

Lab 1 Final CTH

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17-Oct-25

Our Reference: ACLAB_01

LAB REPORT ON THE IDENTIFICATION OF UNKNOWN MATERIALS USING FT-IR ANALYSIS

References. See footnotes and embedded documents section at end of document.

Abstract

This report details the process and results from the FT-IR experiment conducted by the student on 10th October 2025. The experiment was to identify 4 unknown materials provided by the lecturer using spectroscopic analysis.

This experiment will use a PerkinElmer Spectrum 2 with diamond ATR module to scan and test the unknown materials. Although the main tasks involved will be the measuring of the sample absorption using the FT-IR this report will detail the appropriate method used to achieve the results and steps taken in processing and determination of the materials.

Table of Contents

Abstract	1
Table of Contents	2
1. Introduction and Background	3
1.1. Experiment Purpose	4
1.2. Hypothesis	4
1.3. Variables	4
2. Materials and Setup	5
3. Procedure	5
4. Observations and Data	7
4.1. Sample A	7
4.2. Sample B	7
4.3. Sample C	8
4.4. Sample D	8
5. Calculations and Processing	9
5.1. Sample A	9
6. Results & Discussions	10
6.1. Library Identification	10
7. Conclusions	10
8. References	11
9. Annex 1 – Experimental Notes Digital and Physical	12
10. Annex – 2 Raw Results	17
10.1. Sample A	17
10.2. Sample B	19
10.3. Sample C	21
10.4. Sample D	23

1. Introduction and Background

Fourier Transfer Infra-Red (FTIR) is a type of Spectro analysis that uses a beam of infra-red light to ascertain what a sample of a material might be. As the light is bounced through the sample certain wavelengths of the light are absorbed by some molecules and bonds within the sample. The FTIR then observes the light that's coming out of the sample and can plot a graph knowing what is missing from the light. This is the absorption spectrum of a sample. The below absorption spectrum for TNT shows major peaks in the form of wavelength (μm) this can be converted into wave number cm^{-1} using Equation 1.

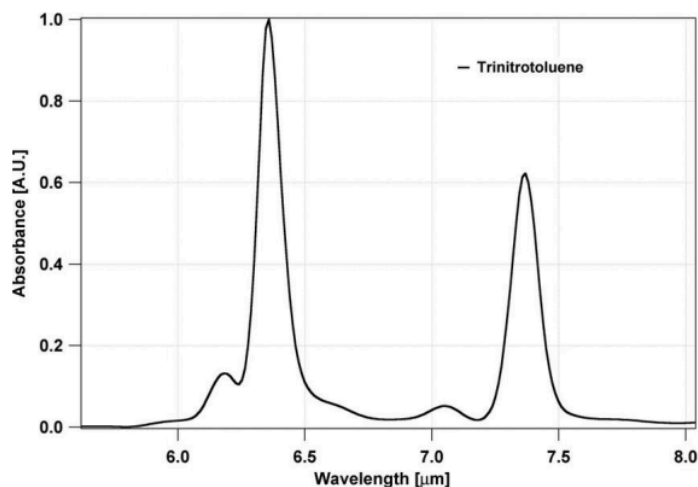


Figure 1 - Absorption Spectrum of TNT [1]

$$\text{Equation 1 - Wavenumber } (\text{cm}^{-1}) = \frac{10^4}{\text{Wavelength } (\mu\text{m})}$$

From Equation 1 ~~we can take~~ ^{it can be taken} the 2 major peaks and 2 minor peaks and convert them into wavenumbers in the table below. From this data the functional groups can be identified. [2] [3] [4]

Wavelength estimate (μm)	Wavenumber approximation (cm^{-1})	Peak Shape	Functional Group
6.3	1587	Strong / Sharp	C=C stretching and or asymmetric NO_2 stretching
7.3	1370	Medium / Sharp	Symmetric NO_2 stretching confirming first peak at 6.3 is Asymmetric NO_2 stretching.
6.2	1613	Weak / Broad	C-H Bending
7.1	1408	Weak / Broad	C-N Stretching

Table 1 - TNT absorption peaks Processing

As Table 1 demonstrates the reading of absorption data can be difficult and heavily specialised. This is the reason that most FTIR experiments use a library of known results to compare against. This provides the user with a quick and accurate method of achieving a result without having to use the basic principles of functional groups to determine the chemical composition.

FTIR is regularly used in Ordnance Munitions and Explosives (OME) as a method of energetics identification, residue analysis and thermal stability analysis. FTIR analysis is used as it has key advantages being non-destructive, highly sensitive, versatile and can be made portable. [5]

Mainly FTIR is used in the identification of materials post incident. For example when an Improvised Explosive Device (IED) has been either recovered, made safe or initiated the identification of the energetic used can support the investigation and help prevent future incidents [6]

1.1.Experiment Purpose *equally important purpose is to develop a SOP for FT-IR analysis of these materials*

The aim of this experiment is to identify the 4 unknown samples using the FT-IR machine to prove the process and identify the materials. The scenario provided by the lecturer is detailed below.

"Following a site inspection at a small materials-testing facility, inspectors recovered a series of labelled reference powders that were reportedly being used in the evaluation of new energetic formulations. The materials are common industrial or laboratory chemicals, but each represents a different class of functional group frequently encountered in the design, manufacture, or degradation of energetic compounds. Before the samples can be cleared for safe disposal, confirmation of their identity and chemical functionality is required." [7]

1.2.Hypothesis

The hypothesis is that the 4 materials will be identified using the FTIR machine and associated material library with a confidence level of above 95%.

1.3.Variables

The below table details the variables identified in this experiment, their type and how they relate to the experiment

Variable Type ¹	Variable	Effect/ example
C	FTIR Technique	The equipment available and therefore the technique used can affect the results KBr Plates vs ATR Crystal.
C	Instrument Calibration	Is the machine calibrated, when and is the experiment using reference materials.
C	Instrument Settings	Settings like the apodization function will alter how much smoothing or background noise is removed from the result.
C	Spectral Resolution	This resolution setting determines how many 'bounces' through the sample the laser does and therefore will impact the readings
D	Absorbance / Transmittance	This is the primary measurement.

¹ I = Independent, D = Dependent, C = Controlled

D	Baseline Characteristics	How much noise exists on the result, this directly reflects how contaminated the sample is. The less noise the purer the sample.
D	Peak Intensity	This correlates to how concentrated the sample is and the strength of certain bonds.
D	Peak Position	This correlates to Bond vibration frequencies.
I	Sample	Which sample is being tested.
I	Sample Composition	What the sample is.
I	Sample Phase	what phase the sample is, S,L or G
I	Sample Thickness	The thickness of the sample can affect.

Table 2 - Experimental Variables

2. Materials and Setup

PPE

Safety Goggles
Nitrile Gloves

Materials

Isopropyl alcohol
Blue Roll
Powdered Sample Materials

Equipment

1 x Sample Container Per sample.
1 x Metal Spatula Per Sample
1 x Perkin Elmer Spectrum 2 with Diamond ATR and associated equipment

Setup

Other than the gathering of appropriate materials no setup is specifically required for this experiment outside of the procedure. If the FTIR is new the manufactures instructions should be followed for initialisation and first use. [8]

3. Procedure

The procedure outlined below details what was performed in the experiment but does not include specifics related to the equipment being used.

- Prepare Sample
 - Place a small amount of the sample in a labelled disposable container.
- Prepare FTIR Machine
 - Start Up Machine
 - Retract foot from sample plate by turning anti clockwise
 - Remove Protective covers from foot and sample plate
- Clean Sample Plate and Foot
 - Rotate foot to clear plate to enable cleaning.
 - Remove foot by pulling down gently.
 - Clean sample plate and foot using IPA and Blue Roll.
 - Re attached foot gently by pushing it back on.
- Perform Background Scan.
 - Rotate Foot to over the sensor
 - Tighten the foot till the ratchet clicks
 - Initiate the background scan on the software.
 - Observe the results for any irregularities to the 'normal' scan. 'If anything makes sense clean and test again'.
 - Once successful test is achieved loosen the foot and rotate the foot out of the way of the sample plate to finish preparation for the sample.
- Load Sample

- Using the metal spatula add a sufficient pile of the material to the sensor until the sensor is covered. The quantity does not matter if the sensor is covered. "This is bucket chemistry" [9]
- Rotate the arm and foot over the sample.
- Tighten foot until the ratchet clicks
- Scan Sample
 - Select Scan
 - Wait for Initial Scan
 - Confirm reading is logical for expected material
 - Select Scan
 - Await Final Scan to complete.
- Initial Processing
 - Change Sample results graph line colour to something 'sensible'
 - Compare result to available Library
 - Observe and note Initial Result
 - Save Files in file format Name: YYYYMMDDHHMM-SAMPLENAME-OPERATOR.csv
 - Repeat from Step 3 for each new sample.
- Initial Results from Library Lookup
 - Sample A Vit C Powder
 - Sample B Guanidine Nitrate
 - Sample C Methyl 3-nitrobenzoate
 - Sample D Acetaminophen (Paracetamol)
- Tidy Up
 - After the final sample has been tested, repeat Steps 3 and 4 till clean.
 - Replace Foot and Plate covers
 - Tighten foot till click.
 - Power down equipment.

the parameters from the handout such as apodisation, S/N ratio, etc are not mentioned

4. Observations and Data

The full results achieved for each sample can be seen in Annex 2 separated by sample, this also details the library search results for each sample. The below section reports the individual spectra for each sample with the associated absorption peaks.

4.1. Sample A

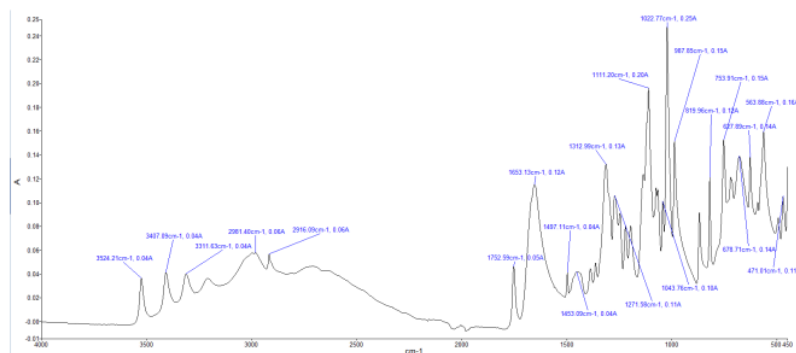


Figure 2- Sample A Spectra

4.2. Sample B

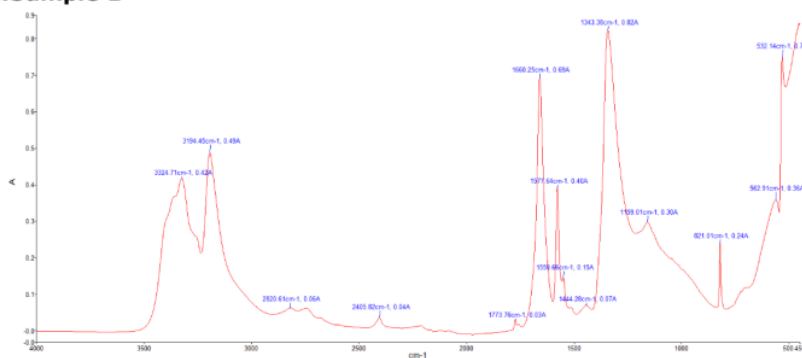
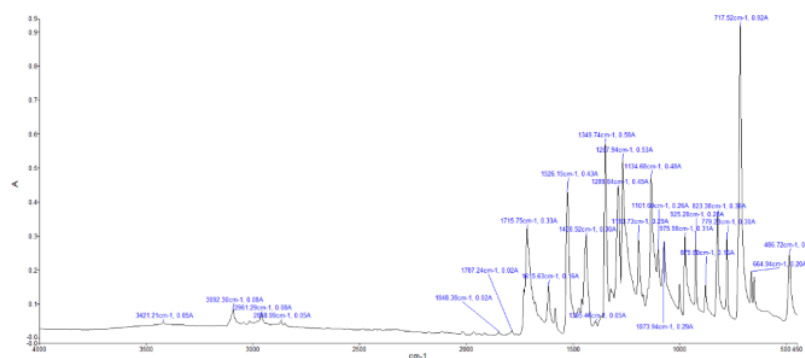
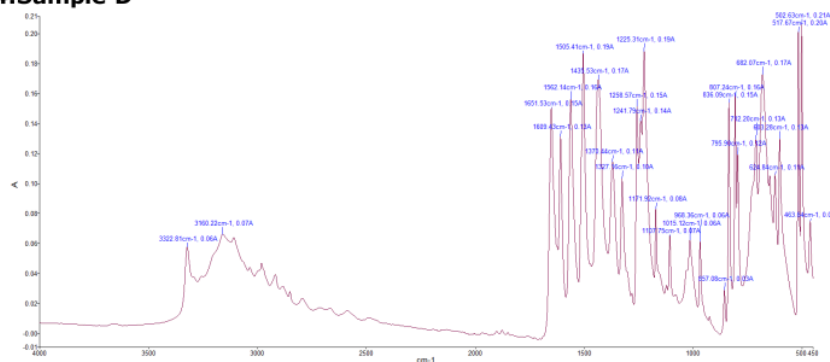


Figure 3 - Sample B Spectra

4.3. Sample C



4.4. Sample D



5. Results Processing

The common method to process and evaluate FTIR spectra is to compare the resultant absorption spectra to a library of known spectra. This is the fastest and most effective way of accurately determining the chemical in a spectrum. Prior to these libraries being available, the reading of spectra results was a valued skill. The sections below detail the major functional groups that can be identified from the sample spectra as this is what would be done when there is no result from a library or chemical is unknown.

Due to the constraints of this report only sample A will be evaluated manually as detailed in the introduction using a list of available functional groups with wave numbers [10].

5.1. Sample A

Wavenumber approximation (cm^{-1})	Peak Shape	Functional Group
3524, 3407, 3311	Sharp	O-H Stretch
2981, 2916	Broad, Medium	C-H Stretch
1732, 1653	Strong, Sharp	C=O Stretch
1497, 1453	Medium	C-H Bending
1271, 1111, 1043	Strong, Sharp	C-O Stretch
987, 819, 753	Strong, Sharp	C-H Bending

Table 3 - Sample A Peaks With Functional Groups

From the above functional groups, these can be mapped to the suspected substance of Ascorbic Acid (Vitamin C). The major groups show the presence of hydroxyl (Alcohol) Groups, Ester Group and a Carbonyl Group. This provides further confidence that the material is correctly identified as Vitamin C.

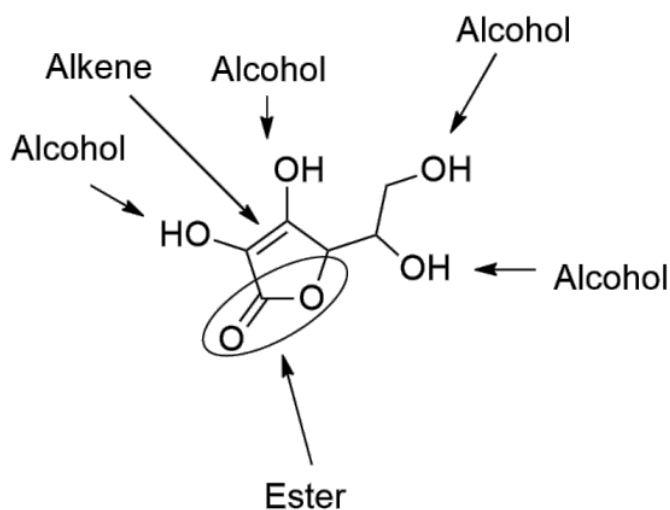


Figure 6 - Ascorbic Acid Functional Groups Diagram [11]

6. Results & Discussions

6.1. Library Identification

Using the available library matching the below results can be concluded.

Sample Name	Determined compound	% Confidence From Library Search	Comments
A	Vitamin C Powder	99.4	High confidence in results
B	Guanidine Nitrate	95.3	Slightly lower confidence than expected. Could re-run.
C	Methyl 3-Nitrobenzoate	52.8	Compound not in library, identified Ethyl 4-nitrobenzoate instead
D	Paracetamol (acetaminophen)	99.3	Hi confidence in results

Table 4 - Library Search Results

The results in Table 4 provide high confidence in the identification of samples A,B and D. With confidence matches all above 95% there is little likelihood of misidentification. Sample 3 came back with a incorrect match with a low confidence. On further investigation it was determined that the correct spectra is not available in the library hence the incorrect result. In addition, as this sample was locally synthesised quality and contamination of the sample are concerns.

7. Conclusions

In conclusion the 4 unknown materials were able to be correctly identified using the FTIR despite sample C not being available in the library. The basic evaluation of the major functional groups within the samples further assured the correct results. FTIR spectrometry is a critical method in the identification of unknown materials within OME and is often used in both lab and field conditions. As a whole the experiment was a success, enabling the safe disposal of the materials from the given scenario.

8. References

- [1] I. G. D. M. P. A. G. T. R. G. Michael B. Pushkarsky*, "High-sensitivity detection of TNT," *PNAS*, vol. 103, no. 52, pp. 19630-19634, 2007.
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- [3] R. O. R. R. Asep Bayu Dani Nandiyanto*, "How to Read and Interpret FTIR Spectroscopy of Organic," *Indonesian Journal of Science & Technology*, vol. 4, no. 1, pp. 97 - 118, 2019.
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- [6] 1. P. a. J. W. R. P. Yongyan Mou, "Detection and identification of explosive particles in fingerprints using attenuated total reflection-Fourier transform infrared spectromicroscopy," *Forensic Science*, vol. 54, no. 4, pp. 739-973, 2009.
- [7] E. Kazimierska, "ACDA6020 LAB #1 FT-IR Analysis and Identification of Organic Materials," 09 10 2025. [Online]. Available: <https://moodle.uwtsd.ac.uk/course/view.php?id=11711>. [Accessed 12 10 2025].
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- [11] WizePrep, "6.1.11 Functional Groups of Vitamin C," [Online]. Available: <https://www.wizeprep.com/online-courses/4146/chapter/6/core/1/11>. [Accessed 16 10 2025].

9. Annex 1 – Experimental Notes Digital and Physical

The below annex details the data and information captured through both digital and written means during the experiment.

Fillable FT-IR Method Template

(complete every field. Where asked to justify a choice, give a short reason, 1–2 sentences.)

1. Safety & sample handling (tick / fill)

PPE required: ☐ Lab coat ☒ Nitrile gloves ☒ Safety glasses ☐ Fume hood if dusty

Hazard notes (brief): No Specific Notes in relation to the Task but unknown chemicals should be treated with sufficient caution

Waste route (how samples / wipes will be disposed):

Most samples present no hazard and therefore contaminated supplies can be disposed of through general waste. Methyl 3-nitrobenzoate contaminated items will be disposed centrally through contaminated waste.

2. Equipment & consumables (list model where applicable)

Item	Make / model (if known)	Qty / Notes
ATR-FTIR spectrometer	Perkins Elmer Spectrum 2	___1___
ATR crystal (type)	X Diamond ☐ ZnSe ☐ Other: _____	___1___
Cleaning solvent	(IPA / EtOH / other)	___500ml___
Micro-spatula / tissue	Blue Tissue and Metal Spatulas	1 Roll + 1 Spatula per sample
PC / software	Spectrum IR	_____
Reference spectra files	Stored in local Library	_____

3. Acquisition parameters (fill and justify)

Spectral range: 4000 – 250 cm^{-1} - This is the capability of the machine.

Resolution: _____ cm^{-1} - Justification: this refers to how many 'bounces' the laser does along the sample

Background scans: 15 scans - Justification: this is considered a statistically relevant number of scans to allow for a more relevant average reading of the sample.

Sample scans: 15 scans - Justification: Same as background.

Apodization function: _____ - Justification: TBC

Pressure/force guidance: (how you will ensure consistent contact)

The ATR has an inbuilt max torque wrench

File naming convention: YYYYMMDDHHMM-SAMPLENAME-OPERATOR.csv

Files to be saved: ☐ native format ☒ .csv ☐ .png/.pdf annotated

4. Step-by-step measurement procedure (numbered)

(Be explicit so another trained student could reproduce your work.)

- A. Prepare Sample
 - i. Place a small amount of the sample in a labelled disposable container.
- B. Prepare FTIR Machine
 - i. Start Up Machine
 - ii. Retract foot from sample plate
 - iii. Remove Protective covers from foot and sample plate
- C. Clean Sample Plate and Foot
 - i. Rotate foot to clear plate to enable cleaning.
 - ii. Remove foot by pulling down gently.
 - iii. Clean sample plate and foot using IPA and Blue Roll.
 - iv. Re attached foot gently by pushing it back on.
- D. Perform Background Scan.
 - i. Rotate Foot to over the sensor
 - ii. Tighten the foot till the ratchet clicks
 - iii. Initiate the background scan on the software.
 - iv. Observe the results for any irregularities to the 'normal' scan. 'If anything makes sense clean and test again'.
 - v. Once successful test is achieved loosen the foot and rotate the foot out of the way of the sample plate to finish preparation for the sample.
- E. Load Sample
 - i. Using the metal spatula add a sufficient pile of the material to the sensor until the sensor is covered. The quantity does not matter if the sensor is covered. "This is bucket chemistry" [9]
 - ii. Rotate the arm and foot over the sample.
 - iii. Tighten foot until the ratchet clicks
- F. Scan Sample
 - i. Select Scan
 - ii. Await for Initial Scan
 - iii. Confirm reading is logical for expected material
 - iv. Select Scan
 - v. Await Final Scan to complete.
- G. Initial Processing
 - i. Change Sample results graph line colour to something 'sensible'
 - ii. Compare result to available Library
 - iii. Observe and note Initial Result
 - iv. Save Files in file format Name: YYYYMMDDHHMM-SAMPLENAME-OPERATOR.csv
 - v. Repeat from Step 3 for each new sample.
- H. Initial Results from Library Lookup
 - i. Sample A Vit C Powder
 - ii. Sample B Guanidine Nitrate
 - iii. Sample C Methyl 3-nitrobenzoate
 - iv. Sample D Acetaminophen (Paracetamol)
- I. Tidy Up
 - i. After the final sample has been tested, repeat Steps 3 and 4 till clean.
 - ii. Replace Foot and Plate covers
 - iii. Tighten foot till click.
 - iv. Power down equipment.

5. Data processing & interpretation policy (state what you will do)

ATR correction: [] Apply [X] Do not apply - Reason: Not Needed

Baseline correction: [] Yes [X] No - Method / settings: None

Smoothing: ☒ None ☐ Savitzky-Golay (window = ____, poly = ____) - Reason: Smoothing from 15 scans and Average

Peak-picking rules: (e.g., pick top 5 peaks > X% absorbance, tolerance $\pm Y \text{ cm}^{-1}$)

Manual _____

Library search use: ☒ Will run library search - acceptance threshold: 95 %

Manual justification requirement: (state how many diagnostic peaks you will cite) ____

6. Quality control / validation checks (tick and comment)

Background collected at start - time: _____ - comment: _____

Blank collected after each sample - comment: Yes per notes and Procedure.

Replicate acquisition performed on sample: ☐ A ☐ B ☐ C ☐ D - results OK? ☐ Yes ☐ No - notes:

ATR crystal cleaned between samples - method: Clean after Test, Re background test, and then next sample

S/N check - main peaks $S/N \geq$ _____ - measured at _____ cm^{-1} - value: _____

If any check fails, describe corrective action: Reclean, Background Scan, and Retest

7. Troubleshooting (two likely problems and mitigation)

Problem 1: Contamination

Action: Reclean, Background Test and Retest

Problem 2: Poor Sample Contact

Action: Retighten till torque drive clicks, retest.

Fillable FT-IR Method Template
(complete every field. Where asked to justify a choice, give a short reason, 1-2 sentences.)

1. Safety & sample handling (tick / fill)
PPE required: ☐ Lab coat ☒ Nitrile gloves ☒ Safety glasses ☐ Fume hood if dusty
Hazard notes (brief):

Waste route (how samples / wipes will be disposed):
General Waste. Sample C - container wipe + bung

2. Equipment & consumables (list model where applicable)

Item	Make / model (if known)	Qty / Notes
ATR-FTIR spectrometer	<u>Perkin Elmer Spectra 2</u>	
ATR crystal (type)	☒ Diamond ☐ ZnSe ☐ Other: _____	
Cleaning solvent	<u>(IPA) / EtOH / other</u>	
Micro-spatula / tissue	<u>blue tissue + spatula</u>	
PC / software	<u>Spectra 2</u>	
Reference spectra files	<u>stored locally</u>	

3. Acquisition parameters (fill and justify)

Spectral range: 4000-250 cm^{-1} - capability of machine

Resolution: _____ cm^{-1} Justification: harmonic dip clear

Background scans: 15 scans - Justification: statistically Relevant

Sample scans: 15 scans - Justification: statistically Relevant

Apodization function: _____ - Justification: 756

Pressure/force guidance: (how you will ensure consistent contact)
in built torque wheel (clicks)

File naming convention: Perkin Elmer Sample Name Spectra 2

Files to be saved: ☐ native format ☒ .csv ☐ .png/.pdf annotated

Figure 7 - Written Experiment Notes Page 1

4. Step-by-step measurement procedure (numbered)
(Be explicit so another trained student could reproduce your work.)

1. A - vitc powder
2. B - glucose nitrate
3. C - not good sample - could Raman - not in library
4. D - paracetamol
5. _____
6. _____
7. _____

5. Data processing & interpretation policy (state what you will do)

ATR correction: ☐ Apply ☒ Do not apply - Reason: not needed

Baseline correction: ☐ Yes ☒ No - Method / settings: no

Smoothing: ☒ None ☐ Savitzky-Golay (window = __, poly = __) - Reason: inbuilt is smooth

Peak-picking rules: (e.g., pick top 5 peaks > X% absorbance, tolerance $\pm Y \text{ cm}^{-1}$)
manucl

Library search use: ☒ Will run library search - acceptance threshold: 95 %

Manual justification requirement: (state how many diagnostic peaks you will cite) _____

6. Quality control / validation checks (tick and comment)

Background collected at start - time: _____ - comment: inhibitor

Blank collected after each sample - comment: no but should or we detected
water

Replicate acquisition performed on sample: ☐ A ☐ B ☐ C ☐ D - results OK? ☐ Yes ☐ No - notes: _____

ATR crystal cleaned between samples - method: yes Always clean + Raman

S/N check - main peaks S/N $\geq$ _____ - measured at _____ cm^{-1} - value: _____ - not needed

If any check fails, describe corrective action: Reclean, backscat, Relect

7. Troubleshooting (two likely problems and mitigation)

Problem 1: contamination

Action: Reclean + Relect

Problem 2: _____

Action: _____

Figure 8 - Written Experiment Notes Page 2

10. Annex – 2 Raw Results

10.1. Sample A

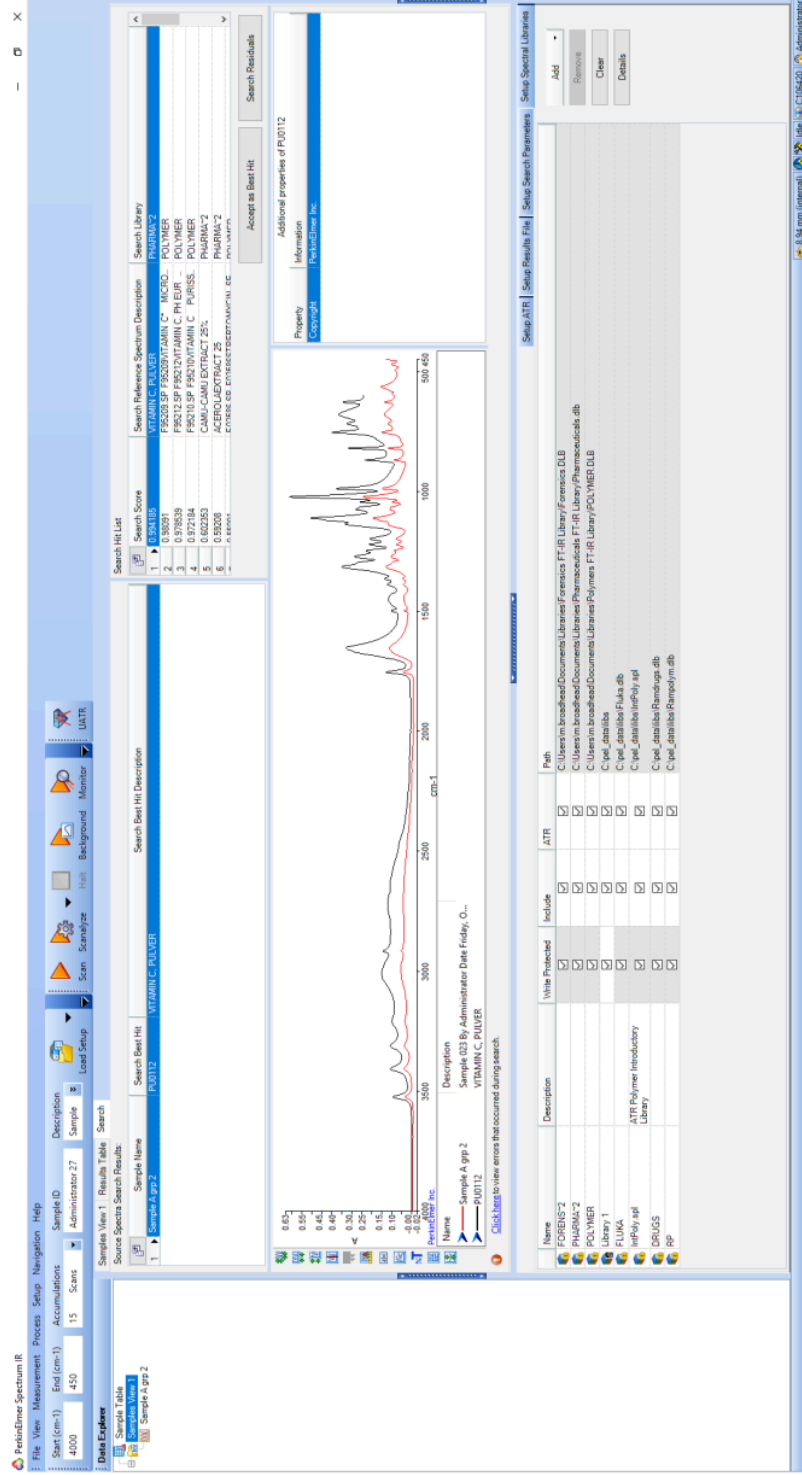


Figure 9 - Sample A Screen Shot

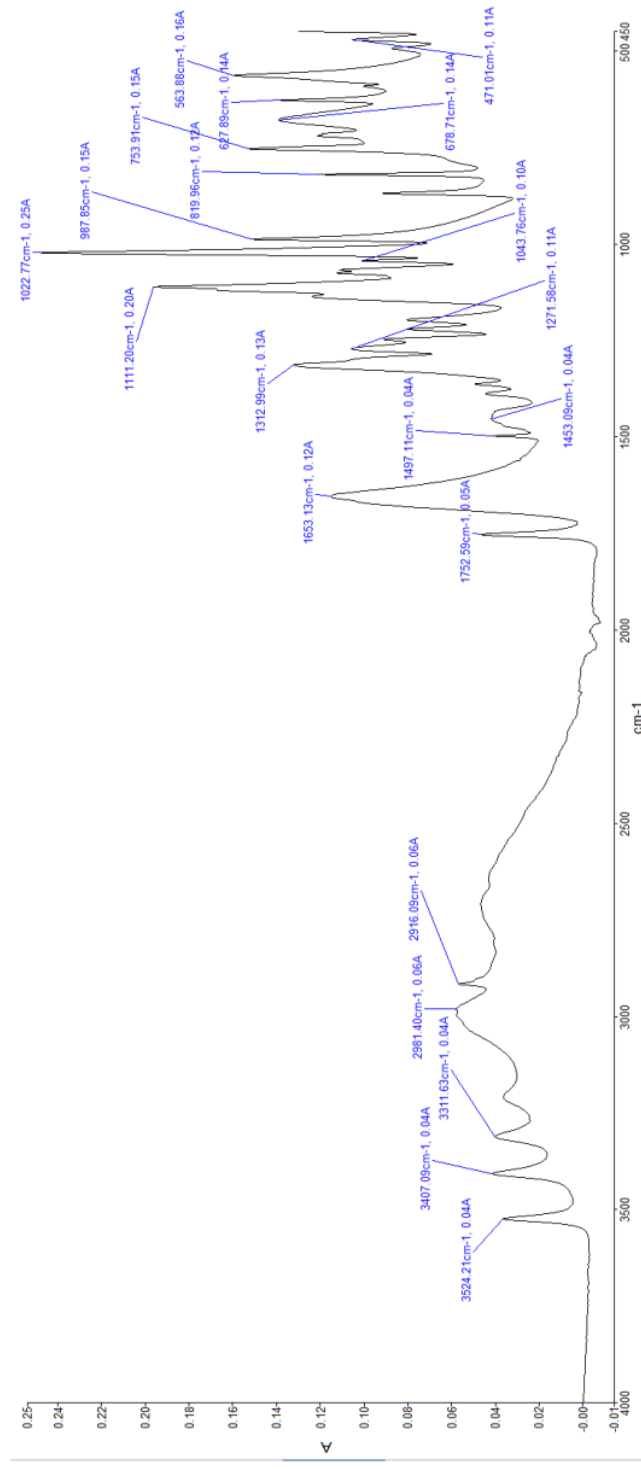


Figure 10 - Sample A Spectra

10.2. Sample B

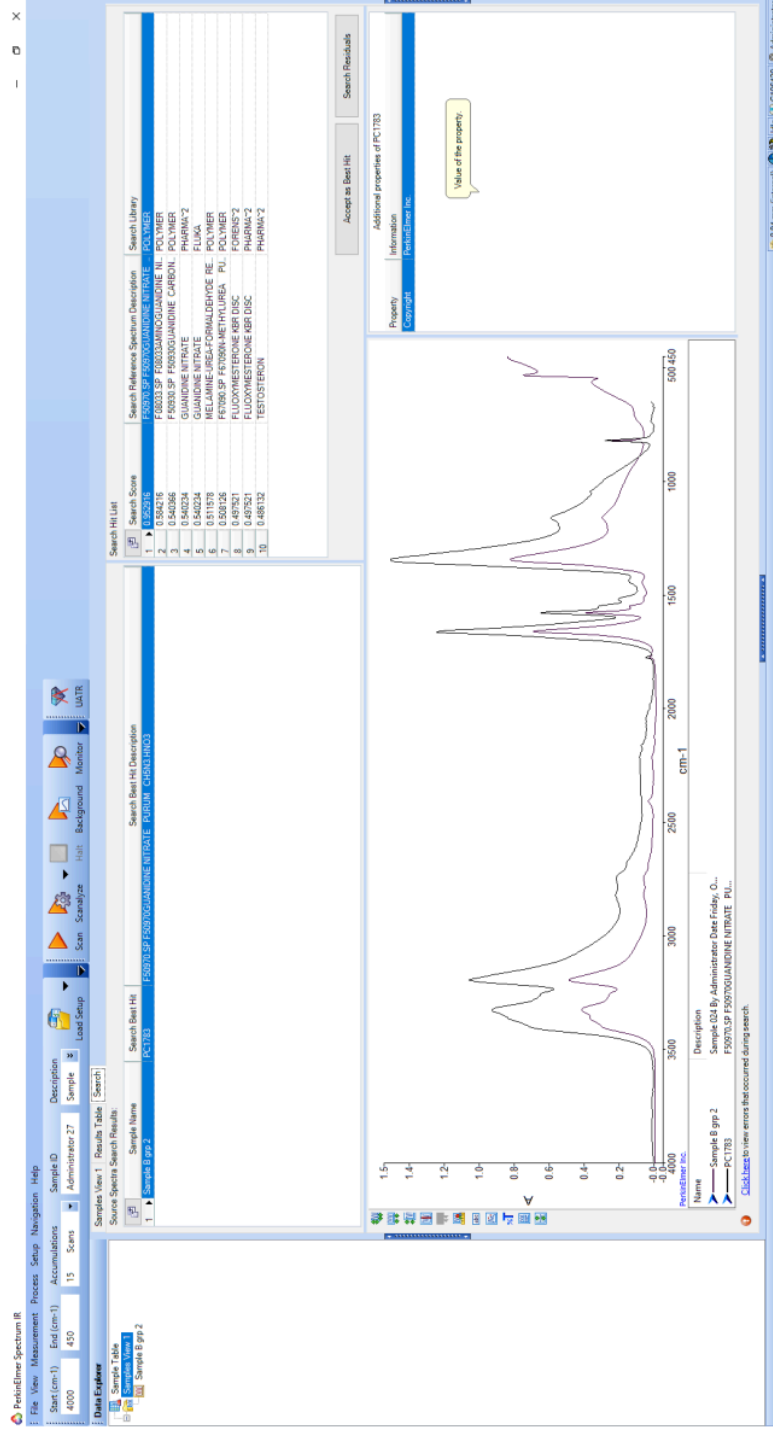


Figure 11 - Sample B Screen Shot

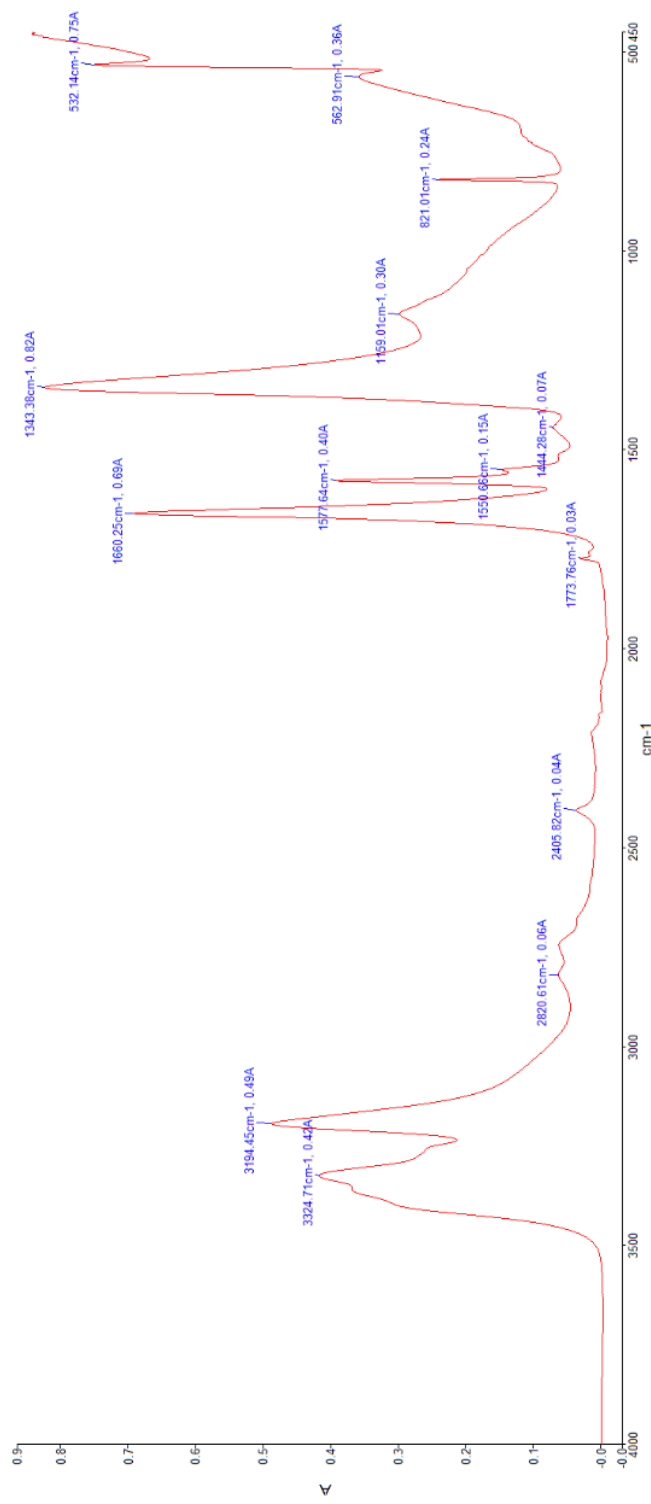


Figure 12 - Sample B Spectra

10.3. Sample C

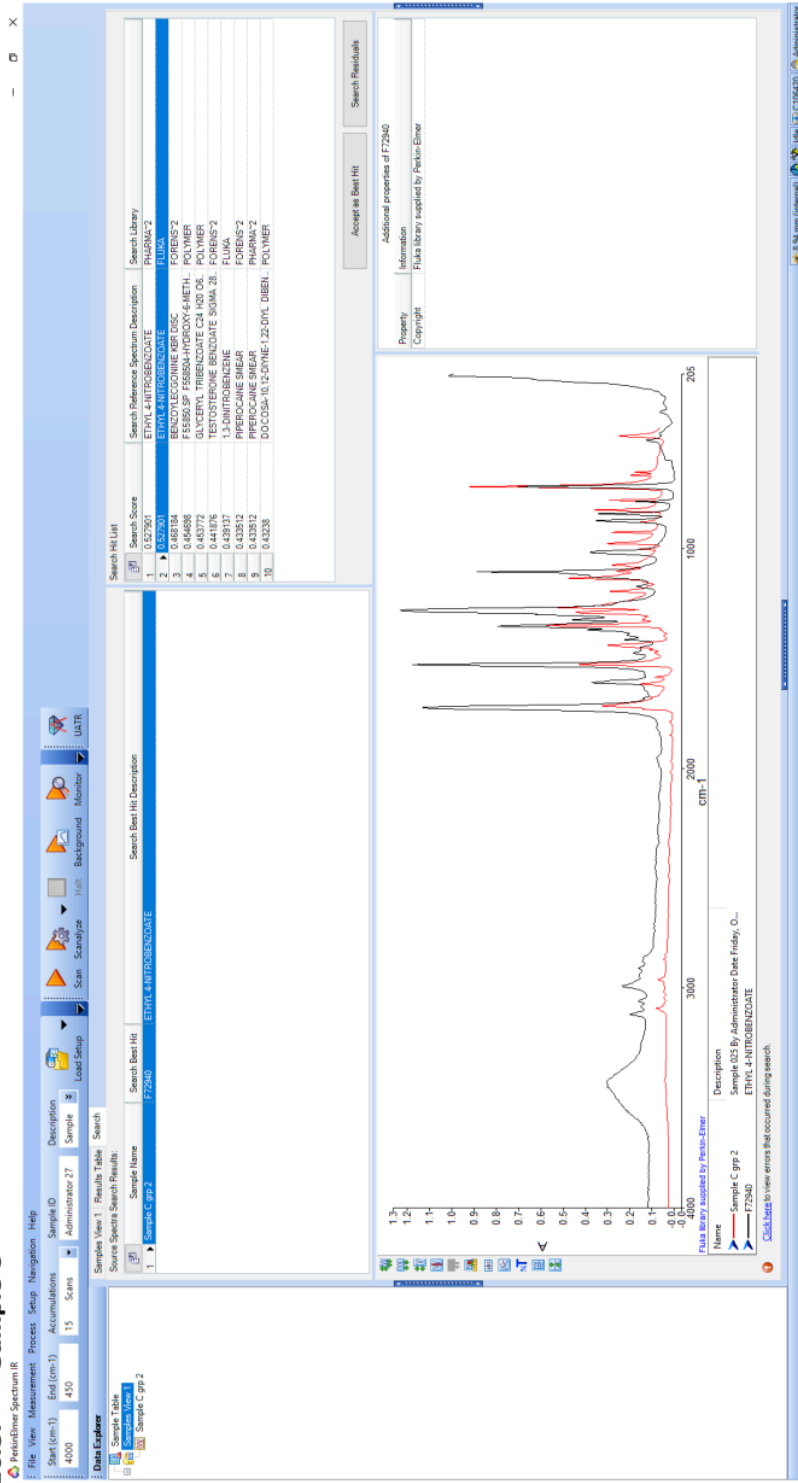


Figure 13 - Sample C Screen Shot

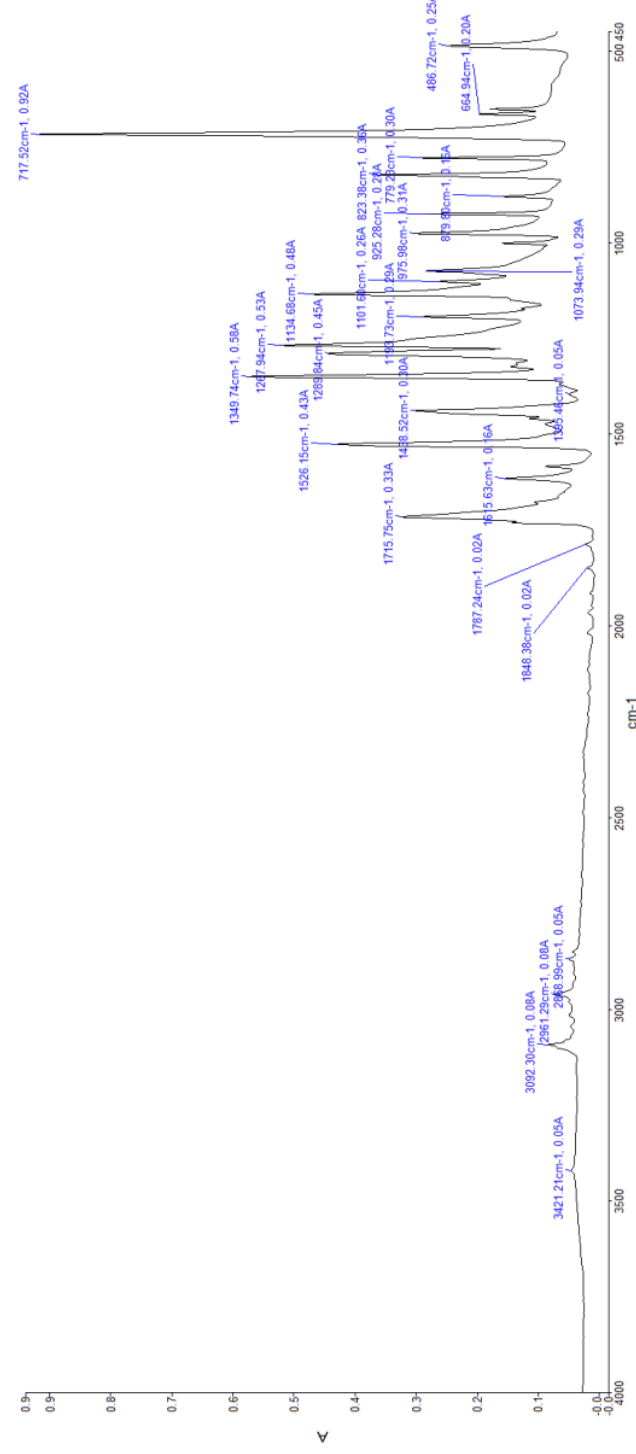


Figure 14 - Sample C Spectra

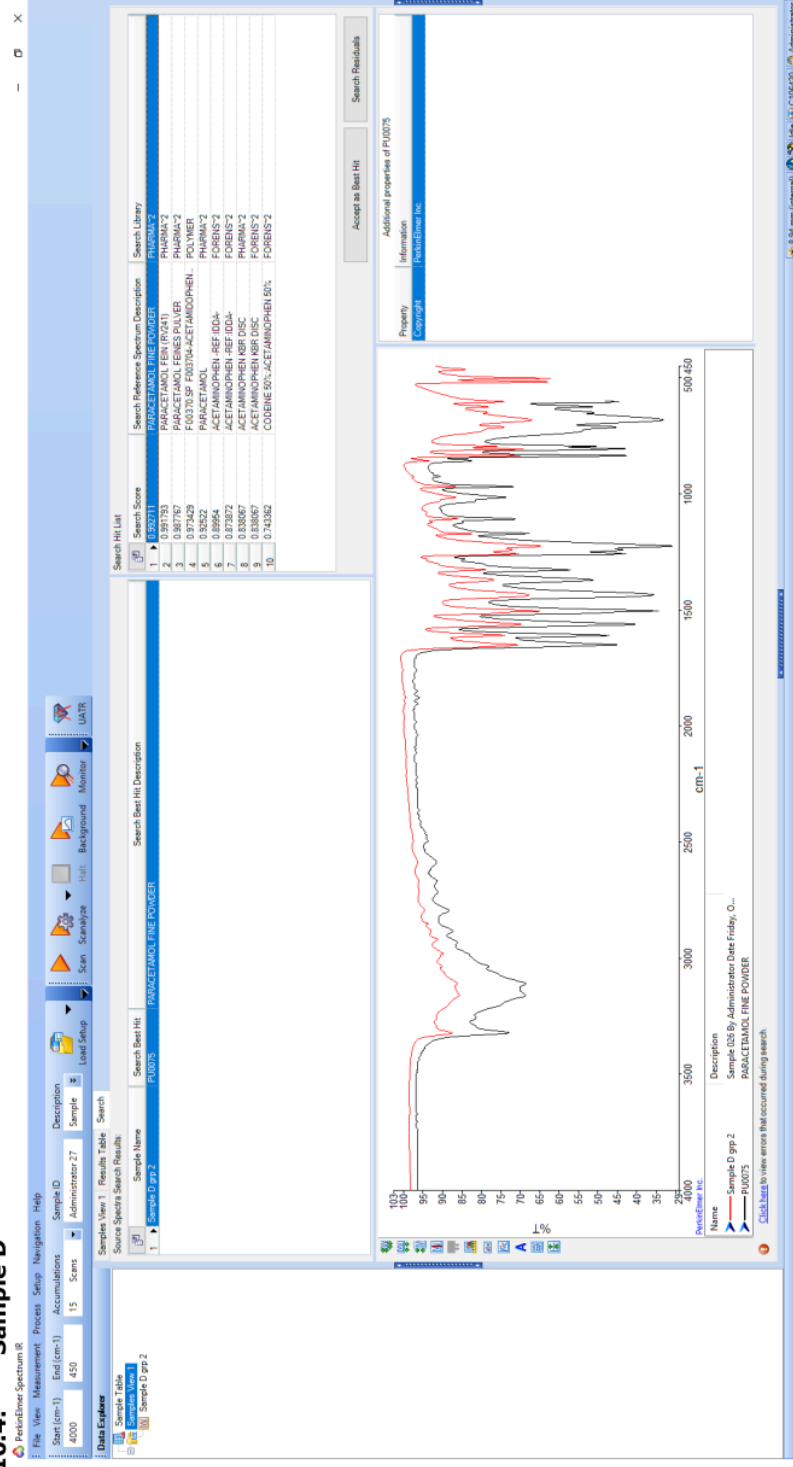
10.4. Sample D

Figure 15 - Sample D Screen Shot

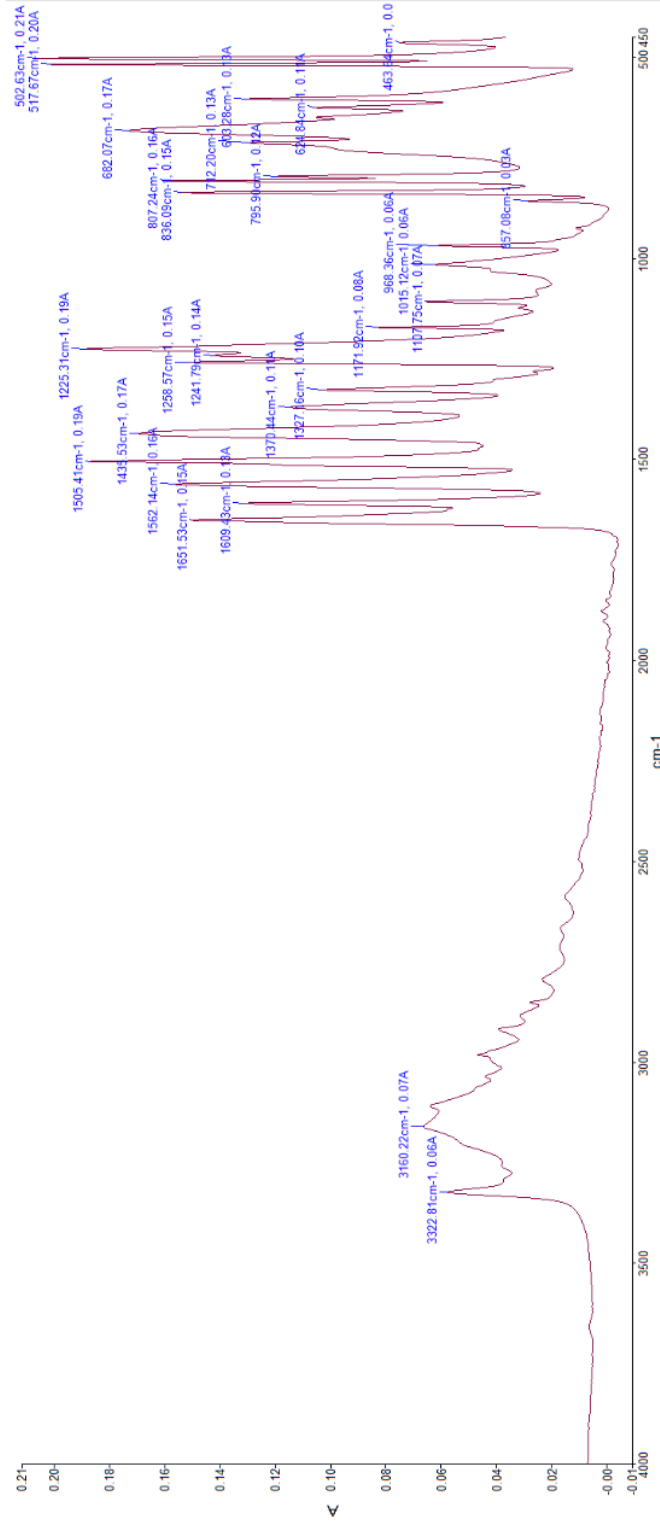


Figure 16 - Sample D Spectra

FINAL GRADE

76/100

GENERAL COMMENTS

Engagement with Literature 13/15

You use a strong range of FT-IR sources, including vendor documentation, textbooks and website tables. IEEE formatting is consistent but there are errors in authors' names.

Knowledge and Understanding 15/20

Good understanding of FT-IR theory, ATR operation, and functional-group identification. The introduction is clear and provides appropriate OME context. However, vibrational modes (stretching, bending, rocking, wagging, twisting), the foundation of FT-IR, are not explained. The introduction also frames the task as identification rather than the main aim: producing a reproducible FT-IR method. Identifying functional groups on the spectra would improve clarity and help interpretation.

Cognitive and Intellectual Skills 15/20

Your analysis is generally good: you identify all four samples correctly, justify functional-group assignments, and correctly explain the low similarity score for sample C. The interpretation is sound, though largely descriptive, and you do not explore the fingerprint region in depth. Comparison to literature values could be more systematic, and only Sample A is fully processed manually. More explicit reasoning around peak shape/intensity and ATR-related shifts would add analytical depth.

Practical Skills 20/30

You completed the provided FT-IR method template in Annex 1, which is excellent but the main body of the report does not contain a complete, properly presented SOP-level method, as required.

Transferable Skills 13/15

Very strong presentation: clear layout, logical structure, high-quality figures and tables. Writing is professional, with good use of diagrams and well-annotated spectra. Minor improvements include avoiding 1st person writing.

Strikethrough.

Text Comment. it can be taken

Strikethrough.

Text Comment. equally important purpose is to develop a SOP for FT-IR analysis of these materials

Text Comment. the parameters from the handout such as apodisation, S/N ratio, etc are not mentioned



incorrect authors' names

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PAGE 16

PAGE 17

PAGE 18

PAGE 19

PAGE 20

PAGE 21

PAGE 22

PAGE 23

PAGE 24
