Supplementary information

for article

**Reflectance FT-IR spectroscopy as a viable option for textile fiber identification**

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Table of contents

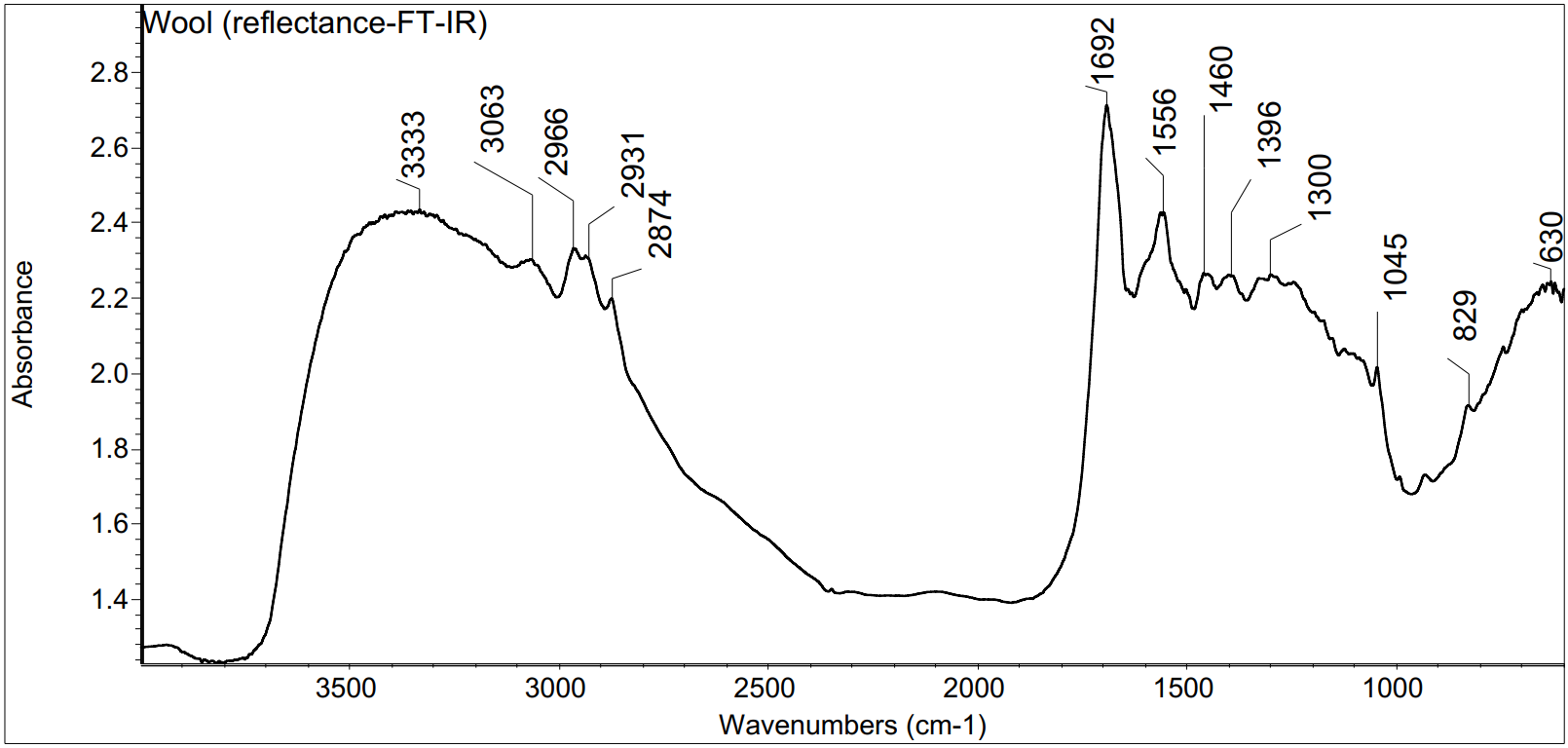
[Example spectra of each fiber class recorded with FT-IR microspectrometer in reflectance mode 2](#_Toc17726422)

[Case-study: Scarf from 20th century 13](#_Toc17726423)

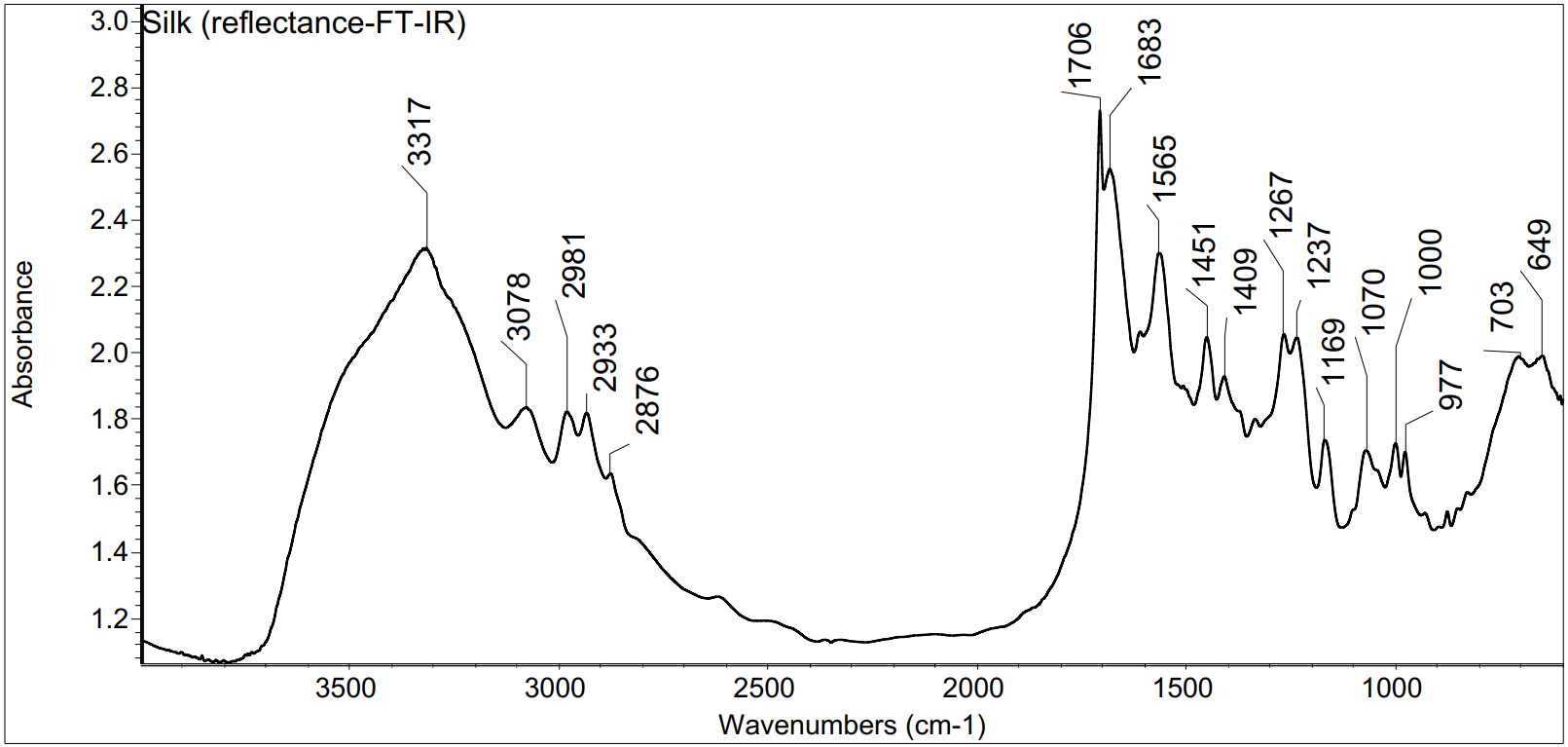
[Case-study: Very small fiber thread from painting on the textile from end of the 20th century 27](#_Toc17726424)

# Spectra of each fiber class recorded with FT-IR microspectrometer in reflectance mode

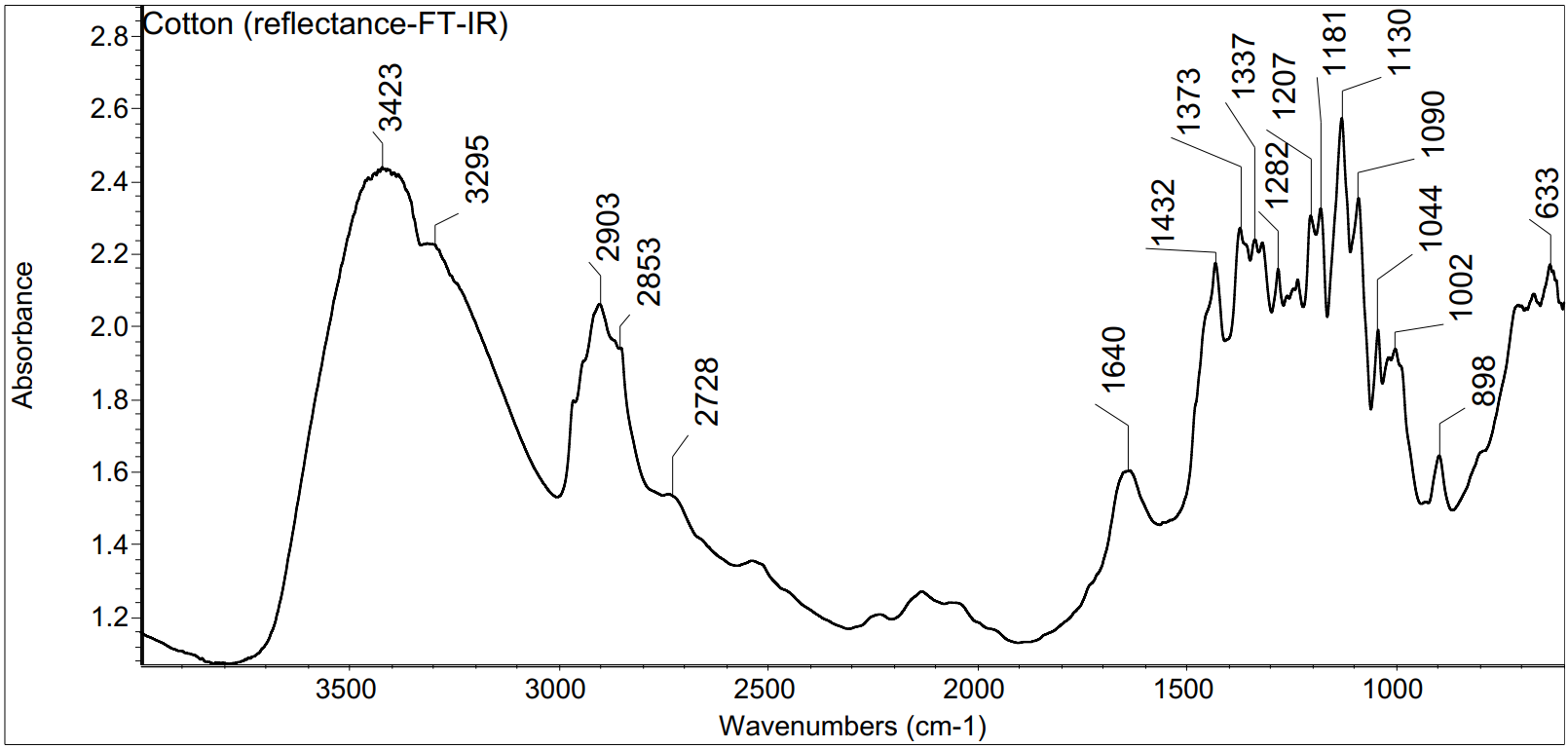
All spectra below are original without any alteration or correction.

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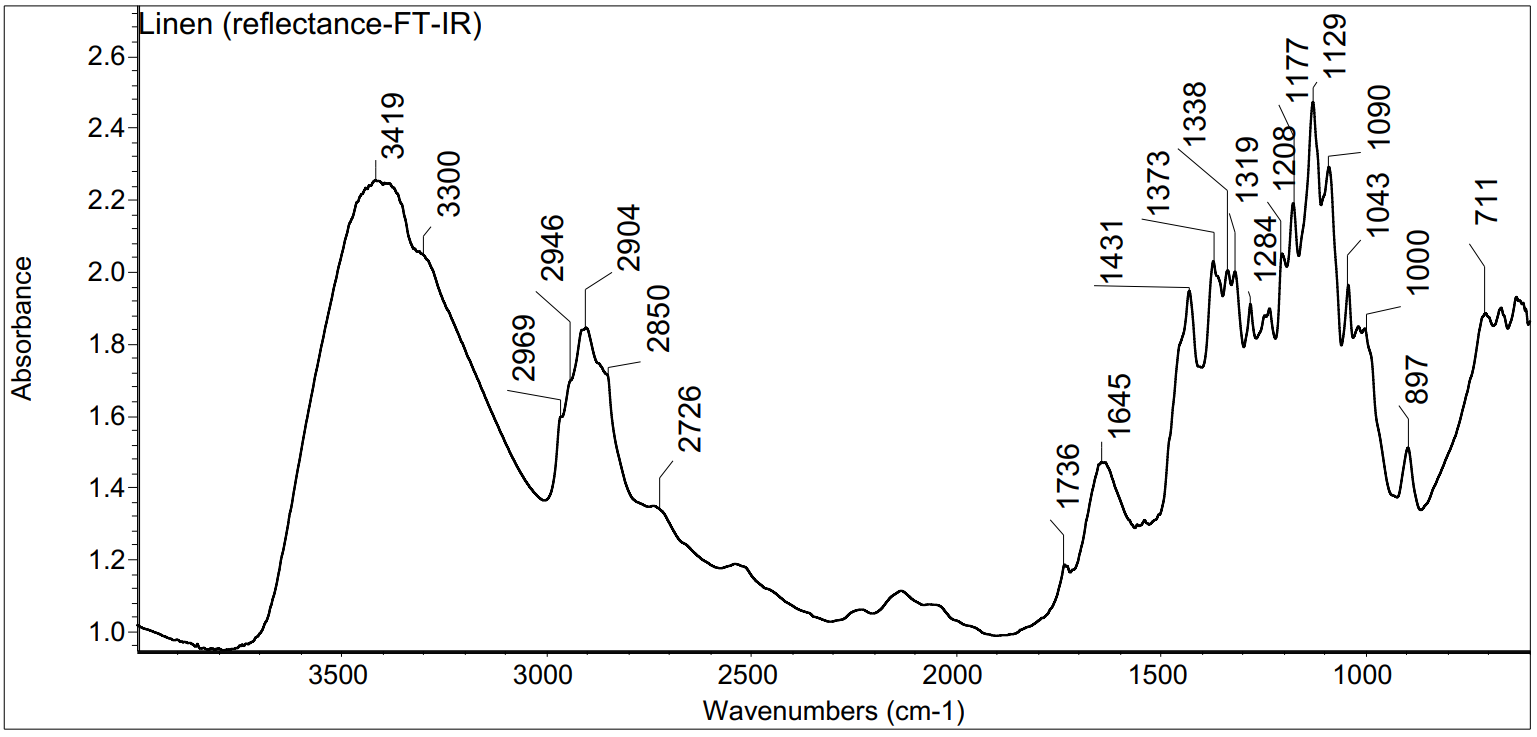
*Figure S1. r-FT-IR spectrum of wool fiber*

**

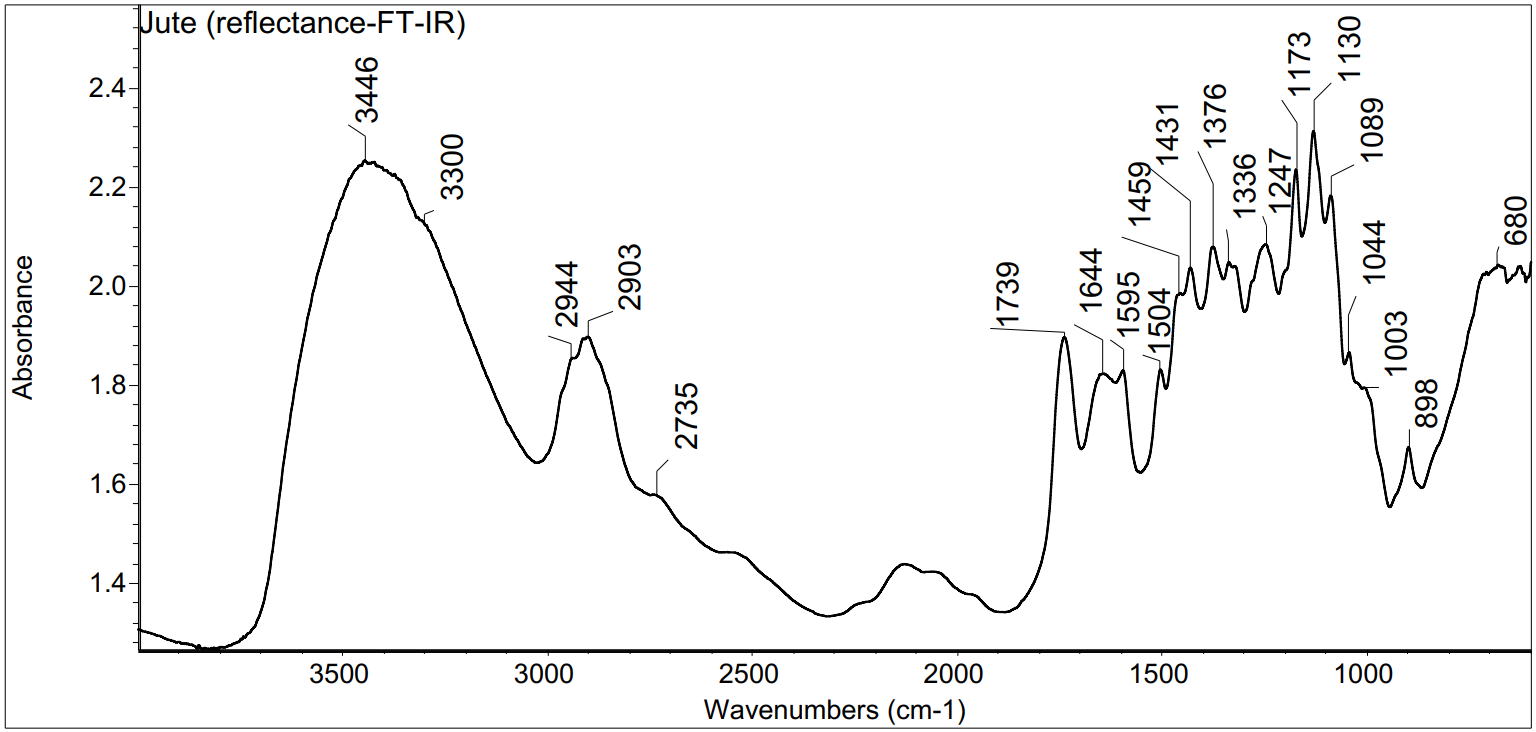
*Figure S2. r-FT-IR spectrum of silk fiber*

**

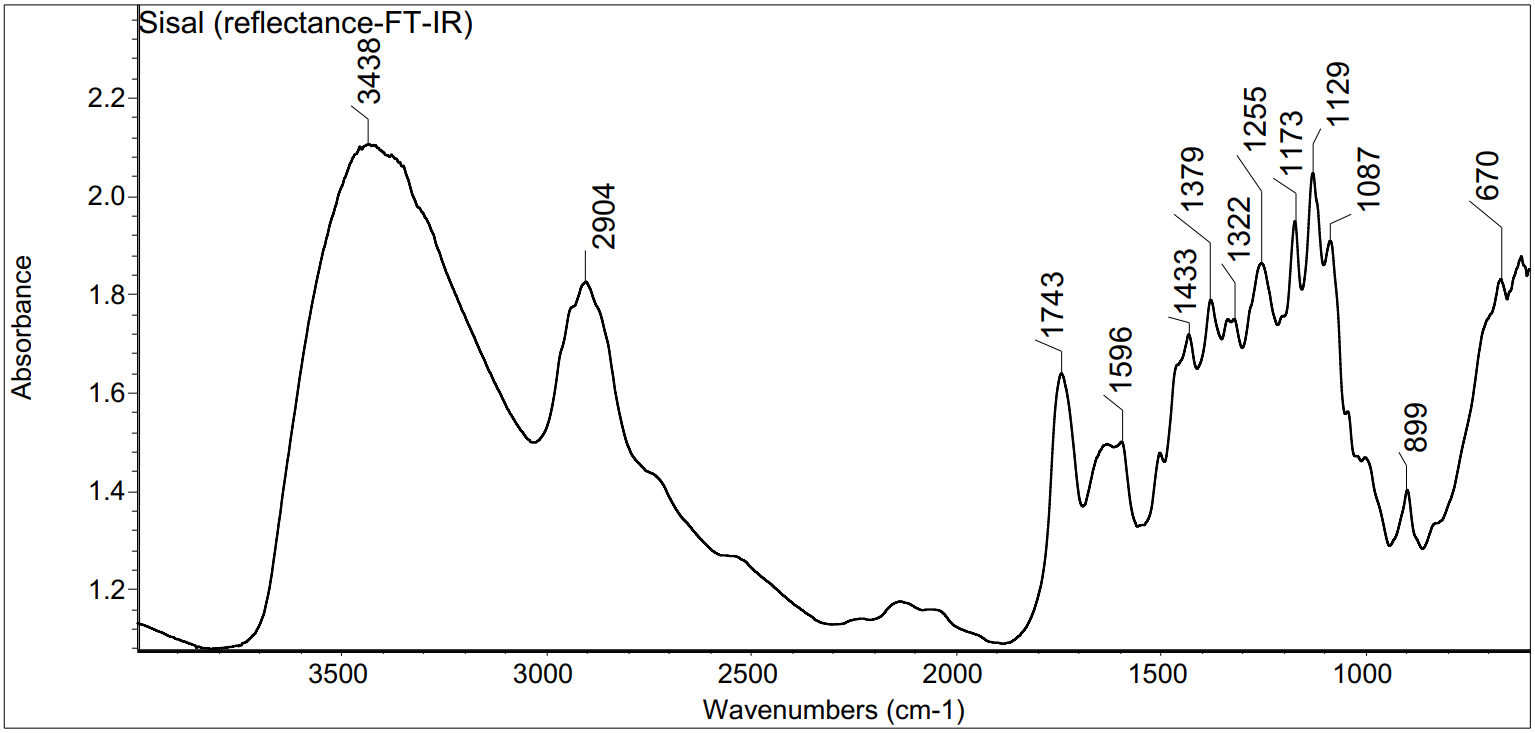
*Figure S3. r-FT-IR spectrum of cotton fiber*

**

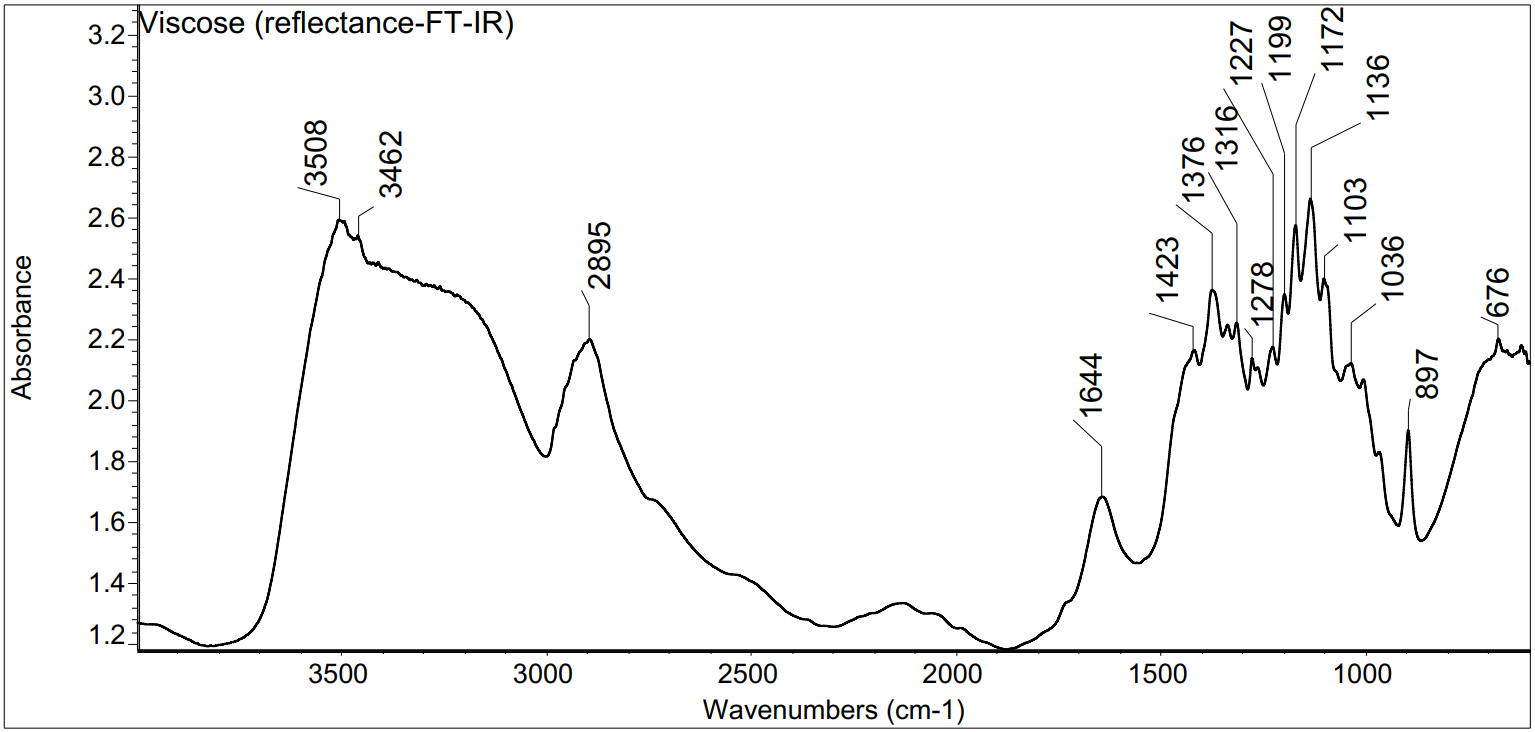
*Figure S4. r-FT-IR spectrum of linen fiber*

**

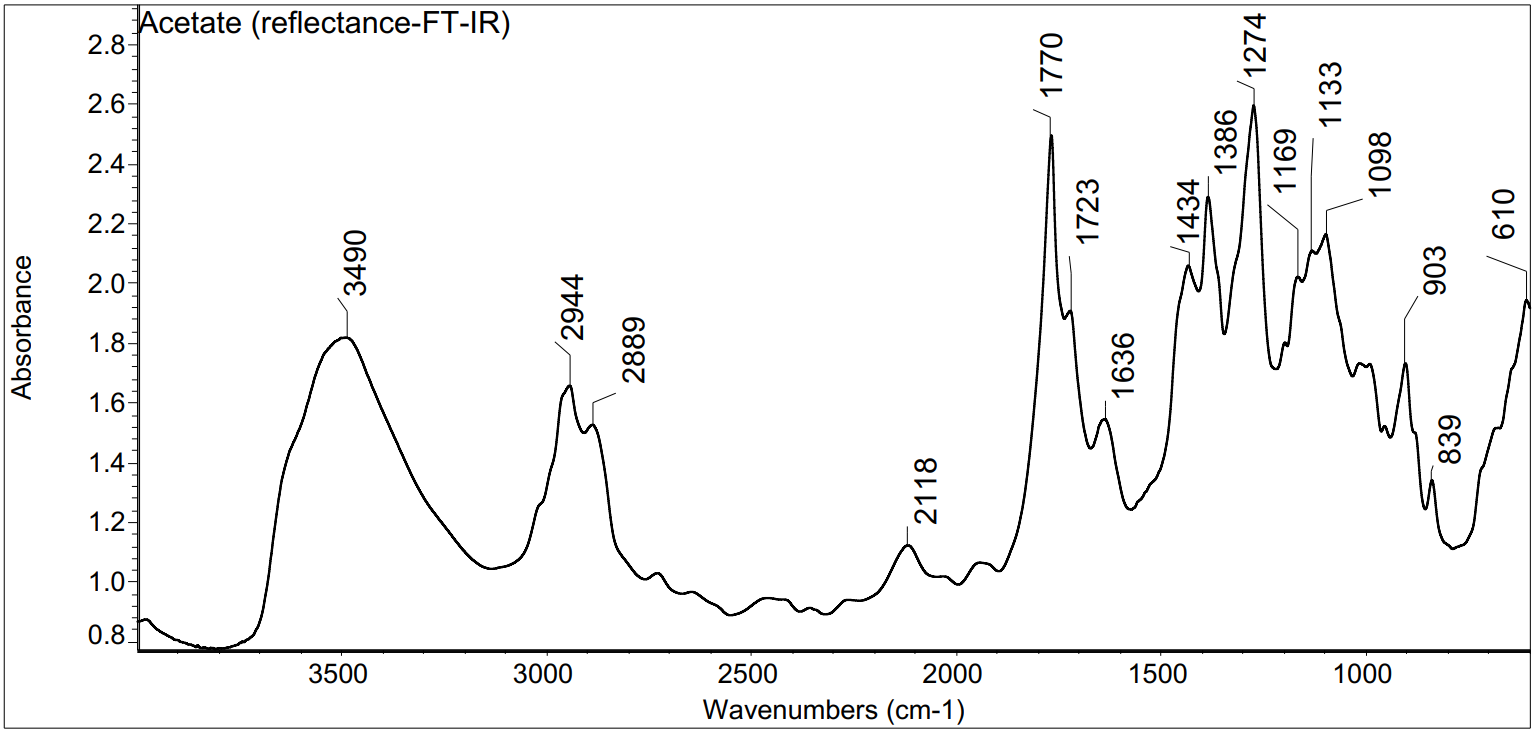
*Figure S5. r-FT-IR spectrum of jute fiber*

**

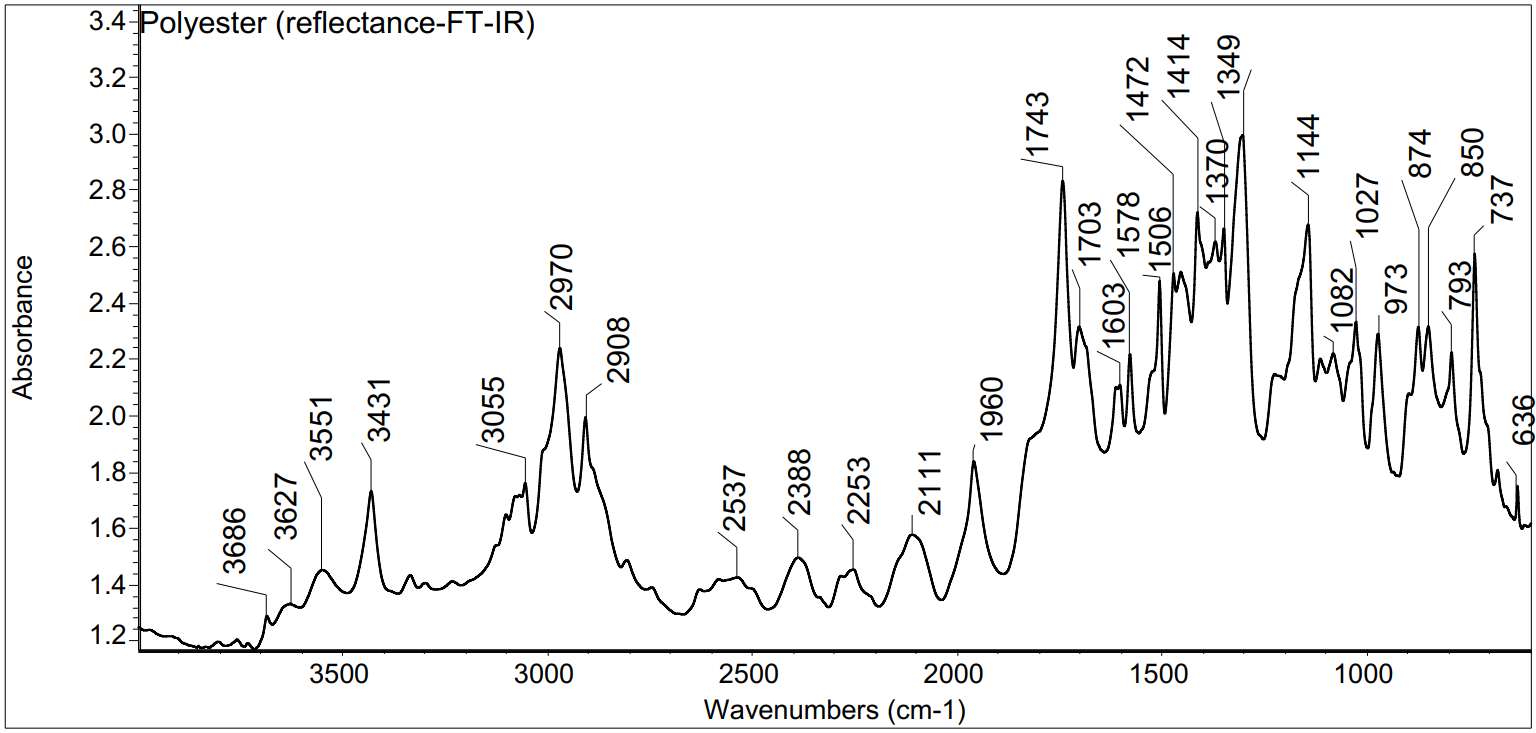
*Figure S6. r-FT-IR spectrum of sisal fiber*

**

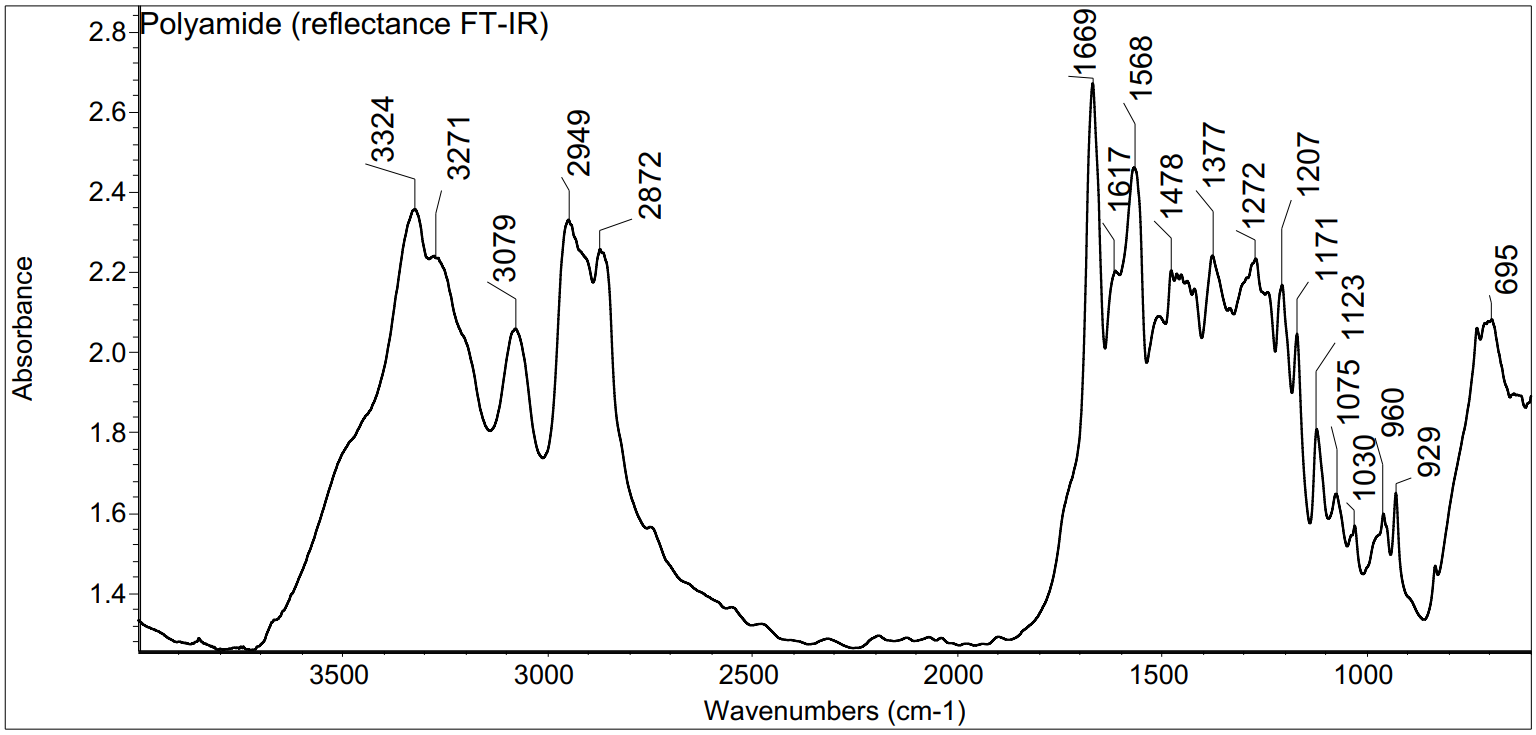
*Figure S7. r-FT-IR spectrum of viscose fiber*

**

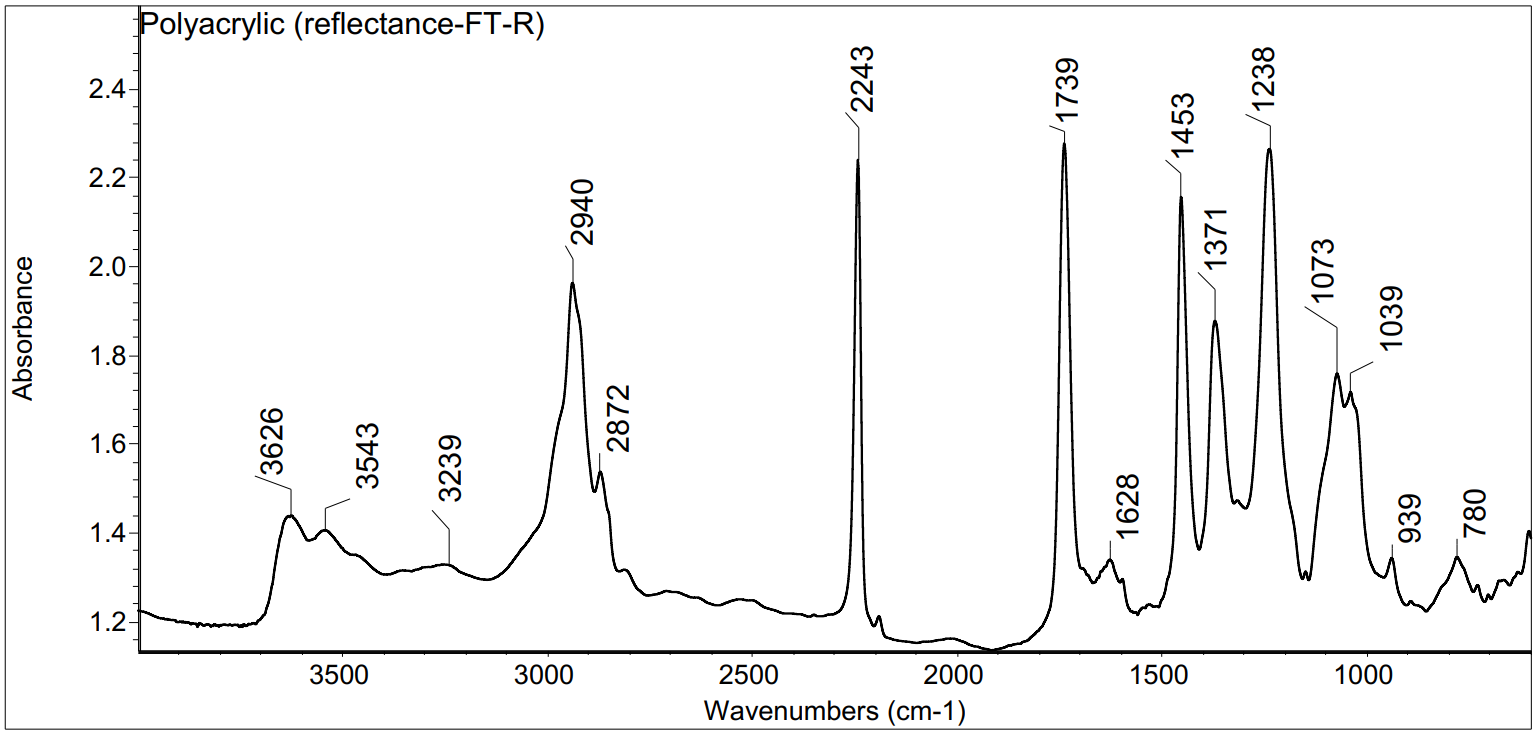
*Figure S8. r-FT-IR spectrum of cellulose acetate fiber*

**

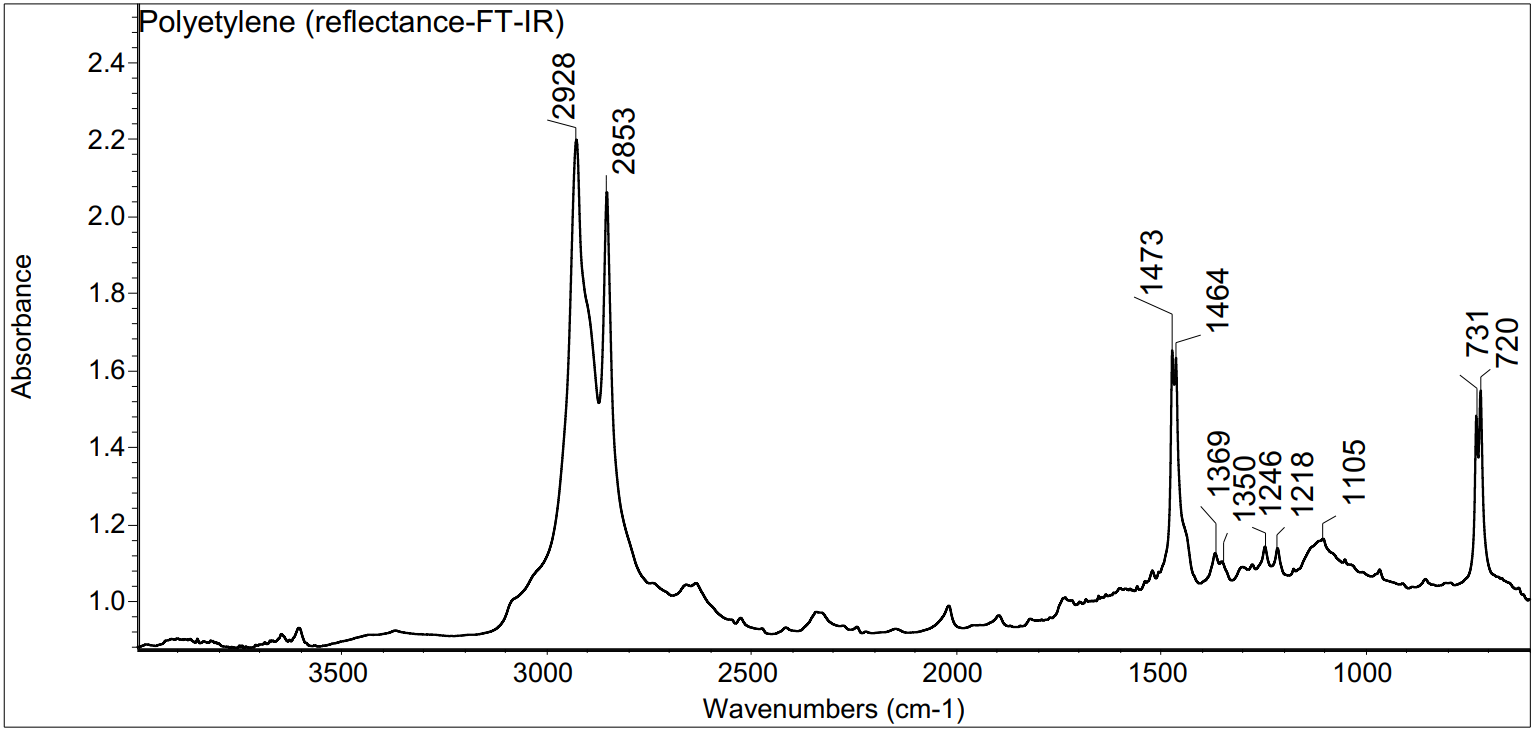
*Figure S9. r-FT-IR spectrum of polyester fiber*

**

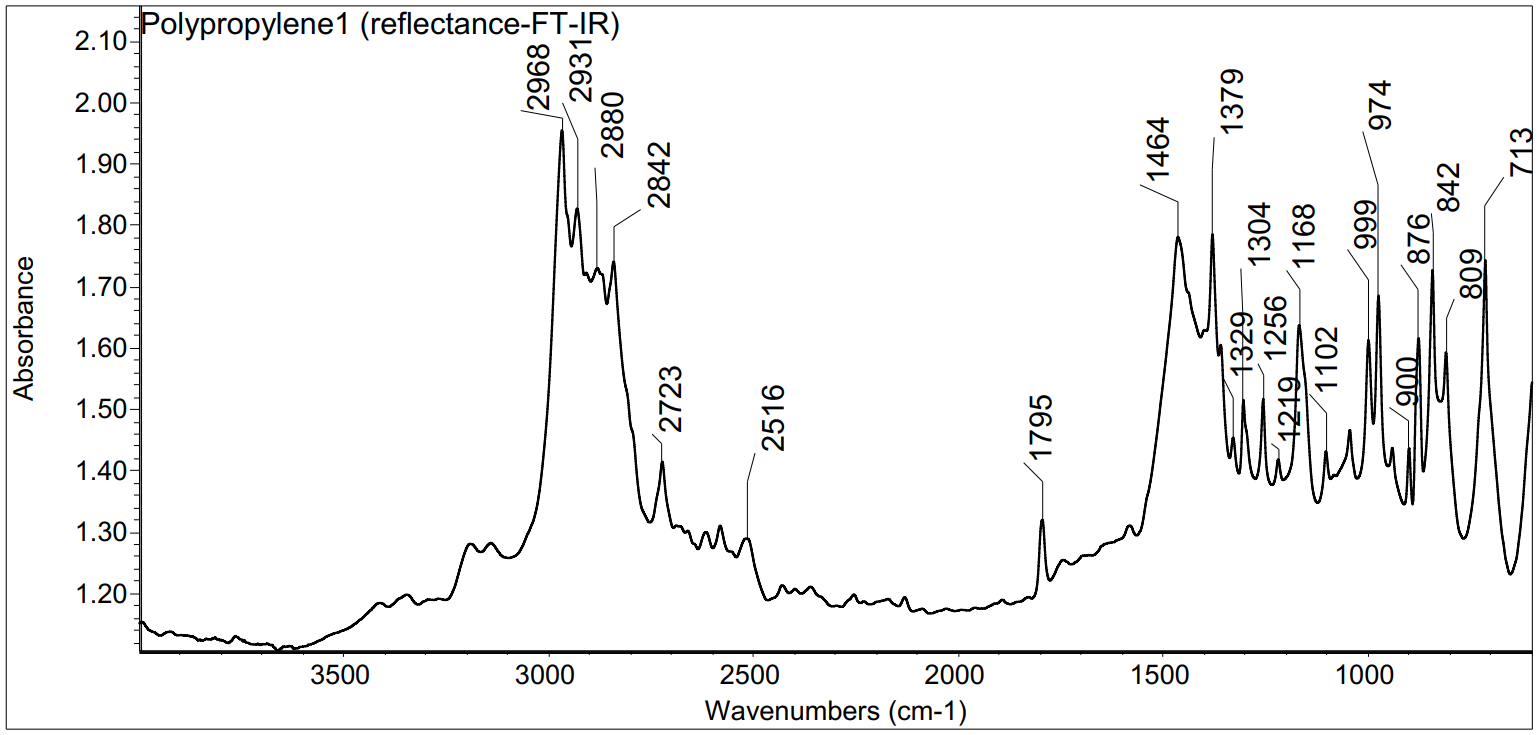
*Figure S10. r-FT-IR spectrum of polyamide fiber*

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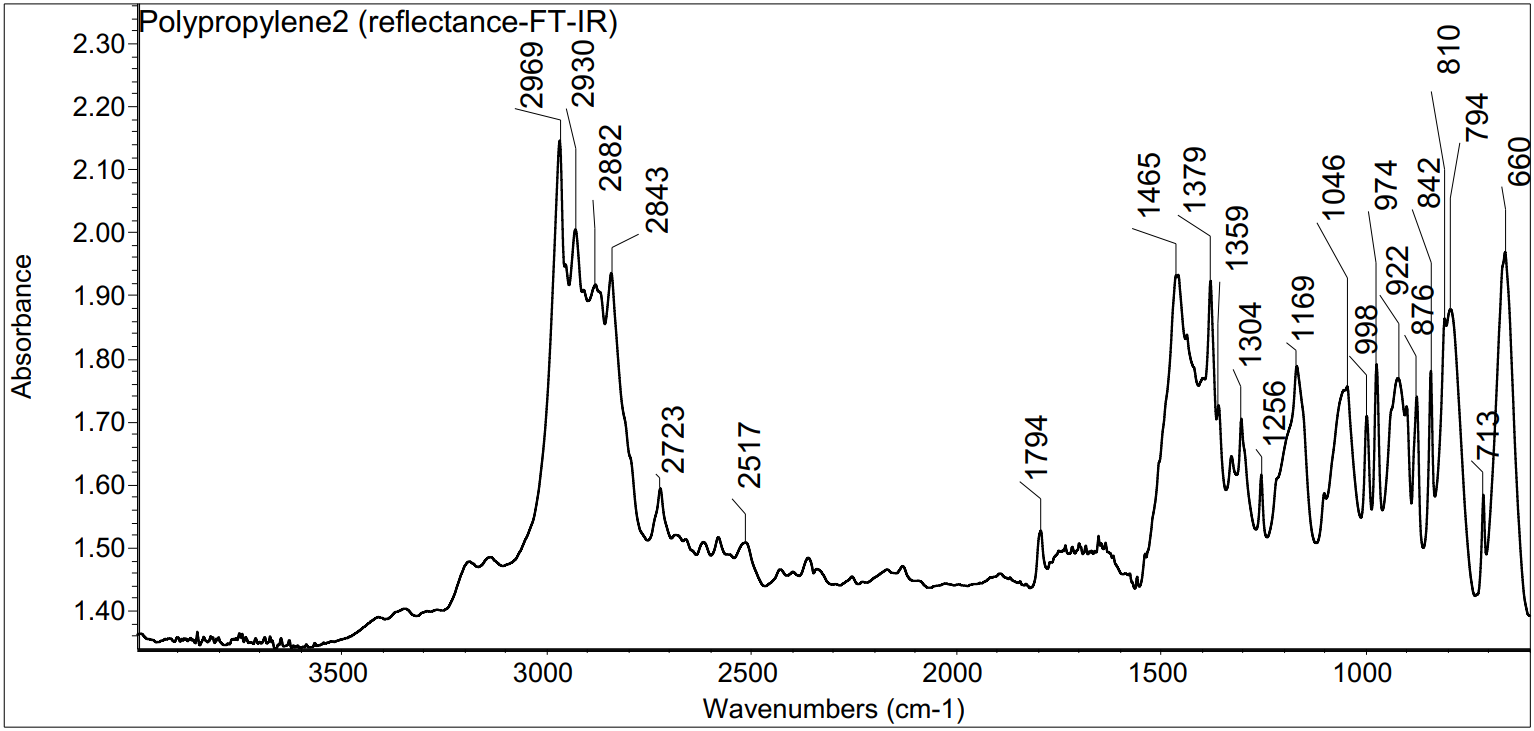
*Figure S11. r-FT-IR spectrum of polyacrylic fiber*

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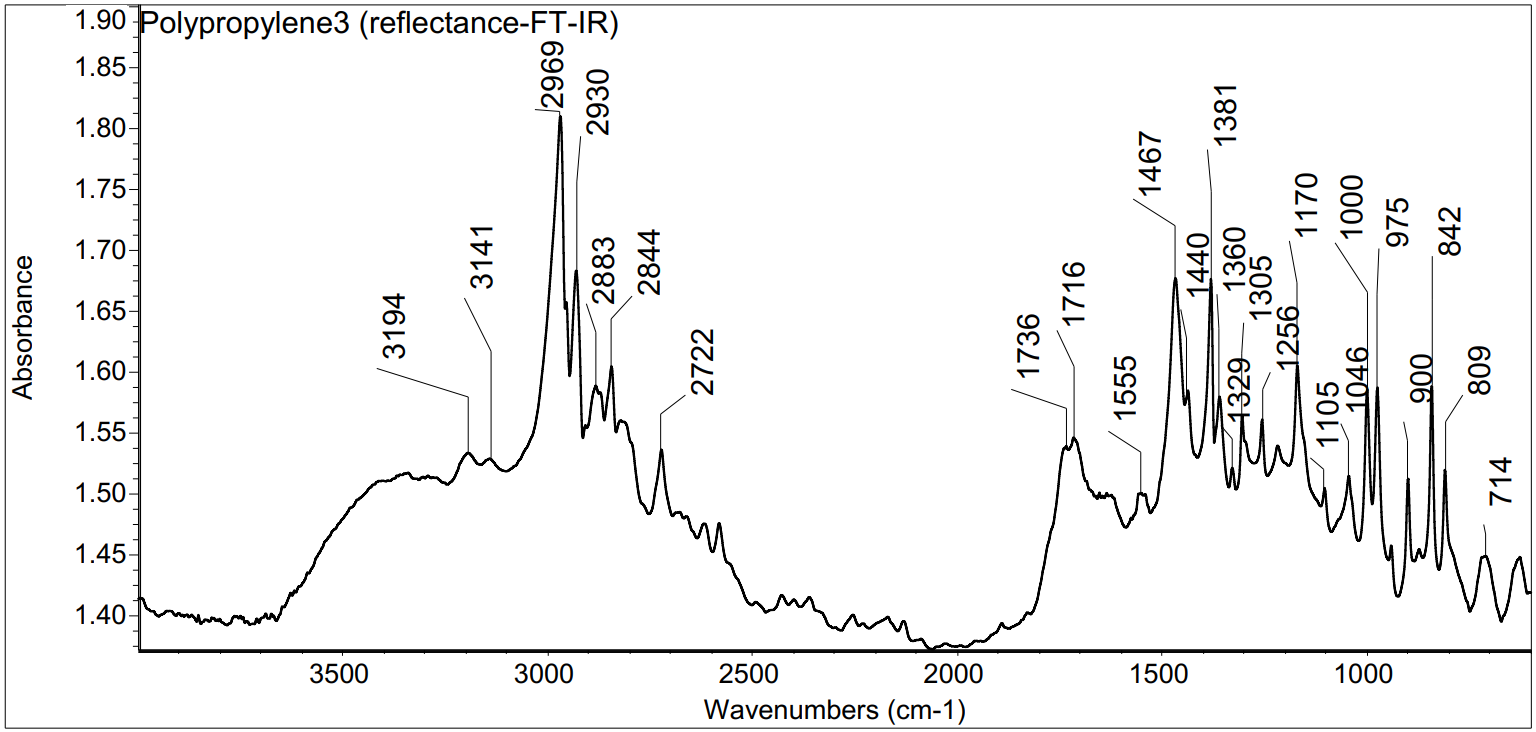
*Figure S12. r-FT-IR spectrum of polyethylene fiber*

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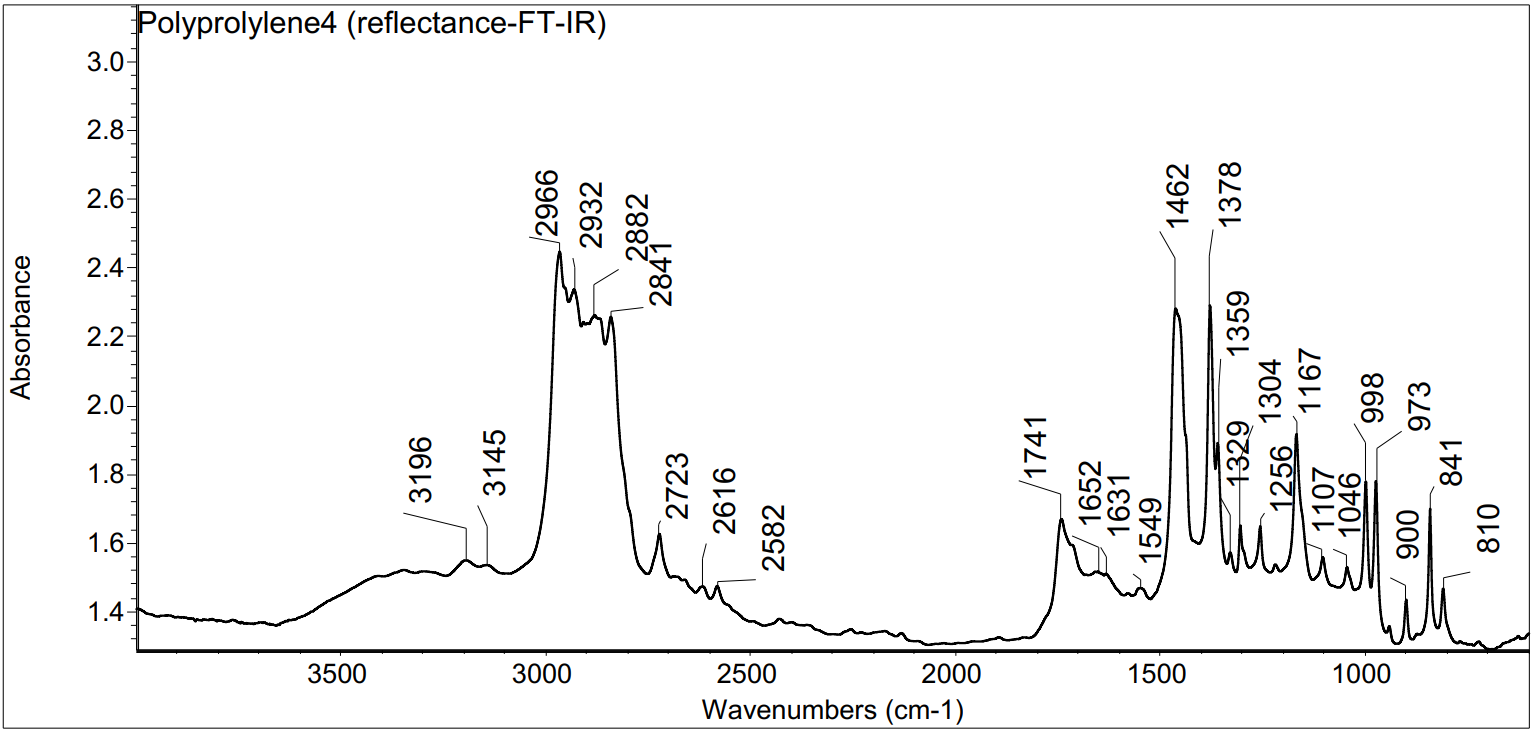
*Figure S13. r-FT-IR spectrum of polypropylene fiber*

**

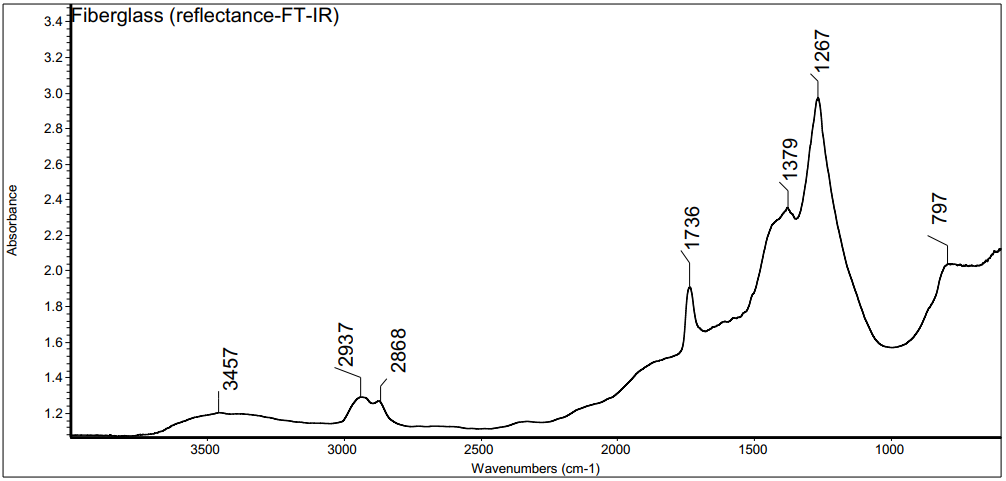
*Figure S14. r-FT-IR spectrum of polypropylene fiber*

**

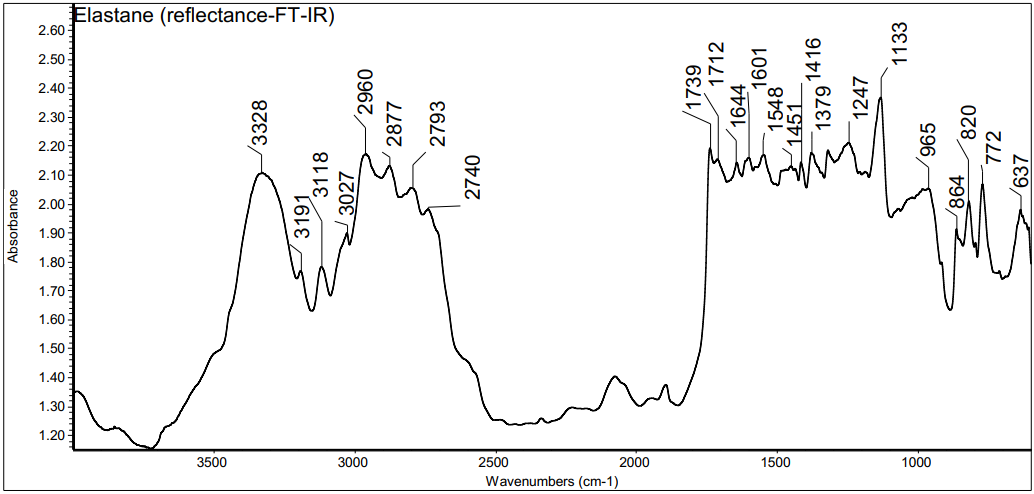
*Figure S15. r-FT-IR spectrum of polypropylene fiber*

**

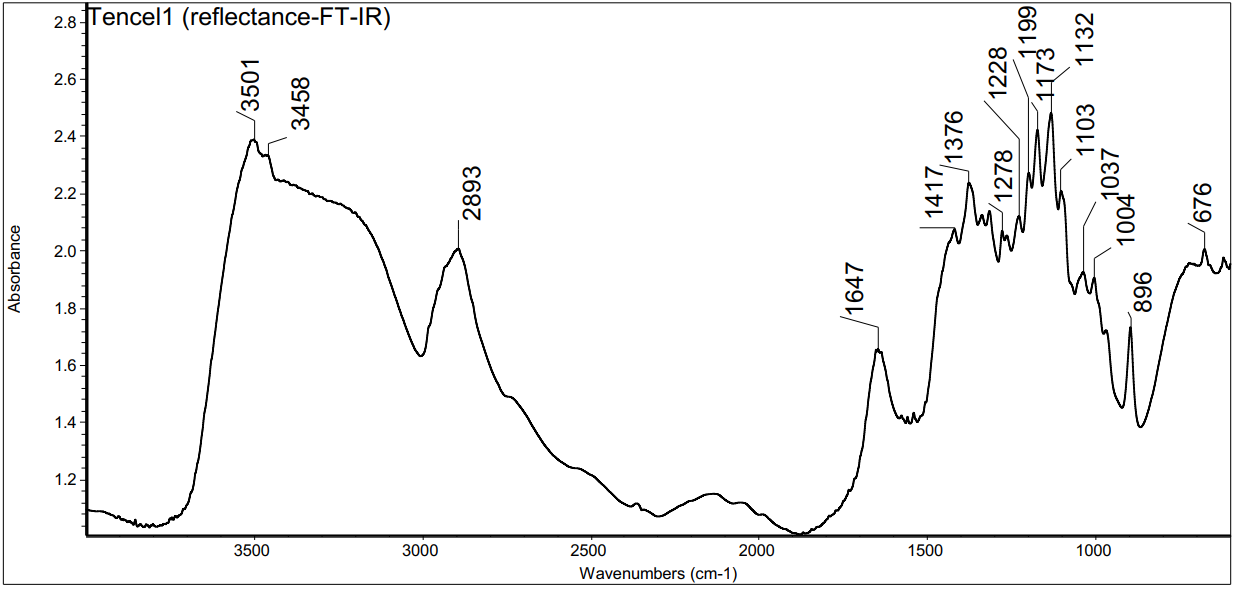
*Figure S16. r-FT-IR spectrum of polypropylene fiber*

**

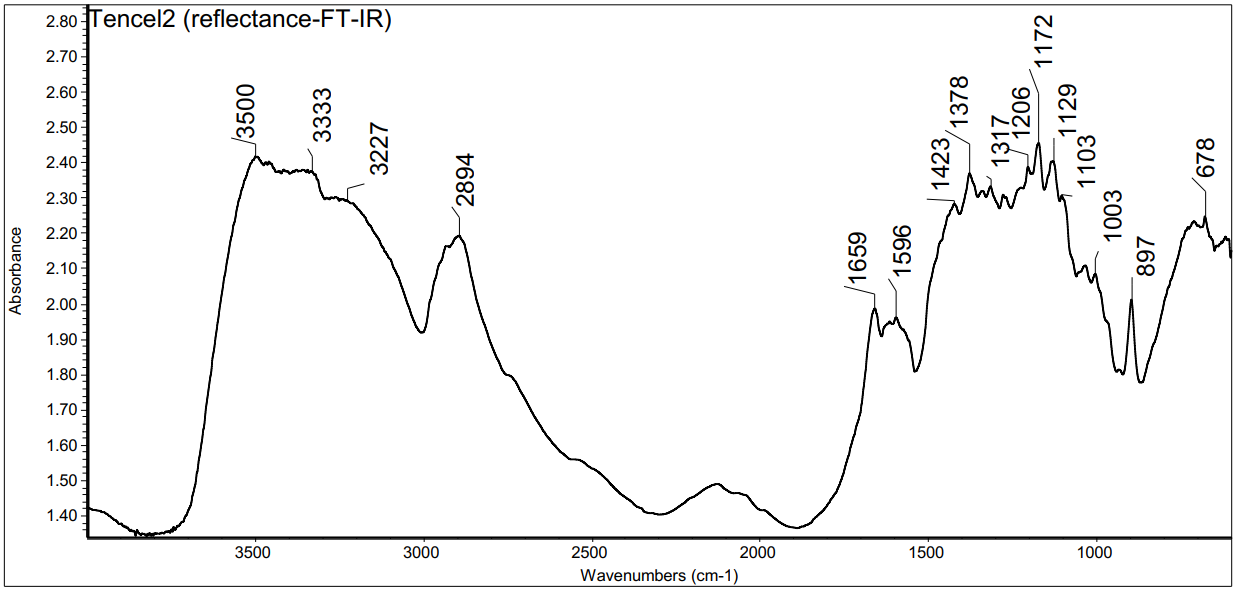
*Figure S17. r-FT-IR spectrum of fiberglass*

**

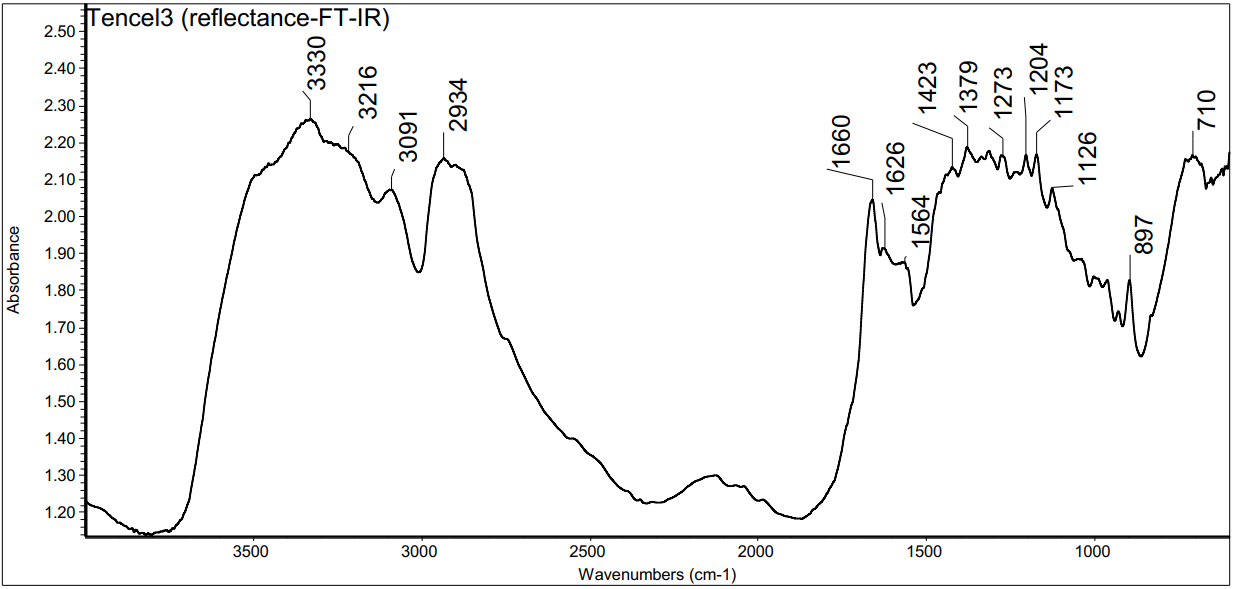
*Figure S18. r-FT-IR spectrum of elastane fiber (deformed due to small fiber diameter)*

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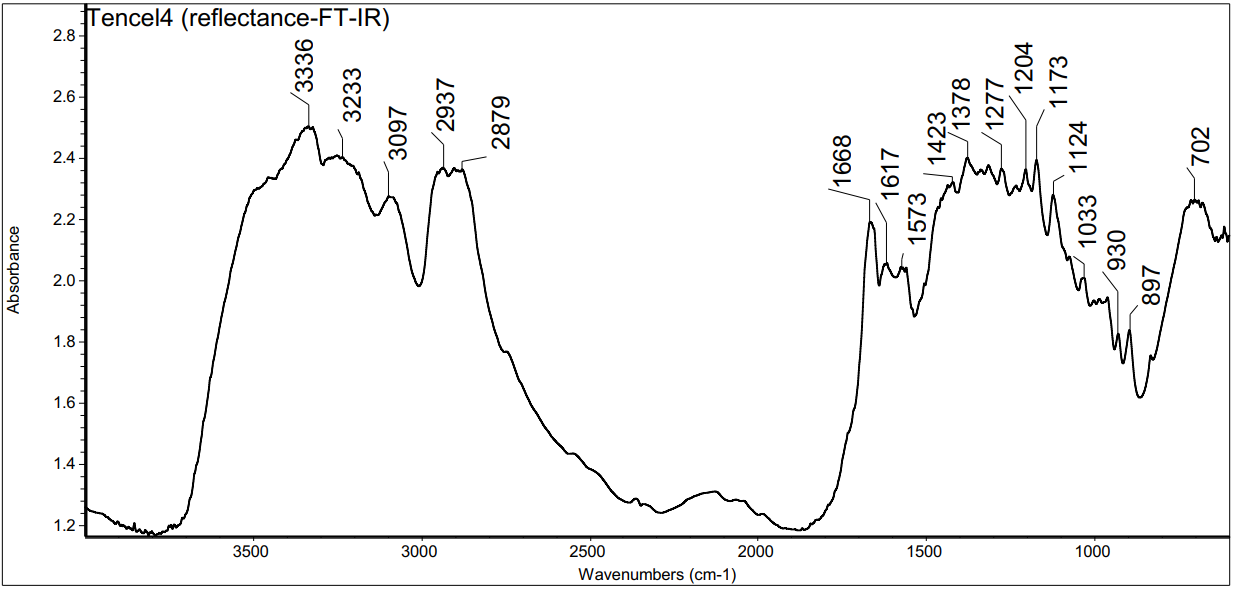
*Figure S19. r-FT-IR spectrum of Tencel*

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*Figure S20. r-FT-IR spectrum of Tencel*

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*Figure S21. r-FT-IR spectrum of Tencel*

**

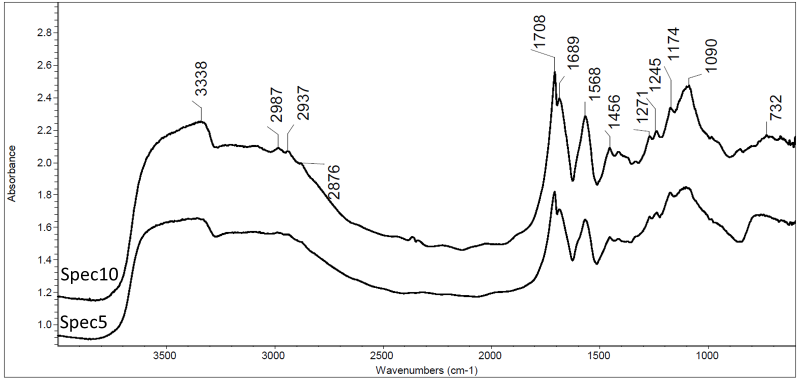
*Figure S22. r-FT-IR spectrum of Tencel*

# Case-study: Scarf from 20th century

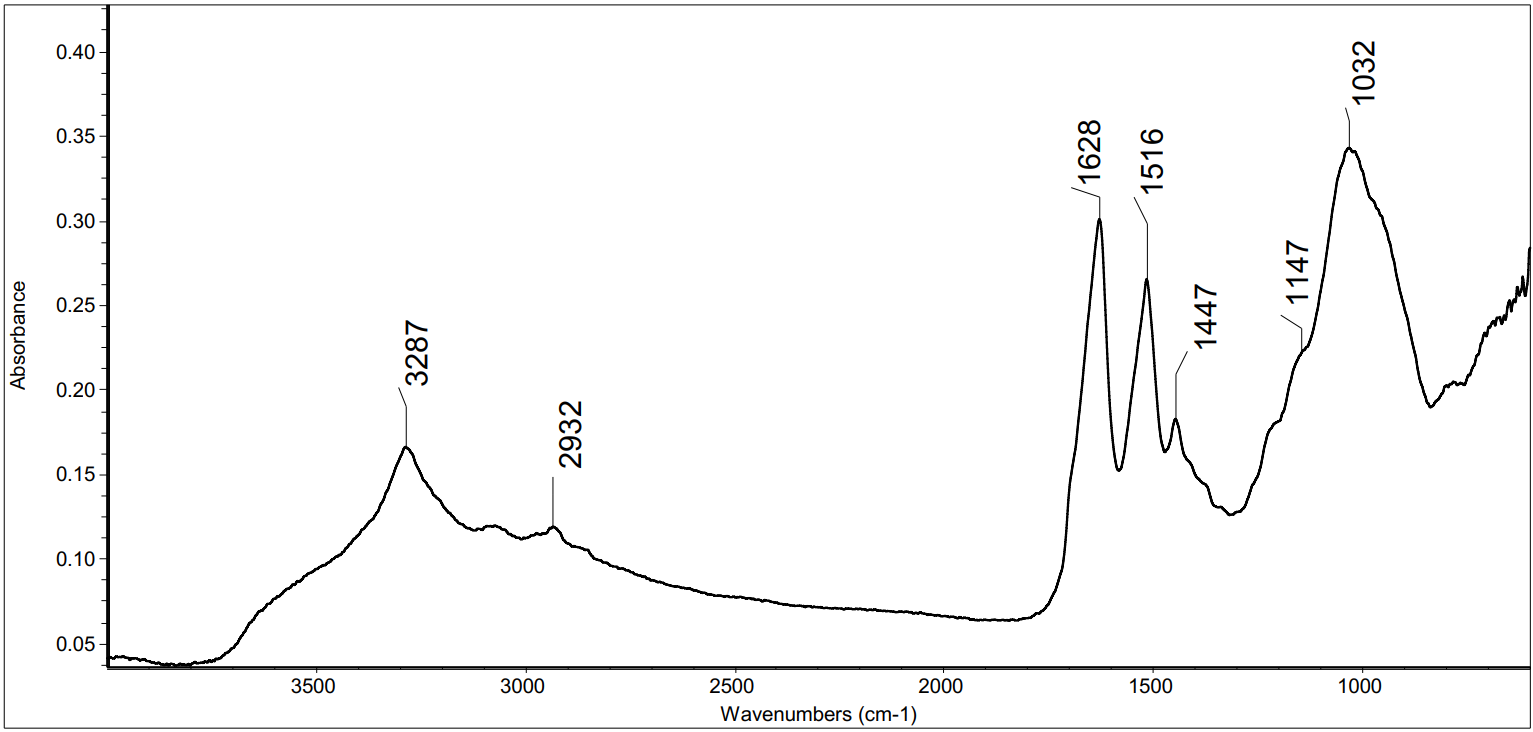
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*Figure S23. Photo of the analyzed scarf with the locations of the samples (Photo from the Conservation and Digitization Centre Kanut).*

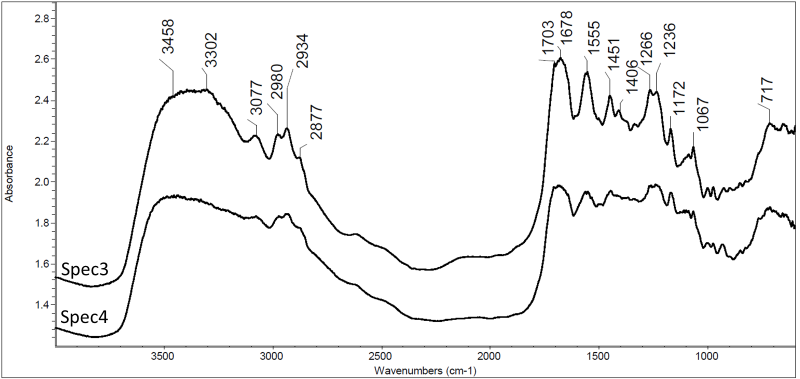
|  |  |  |
| --- | --- | --- |
| Sample nr | Microscope picture of the sample | Microscope picture of fibers |
| *1* |  |  |
|  | *Figure S24. Sample 1* | *Figure S25. Sample 1* |
| *2* |  |  |
|  | *Figure S26. Sample 2* | *Figure S27. Sample 2* |
| *3.1* |  |  |
|  | *Figure S28. Sample 3.1* | *Figure S29. Sample 3.1* |
| *3.2* |  |  |
|  | *Figure S30. Sample 3.2* | *Figure S31. Sample 3.2* |
| *4* |  |  |
|  | *Figure S32. Sample 4* | *Figure S33. Sample 4* |
| *5.1* |  |  |
|  | *Figure S34. Sample 5.1* | *Figure S35. Sample 5.1* |
| *5.2* |  |  |
|  | *Figure S36. Sample 5.2* | *Figure S37. Sample 5.2* |

**

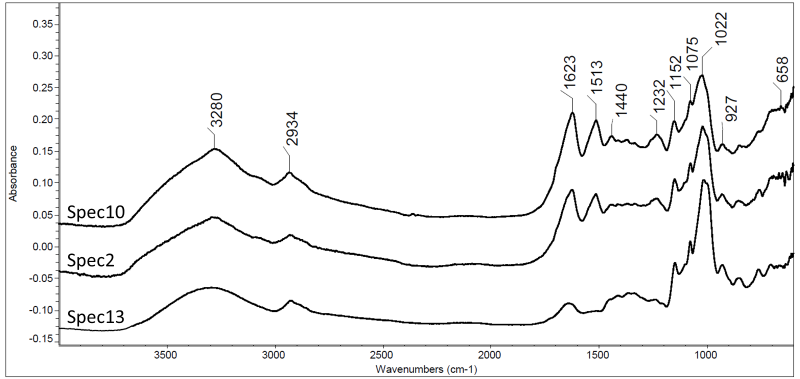
*Figure S38. Examples of r-FT-IR spectra of sample 1. Two spectra are presented to show the spectral differences within the sample.*

**

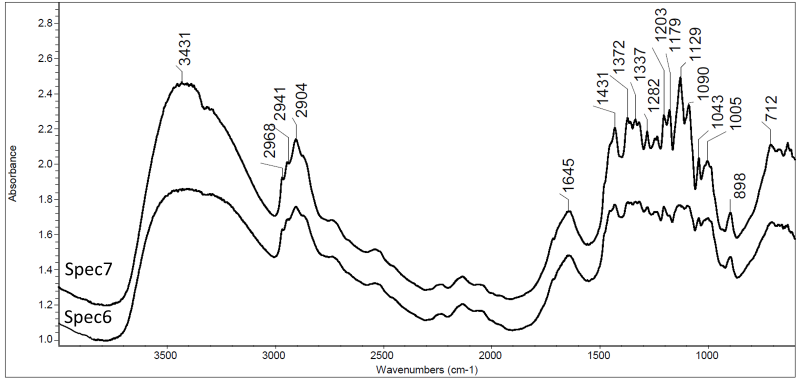
*Figure S39. Example of mATR-FT-IR spectrum of sample 1*

**

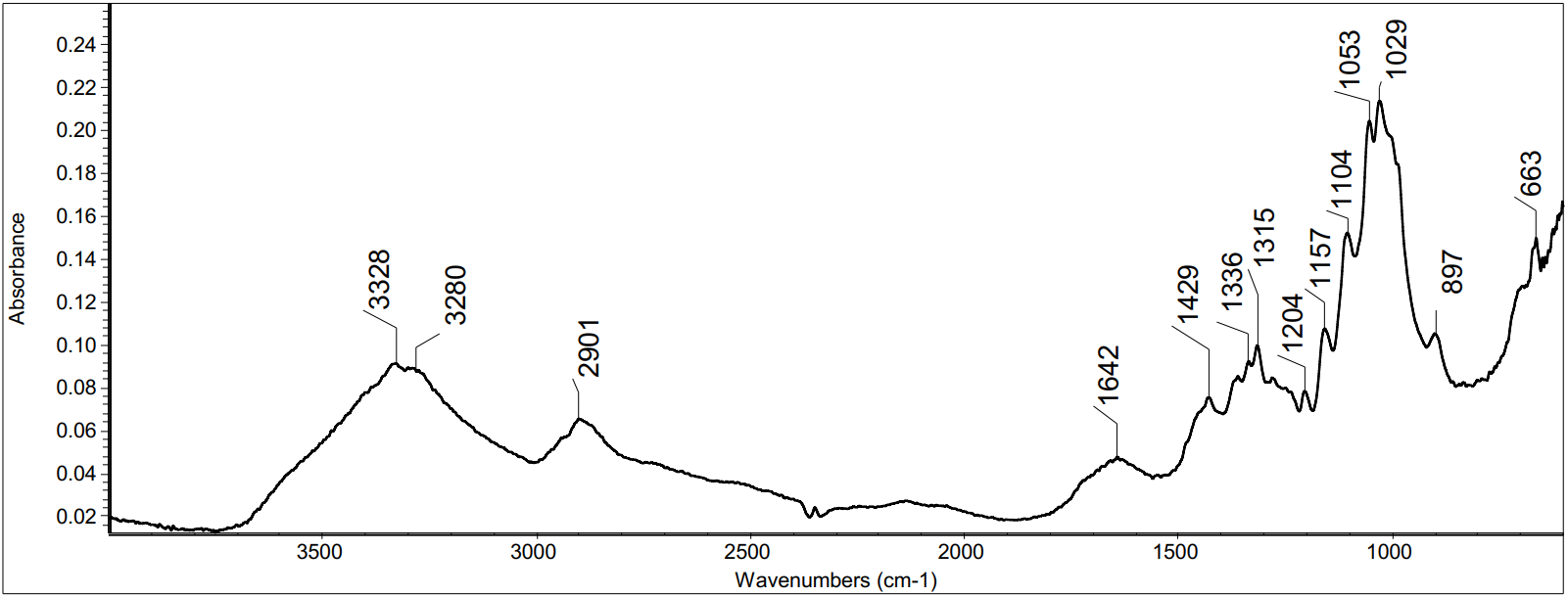
*Figure S40. Examples of r-FT-IR spectra of sample 2. Two spectra are presented to show the spectral differences within the sample.*

**

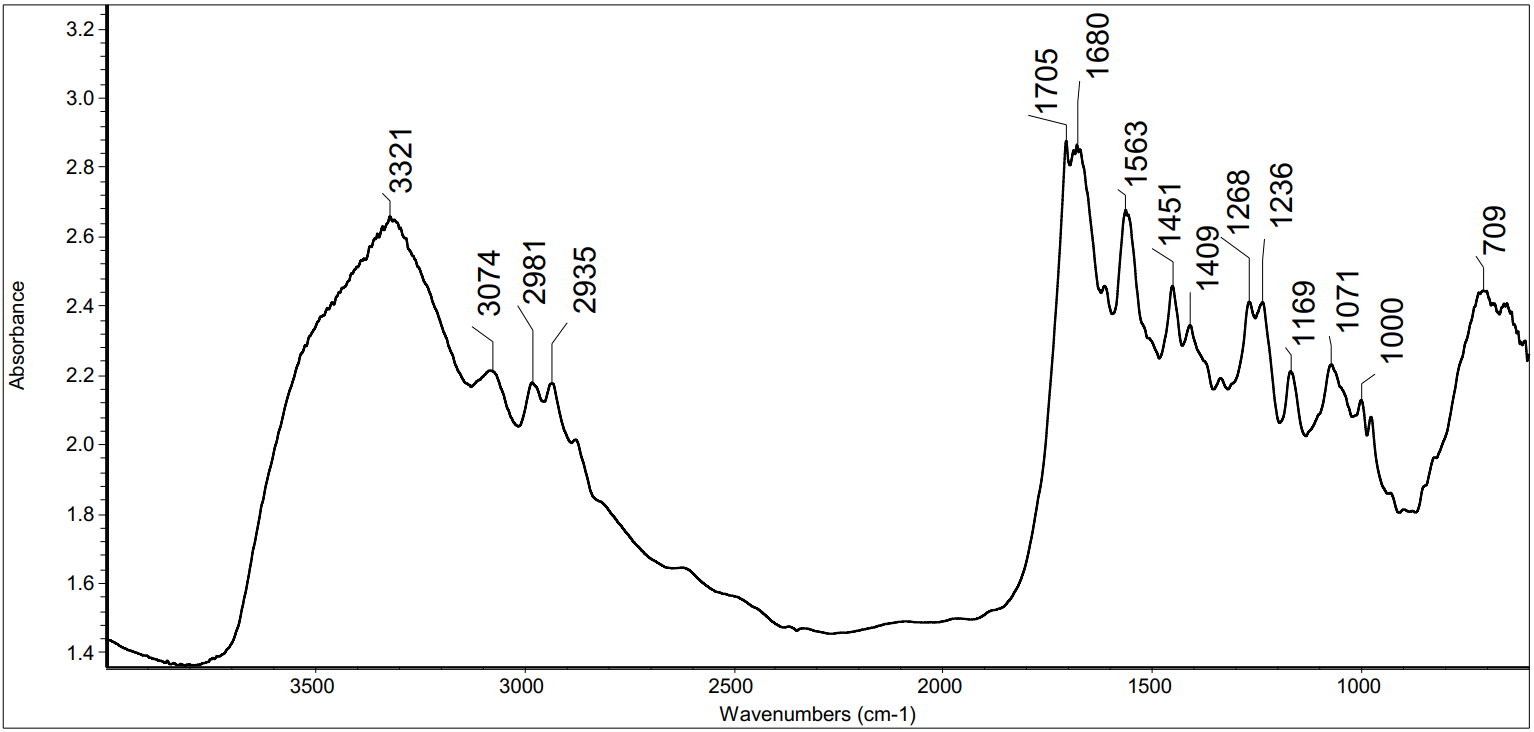
*Figure S41. Examples of mATR-FT-IR spectra of sample 2. Three spectra are presented to show the spectral differences within the sample*

**

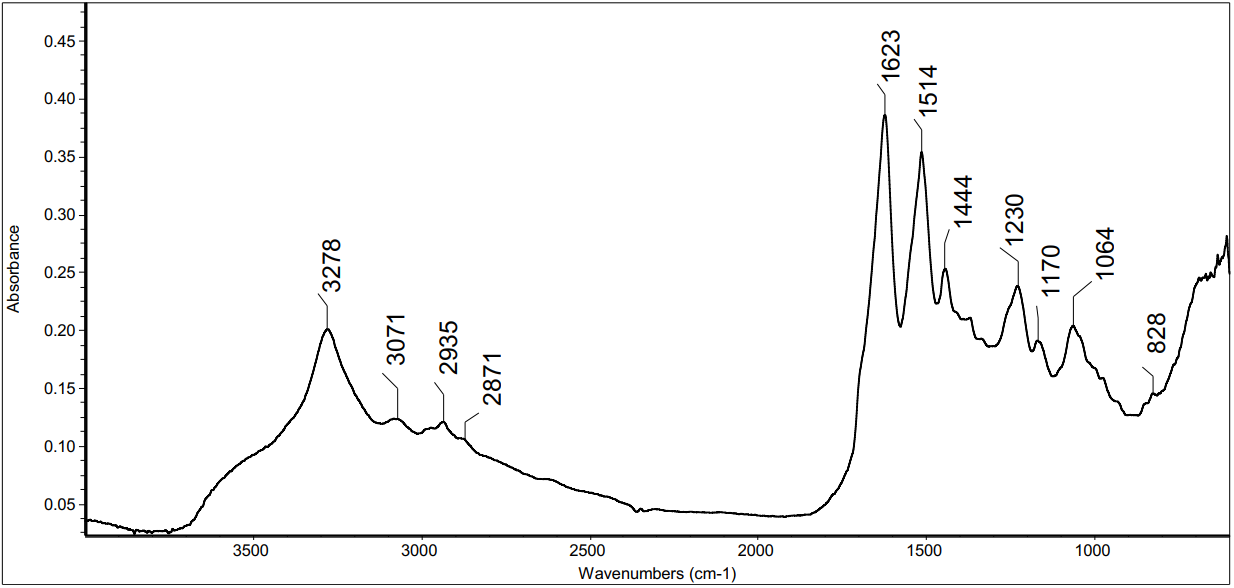
*Figure S42. Examples of r-FT-IR spectra of sample 3.1. Two spectra are presented to show the spectral differences within the sample*



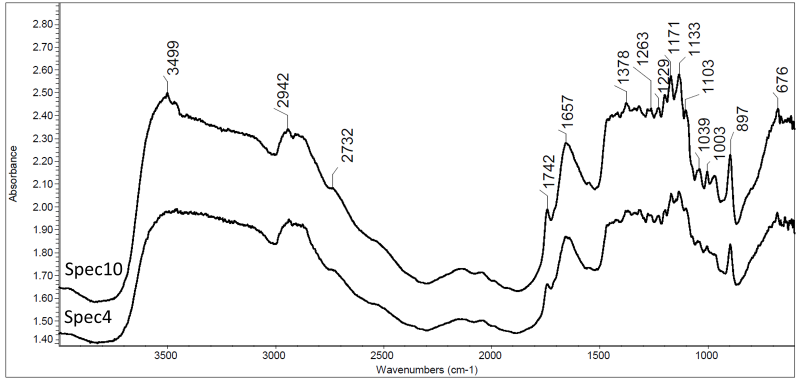
*Figure S43. Examples of mATR-FT-IR spectra of sample 3.1.*

**

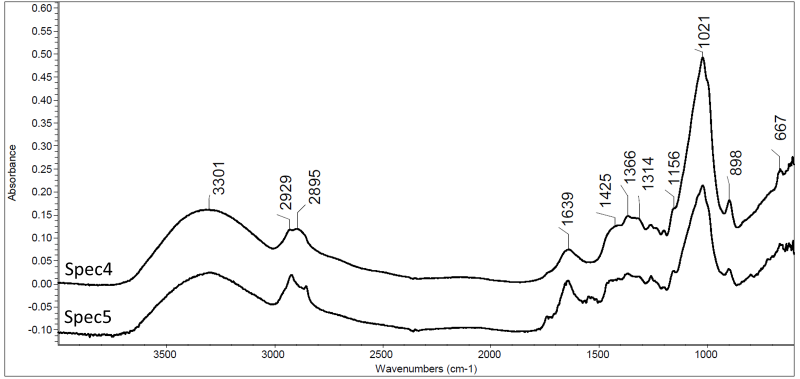
*Figure S44. Example of r-FT-IR spectrum of sample 3.2*

**

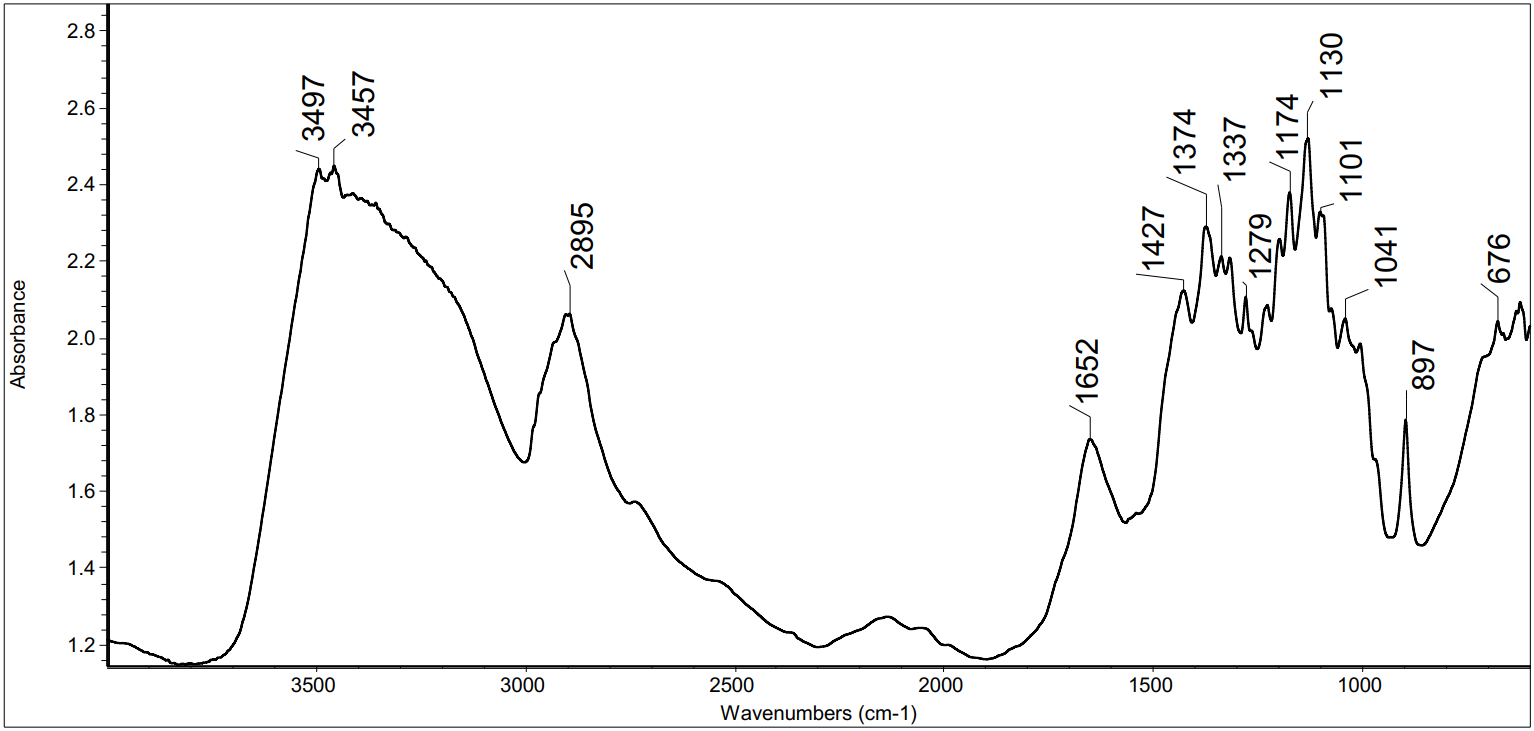
*Figure S45. Examples of mATR-FT-IR spectra of sample 3.2*

**

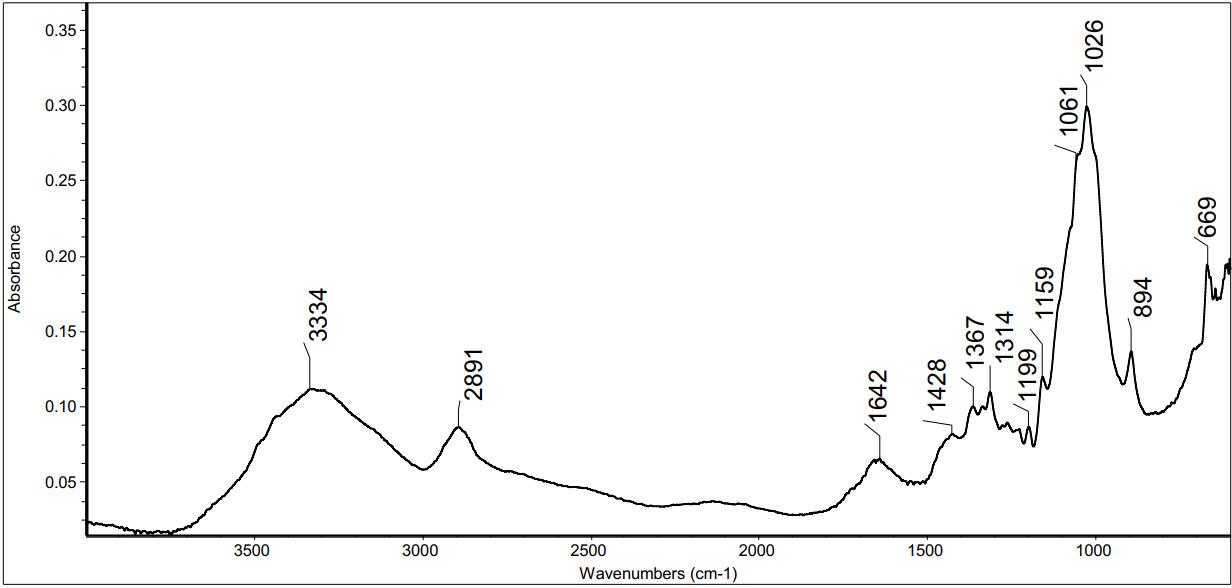
*Figure S46. Examples of r-FT-IR spectra of sample 4. Two spectra are presented to show the spectral differences within the sample.*

**

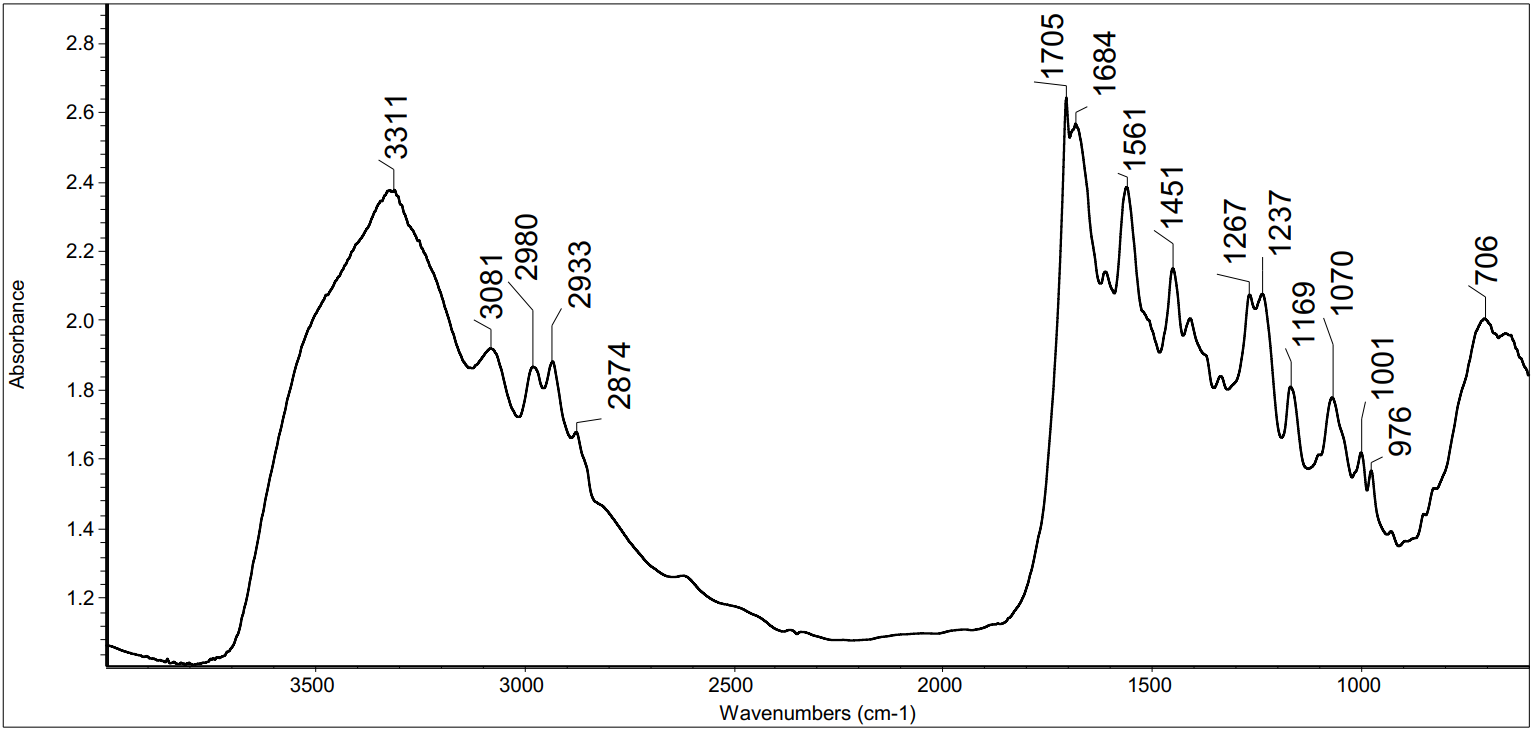
*Figure S47. Examples of mATR-FT-IR spectra of sample 4. Two spectra are presented to show the spectral differences within the sample.*

**

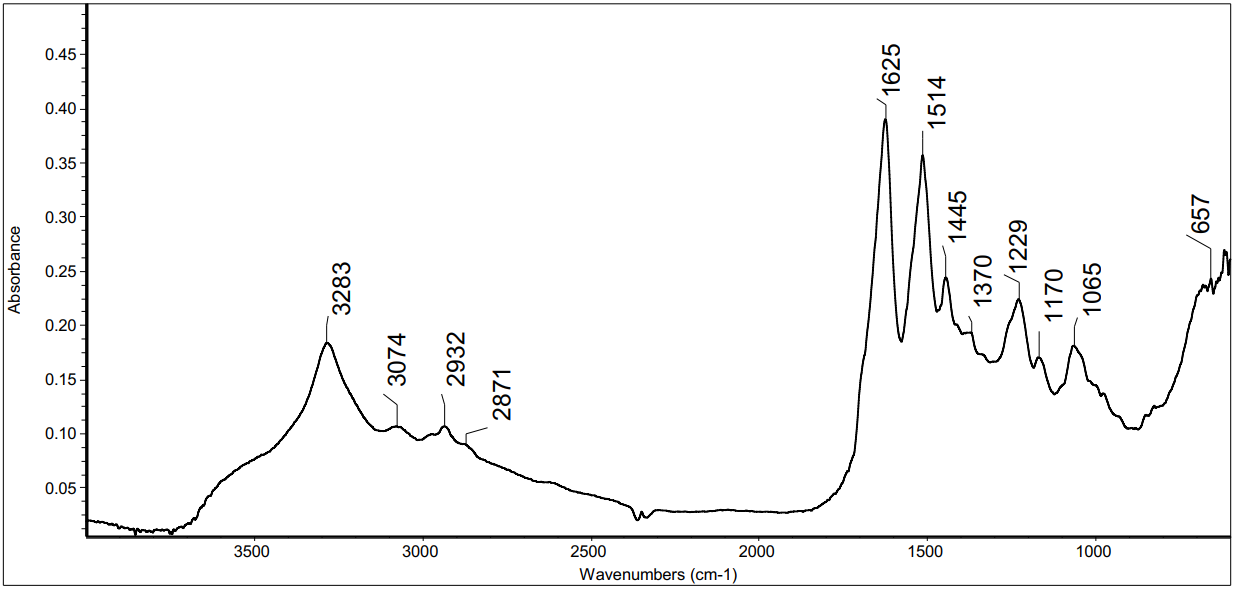
*Figure S48. Example of r-FT-IR spectrum of sample 5.1*

**

*Figure S49. Examples of mATR-FT-IR spectra of sample 5.1*

**

*Figure S50. Example of r-FT-IR spectrum of sample 5.2*

**

*Figure S51. Examples of mATR-FT-IR spectra of sample 5.2*

*Table 1. Classification results with r-FT-IR. The smaller the PCA score is for DA the more accurate the result. The bigger the accuracy score (max 1.00) is for random forest the more accurate the result*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sample nr | Measured spectra | **Class (Discriminant analysis)** | PCA scores | **Class (Random forest)** | Accuracy scores |
| **1** | Spec 1 | jute | 3.27 | wool | 0.24 |
|  | Spec 2 | jute | 3.62 | jute | 0.27 |
|  | Spec 3 | jute | 3.53 | jute | 0.30 |
|  | Spec 4 | jute | 3.63 | jute | 0.29 |
|  | Spec 5 | jute | 3.36 | jute | 0.35 |
|  | Spec 6 | jute | 3.37 | jute | 0.29 |
|  | Spec 7 | jute | 3.34 | jute | 0.30 |
|  | Spec 8 | jute | 3.19 | jute | 0.29 |
|  | Spec 9 | jute | 3.58 | jute | 0.30 |
|  | Spec 10 | jute | 3.55 | jute | 0.28 |
|  | Spec 11 | jute | 3.69 | jute | 0.28 |
|  | Spec 12 | jute | 3.34 | jute | 0.33 |
|  | Spec 13 | jute | 3.37 | jute | 0.33 |
|  | Spec 14 | jute | 4.05 | jute | 0.24 |
|  | Spec 15 | jute | 3.29 | jute | 0.28 |
|  | Spec 16 | jute | 2.13 | jute | 0.31 |
| **2** | Spec 1 | silk | 2.51 | jute | 0.59 |
|  | Spec 2 | silk | 1.61 | jute | 0.31 |
|  | Spec 3 | jute | 2.64 | silk | 0.89 |
|  | Spec 4 | wool | 2.54 | jute | 0.43 |
|  | Spec 5 | jute | 2.17 | jute | 0.35 |
|  | Spec 6 | silk | 2.57 | jute | 0.6 |
|  | Spec 7 | silk | 1.77 | jute | 0.29 |
|  | Spec 8 | jute | 2.65 | silk | 0.68 |
|  | Spec 9 | wool | 2.61 | jute | 0.4 |
|  | Spec 10 | cotton | 0.83 | jute | 0.34 |
| **3.1** | Spec 1 | jute | 1.16 | linen | 0.49 |
|  | Spec 2 | cotton | 1.1 | linen | 0.57 |
|  | Spec 3 | jute | 1.37 | cotton | 0.68 |
|  | Spec 4 | jute | 1.99 | linen | 0.67 |
|  | Spec 5 | jute | 1.77 | jute | 0.46 |
|  | Spec 6 | cotton | 0.77 | linen | 0.42 |
|  | Spec 7 | jute | 1.36 | cotton | 0.65 |
|  | Spec 8 | silk | 2.87 | linen | 0.66 |
| **3.2** | Spec 1 | silk | 1.55 | silk | 0.7 |
|  | Spec 2 | silk | 1.15 | silk | 0.95 |
|  | Spec 3 | silk | 1.58 | silk | 0.99 |
|  | Spec 4 | silk | 1.47 | silk | 0.99 |
|  | Spec 5 | silk | 1.37 | silk | 0.99 |
|  | Spec 6 | silk | 1.33 | silk | 0.93 |
|  | Spec 7 | silk | 0.92 | silk | 0.92 |
|  | Spec 8 | silk | 0.98 | silk | 0.99 |
|  | Spec 9 | silk | 1.67 | silk | 0.99 |
| **4** | Spec 1 | jute | 1.38 | jute | 0.37 |
|  | Spec 2 | jute | 1.42 | jute | 0.41 |
|  | Spec 3 | jute | 1.59 | wool | 0.37 |
|  | Spec 4 | jute | 1.35 | wool | 0.28 |
|  | Spec 5 | jute | 1.62 | wool | 0.41 |
|  | Spec 6 | jute | 1.92 | wool | 0.37 |
|  | Spec 7 | jute | 1.46 | wool | 0.29 |
|  | Spec 8 | jute | 1.78 | viscose | 0.31 |
|  | Spec 9 | jute | 1.92 | viscose | 0.26 |
|  | Spec 10 | jute | 1.35 | jute | 0.44 |
|  | Spec 11 | jute | 1.46 | viscose | 0.27 |
|  | Spec 12 | jute | 1.49 | wool | 0.27 |
| **5.1** | Spec 1 | cotton | 1.13 | cotton | 0.49 |
|  | Spec 2 | viscose | 1.08 | cotton | 0.42 |
|  | Spec 3 | viscose | 0.82 | viscose | 0.49 |
|  | Spec 4 | viscose | 1.29 | viscose | 0.61 |
|  | Spec 5 | viscose | 1.07 | linen | 0.34 |
|  | Spec 6 | viscose | 1.12 | cotton | 0.37 |
|  | Spec 7 | cotton | 0.83 | cotton | 0.55 |
|  | Spec 8 | cotton | 1.29 | cotton | 0.49 |
|  | Spec 9 | jute | 1.1 | cotton | 0.4 |
|  | Spec 10 | jute | 1.24 | cotton | 0.47 |
|  | Spec 11 | jute | 1.01 | cotton | 0.47 |
|  | Spec 12 | cotton | 1.06 | cotton | 0.54 |
|  | Spec 13 | cotton | 1.11 | cotton | 0.44 |
|  | Spec 14 | jute | 0.93 | cotton | 0.49 |
| **5.2** | Spec 1 | silk | 1.03 | silk | 0.97 |
|  | Spec 2 | silk | 1.69 | silk | 0.93 |
|  | Spec 3 | silk | 1.19 | silk | 0.96 |
|  | Spec 4 | silk | 1.03 | silk | 0.98 |
|  | Spec 5 | silk | 1.56 | silk | 0.97 |
|  | Spec 6 | silk | 1.42 | silk | 0.96 |
|  | Spec 7 | silk | 1.44 | silk | 0.96 |
|  | Spec 8 | silk | 1.45 | silk | 0.98 |
|  | Spec 9 | silk | 1.2 | silk | 0.95 |
|  | Spec 10 | silk | 1.29 | silk | 0.94 |

Table 2. *Classification results with mATR-FT-IR. The smaller the PCA score is for DA the more accurate the result. The bigger the accuracy score (max 1.00) is for random forest the more accurate the result*

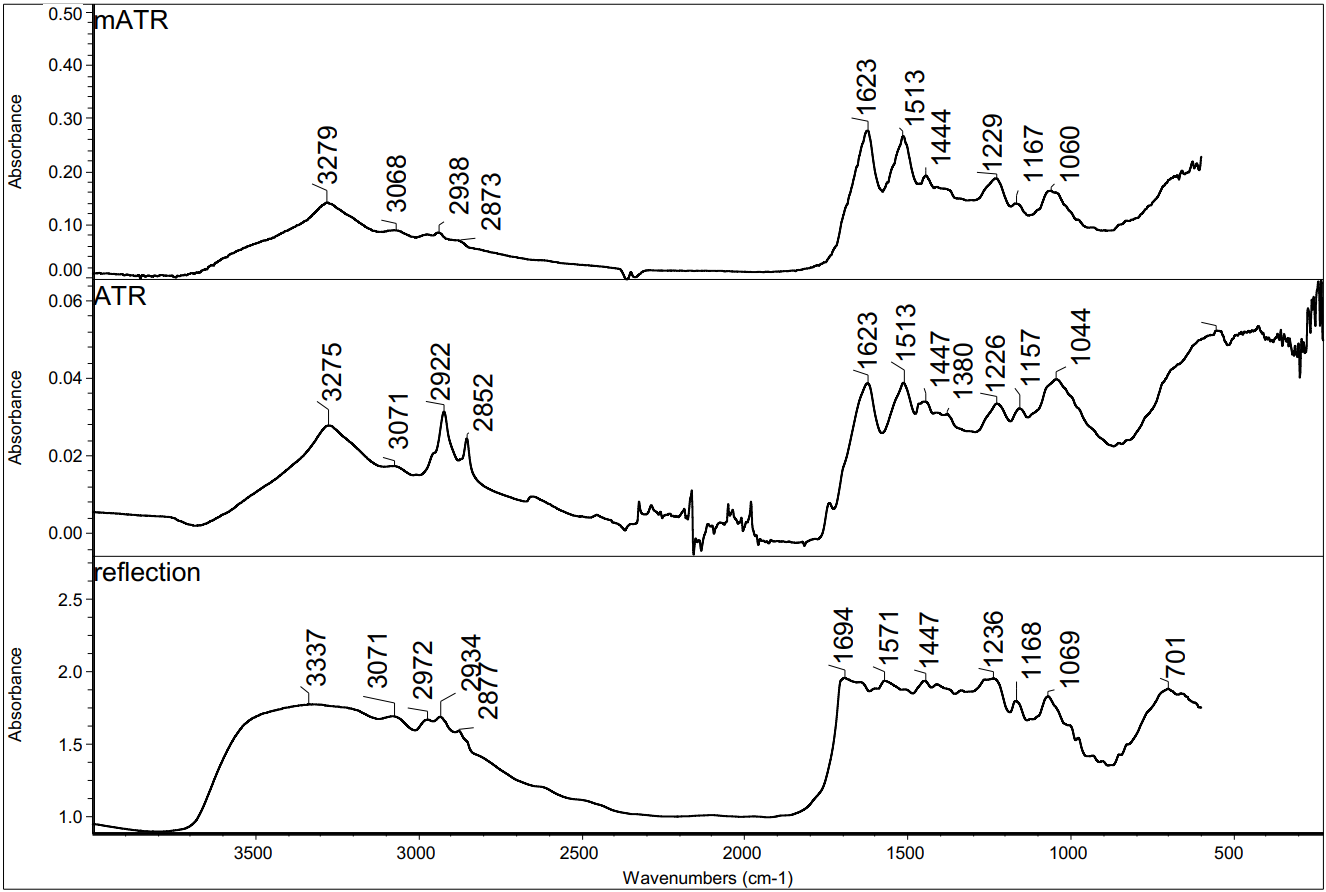
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sample nr | Measured spectra | **Class (Discriminant analysis)** | PCA scores | **Class (Random forest)** | Accuracy scores |
| **1** | Spec 1 | polyacrylic | 2.14 | silk | 0.29 |
|  | Spec 2 | polyacrylic | 1.88 | silk | 0.33 |
|  | Spec 3 | polyacrylic | 1.59 | silk | 0.49 |
|  | Spec 4 | polyacrylic | 1.87 | sisal | 0.27 |
|  | Spec 5 | polyacrylic | 2.21 | sisal | 0.25 |
|  | Spec 6 | polyacrylic | 2.17 | sisal | 0.28 |
|  | Spec 7 | polyacrylic | 2.17 | sisal | 0.27 |
|  | Spec 8 | polyacrylic | 1.68 | silk | 0.48 |
|  | Spec 9 | polyacrylic | 1.67 | silk | 0.52 |
|  | Spec 10 | polyacrylic | 2.05 | silk | 0.35 |
|  | Spec 12 | polyacrylic | 2.22 | sisal | 0.27 |
|  | Spec 13 | polyacrylic | 1.79 | silk | 0.54 |
|  | Spec 14 | polyacrylic | 1.82 | silk | 0.32 |
| **2** | Spec 1 | jute | 1.81 | sisal | 0.34 |
|  | Spec 2 | polyacrylic | 2.04 | sisal | 0.38 |
|  | Spec 3 | polyacrylic | 1.86 | sisal | 0.35 |
|  | Spec 4 | jute | 2.16 | sisal | 0.34 |
|  | Spec 5 | polyacrylic | 2.34 | viscose | 0.54 |
|  | Spec 6 | jute | 1.69 | sisal | 0.28 |
|  | Spec 7 | polyacrylic | 2.34 | sisal | 0.26 |
|  | Spec 8 | polyacrylic | 2.26 | sisal | 0.29 |
|  | Spec 9 | polyacrylic | 2.25 | sisal | 0.4 |
|  | Spec 10 | polyacrylic | 2.11 | sisal | 0.27 |
|  | Spec 11 | polyacrylic | 1.8 | sisal | 0.38 |
|  | Spec 12 | polyacrylic | 1.95 | sisal | 0.36 |
|  | Spec 13 | jute | 2.16 | viscose | 0.61 |
|  | Spec 14 | jute | 2.14 | viscose | 0.66 |
|  | Spec 15 | polyacrylic | 2.22 | silk | 0.42 |
|  | Spec 16 | polyacrylic | 2.29 | sisal | 0.24 |
|  | Spec 17 | polyacrylic | 2.27 | sisal | 0.33 |
|  | Spec 18 | jute | 1.86 | viscose | 0.54 |
|  | Spec 19 | jute | 1.69 | sisal | 0.36 |
|  | Spec 20 | jute | 1.61 | sisal | 0.39 |
| **3.1** | Spec 1 | jute | 0.99 | linen | 0.365 |
|  | Spec 2 | cotton | 1.01 | cotton | 0.34 |
|  | Spec 3 | jute | 1.45 | jute | 0.45 |
|  | Spec 4 | jute | 0.78 | jute | 0.49 |
|  | Spec 6 | jute | 1.05 | linen | 0.285 |
|  | Spec 7 | jute | 1.7 | jute | 0.29 |
| **3.2** | Spec 1 | silk | 1.14 | silk | 1 |
|  | Spec 2 | silk | 1.5 | silk | 1 |
|  | Spec 3 | silk | 1.66 | silk | 0.86 |
|  | Spec 4 | silk | 1.49 | silk | 0.99 |
|  | Spec 5 | silk | 1.82 | silk | 0.74 |
|  | Spec 6 | silk | 1.42 | silk | 0.99 |
| **4** | Spec 1 | jute | 1.35 | viscose | 0.63 |
|  | Spec 2 | jute | 1.54 | viscose | 0.55 |
|  | Spec 3 | jute | 1.49 | viscose | 0.57 |
|  | Spec 4 | jute | 1.72 | viscose | 0.6 |
|  | Spec 5 | jute | 1.96 | jute | 0.31 |
| **5.1** | Spec 1 | jute | 1.26 | viscose | 0.49 |
|  | Spec 2 | viscose | 1.25 | viscose | 0.92 |
|  | Spec 3 | jute | 1.12 | viscose | 0.78 |
|  | Spec 4 | jute | 1.1 | viscose | 0.63 |
|  | Spec 5 | jute | 0.9 | viscose | 0.64 |
|  | Spec 6 | jute | 1.55 | viscose | 0.51 |
| **5.2** | Spec 1 | silk | 1.08 | silk | 0.99 |
|  | Spec 2 | silk | 1.29 | silk | 0.97 |
|  | Spec 3 | silk | 1.41 | silk | 0.97 |

# Case-study: Very small fiber thread from painting on the textile from the end of the 20th century

**

*Figure S52. Photo of analyzed object. The red circle at the bottom of the painting shows where analyzed sample was taken (Photo made by Nele Ambos).*

|  |  |  |
| --- | --- | --- |
|  |  |  |
| *Figure S53. Picture of the analyzed fiber on ATR diamond crystal.* | *Figure S54. Microscope picture of the fibers* | *Figure S55. Microscope picture of the fibers* |

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*Figure S56. FT-IR spectra of analyzed paint fiber. Spectra are recorded using FT-IR microspectrometer in ATR mode, ATR-FT-IR spectrometer and FT-IR microspectrometer in reflectance mode.*

Table 3*. Classification results with mATR-FT-IR. The smaller the PCA score is for DA the more accurate the result. The bigger the accuracy score (max 1.00) is for random forest the more accurate the result*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Measured spectra | **Class (Discriminant analysis)** | PCA scores | **Class (Random forest)** | Accuracy scores |
| Spec 1 | silk | 2.34 | silk | 0.99 |
| Spec 2 | silk | 2.07 | silk | 0.95 |