

## FTIR and Raman Proficiency Program

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### Summary Report for September 2019 FTIR Testing Event

The September 2019 FTIR testing event had one liquid and two powder unknowns. **FTIR19-7** was an ion-exchange resin, specifically Dowex®50WX8. This is a fine white powder material that is used as its name implies, as an ion-exchange resin. Ion-exchange is trapping ions out of some matrix, for purposes that include separation, purification (water softeners), and decontamination. Ion-exchange refers to a class of compounds, and some can be proprietary in their composition. This specific brand is a bead form, and contains cross-linked styrene sulfonates and divinylbenzenes. This compound was selected because it is listed in the Smiths common chemicals library and has a well-established IR spectrum. Figure 1 shows the structure of the material.

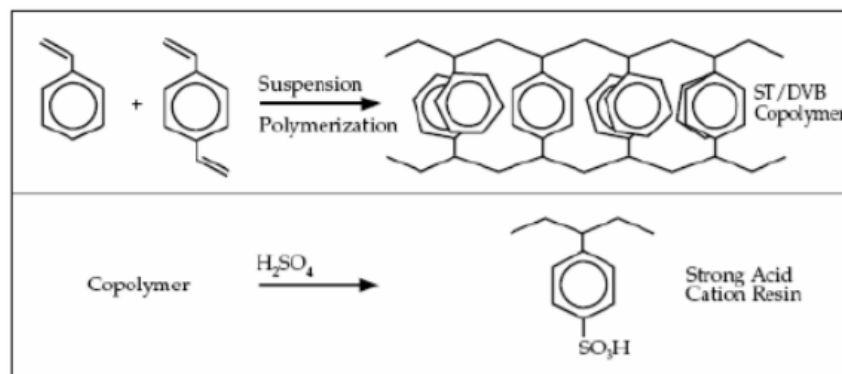
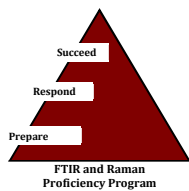


Figure 1. Dowex ion-exchange resin

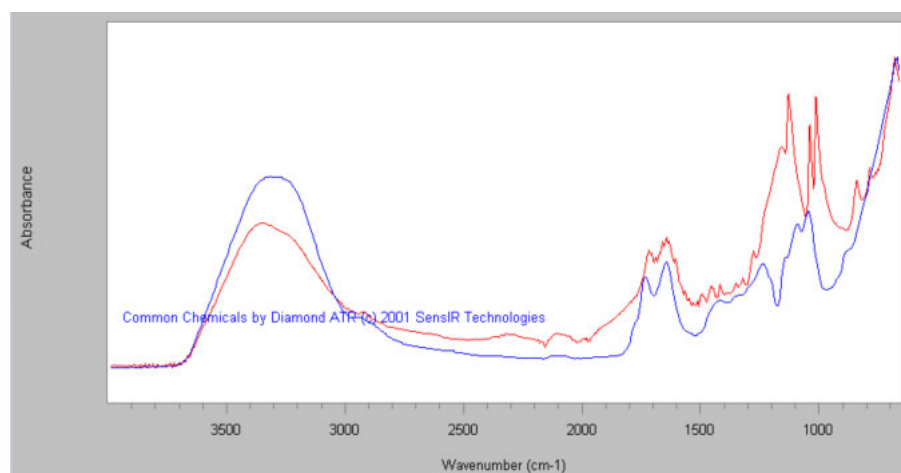
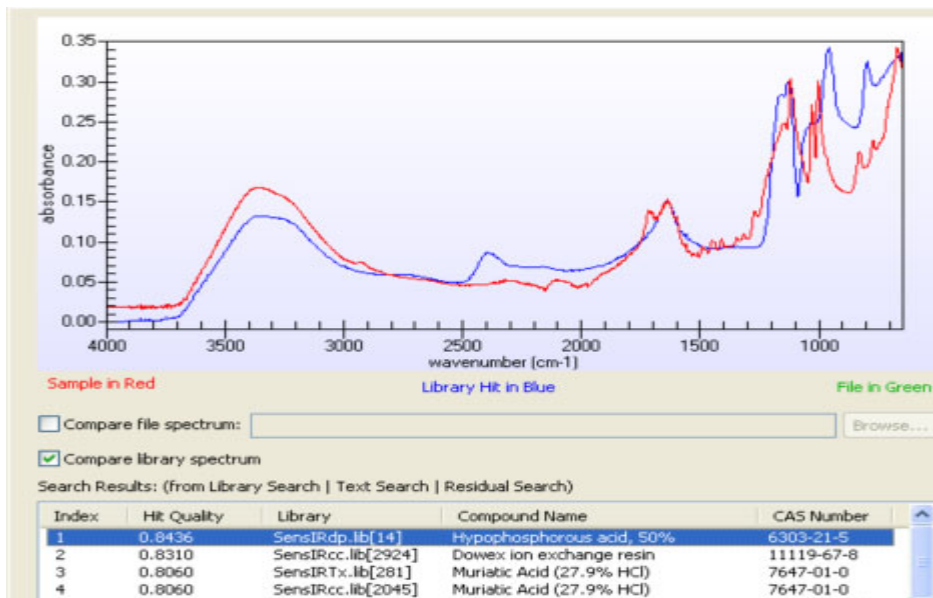
Analysis with the instrument was straightforward on this sample, but our instruments did not match on the first hit. On one instrument the first hit was consistently Hypophosphorous acid, and on the other it was gluconic acid. On the first instrument, Dowex ion exchange resin was consistently hit #2. On the other instrument, it was not among the first 10 hits. We tested our sample directly and immediately out of the container, so we couldn't find a reason for the spectrum not to match up with the library. With a text search, we could see that the spectrum matched up decently well up to 1500 cm<sup>-1</sup>, but as a whole didn't look too good. On our first instrument, the top three hits were different enough from each other that one would have an issue arriving at a consensus on the class of compound present. The majority of participants did not identify this compound, and it was considered non-graded. This may be another example of a vendor listing compounds to beef up its library, but in a practical sense not being very trustworthy on the results.



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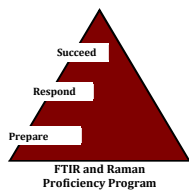
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Quality	Memo	LibName	LibIndex
.248951	<b>Gluconic acid</b>	<b>sensircc.lib</b>	<b>996</b>
.248951	Gluconic acid	sensircc.lib	996
.261213	Glutaric dialdehyde	sensircc.lib	1622
.261213	Glutaric dialdehyde	sensirtx.lib	189

Figure 2. Library match for FTIR19-7 on two instruments



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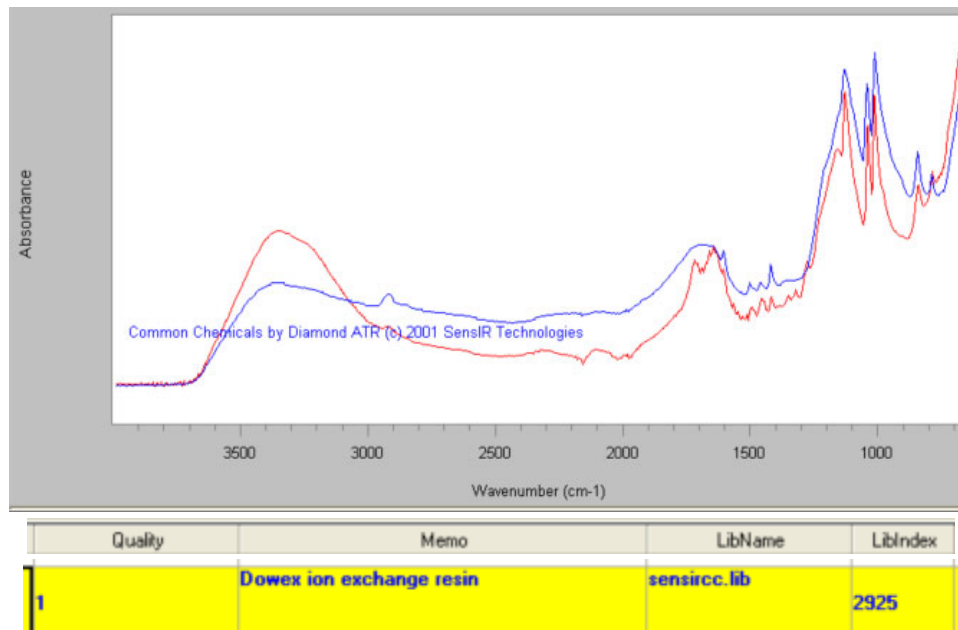


Figure 3. Text search library comparison for FTIR19-7 on instrument #2

FTIR19-8 was dimethyl phthalate. This clear, slightly viscous liquid is used in insect repellent.

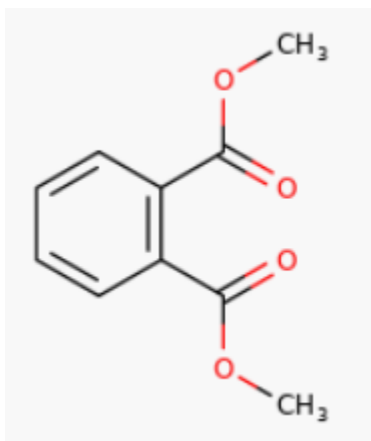
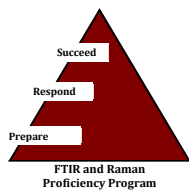


Figure 4. Dimethyl Phthalate

Analysis with the instrument was the standard liquid testing, where we put a drop over the ATR diamond tip and don't apply any pressure with the press. The spectrum matched up near perfectly with the library match. The Smiths common chemicals library contained dimethyl phthalate.



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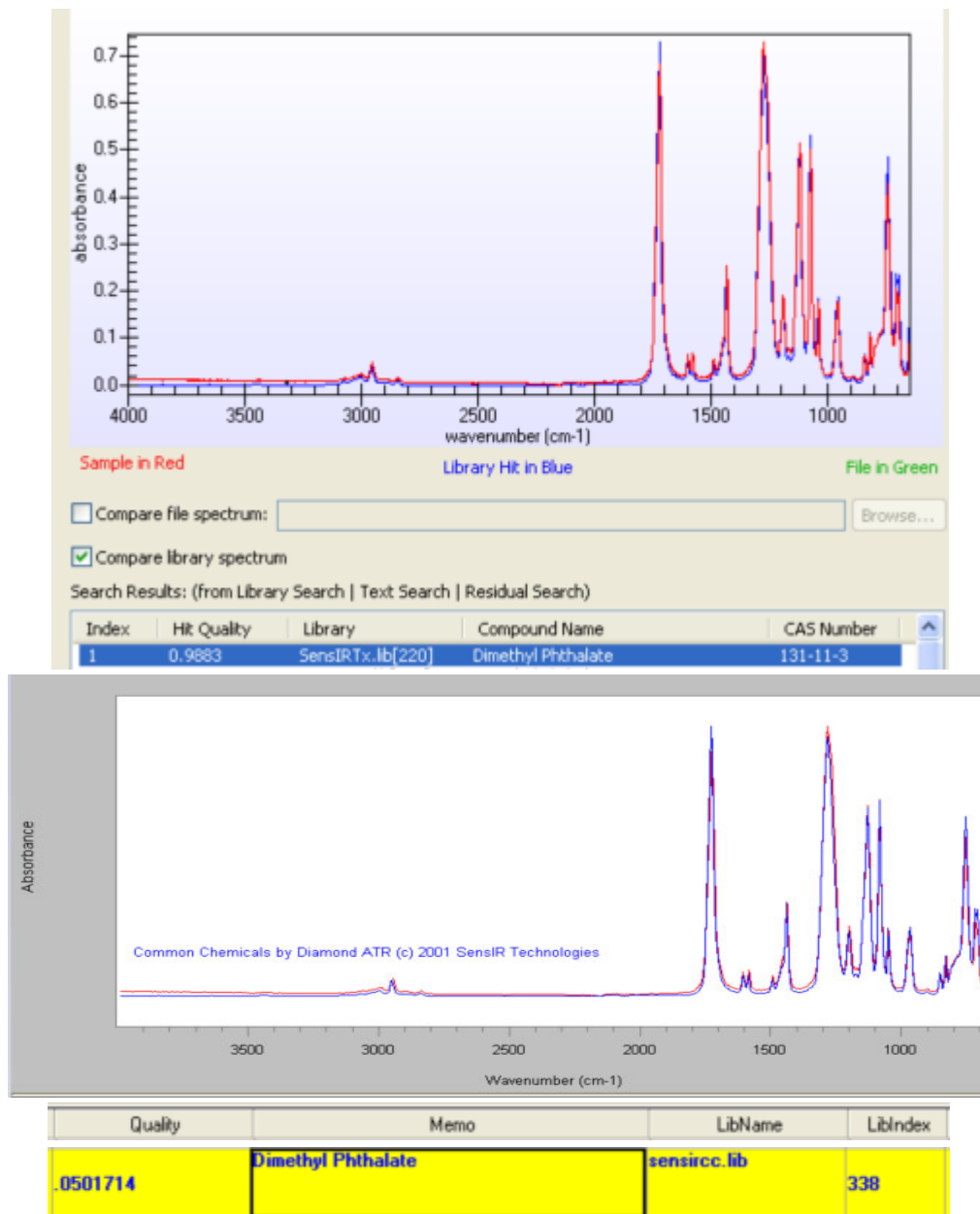
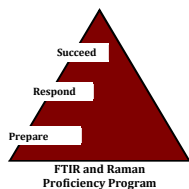


Figure 5. Library match for FTIR19-8 on two instruments

The majority of participants were able to correctly identify this.



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**FTIR19-9** was ammonium acetate. This is a white powder with large crystals. This compound is used in laboratories in buffer solutions, and can also be used in organic synthesis, as a de-icing agent, and as a food additive in some countries.

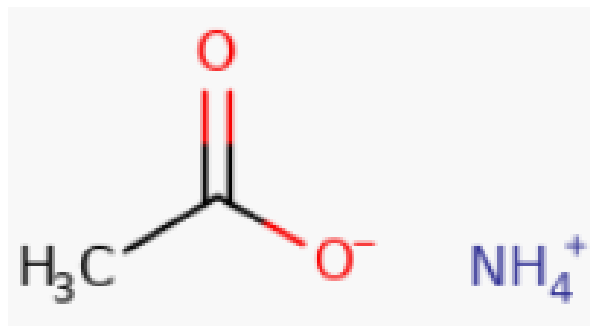
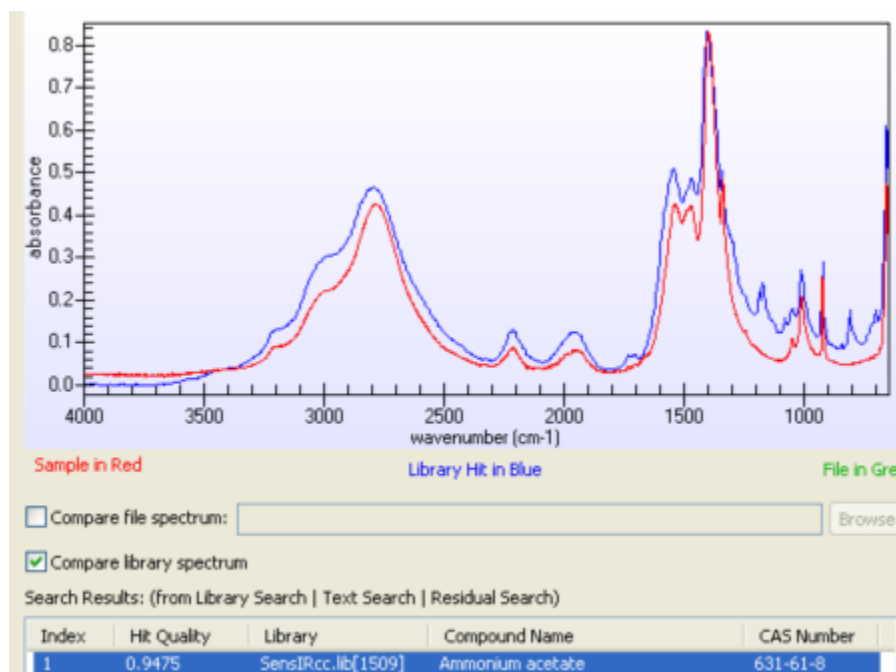
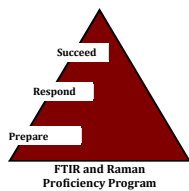


Figure 6. FTIR19-9

Testing this sample was straightforward and our instrument consistently gave a high quality match for ammonium acetate. The Smiths common chemicals library contained ammonium acetate.





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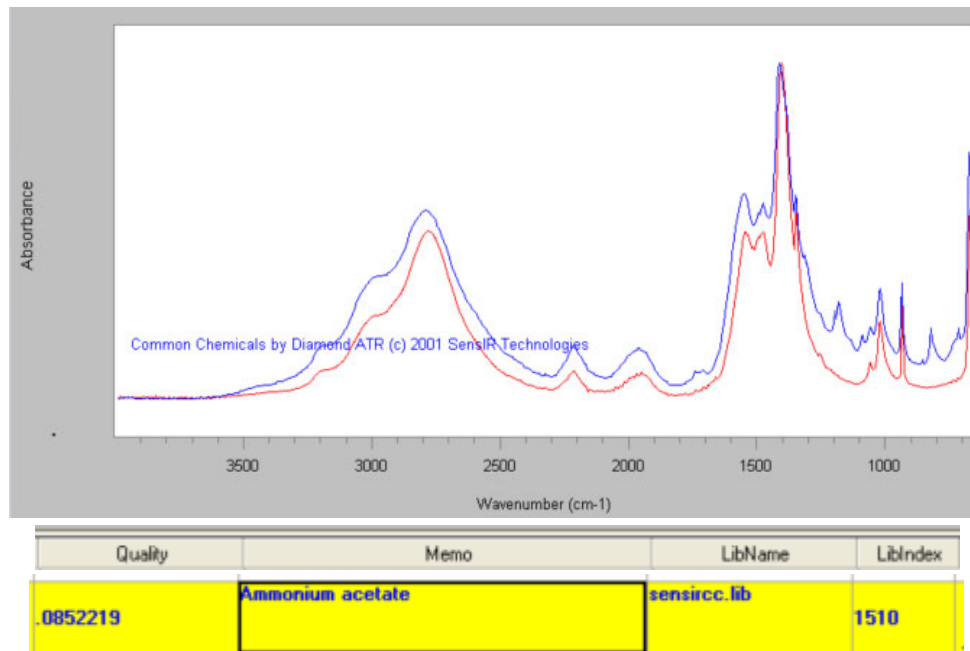


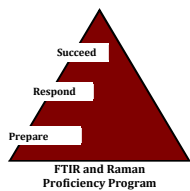
Figure 7. Library match for FTIR19-9 on two instruments

The majority of participants either correctly identified this or identified it as some acetate.

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,

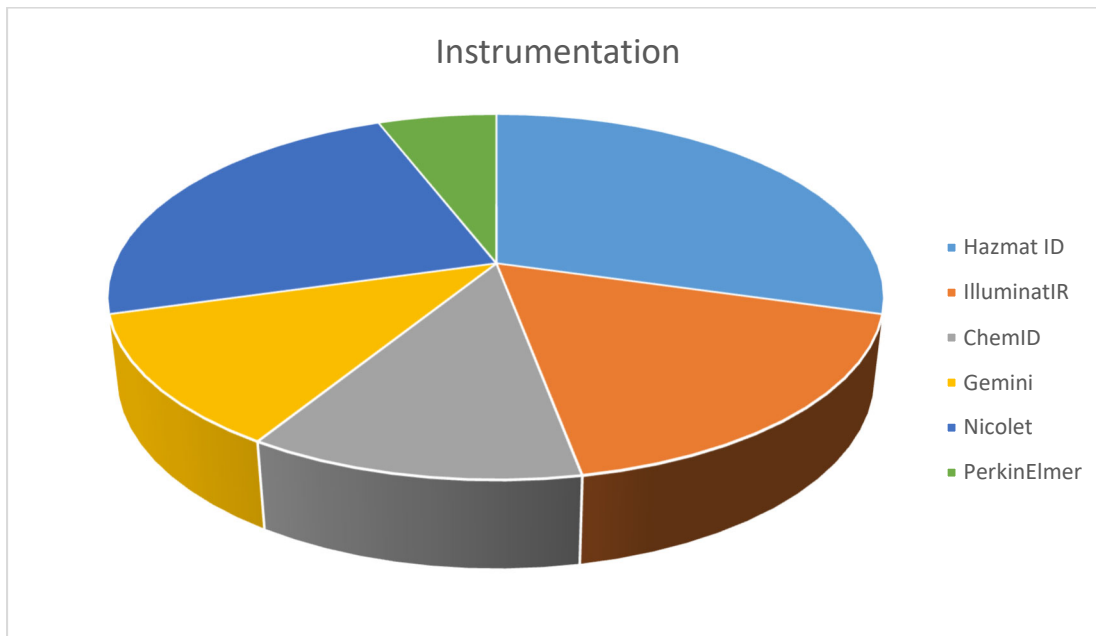
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### Event Performance:

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

PT ID	Compound	Match	Partial Match	No Match	Comments
FTIR19-7	Dowex Ion-exchange Resin	5%	-	95%	Not graded
FTIR19-8	Dimethyl Phthalate	100%	-	-	
FTIR19-9	Ammonium Acetate	80%	15%	5%	