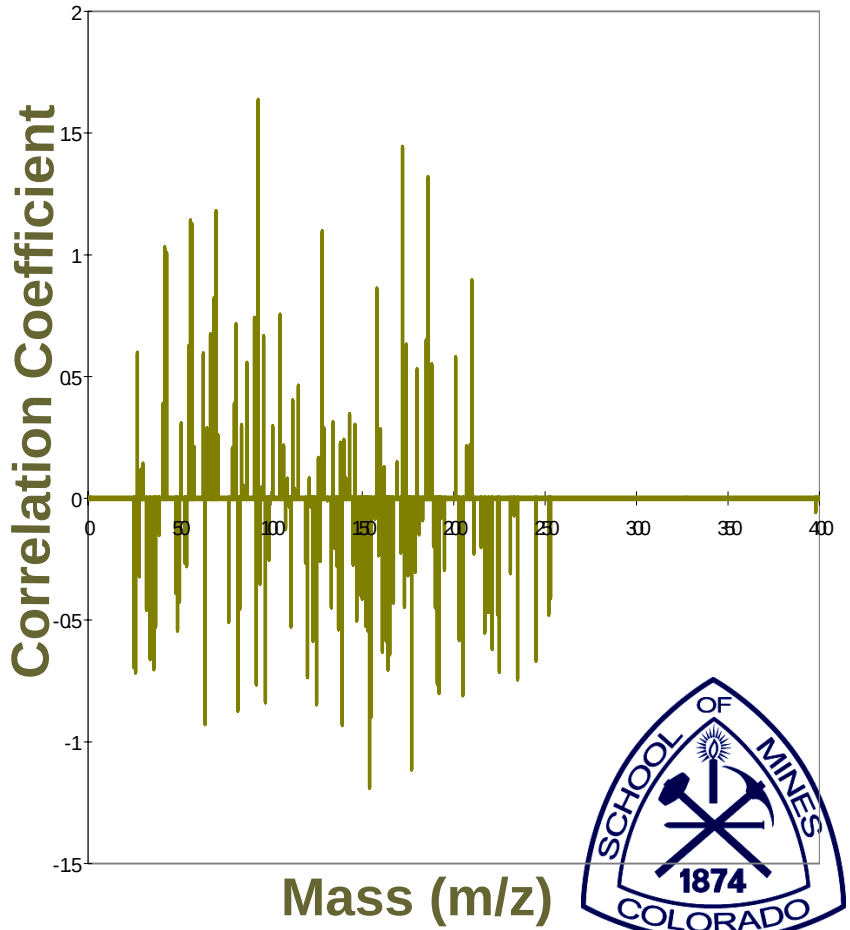




SCHOOL OF MINES
1874
COLORADO

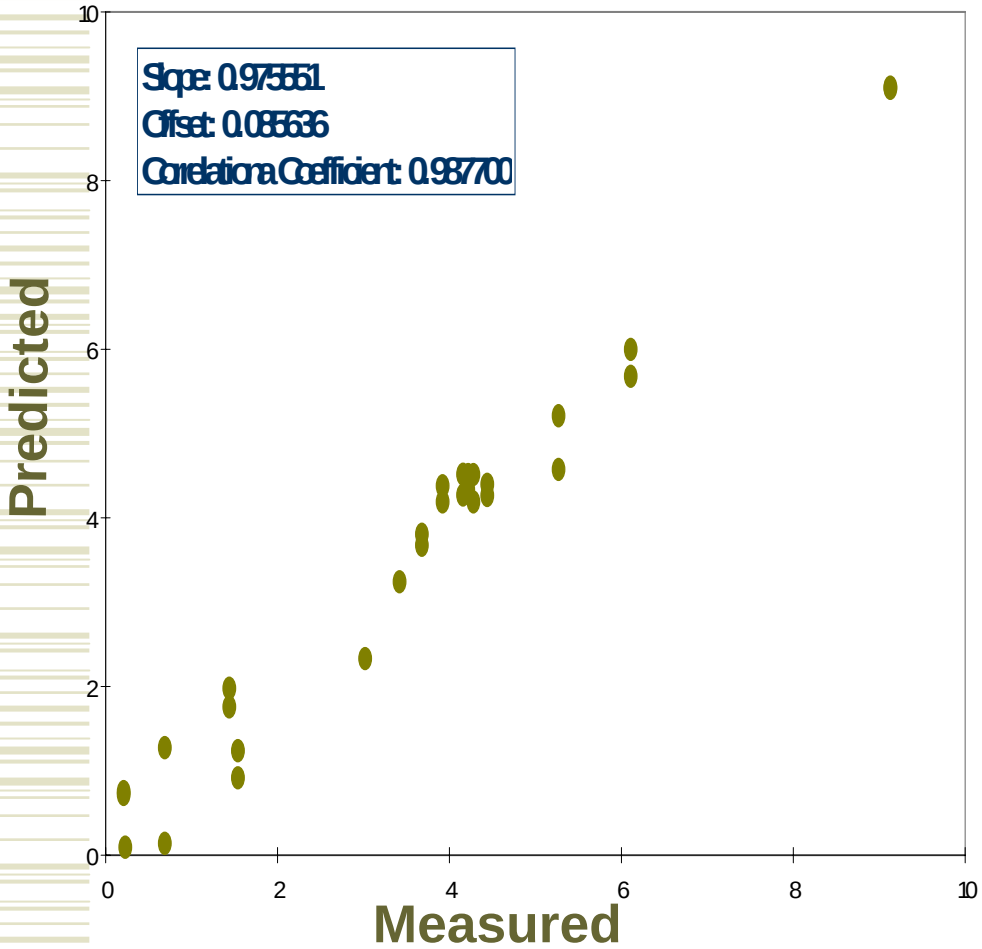
PLS Regression Analysis: Asphaltenes

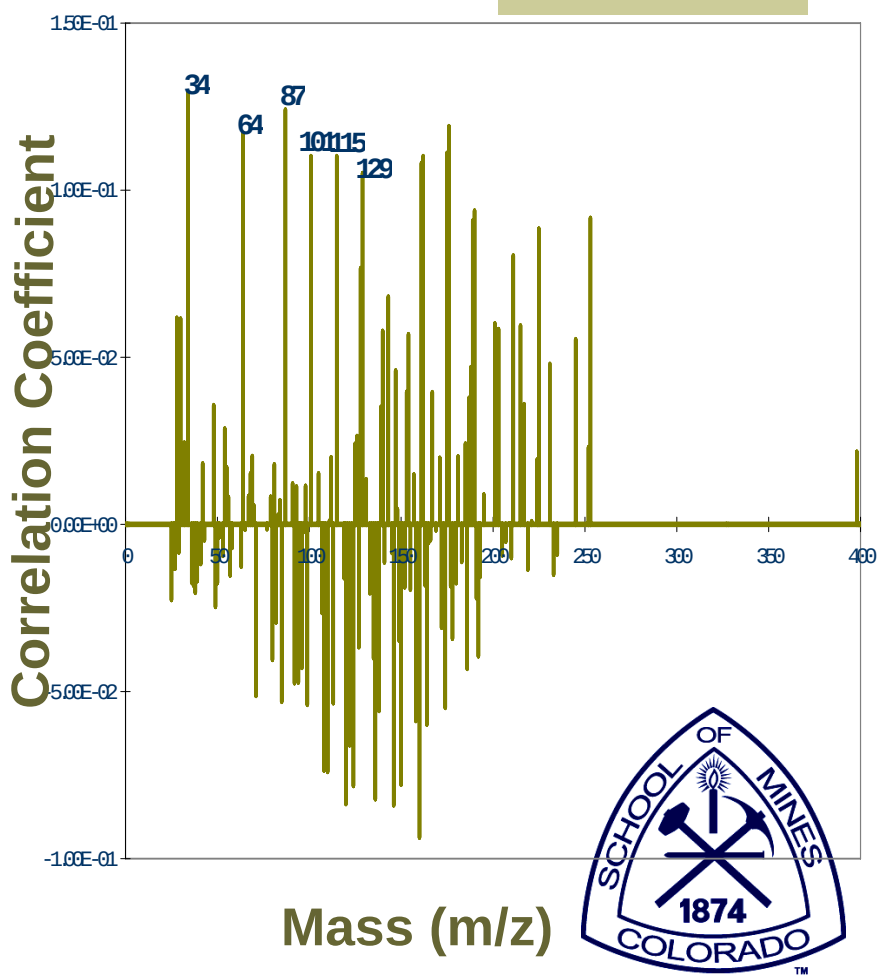




SCHOOL OF MINES 1874 COLORADO

PLS Regression Analysis: Sulfur





SCHOOL OF MINES 1874 COLORADO

Summary

- 20 HC samples were classified into three groups.
- Characteristic component of each group was extracted.
- Composition of components of each group was calculated.
- Py-MBMS were successfully used to predict five geochemical compositions in the samples.

Conclusion

- **Using Pyrolysis, MBMS and Multivariate Analysis could a tool to rapidly characterize different types of alternative hydrocarbon resources.**