



CONDOM TRACE EVIDENCE ANALYSIS MANUAL VERSION 2.0

Effective date: February 8, 2005

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FORENSIC BIOLOGY CONDOM TRACE EVIDENCE ANALYSIS MANUAL

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1. GENERAL GUIDELINES		
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1. All reagents are available pre-made and quality control checked. Do not use supplies that have not been quality control checked.
2. In general, semen analysis (AP, sperm identification, or p30 ELISA) is done prior to lubricant analysis. The analysis of amylase and other body fluids should also precede lubricant analysis.
3. Scissors and other cutting instruments must be cleaned with 10% bleach followed by 70% ethanol and dried before each cutting of a swab, including blanks. They must not contact any “greasy” or silicone-based lubricants before sampling the swabs. Clean scissors between samples. New razor and scalpel blades must not be used without first being cleaned as they may be coated with a lubricant.
4. An adhesive is used to attach cotton to the stick of a swab. These adhesives may produce an infrared spectrum, even at low concentrations, that can interfere with the spectrum of polydimethylsiloxane (PDMS). Therefore, when removing a portion of the cotton material, do not contact the stick with the scissors.
5. To reduce the amount of purge time required to reduce the absorption peaks due to carbon dioxide and ambient moisture, do not breathe into the sample compartment when changing samples. Use the compartment window when possible and make sample changes quickly.
6. **Negative controls are necessary to detect any interfering peaks from the extraction solvent, scissors, swabs, and/or any other extraneous contaminants.**
7. **Perform ALL methylene chloride extractions under an operating chemical fume hood, not a biohazard hood.**

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1. Start-up

- a. Startup of system, OMNIC E.S.P. software, and diagnostics check

NOTE: This procedure assumes some knowledge of the Windows[®] operating system.

- 1) **NOTE: The IR bench is left on at all times to maintain stability within the instrument and eliminate warm-up.** Turn on the computer and monitor. Check that the Nicolet Magna-IR 650 Series II bench is turned on and ready to collect spectra. The Power indicator light, at the top front left of the instrument, should be lit. If the indicator light is not lit, check the power switch at the rear of the instrument and the power cord to ensure that the connections are intact.
- 2) A prompt for the network connection appears. Enter your login name and password.
- 3) Double click the OMNIC E.S.P. icon on the computer desktop.
- 4) Click the Collect option on the menu bar.
- 5) Click on Advanced Diagnostics....

This verifies that the components of the instrument are operating properly. If there are any components with a red slash through it, refer to the **Troubleshooting** section.

- 6) Click the Report button. Click the View More button. Click the Print button. Click the Return button twice. Click the close window button at the top right of the window.

Store this report in the *FT-IR Instrument Usage Log, Maintenance, & Diagnostics Records* binder under the *Diagnostics* section.

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b. Experiment setup

- 1) In the **Experiment** title bar, which is just above the toolbar, make sure **Lubricant Analysis** method is selected for running samples. **Blank Card Analysis** may be selected if checking blank cards only. The blank card analysis has fewer scans, otherwise they are the same parameters.
- 2) In the *FT-IR Instrument Usage Log, Maintenance & Diagnostics Records* binder under the *Usage Log* section, enter the date, instrument start time, purpose of usage, and your initials.

NOTE: Remember to fill in the *Time Elapsed* column when finished with the system along with any comments concerning the instrument's operation.

c. Verification of collection parameters

- 1) To verify that the collection settings are correct, click the **Collect** option on the toolbar and select **Experiment Setup....** The following list contains the parameter settings for the collection of spectra. Compare each value with those listed below.

Collect

No. of Scans: 32 for Lubricants Analysis or 15 for Blank Card Analysis

Resolution: 2

Data spacing: 0.482cm⁻¹

Final format: Absorbance

Correction: None

Automatic atmospheric correction

Preview data collection

File Handling

Save interferograms

Background Handling

Collect background after 10 minutes

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Bench

Gain: Autogain

Velocity: 0.6329

Aperture: 69

Min/Max

Sample Compartment: Main

Detector: DTGS KBr

Beamsplitter: KBr

Source: IR

Accessory: None

Window material: None

Spectral Range

Saved: 4000-400

Single beam

Tone

Quality

Use spectral quality checks (should be deselected).

Advanced

Zerofilling: 1 Level

Apodization: Happ-Genzel

Phase correction: Mertz

Single-sided interferogram

Reset bench at start of collection

Diagnostics

The printout from Advanced Diagnostics... provides the necessary information needed to determine that all systems are running properly.

- 2) If the settings are correct, the software is ready to collect spectra. Proceed to the section **Collection of spectra**. Click OK to proceed.

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2. Collection of spectra

a. Removing and placing IR cards in the sample holder

- 1) On either side of the sample chamber are two levers. Flip them up.
- 2) Open the window to the sample chamber by sliding the cover toward the back of the instrument and remove or place any IR cards in the sample holder.
- 3) Close the window by sliding the cover toward the front of the instrument. Flip both levers down.

NOTE: The levers are kept in the raised position when the cover is open so that the purge is maintained in the rest of the instrument.

b. Collection of the background spectrum

A background spectrum should be collected every ten (10) minutes or as necessary. Certain actions on the part of the analyst may require the collection of background spectra more frequently.

- 1) The sample chamber should be empty. If not, remove any IR cards in the sample chamber following the instructions in the section **Removing and placing IR cards in the sample holder**.
- 2) Click the Col Bkg (Collect Background) button on the toolbar.
- 3) A Confirmation window appears. It reads:
Background
Please prepare to collect the background spectrum

Click OK.
- 4) A Confirmation window appears after the background has been collected. It reads:
Data collection has stopped.
Add to Window 1?

Click No.

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c. Collection of spectra from blank IR cards

This section describes the collection of spectra from the IR cards before application of the samples. These negative controls show that the IR cards do not contribute to the PDMS spectrum. Either Lubricants Analysis or Blank Card Analysis may be used to check the cards. **Every IR card is checked before sample application! Discard any cards that contain detectable contaminants!**

- 1) Place a blank IR card (3M Type 61 polyethylene) into the chamber following the instructions in the section **Removing and placing IR cards in the sample holder**.
- 2) Click the Col Smp (Collect Sample) button on the toolbar.
- 3) The Collect Sample window appears. It reads:
Enter spectrum title.
- 4) For the spectrum title: Click OK to enter default date and time.
- 5) A Confirmation window appears which reads:
Sample
Please prepare to collect the sample spectrum.
Click OK.
- 6) A Confirmation window appears after the spectrum has been collected. It reads:
Data collection has stopped.
Add to Window 1?
Click Yes.
- 7) **CHECK THE BLANK CARD SPECTRUM FOR CONTAMINANTS.**

The spectrum should appear similar to Figure 1 on the following page.

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- 8) Change the display limits by selecting Display Limits... in the View menu and set the X-Axis Limits from a Start: value of 1300 to an End: value of 700. Click OK.
- 9) Click on the View menu and select Full Scale.
- 10) The spectrum ($1300-700\text{cm}^{-1}$) should appear similar to the spectrum on the following page. The two peaks between $750-700\text{cm}^{-1}$ are from polyethylene.

If similar, remove the IR card and continue to step 11.

If there are any other peaks, remove the card and **discard** it. Start at step 1 with a new card.

- 11) Remove the blank card from the sample chamber. Store the IR card in a clean, dry place until the sample is ready to be applied to the card.
- 12) Select the spectrum card blank from the list. Once the spectrum title is highlighted, press the Cut button on the toolbar.
- 13) Repeat steps 1-12 until all the blank cards have been checked for contaminants (change the Display Limits back to $4000-400\text{cm}^{-1}$).

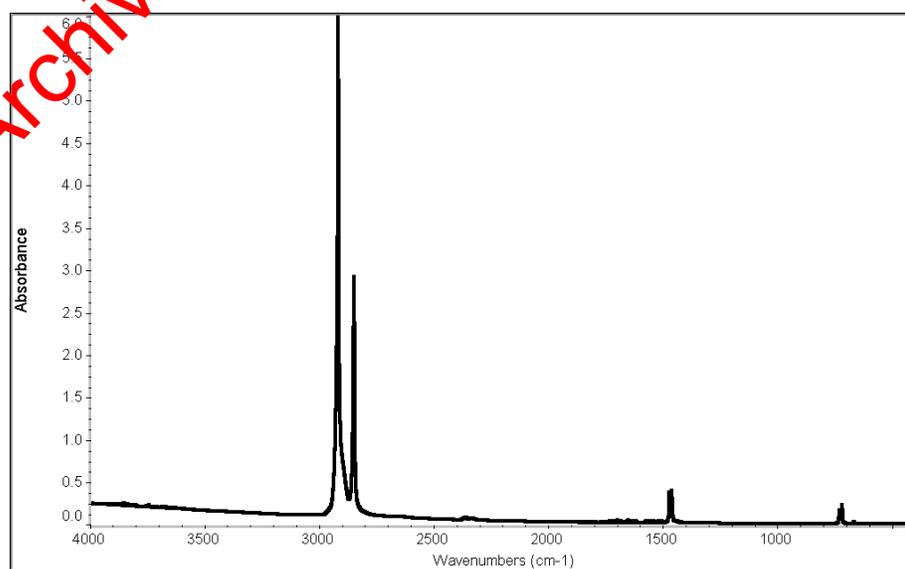


Figure 1a: Spectrum of polyethylene IR card in the $4000-400\text{cm}^{-1}$ region.

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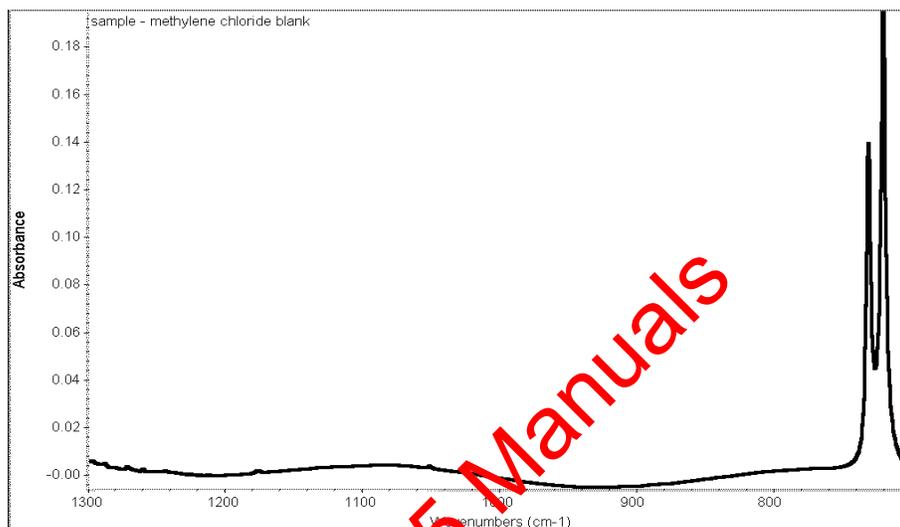


Figure 1b: Spectrum of polyethylene IR card in the 1300-700 cm^{-1} region.

- d. Preparation of extraction negative (methylene chloride blank), positive control, and sample extracts

The purpose of the extraction negative control (reagent blank) is to verify that the solvent does not contain any infrared active species that may interfere with the detection of PPMS. The purpose of the positive control is to demonstrate the effectiveness of the extraction.

NOTE: These steps **MUST** be performed under a chemical fume hood.

- 1) Prepare an extraction negative tube by labeling an empty 1.5mL microcentrifuge tube as such.
- 2) Obtain a positive control tube and note the lot number on the extraction worksheet.

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- 3) With a fine tipped marker, label each checked, blank IR card with the appropriate identifier (extraction negative, positive control, or sample identifier (FB number, swab type, and IA's initials)). Check off the appropriate box on extraction worksheet.

NOTE: Each card must contain the date it was prepared and the initials of the individual preparing the cards.

- 4) Place all tubes in the order listed on the extraction worksheet.
- 5) Place the IR sample cards in the same order as the tubes. Have a witness check the tubes and cards and initial the extraction worksheet.
- 6) Pipette approximately 5mL of methylene chloride into a labeled, working stock tube.

NOTE: Whenever pipetting methylene chloride, the pipet tip must be "conditioned" by pipetting the solvent up and down about 5-10 times before dispensing. If this is not done, the methylene chloride will leak out of the tip immediately.

- 7) Pipette 75 μ L of methylene chloride into each tube. Ensure that the entire sample is covered in solvent. Close each tube tightly to minimize evaporation.
- 8) Mark the level of the meniscus on the side of each tube with a fine tipped marker.

- e. Deposition of samples onto IR sample cards

NOTE: This **MUST** be performed under a chemical fume hood.

- 1) Place each IR sample card onto an elevated surface, ensuring that the membrane does not touch any other surface or solution.

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- 2) Vortex the appropriate sample tube for 15 seconds.

NOTE: Check the meniscus of the PDMS standards to ensure that the solvent levels are not lower than were previously marked. Add sufficient methylene chloride to raise the level to the previously marked meniscus for samples that have experienced solvent loss. Vortex the affected sample tube(s) for 15 seconds.

- 3) With a pipet and an aerosol resistant tip (ART), take 3-5 μ L of the extract and place **onto the center** of a labeled IR card. Allow the solvent to dry. Take another 3-5 μ L of the extract and place onto the same part of the IR card. Allow the solvent to dry. Repeat until all of the extract has been delivered to the card. Squeeze as much of the solvent out of the substrate as possible. Repeat for each card labeled for samples and blanks.

NOTE: It is important that most of the solvent is concentrated at the center of the IR card window because the infrared beam passes through near the center (adjacent to the red laser beam). This area must contain a significant amount of the sample for an accurate spectrum to be collected.

- 4) After the methylene chloride has evaporated, wait 10 minutes to allow residual moisture to evaporate. Once dry, the samples are ready for IR analysis.
- 5) Dispose of sample tubes containing the substrate.

f. Collection of control and sample spectra

- 1) **Ensure Lubricant Analysis is selected in Experiment title bar.** Collect a new background spectrum. The background level should be checked every ten minutes, or more frequently, if required.
- 2) Begin to collect spectra for each card. Follow the instructions in the section **Removing and placing IR cards in the sample holder.**
- 3) Place an IR card with a sample into the chamber.
- 4) Click the Col Smp (Collect Sample) button on the toolbar.

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- 5) The Collect Sample window appears. It reads:

Enter spectrum title:

For the spectrum title, enter the sample identifier as it appears on the IR card and the worksheet. Click OK.

- 6) A Confirmation window appears which reads:

Sample
Please prepare to collect the sample spectrum.

Click OK.

- 7) A Confirmation window appears after the spectrum has been collected. It reads:

Data collection has stopped.
Add to Window 1?

Click Yes.

- 8) Remove the IR card from the sample chamber and place the next IR sample card into the chamber.

Repeat sample collection steps 4-8 for all sample cards.

- 9) After collecting spectra for all sample cards, the spectra should be baseline corrected. For the Automatic Baseline Correction function to baseline correct the entire spectrum, the X-Axis Limits (*i.e.*, wavenumbers) must extend from 4000-400 cm^{-1} . If the X-Axis Limits are not from 4000-400 cm^{-1} , then select Display Limits... in the View menu and enter 4000 as the Start: value and 400 as the End: value.

NOTE: Automatic baseline correction must be performed with the spectrum displayed as an *Absorbance* spectrum.

- 10) From the Edit menu, choose Select All. All the spectra should now be displayed in red.

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- 11) Click on Process on the menu bar and select Automatic Baseline Correct.

Spectra that have been baseline corrected have an asterisk (*) preceding the name of the spectrum.

- 12) The original uncorrected spectra should be deleted from the window by using the select and cut method. Click on the down arrow to the right of the sample name window. A pull-down list of all the spectra in the window will be displayed. Cut all of the spectra (using scissor function) that are not baseline corrected (spectra without asterisks).
- 13) The asterisk (*) should be removed from the name of the baseline corrected spectra before saving. Click on each sample name and delete the asterisk (*).
- 14) Save the baseline corrected spectrum:
 - a) Click on File and select Open....
 - b) Click the button **Create New Folder** and name it with the appropriate extraction set date and time. Click off the folder.
 - c) Close the Open window.
 - d) Select all of the baseline corrected spectra to save into the folder. From the Edit menu, choose **Select All**. All of the spectra should be displayed in red. Click on File and select **Save A**s....
 - e) Open the extraction set folder for the appropriate extraction. Click "Set file name to title" and click Save. Repeat step e for each sample.
 - f) Click on File and Select Open
 - g) Select the new extraction dated folder and drag it, by holding the left mouse button down, into the Files FB folder
 - h) Open the Casework Files FB file and select the extraction folder and drag it into the appropriate Casework folder. Close the Open window.
- 15) Continue with the **Analysis of Spectra** section.

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g. Storage of spectral data

The following printouts (hard copies) must be kept with each case file:

- Positive PDMS control
- Extraction negative
- All casework samples

Digital archives (computer) can be deleted of six months after the extraction was performed.

3. Analysis of spectra

The purpose of the analysis is to provide results concerning the identity of any compounds detected in casework samples. The analysis includes overlaying the sample and PDMS standard spectra and performing spectral subtraction and library searches, if needed.

In order to analyze one spectrum at a time, each spectrum will be moved to its own analysis window.

- 1) Highlight the spectrum to be analyzed by opening the sample name window (down arrow to the right of the sample name) and clicking on the name of the selected spectrum.
- 2) Using the “cut” function (scissor icon), cut the selected spectrum.
- 3) Move the spectrum to a new window by clicking on the Window menu. Select **New Window**. Name the new window with the appropriate sample identifier. Click **OK**. A blank window should appear.
- 4) Hit “Paste.” The selected spectrum should appear in the window.
- 5) Once all spectra are in their own window, visually examine each spectra in full scan region and the fingerprint region. The positive control should resemble the figures 2a and 2b (below). The extraction negative appear should similar to figures 2c and 2d.

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- 6) Overlay a copy of a PDMS standard spectrum to compare to unknown spectra. Open the positive control window (or a PDMS standard from the library) click on Copy from the Edit menu. Close PDMS standard window. Open unknown sample window and paste PDMS standard spectra. Determine if it appears that PDMS is present.
 - 7) If the unknown sample does not resemble PDMS or appears to contain a trace amount of PDMS, perform a library search. **See section b Library Searches below.**
 - 8) After analyzing each spectra, print the spectra. **See Section d Printing Spectra.**
- a. Standard PDMS and Extraction Negative Spectra

The spectrum of PDMS should appear similar to the spectra below. There should be four peaks that are around 1262, 1096, 1020, and 801 cm^{-1} .

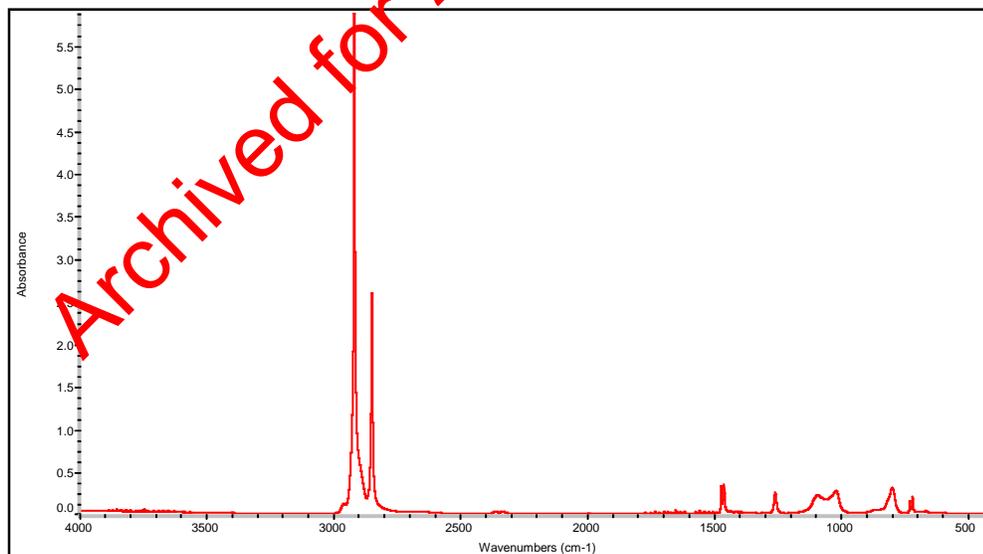
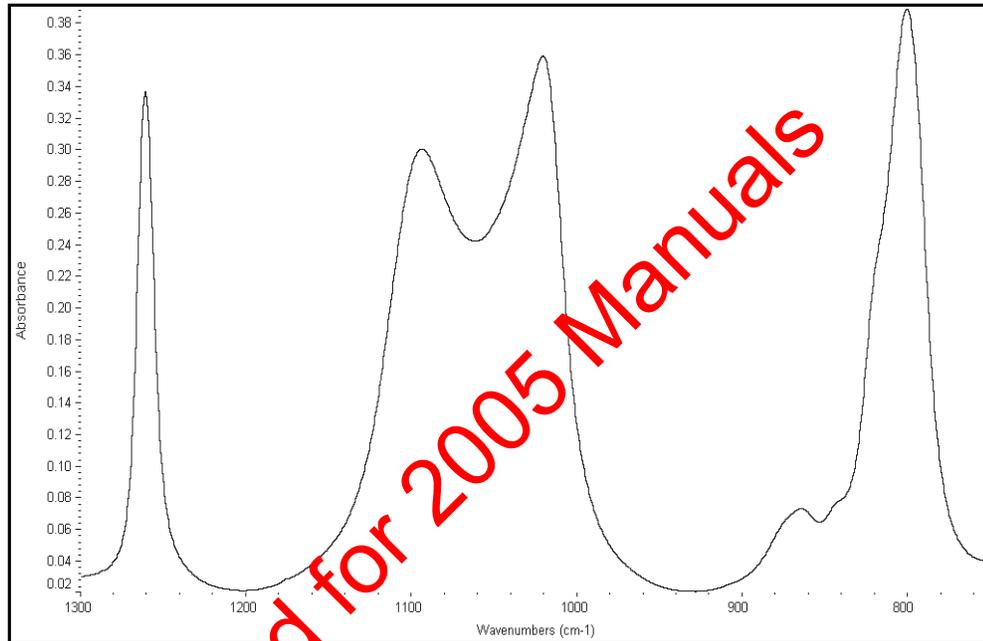


Figure 2a: Spectrum of PDMS in the 4000-400 cm^{-1} region

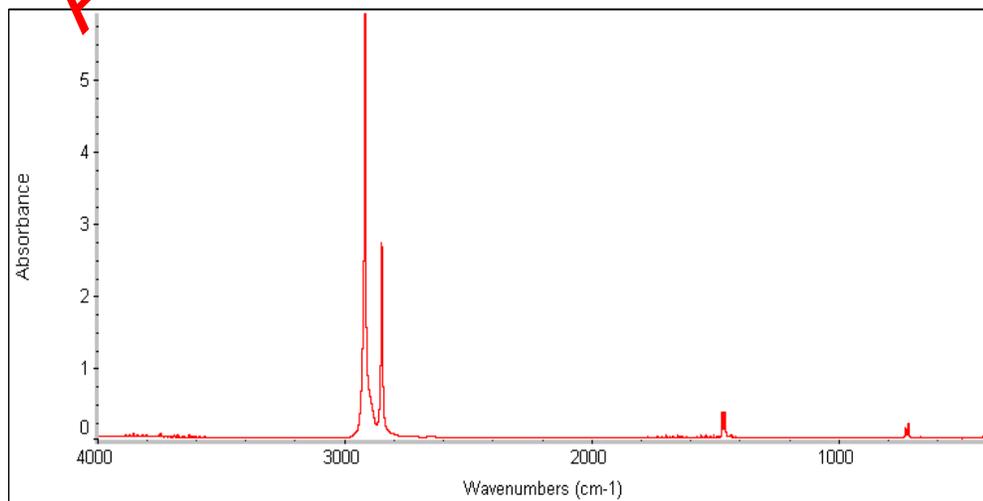
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The spectra of the Extraction Negative should appear as the spectra below.

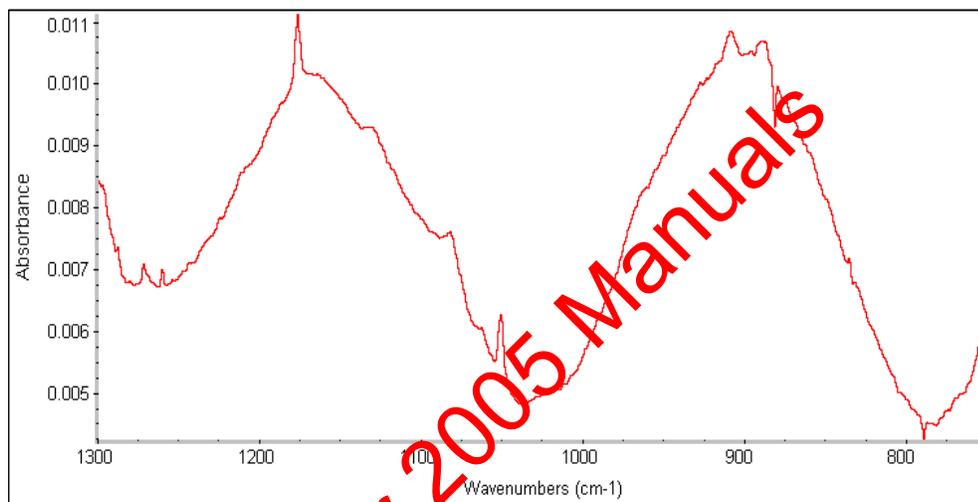


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b. Library Searches

Perform a library search on those spectra that appear to contain only trace amounts of PDMS or do not resemble PDMS (no library search is required for spectra that resemble the positive PDMS control spectra):

- 1) Make sure that the display limits are set for 1300-750 cm^{-1} . If not, change the display limits by selecting **Display Limits...** in the **View** menu, and set the X-Axis Limits from a **Start:** value of 1300 to an **End:** value of 750. Click OK.
- 2) Click the **Full Scale** button.
- 3) Select the **Library Setup...** option in the **Analyze** menu. A **Library Setup** window appears.

In the **Search Libraries** folder, select the **Sample Libraries** from the list of Available search libraries and groups: and then click the **Add** button.

NOTE: Ensure that the PDMS Standards Library is searched.

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In the *Extended Search* folder, the Use extended search box should NOT be checked.

In the *Search Results* folder, the Configure search results button should be checked and the Search type: box, Correlation should be selected.

In the *QC Libraries* folder, no libraries should appear under the QC libraries and groups:.

In the *Search Regions* folder, the Use spectral regions button should be checked. Input the values 1300 under the Start column and 750 under the End column. A shaded area should appear in the displayed spectrum corresponding to the selected area.

- 4) Click OK.
- 5) Click the Search button. A display of search results in the 1300-750cm⁻¹ range will appear. The display will include a list of the top ten matches based on the match value for each compound and a spectrum for the top three matches.

NOTE: Search compares the selected library spectra to that of the unknown spectrum and displays the spectra that most closely match the unknown.

- 6) Compare every spectrum (search result) whose match value is ≥ 80 to the sample spectrum. If a PDMS spectrum (search result) is listed with a match value of ≥ 80 , the sample may contain PDMS. Make a note of any PDMS spectra that yield a match value of ≥ 80 to the sample. Do not print the search results.

NOTE: Library search results may assist in preliminarily identifying trace amounts of PDMS or other unknown compounds. If a preliminary identification is made, a known standard must be run and compared directly with the unknown spectrum. No definite conclusions can be drawn from a library search alone.

- 7) Click the Close button.

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c. Subtraction of Spectra

Overlapping peaks are possible. Absorption bands that are partially overlapped may appear as a broad band with two maxima or with a principal maximum and smaller second maximum on either face of the principal peak. Frequently, overlapping peaks appear as an absorption band with a shoulder.

One spectrum may be subtracted from another in instances where an interfering component may be present in a sample. The spectrum of the interfering component is subtracted from the sample spectrum with a normalizing factor which is user defined. For example, if a sample spectrum contains the cotton swab glue and the lubricant PDMS then the spectral features that arise from this glue can be removed to reveal PDMS more clearly. Spectral subtraction must be done with BOTH spectra in absorbance format.

- 1) Retrieve the suspected interfering component spectrum from the library. From the Analyze menu, select Library Manager....
- 2) Click on **Search Libraries**. Click on **PDMS standards**.
- 3) Select the standard spectrum (previously noted standard spectrum with the highest match value) and click the **Add to Window** button.
- 4) In the **Add to Window** window, select **Add to Window1** and click the **Add** button. Close the **Library Manager** window.
- 5) From the **Edit** menu, select **Select All**. This will select all of the spectra present in the window. As an alternative, press **Ctrl+W**.
- 6) Press the **Absorbance** button to convert the sample spectrum to an absorbance scale.
- 7) Change the display limits to $1400-750\text{cm}^{-1}$ by selecting **Display Limits...** in the View menu, and set the **X-Axis Limits** from a **Start:** value of 1400 to an **End:** value of 750. Click **OK**.

NOTE: If the interfering component is glue from a cotton swab, there may be an absorption peak at approximately 1373cm^{-1} . This peak can be utilized as a reference peak in the subtraction process. This peak is NOT unique to cotton swab glue, however, its absence in a PDMS spectrum makes it a practical reference peak.

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- 8) Click the **Full Scale** button.
 - 9) From the **Process** menu, select **Subtract...**
 - 10) Ensure that the sample spectrum is the top spectrum in the window. If not, click the double-headed arrow button at the right to swap the spectra.
 - 11) Adjust the **Factor** bar by sliding the button up or down the scale until the reference peak at 1373cm^{-1} disappears (or flattens). The **Coarser** and **Finer** buttons can be used to increase/decrease the normalizing factor.
 - 12) Once the interfering component has been removed from the sample spectrum, add the spectrum to a new window. Select the **Add to new window** and click the **Add** button.
 - 13) A **New Window** window appears which reads:
Enter a title for the window:
 - 14) For the title of the new window, type **Subtraction result**. Click **OK**. The subtracted spectrum will appear in a new window.
 - 15) Proceed to the section **Printing sample spectra and standard PDMS spectra** to print the subtracted spectrum.
- d. **Printing Sample Spectra and PDMS Standard Spectra**
- All casework sample spectra **MUST** be printed for every case file. Additionally, a standard PDMS spectrum (positive control) and extraction negative control **MUST** be printed for every case file.
- 1) Press the **% Transmittance** button to convert the sample spectrum to a transmittance scale.
 - 2) Place the cursor in the title bar and remove the asterisk in front of the sample title by deleting it (an asterisk indicates that the sample has been baseline corrected).
 - 3) From the **Report** menu, select **Preview/Print Report...**

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- 4) Press the Print button and click OK.
 - 5) On the printed report, put your initials in the space for analyst.
 - 6) Indicate PDMS detected, not detected, or inconclusive in the results space.
 - 7) Give extraction worksheet and all sample and control reports to a supervisor for review.
 - 8) File original paperwork in appropriate binder after photocopying.
 - 9) When finished with all samples, fill in the *Time Ended* column of the *FT-IR Instrument Usage Log*.
4. Interpretation of spectra – General Guidelines
- a. Each peak represents absorption of infrared energy by a molecular bond or functional group (see table of **Characteristic Infrared Absorptions of Various Functional Groups**).
 - b. The peak area is related to the concentration of the IR active species.
 - c. The degree of peak broadening is determined by a combination of the following factors:
 - Instrument resolution
 - Different vibrational energy states of a molecular bond
 - Intermolecular and intramolecular interactions
 - d. The extraction negative spectrum should appear similar to Figures 1a and 1b. If additional peaks are present, the methylene chloride has been contaminated and the extracted samples must be discarded. Each sample must be re-cut and taken through the extraction process again using fresh quality control checked methylene chloride.

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- e. The positive control spectrum must be compared to the spectra in the PDMS Standards Library and it should appear similar to one of the archived PDMS standards (and Figures 2a and 2b). The spectrum must possess the four characteristic peaks in the fingerprint region that are around 1262, 1096, 1020, and 801 cm^{-1} and the rest of the spectrum must appear similar. If the positive control spectrum does not appear similar to any of the archived PDMS standards, the extracted samples must be discarded. Each sample must be re-cut and taken through the extraction process again using fresh quality control checked PDMS positive control.
- f. Sample spectra that appear similar to the PDMS positive control spectrum (and Figures 2a and 2b) likely contain PDMS. The spectrum must possess the four characteristic peaks in the fingerprint region that are around 1262, 1096, 1020, and 801 cm^{-1} and the rest of the spectrum must appear similar.
- g. Sample spectra that appear similar to the extraction negative spectrum (Figures 1a and 1b) can be considered negative for the presence of PDMS. However, the absence of characteristic peaks does not mean that the compound is not in the sample. An appropriate description of a negative result is “the compound was not detected.”
- h. Sample spectra that appear similar to the PDMS positive control spectrum (with the four characteristic absorption peaks) yet possess additional absorption peaks are indicative of a mixture. Mixtures **MUST** be interpreted with caution.
- i. Sample spectra that do not resemble the PDMS positive control spectrum nor the extraction negative spectrum yet possess absorption peaks indicate that some chemical compound(s) is (are) present in the sample. The library search may assist in a preliminary identification of the compound(s).
- j. After reviewing spectra and printing, indicate PDMS detected or not detected in the “result” section of the printed report. Give all paperwork to the FTIR supervisor for review.

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5. Troubleshooting

For simple troubleshooting of the spectrometer and software, follow the instructions outlined below.

- a. Click on Help and select Spectrometer Help Topics.
- b. Double click on Troubleshooting.
- c. Search this section for the problem and solution.

For problems that are beyond the scope of the analyst, contact Thermo Nicolet and schedule an appointment with a Field Service representative.

Characteristic Infrared Absorptions of Various Functional Groups		
Functional Group	Frequency Range (cm ⁻¹)	Intensity
C-H (alkyl)	2853-2962	Medium-strong
=C-H (alkenyl)	3010-3095	Medium
≡C-H (alkynyl)	~3300	Strong
C=C	1620-1680	Variable
C≡C	2100-2260	Variable
-CH(CH ₃) ₂	1365-1370, 1380-1385	Strong, strong
-C(CH ₃) ₃	~1365, 1385-1395	Strong, medium
R-CH=CH ₂	905-920, 985-1000	Strong, strong
R ₂ C=CH ₂	880-900	Strong
<i>cis</i> -RCH=CHR	675-730	Strong
<i>trans</i> -RCH=CHR	960-975	Strong
O-H (alcohols and phenols, dilute solutions)	3590-3650	Variable and sharp
O-H (alcohols and phenols, H bonded)	3200-3550	Strong and broad
O-H (carboxylic acids, H bonded)	2500-3000	Variable and broad
C=O (aldehydes)	1690-1780	Strong
C=O (ketones)	1680-1750	Strong
C=O (esters)	1735-1750	Strong

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Characteristic Infrared Absorptions of Various Functional Groups		
Functional Group	Frequency Range (cm ⁻¹)	Intensity
C=O (carboxylic acids)	1710-1780	Strong
C=O (amides)	1630-1690	Strong
Aromatic-H	~3030	Variable
-N-H	3300-3500 (one peak)	Medium
-N-H ₂	3300-3500 (two peaks)	Medium
C≡N	2220-2260	Medium
Si-H	2100-2360	Strong
Si-OR	1000-1100	Strong and broad
Si-CH ₃	1250-1100	Strong and sharp

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Refer to the Case Management Manual for the general guidelines for writing laboratory reports. The template reports contain many pre-written sentences to guide explanations and interpretations of results.

1. For the majority of cases, the following type of summary is sufficient:

“Polydimethylsiloxane (PDMS), a chemical used in many domestic condom lubricant preparations, was (not) detected.”

2. Complicated or unusual cases involving additional absorption peaks can be difficult to write. The template reports are a place to start and many valuable insights can be gained by reading previous reports covering similar cases. It is a good idea for each analyst to maintain a file of his or her complicated reports for future reference.

For cases involving mixtures:

“Additional peaks were present in the sample. PDMS may be a component of this mixture.”

For cases involving identifiable organic compounds:

“Polydimethylsiloxane (PDMS), a chemical used in many domestic condom lubricant preparations, was not detected.”

For cases involving unidentifiable organic compounds:

“Polydimethylsiloxane (PDMS), a chemical used in many domestic condom lubricant preparations, was not detected.”

3. Qualitative statements may be part of the summary. They are used for probative samples when:
 - a. The sample is apparently unmixed.
 - b. The sample could be a mixture of two or more components, including PDMS.

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