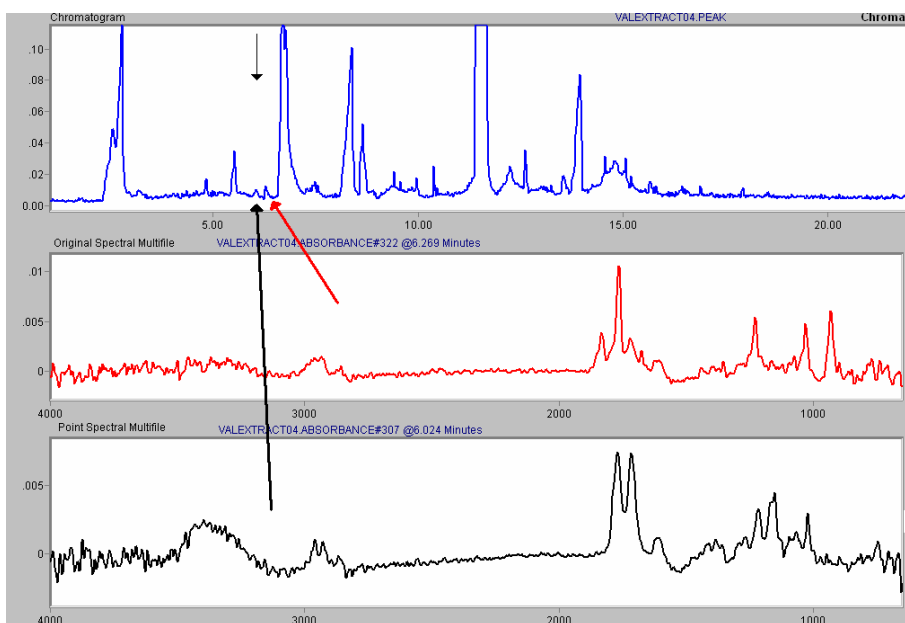




Reduction of Spectral Noise through Post-run Scanning

Since the DiscovIR instrument obtains IR spectra of chromatographic peaks by depositing them on a cryogenic disk, they remain on the disk after the initial spectra are taken. This enables additional IR scanning, which can significantly improve the spectral quality of the marginal components of low concentration. This note demonstrates how excellent spectra may be obtained even of components near the detection limit.

The noise of an FTIR spectrum decreases as the square root of the number of scans. Thus by investing a bit of time scanning the deposit after the run is complete, it is possible to gain a factor of 10 to 100 in signal to noise ratio, which translates to sensitivity. The screen below shows a chromatogram from the DiscovIR-GC of an essential oil flavor, with the spectra of two minor peaks highlighted by the arrows. These components are about 1% of the concentration of the major components, and represent the range of one to three nanograms each. The spectra, while informative, show significant noise. Post-run scanning improves the spectral quality, as shown on the next page.





Reduction of Spectral Noise through Post-run scanning

The most convenient way to collect additional scans is by defining a table of the peaks of interest, and having the instrument rescan them automatically. The dialog screen for this purpose is shown below, with the two peaks defined for rescanning. The chemist defines the peak and background retention times, as well as the number of scans (or signal to noise ratio) desired. Up to ten peaks may be processed in a batch. The two peaks of this example are shown below, comparing the original with the post-run spectra.

Peak #	Peak Time	+ Scans - S/N ratio	Seek Band	Backgrounds
1	6.04	200	0	
2	6.27	200	0	5.5 6.5

2 peaks defined

Buttons: Save, Next Peak, Previous Peak, Erase Peak, Erase Table, Auto

Left edge display: 4000, Max display: 0, Chrom left: 1.195
Right edge display: 650, Min display: 0, Chrom right: 6.004

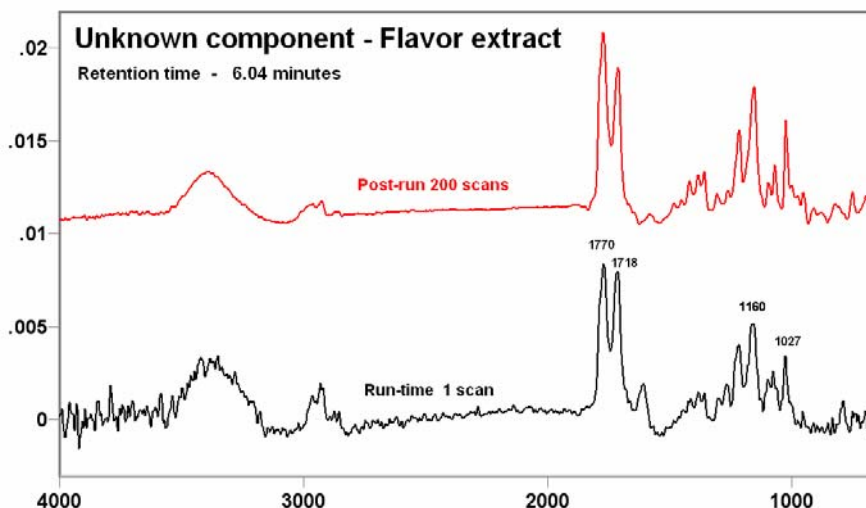
Equal = Autoscale, To set hit ENTER key

Change Run Number: Run 1, C:\Data\Junktest mix

Base of file name: NewSpec

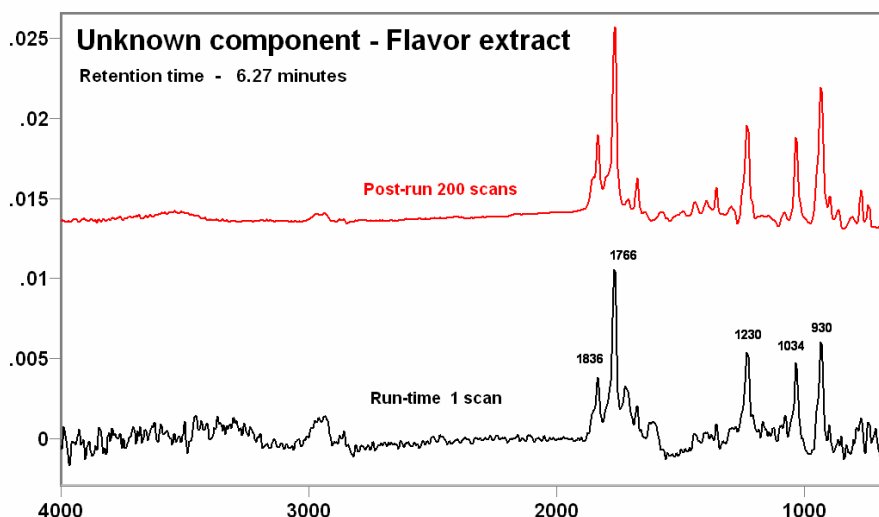
Browse Path: C:\Data\Esesential Oil, Scans/Set: 50

Comment: 60/1/6/120/15/250/5 15m DB1 1 uL split 1%7

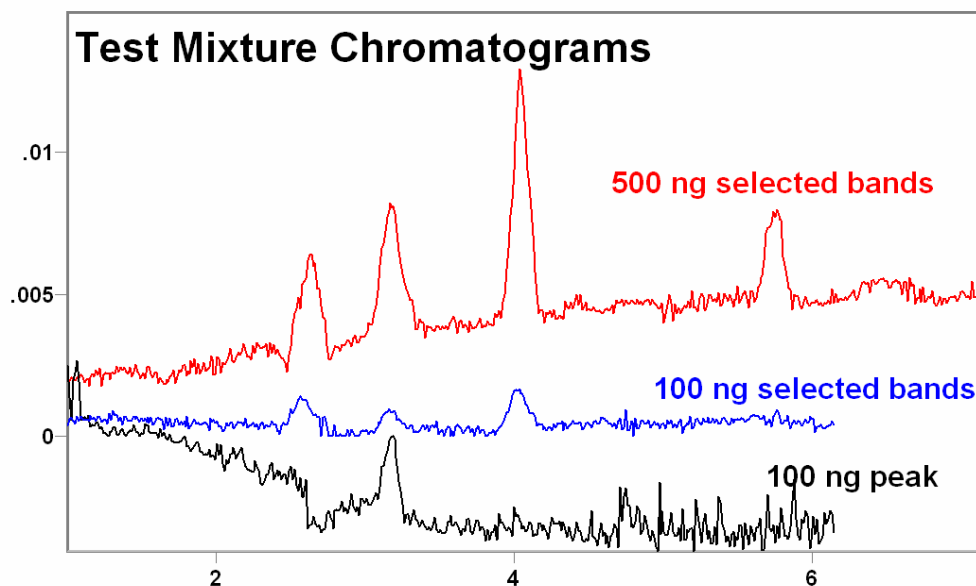




Reduction of Spectral Noise through Post-run scanning



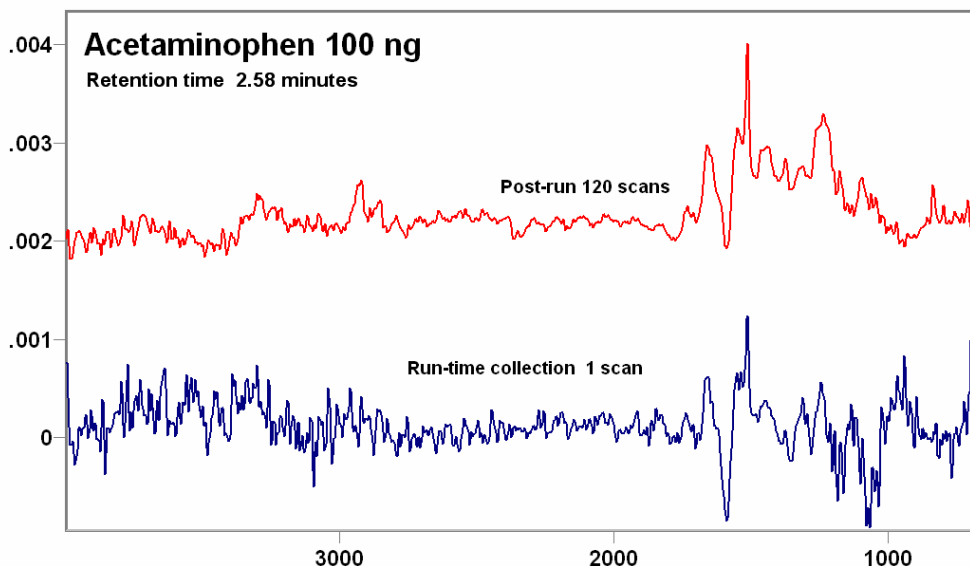
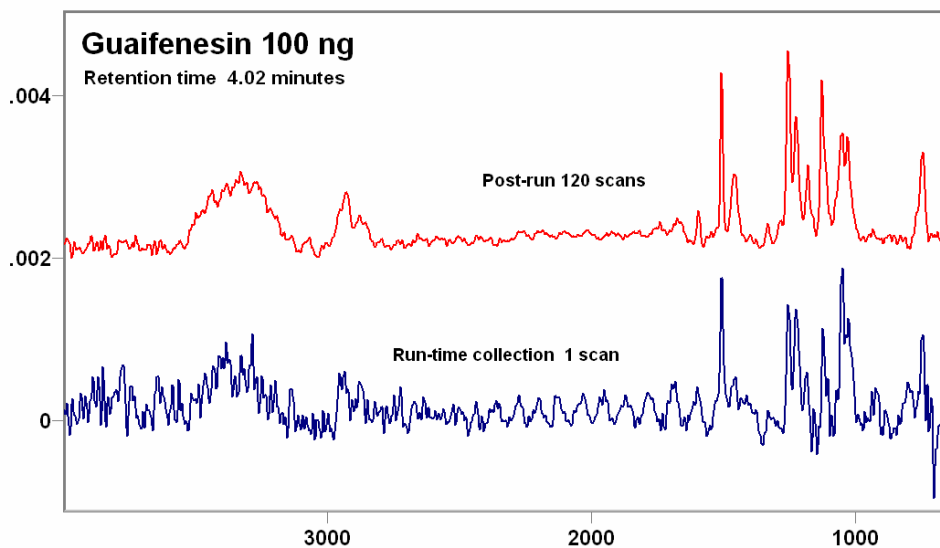
Another example, this time from the DiscovIR-LC, is shown below. A mixture run at 500 ng on-column shows four distinct peaks. At 100 ng, the chromatographic peaks are buried in the noise, but can be extracted using selected band chromatograms. Examples of spectral improvement through post-run scanning are shown next page.





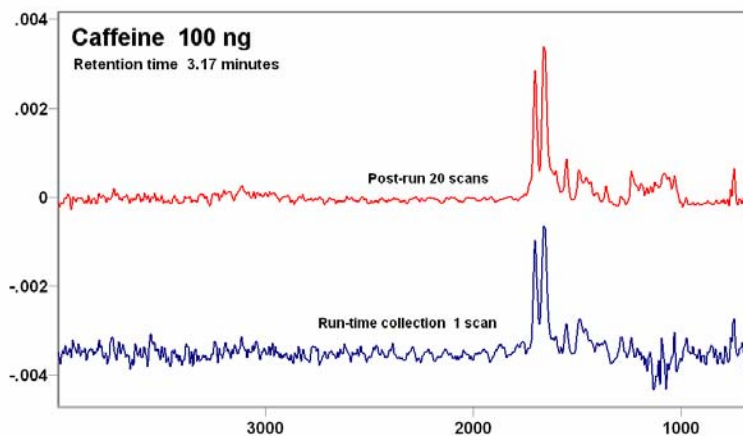
Reduction of Spectral Noise through Post-run scanning

Note on the spectra of Guaifenesin and Acetaminophen below, the absorbance levels of the major bands in the spectra are approximately two (2) milli-absorbance units. Post-run scanning reduces the peak to peak noise from the original 0.5 to 0.05, improving the signal to noise ratio (S/N) from 4 to 40. For Caffeine on the next page, the signal level is three (3) milli-absorbance units, so its S/N improves from the original 6 to a final 60.





Reduction of Spectral Noise through Post-run scanning



With a slightly higher injected amount, at 200 ng each, post-run scanning produces library quality spectra, as shown below.

