Chemometrics

Application Overview

Aligning NMR

Demonstration of the LineUp™ alignment technology to standardize data

Summary

Nuclear Magnetic Resonance can be used in a variety of applications where a rapid evaluation of a complex mixture is required. This brief addresses the x-axis shift problem common to NMR, a problem that is often blocking the deployment of the instrument for routine screening applications. In this case, NMR is used to profile the aromatic fraction separated during the petroleum refining process. We use a chemometric alignment tool based on correlation optimized warping to eliminate the shifting of the spectrum as an alternative to the binning approach that is in common use. An advantage of this approach is that the spectrum retains far more of the detailed features that are critical to an effective evaluation of the fraction when compared to binning.

Plotting the NMR instrument runs for a series of aromatics gives us the data shown in Figure 1 below. The data shows defined clusters that are largely consistent from one run to another, but it is difficult in these data to assess true chemical differences automatically, necessitating a manual evaluation step.

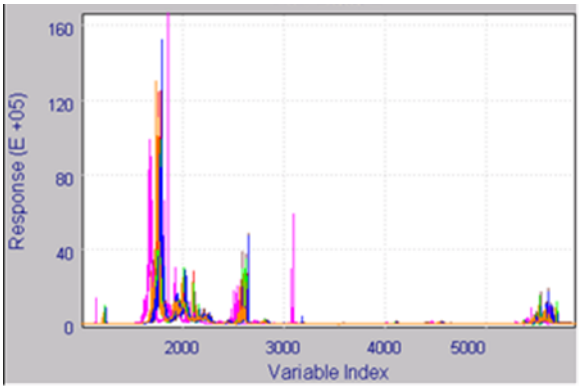

Figure 1: The original QC NMR raw data on the aromatic fractions

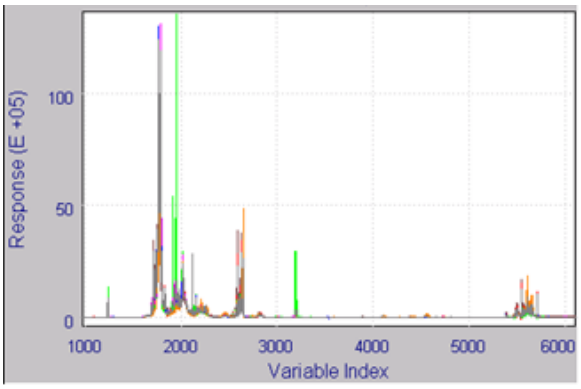

Figure 2: The same NMR runs after alignment with LineUp software

The LineUp software is designed to handle this x-axis shift. The software can be called immediately after data acquisition, even integrated into the method so that it runs automatically with every sample tested. The result is that the original data is preserved and a companion NMR trace is generated that has shift eliminated. The LineUp files generated for the data in Figure 1 are shown in Figure 2.

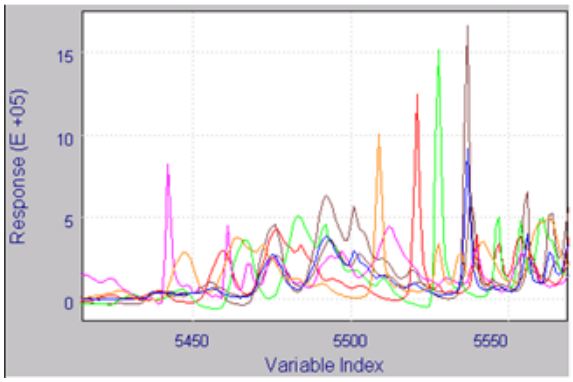

Figure 3: Zooming in on one of the NMR peak clusters (original spectra above, aligned spectra below)

Zooming in on one of the primary peak clusters of the unaligned data shows the need for the LineUp approach (see Figure 3).

The x-axis shifting is so large in these data sets that it is extremely difficult to compare the overlaid traces. Using the alignment, however, traces can be compared directly and small differences can be spotted, even automatically flagged using the Pirouette/InStep system.

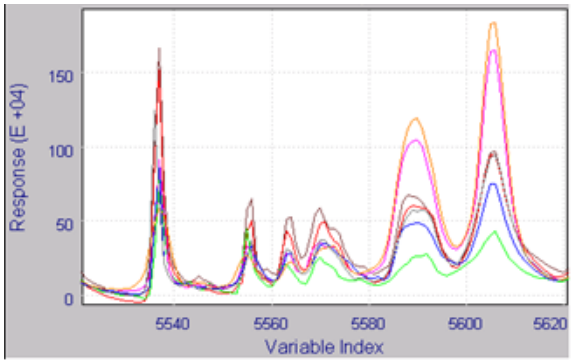

Figure 4: Zooming in on several of the aligned NMR peaks (not the same scale as in Figure 3.)