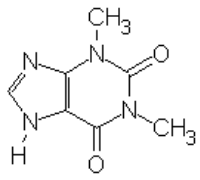
DiscovIR-LC ™
Deposition and Detection System

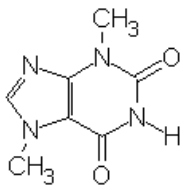
Application Note 023
January 2008

Getting quality LC-IR spectra from 1% mixture components

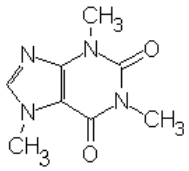
Demonstrating how the DiscovIR-LC instrument can achieve quality IR spectra from minor components, we work with a mixture of methyl xanthines. These compounds are natural products. The compounds used in this study are found in significant quantities in green tea. We set the concentrations to range over two orders of magnitude.



Theobromine
1,3-dimethylxanthine
0.2 mg/mL



Theophylline
3,7-dimethylxanthine
2 mg/mL



Caffeine
1,3,7-trimethylxanthine
0.02 mg/mL

Column:	guard + Eclipse C-18 50 mm x 46 mm, 5 um silica
Mobile phase:	Water with 0.1% formic acid / Acetonitrile
Gradient:	5 -14% acetonitrile over 6 minutes
Injection volume:	40 uL
Nebulizer:	14 W
Carrier gas:	200 cc nitrogen
Disk Speed:	6 mm/min
Temperatures:	-5 °C Disk
	1 °C Condenser
	180 °C Cyclone
Pressures:	3.7 torr Chamber
	195 torr Cyclone

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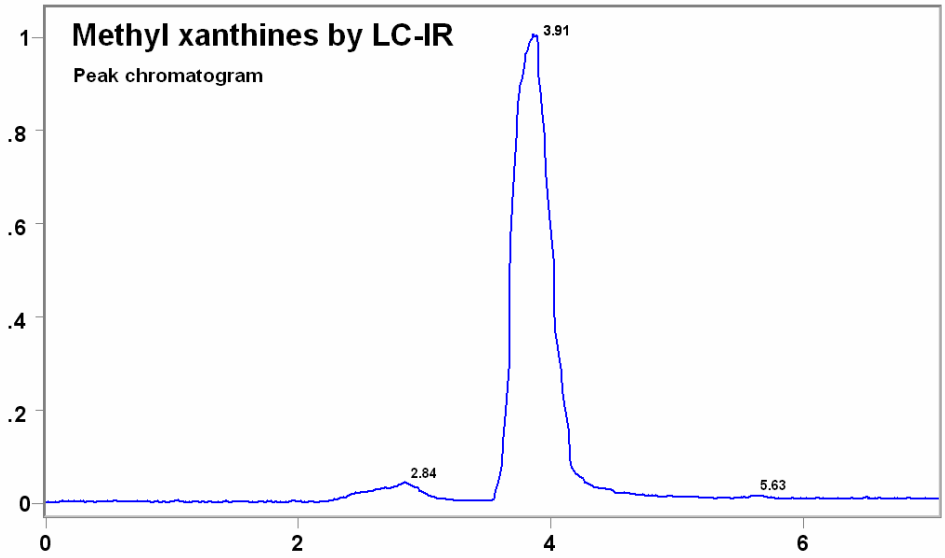
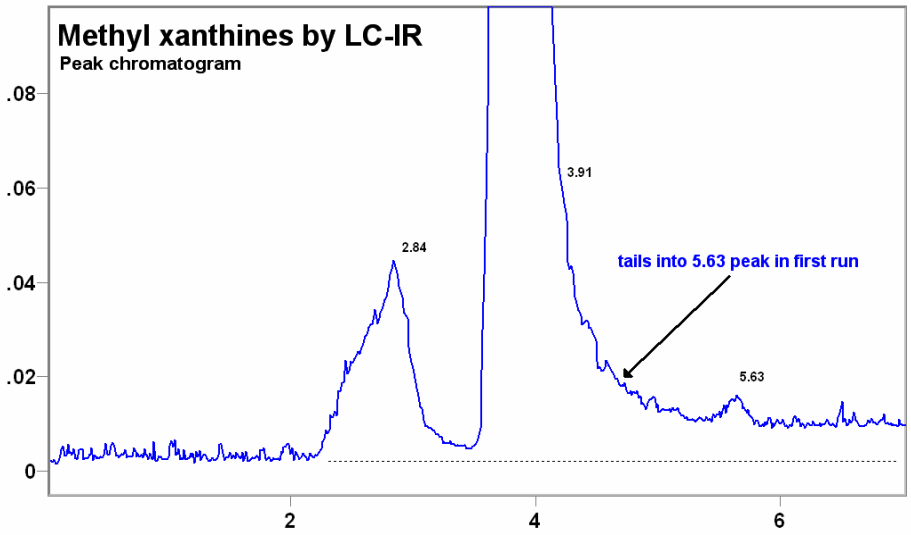
Under the given chromatographic conditions, the compounds elute within a three minute retention time window, with the least concentrated component (caffeine) following the most concentrated one (theophylline). As seen from the chromatograms below (top is full scale, bottom is expanded), the major theophylline peak tails a bit into the caffeine. This tailing was easily removed by subtracting the front edge of the caffeine peak from the main body, giving good quality run-time spectra from all three components, as shown from the spectra on the next page.





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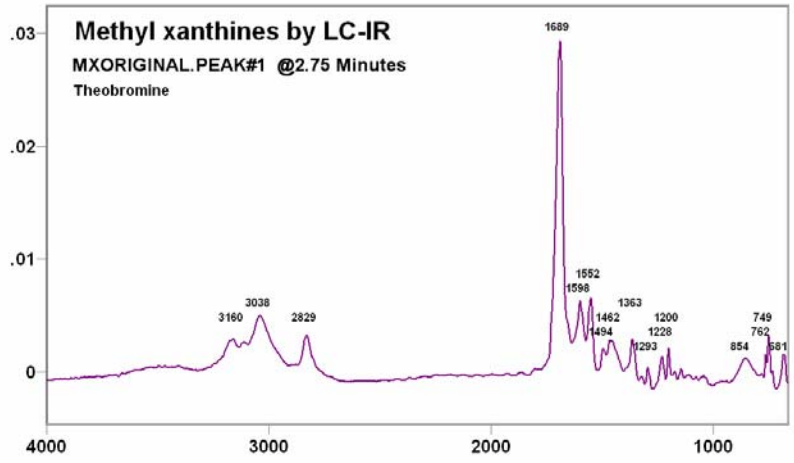

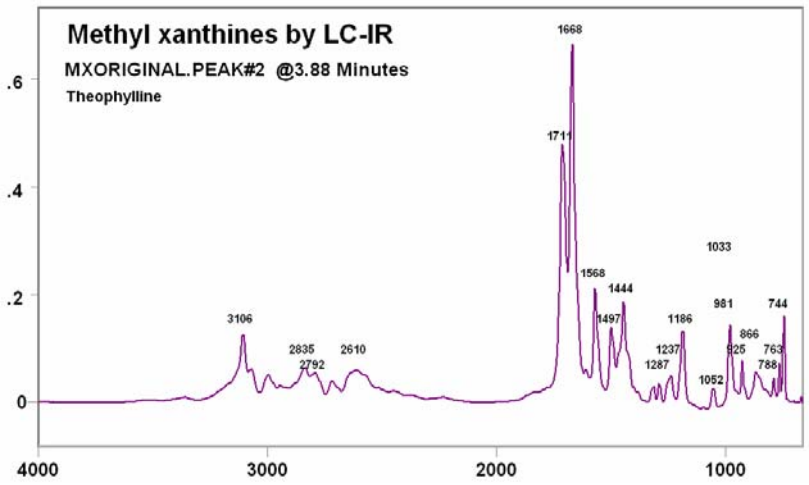

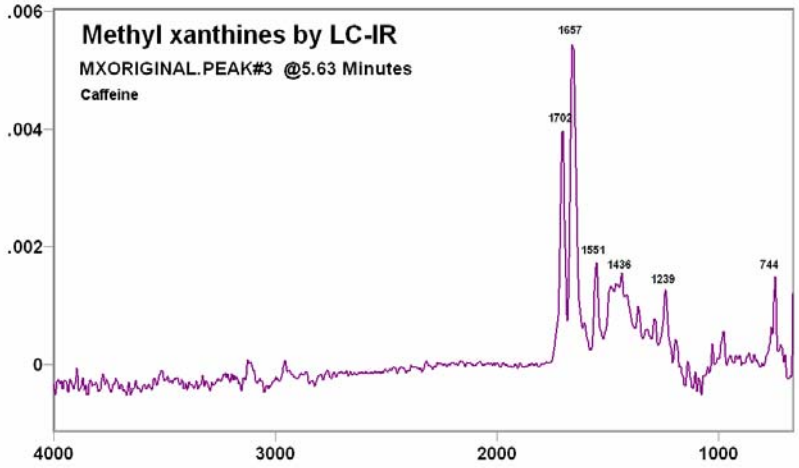

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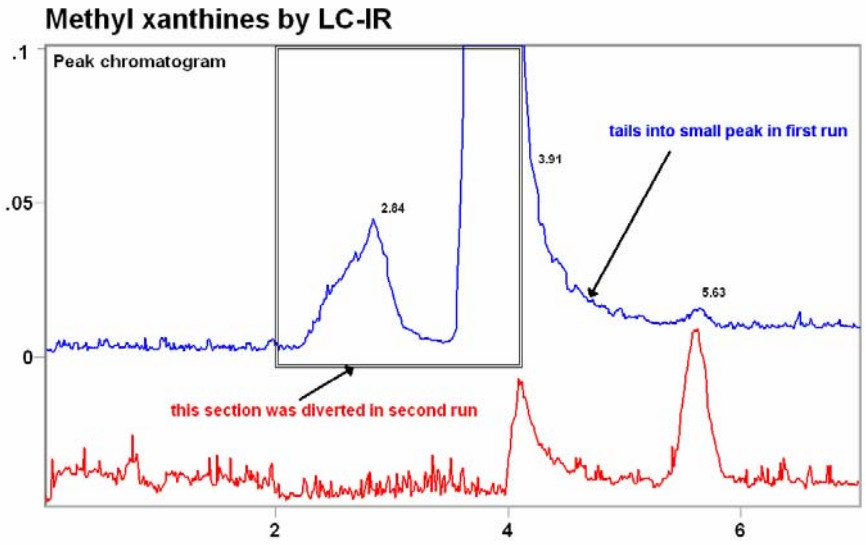
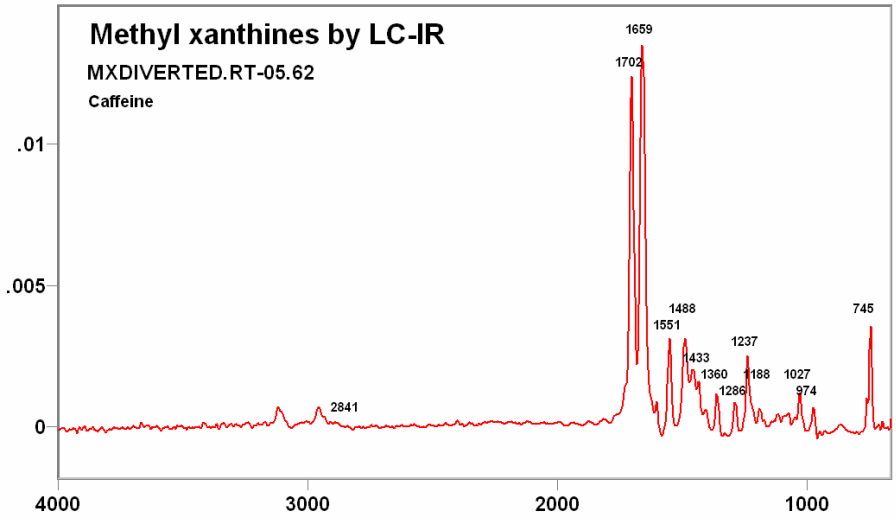
We may get an even better spectrum of the 1% minor component by eliminating the interfering tail from the major component. This is accomplished by plumbing the system in series as LC column – UV detector – divert valve – DiscovIR. The divert valve may be switched momentarily to send the major peak to waste, as shown by the data from the second run below.





Conclusion

This note demonstrates the good quality of spectra obtainable from a run-time analysis of a component at a concentration of 1% of the major component, as well as the technique of diverting the major component in the case where it interferes with the minor one.