

FTIR and Raman Proficiency Program

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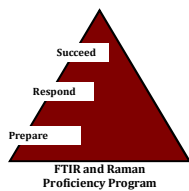
Summary Report for June 2017 FTIR Testing Event

The June 2017 FTIR testing event had three powder samples. **FTIR17-4** was a protein sample. This particular sample was the Becton Dickinson BBL™ Beef Extract Powder. This is a dull, yellowish extremely fine powder that becomes airborne very easily. It is a complex mixture of proteins, peptides, organic acids, minerals, vitamins, and nucleotide fractions. It is used as culture media when growing bacteria, and has a strong odor similar to protein powders.



The ideal response for this PT program for this sample is protein or similar. Again, if responding to a threat letter or a discovered powder, the point would be to consider the possibility of an organism being present and taking appropriate precautions. On our instrument we obtained the typical protein spectrum with the wide peak from 3500 to 2500. Our first match was tryptone from our common chemicals library, and based on the appearance of the powder and the nice spectrum match, we didn't perform any residual searches. In this software the lower the quality index, the better the match (range is 0 – 1.4).

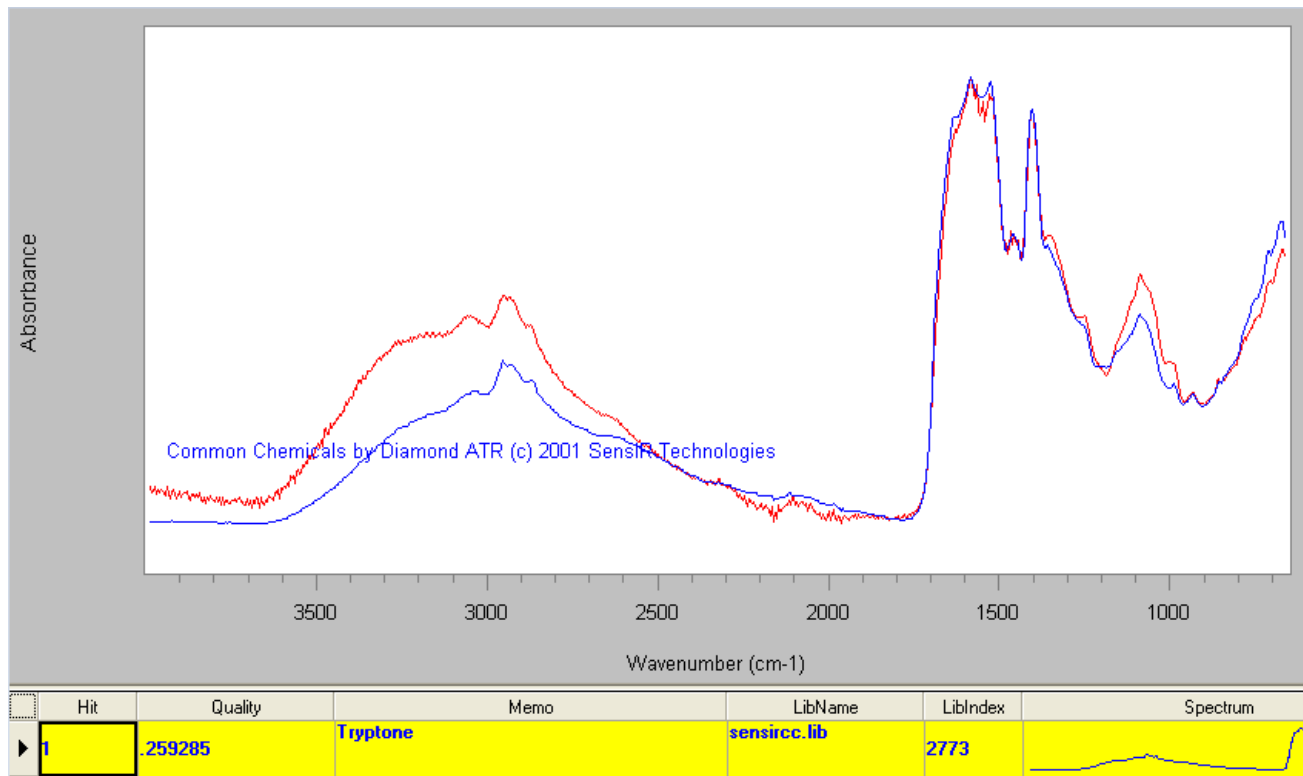
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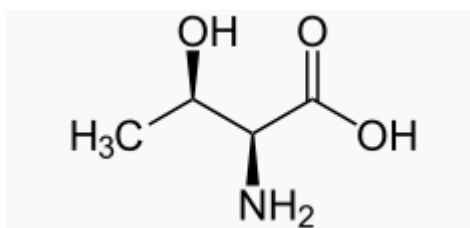
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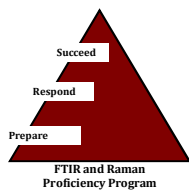
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The majority of participants correctly identified this as a protein, and most also submitted the specific protein their instrument matched with. This varied quite a bit and reflects either the number of different proteins present in the sample or the variability of instruments trying to identify proteins.

FTIR17-5 was L-threonine, an essential amino acid to humans that must be ingested and obtained through diet. This is a white, very crystalline powder with long crystals. It can be crushed into a more powdery form.





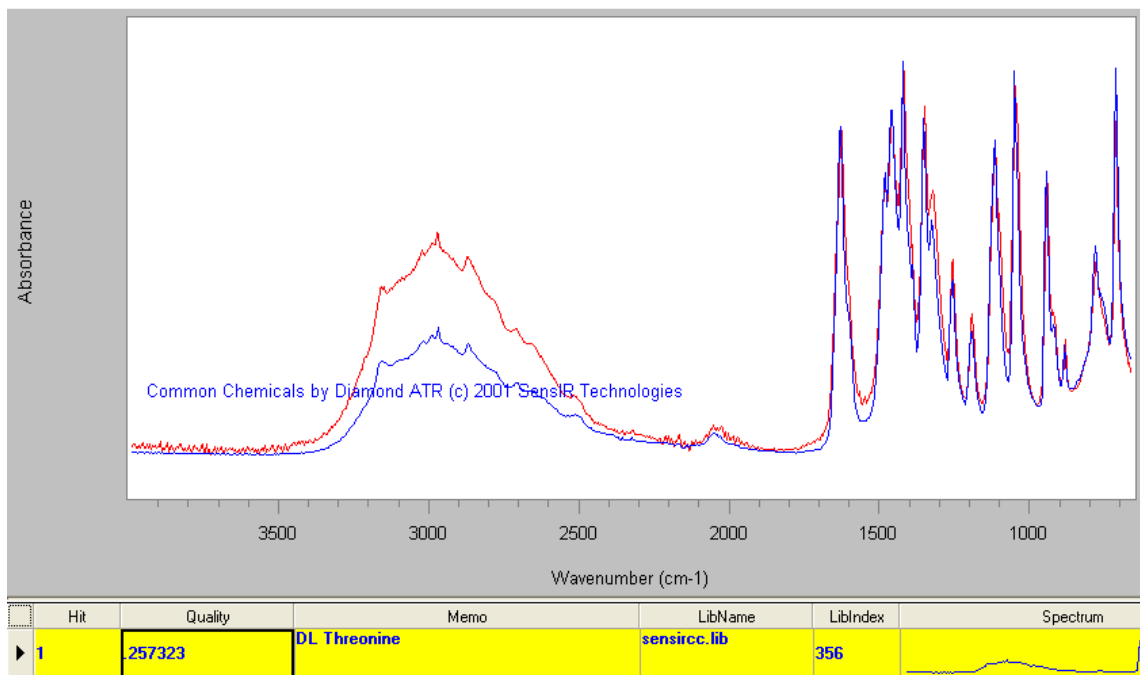
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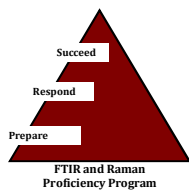
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There are multiple isomers of threonine, and this sample contained L-threonine at 98%. However, the entries in our common chemicals library were for a DL-threonine mixture. Our instrument gave a near-perfect spectral match.





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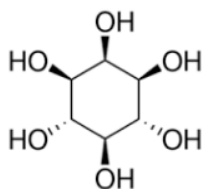
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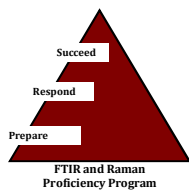
What was surprising was the quality of the match. A 0.257 quality match is just above 80%, and here the range under 2000 looks like it should be closer to 95%. Either way, DL Threonine from the common chemicals library was consistently the first match. The majority of participants correctly identified this.

FTIR17-6 was inositol. This white crystalline powder resembled the threonine, with the long crystals present.



Inositol is a sugar alcohol, and structurally is cyclohexane with 6 alcohol groups attached.



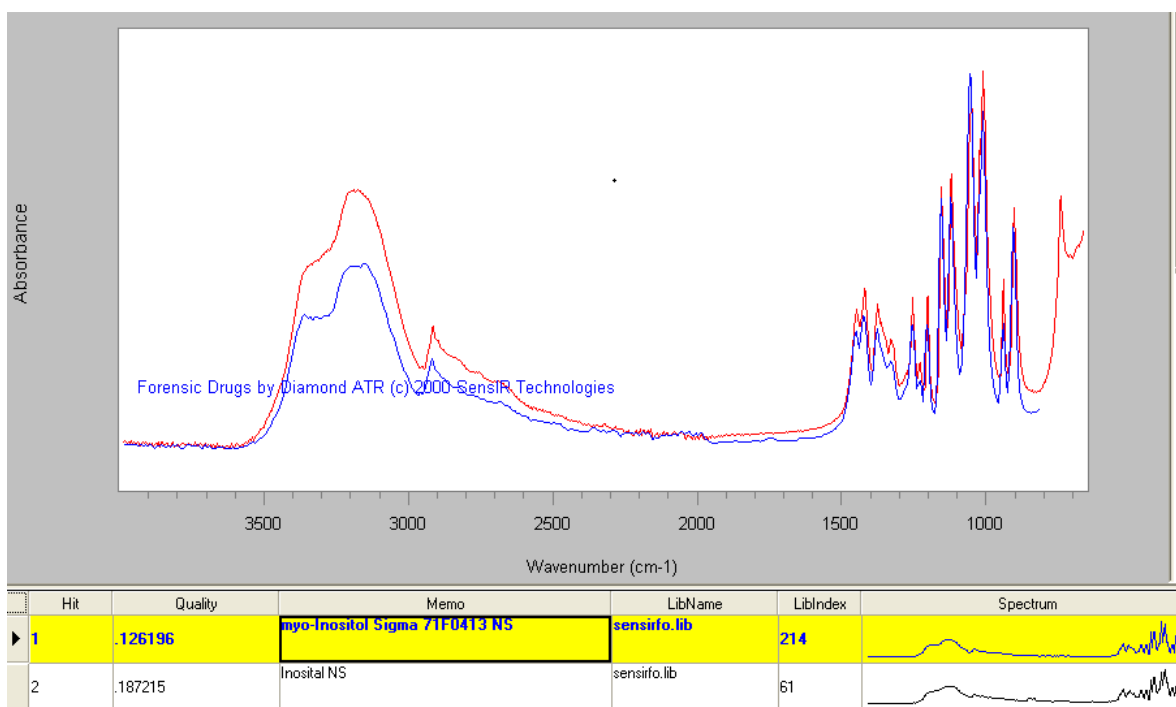


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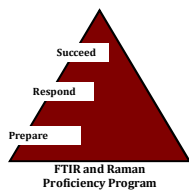
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Inositol is used in the body as a secondary messenger and as a component in some structural lipids. It can be produced by the body from glucose. There are some industry applications for inositol, but it is most commonly encountered as a cutting agent for cocaine. It is less sweet than sucrose and this contributes to it being a good adulterant. When encountered as an adulterant, our microscope has been able to resolve its crystals compared to cocaine crystals and obtain two different spectra. For this sample our instrument consistently matched with inositol compounds from the Smiths forensics library. A side note for this is that the Smiths library entry stops at around 800 cm^{-1} , which leaves off one more peak.



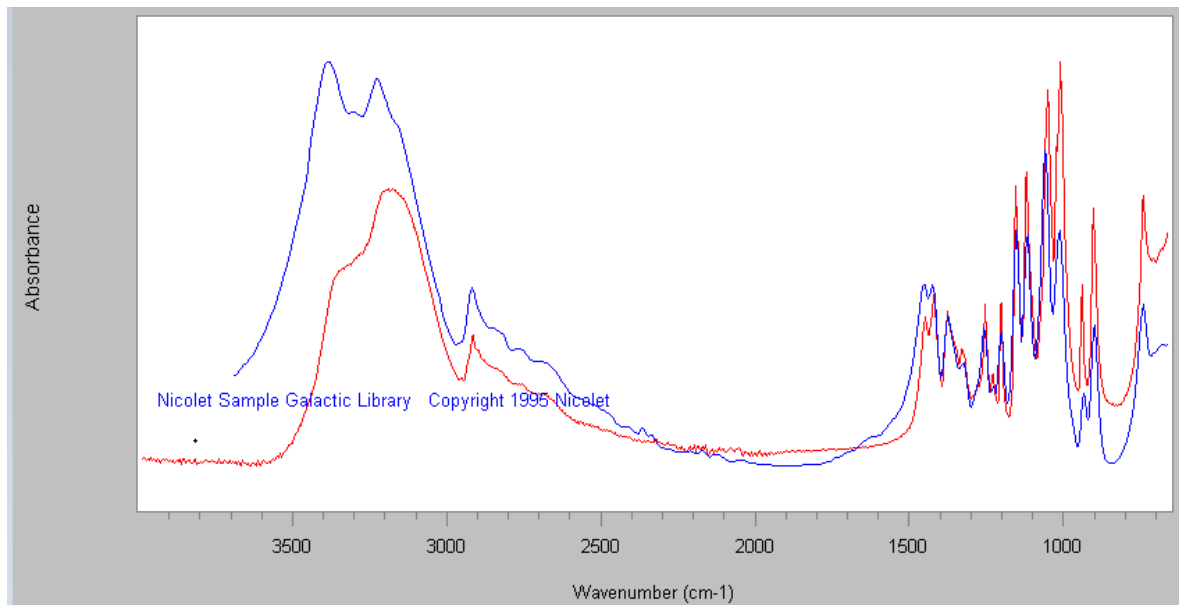
This doesn't make much of a difference for this sample, but we had another library with inositol that had a wider range and included that last peak. It was in a KBr prep but still matched very well.



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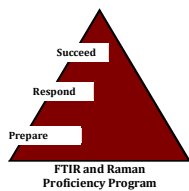


We have seen for some other compounds, notably methamphetamine, that there are some very discreet peaks in that range, and the majority of our library entries did not go down to that range. We had one library with a methamphetamine spectra that did have this extended range and contained these two peaks, and this is quite helpful for a confident identification. The majority of participants correctly identified inositol.

Individual results can be found on the nphl.org website. Log in to the FTIR Program portal and enter facility ID. Click on the report for this event and a pdf file will be generated. The next event will be for the month of September. As always, please contact us with any questions.

Regards,

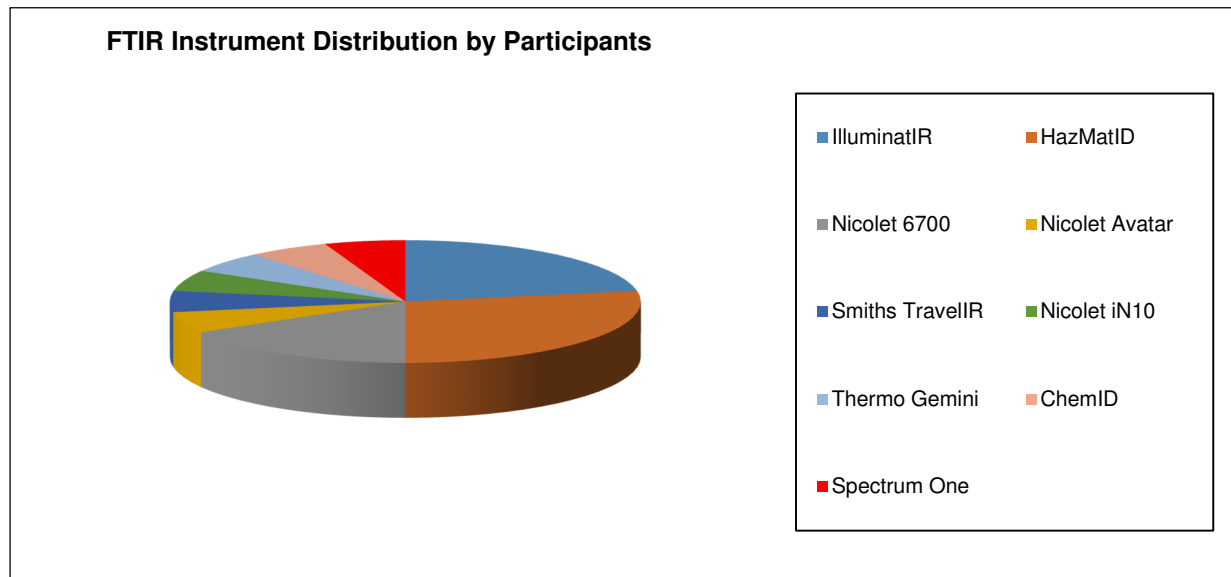
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Event Performance:

A summary of results reported is shown in the following table:

PT ID	Compound	Match	Partial Match	No Match	Comments
FTIR17-4	Protein	80%	11%	6%	Some reported No Result
FTIR17-5	L-Threonine	83%	-	11%	Some reported No Result
FTIR17-6	Inositol	90%	-	6%	Some reported No Result