University of Saskatchewan

Department of Chemistry

CHEM-420

MODULE 2

HANDS-ON EXERCISE

DUE: February 12, 2024

Exercise

In this exercise you will explore a hyperspectral mid-infrared dataset utilizing the tools provided in Quasar. You will go through some basic pre-processing steps followed by a simple analysis looking at infrared band integrations and mapping followed by more advanced analysis tools like PCA and k-Means.

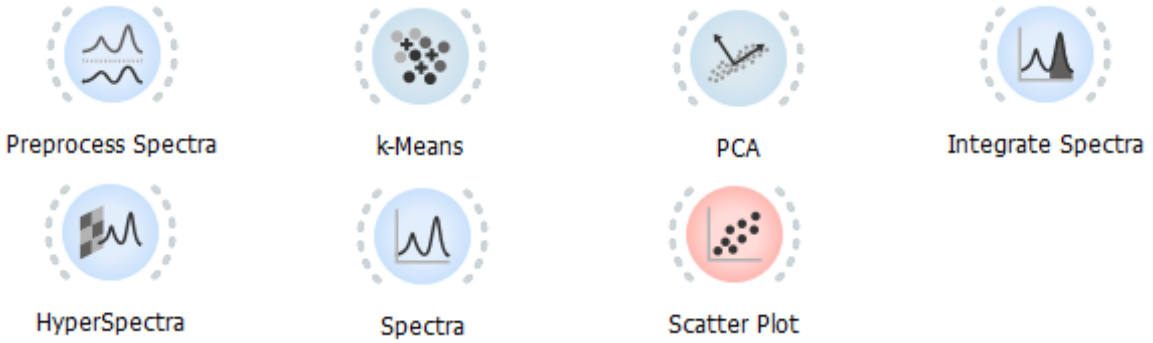
You will submit a copy of your Quasar Canvas Workflow and short summary (200 words) of your analysis through the USask Canvas Course Webpage by the end of the day February 12, 2024.

Dataset

Liver cirrhosis – spectral image: Liver is the organ in charge of food and drug detoxification, cholesterol, lipids and glycogen synthesis. In case of cirrhosis, some parts of the liver become isolated in nodules by fibrotic tissue rich in collagen. The infrared map was recorded at the intersection between several cirrhotic nodules. The Fourier transform infrared spectroscopy (FTIR) measurement was performed in trans-reflection mode from a 10 µm thick section at 8x8 µm² spatial resolution. The data was imaged by Dr. Christophe Sandt.

Tools

Below are some of the tools in Quasar that you will need to use to demonstrate a workflow containing: band integrations, PCA and k-Means results.



Questions

There are no formal questions to answer in this exercise, but consider the questions listed below as potential points to address or include in your short summary write-up or workflow canvas.

- What band integrations did you choose to use and why? (Hint: Reference listed below describes some of those broad biological structures that are routinely analyzed from mid-infrared chemical maps)
- The hyperspectral widget allows you to plot a map as an RGB map by selecting 3 different components as intensity of red, green, blue overlays (can be integrated bands, or principal components). How do results compare between analyses?

- The output of k-Means can be analyzed in the hyperspectral widget by looking at by displaying the cluster output as a 'type'. How does it compare to the integrations? PCA?
- With respect to PCA, in the Loadings (spectra) – are there significant contributions from certain bands in the principal components? Do the Scores show anything interesting (use a Scatter plot)
- What sort of pre-processing did you use? Would it be appropriate to do a baseline correction technique?

References

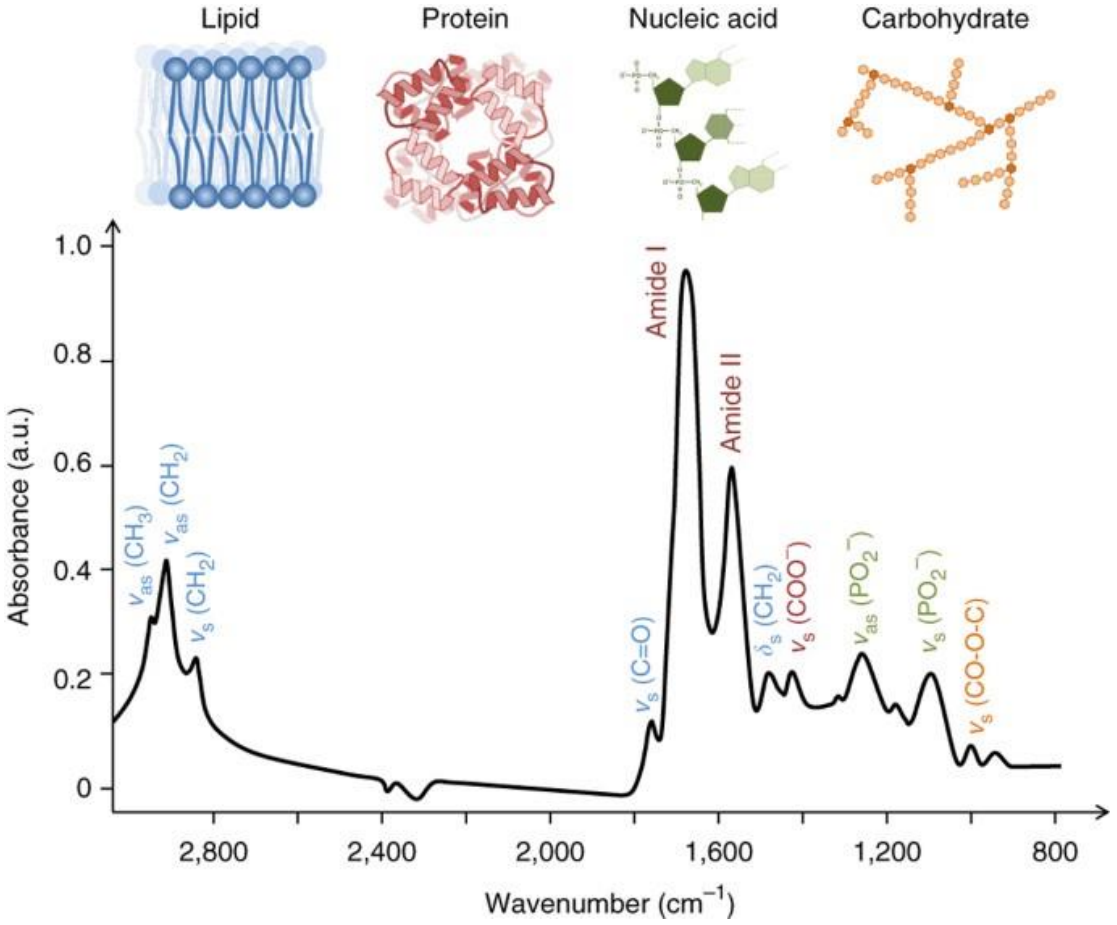


Figure 1: Typical biological spectrum showing biomolecular peak assignments from 3,000–800 cm−1, where ν = stretching vibrations, δ= bending vibrations, s = symmetric vibrations and as = asymmetric vibrations. (Baker, M., Trevisan, J., Bassan, P. et al. Using Fourier transform IR spectroscopy to analyze biological materials. Nat Protoc 9, 1771–1791 (2014). https://doi.org/10.1038/nprot.2014.110)