

FTIR and Raman Proficiency Program

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Summary Report for September 2018 FTIR Testing Event

The September 2018 FTIR testing event had two liquids and one powder. **FTIR18-7** was store brand olive oil. Like other brands of olive oil, this was a relatively clear, greenish oil. Most FTIR libraries have various plant oils in them, and it appears that the spectrum is based on the fatty acid composition of the oils. Some have very similar compositions, and thus have very similar FTIR spectra, as we saw with some results. The top three fatty acids in olive oil are oleic, linoleic, and palmitic. Figure 1 shows our match for the sample, which repeatedly gave olive oil as the first match and had good quality. The match is from the Smiths Common Chemicals library.

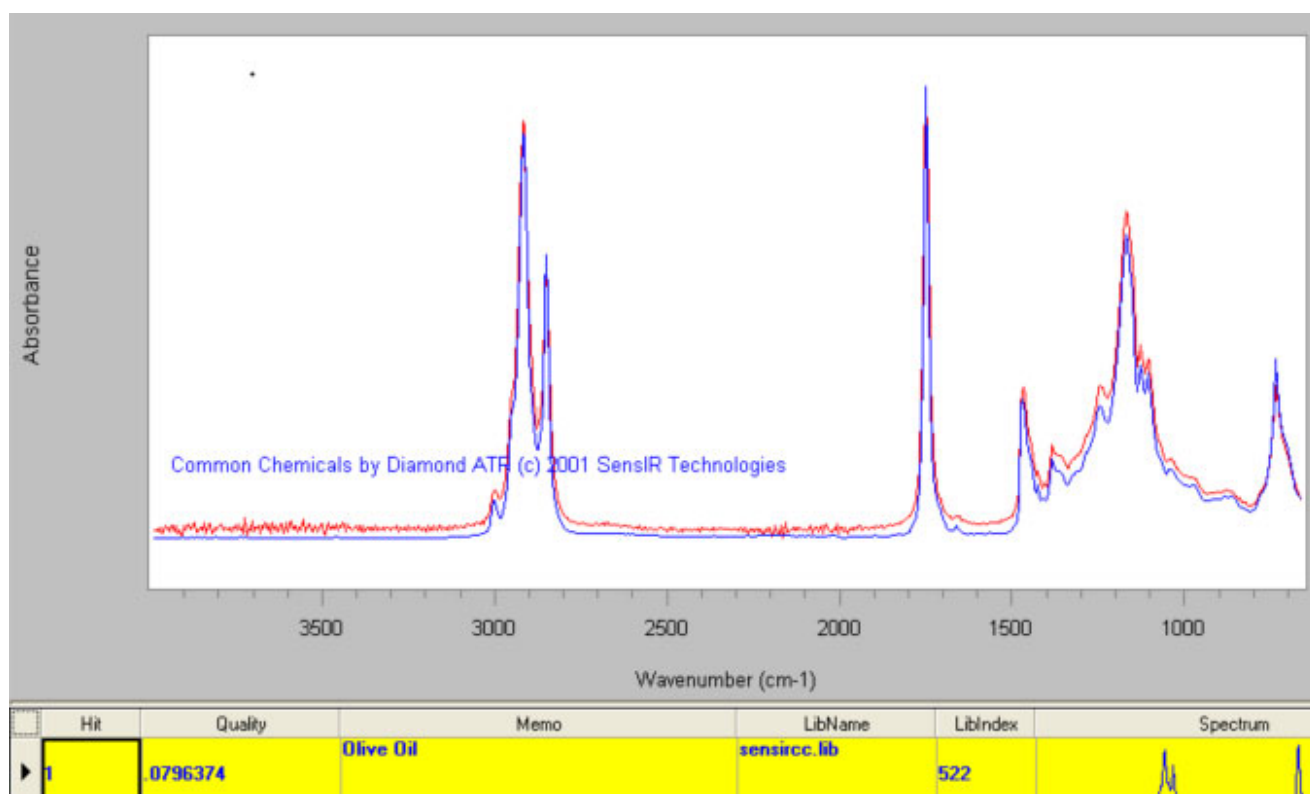


Figure 1. Olive Oil

Another oil that gives a similar spectrum is cottonseed oil, which has the same top three fatty acids. Figure 2 shows the spectrum comparison to the sample.



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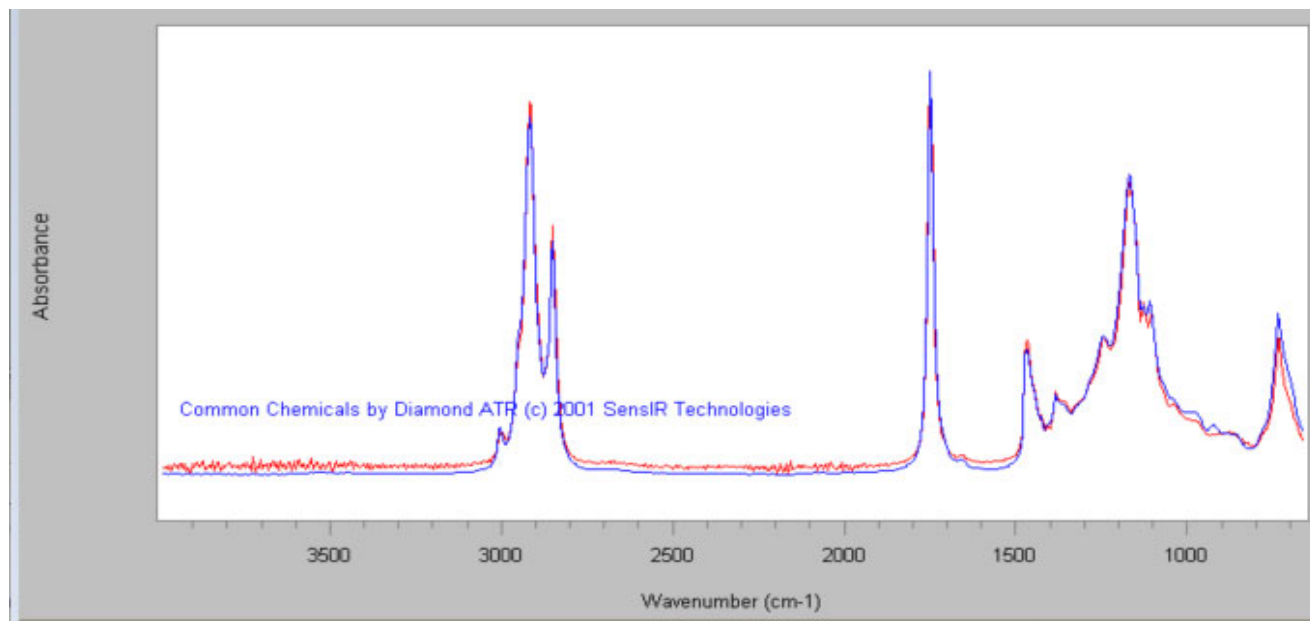


Figure 2. Cottonseed Oil

Our two different FTIR programs gave different top matches, which were either olive oil or cottonseed oil. The difference is of little consequence, as all of the first 10 matches with either software were plant-based oils. All participants either identified this as olive oil or another plant-based oil. An important aspect of an oil is that non-water-soluble compounds can be put in them. Some places have solubility tests as part of their initial exams, and receiving an oil compared to water would have to be accounted for.

FTIR18-6 was inosine. It was a white powder. Inosine is a nucleoside made of hypoxanthine and ribose. It has functions involved in DNA and RNA biochemistry.

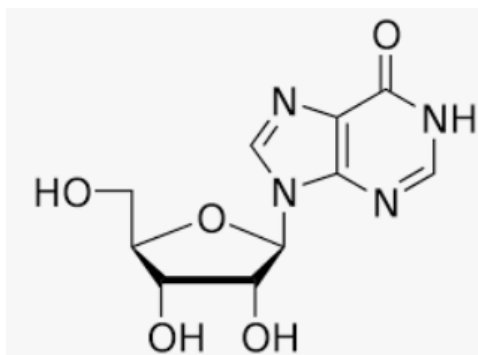
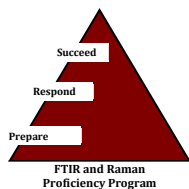


Figure 3. Inosine



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We saw a decent amount of variety in our instruments when testing this sample. Inosine is in the Smiths Common Chemicals library, and the sample was 99% pure, but we did not consistently get inosine as the best match. Most commonly, xanthosine was the first match. As can be seen in Figure 4, xanthosine is a nucleoside that is very close in structure to inosine, with just one extra carbonyl group.

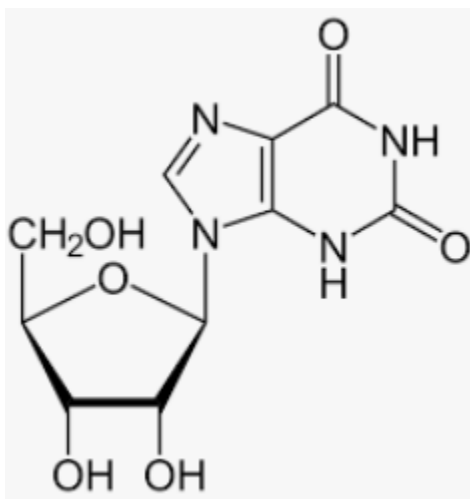
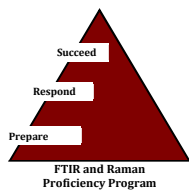


Figure 4. Xanthosine

None of our programs or instruments gave a high quality match. Two immediate analyses returned xanthosine and then inosine, and both had similar qualities.



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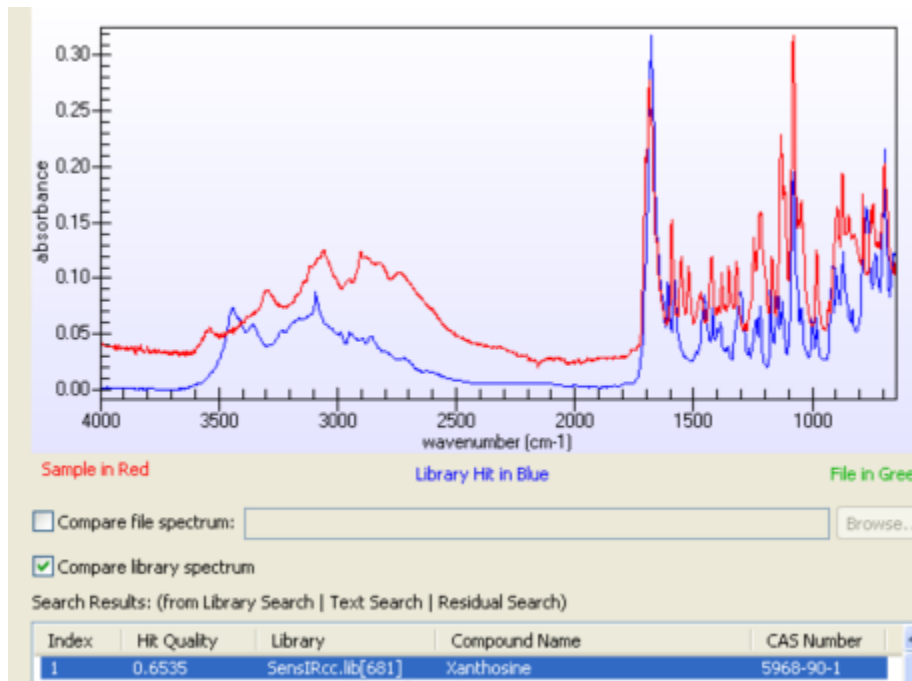


Figure 5. First analysis of inosine

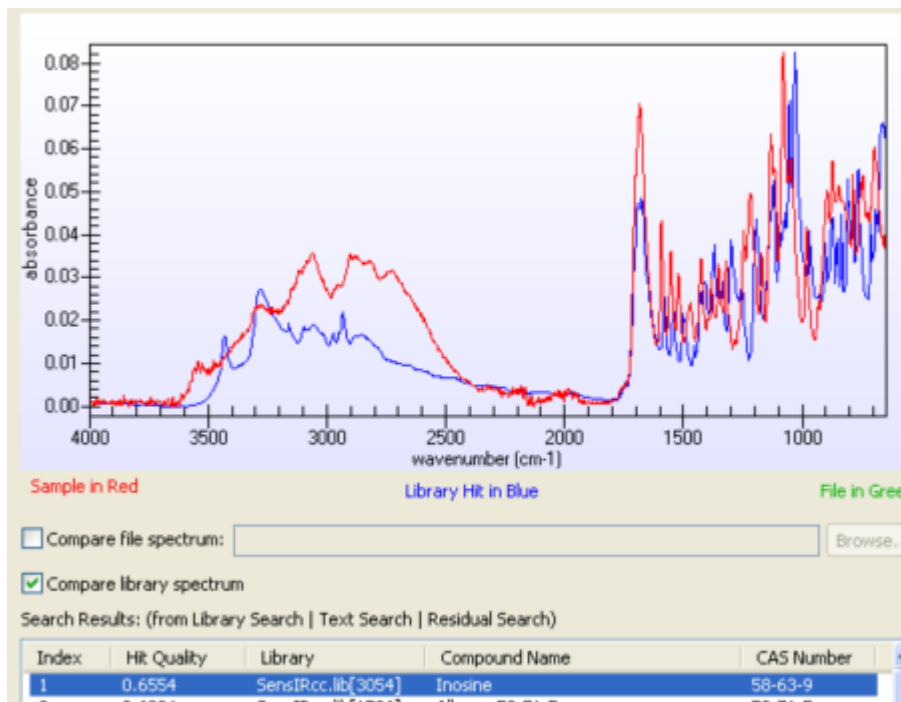
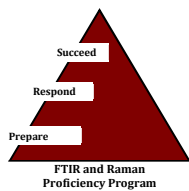


Figure 6. Second analysis of inosine



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The majority of participants identified this as either inosine, some component of the nucleoside, or as xanthosine. It seems to show that most instruments can't reliably differentiate the single carbonyl difference between xanthosine and inosine. Even if the impurity in the sample is xanthosine, at 1 percent it shouldn't be as predominant in the results.

FTIR18-9 was diethyl adipate (diethyl hexanedioate). It is a clear liquid with a little viscosity. It is primarily used in the cosmetic industry.

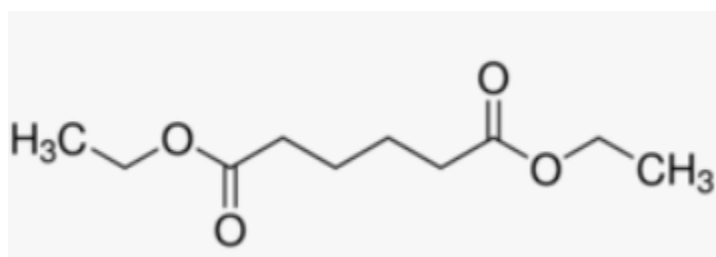


Figure 7. Diethyl adipate

Both of our instruments gave good matches for this. It has a similar spectrum to diethyl glutarate, but diethyl adipate was always the top match. The majority of participants identified this as diethyl adipate.

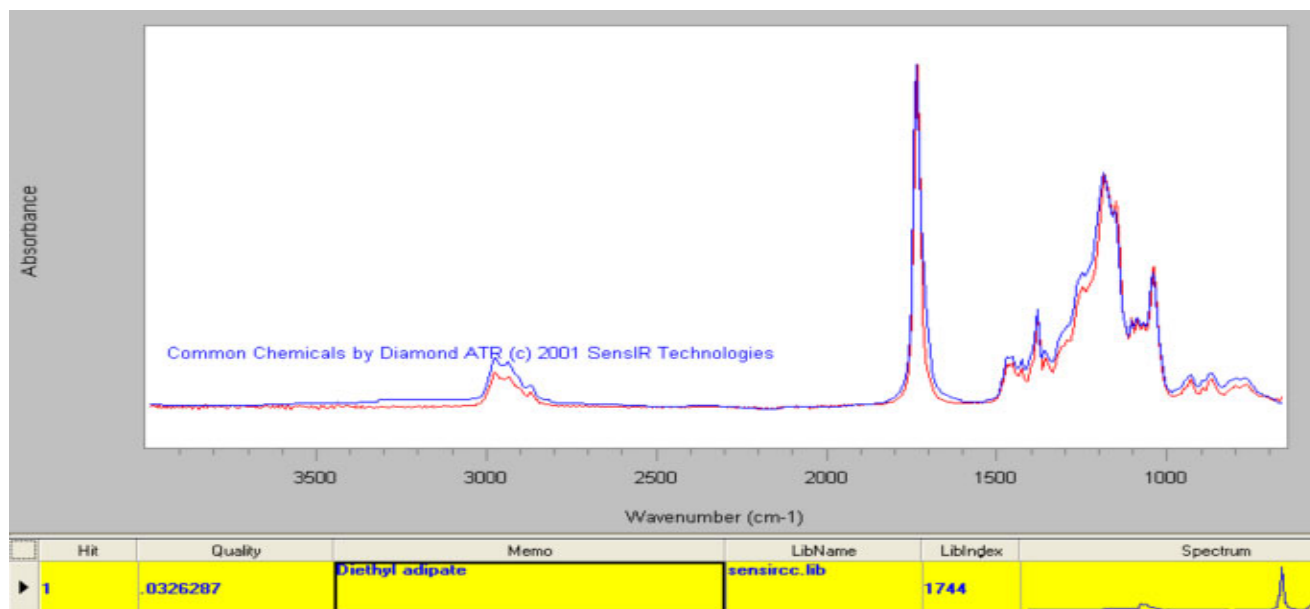
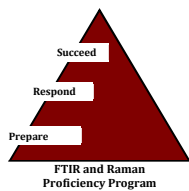


Figure 8. Diethyl adipate spectrum



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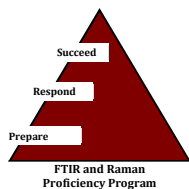
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Individual results can be found on the nphl.org website. Log in to the FTIR Program portal and enter facility ID. Click on the report for this event and a pdf file will be generated. As always, please contact us with any questions.

Regards,

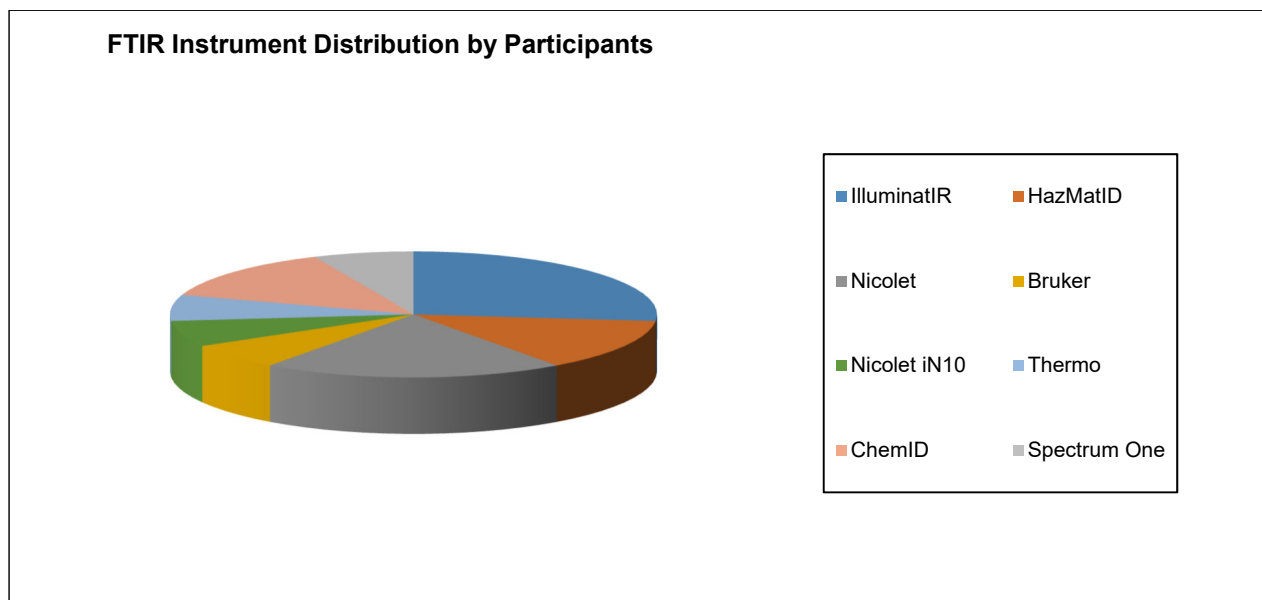
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Event Performance:

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

PT ID	Compound	Match	Partial Match	No Match	Comments
FTIR18-7	Olive Oil	93%	7%	-	
FTIR18-8	Inosine	87%	-	13%	
FTIR18-9	Diethyl adipate	80%	-	20%	