

Automatic Baseline Correction

When performing Raman spectroscopy, it is some times the case that spectra can be contaminated by fluorescence. Working in the near infrared excitation (785 nm) radically reduces the observance of sample fluorescence, often known as auto-fluorescence.

Some samples may still exhibit fluorescence, even when using 785 nm excitation, or in certain examples a shorter wavelength may be in use. In cases such as these, baseline correction can be employed to remove this fluorescence baseline and cosmetically improve the spectra.

When performing high throughput Raman or when acquiring Raman chemical images, it is easy to end up with tens of thousands of Raman spectra. Due to the volume, manually baseline correcting these spectra is simply not possible. What is required is an automated baseline correction algorithm.

Several baseline techniques exist, but these are designed for either user intervention or designed for baseline correction of FT-IR spectra. These techniques cannot be successfully applied to Raman.

Figure 2 shows the spectrum from Figure 1 automatically baseline corrected using an FT-IR software algorithm. These results are not ideal.

The PerkinElmer® Spectrum™ software incorporates a technique which fits a high order polynomial curve to the data, as shown in Figure 3. The software then analyzes the original spectrum and the polynomial, and generates a new “spectrum” (shown in Figure 4), which is made of the original spectrum, with all data-points more intense than the polynomial removed. This resulting spectrum is the software’s first approximation at the fluorescent baseline. This polynomial fitting is repeated, this time using the first pass baseline as the starting point. This process is repeated up to 30 times, resulting in a polynomial

Author

Andrew Dennis BSc, Ph.D.
PerkinElmer
1 Chlorine Gardens
Belfast, N. Ireland
BT9 5DJ

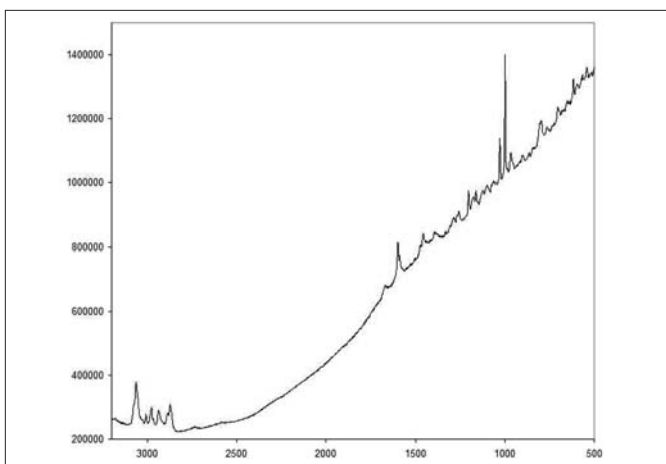


Figure 1. Typical fluorescent spectrum.

which “hugs” the baseline of the original spectrum. Subtraction of the final polynomial from the original spectrum yields the baseline corrected spectrum (see Figure 5).

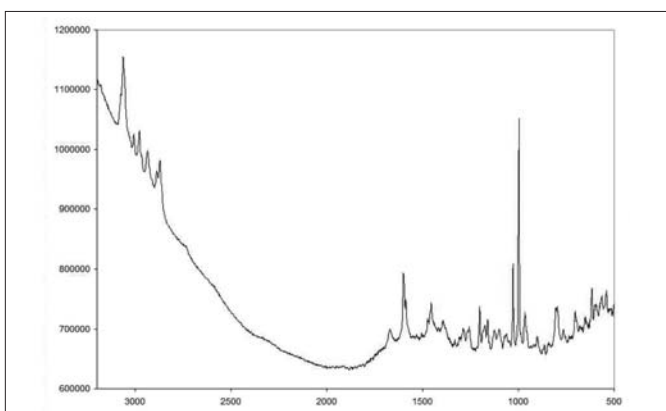


Figure 2. AI Autobaseline correction.

Although this technique is not perfect, it is very good, does not result in spectral artifacts, is highly reproducible and also fully automated. This auto baseline correction technique is incorporated into the Spectrum software, and can be applied in real time while either chemical image or high throughput data is being collected, or while a reaction is being monitored.

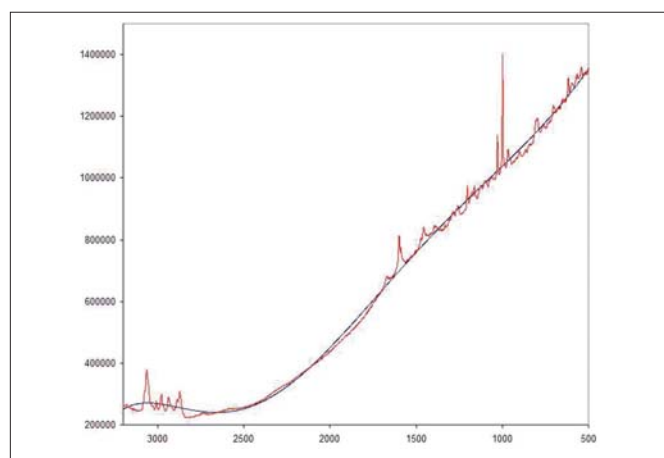


Figure 3. First pass polynomial.

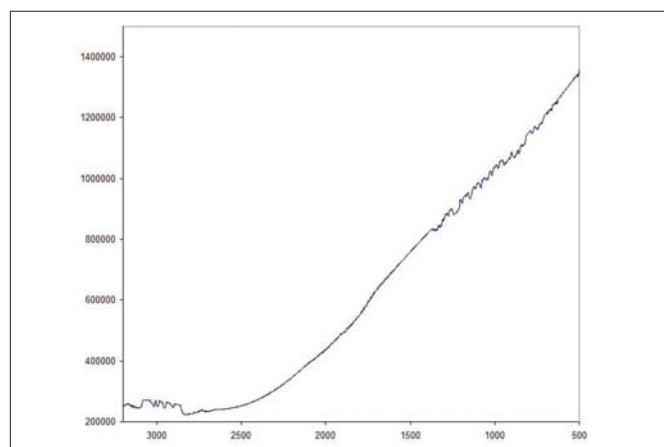


Figure 4. First pass baseline.

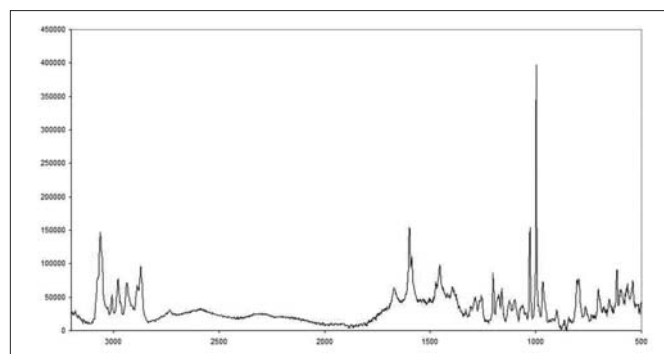


Figure 5. Auto-baseline corrected spectrum.