

University of Saskatchewan
Department of Chemistry

CHEM-420
MODULE 2
ASSIGNMENT

DUE: March 04, 2024

You will submit your answers to the following questions through the USask Canvas Course Webpage by 4PM - March 04, 2024.

1. (/15) Compare and contrast:
 - a. μ -FTIR and O-PTIR
 - b. AFM-IR and n-SNOMS
 - c. Supervised and Unsupervised Data Analysis
2. (/5) In our lab sessions we explored k-Means data analysis tool as a way to classify our data.
 - a. What is k-Means and how does it work?
 - b. What type of data is it best used on?
3. (/5) In class we discussed how PCA could be used to reduce noise in a dataset. Describe this process.
4. (/5) In a standard Fourier Transform Infrared (FTIR) Spectrometer, a HeNe laser (633nm) is typically used as an internal reference.
 - a. What function does this reference laser have?
 - b. Could we use a 532nm diode laser instead? What differences would there be?
5. (/20) Please read this article and answer the questions below.

Micro to Nano: Multiscale IR Analyses Reveal Zinc Soap Heterogeneity in a 19th-Century Painting by Corot; Xiao Ma, Georges Pavlidis, Eoghan Dillon, Victoria Beltran, Jeffrey J. Schwartz, Mathieu Thoury, Ferenc Borondics, Christophe Sandt, Kevin Kjoller, Barbara H. Berrie, and Andrea Centrone; Anal. Chem. 2022, 94, 7, 3103–3110 (doi.org/10.1021/acs.analchem.1c04182).

- a. In this work a variety of infrared methods (μ -FTIR, O-PTIR, PTIR) were used to study the distribution of chemical species in the top-most paint layer of a painting. Describe how the authors performed the measurements (workflow) and the importance of this multiscale approach in their analysis.
- b. Excluding infrared spectroscopic techniques, what other techniques could help these researchers in this work?
- c. Provide an example research problem where a similar multiscale approach could be used.