Supplementary information

for article

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

Pilleriin Peets, Karl Kaupmees, Signe Vahur, Ivo Leito

University of Tartu, Institute of Chemistry, 14a Ravila str, 50411 Tartu, Estonia

Corresponding author: e-mail: pilleriin.peets@ut.ee

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

All spectra below are original without any alteration or correction.

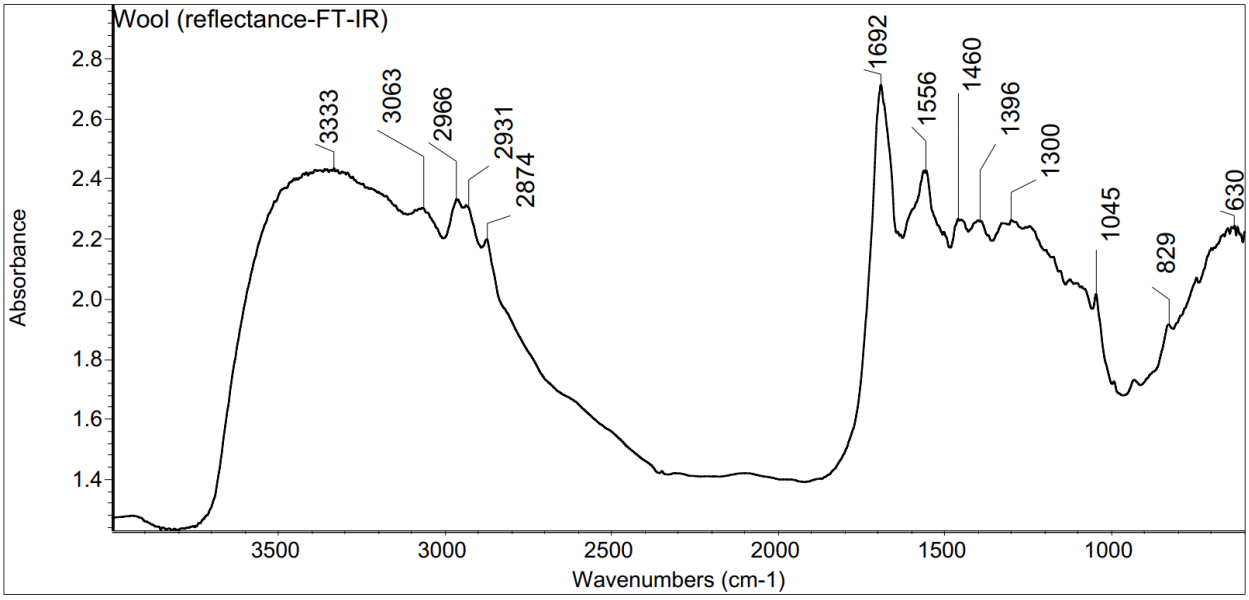


Figure S1. r-FT-IR spectrum of wool fiber

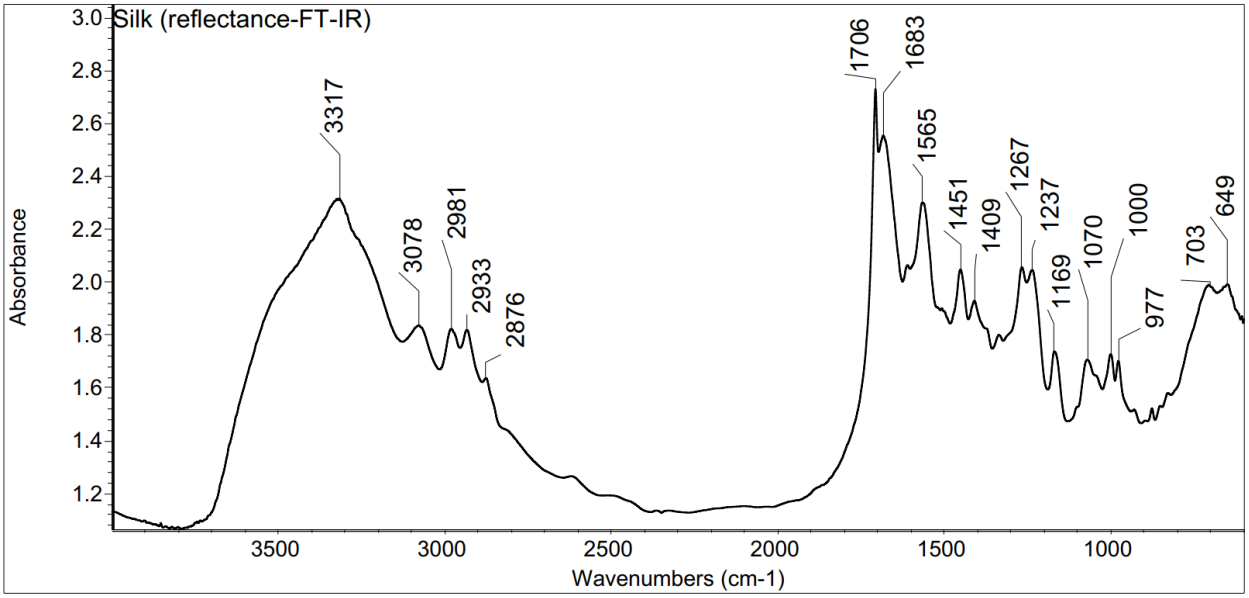


Figure S2. r-FT-IR spectrum of silk fiber

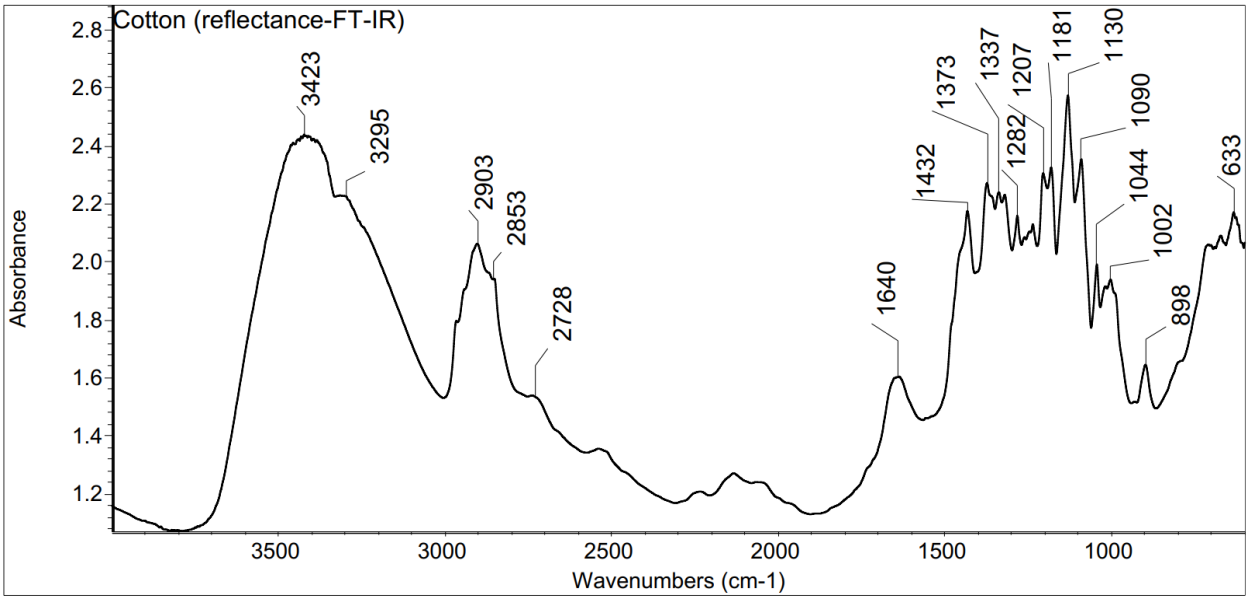


Figure S3. r-FT-IR spectrum of cotton fiber

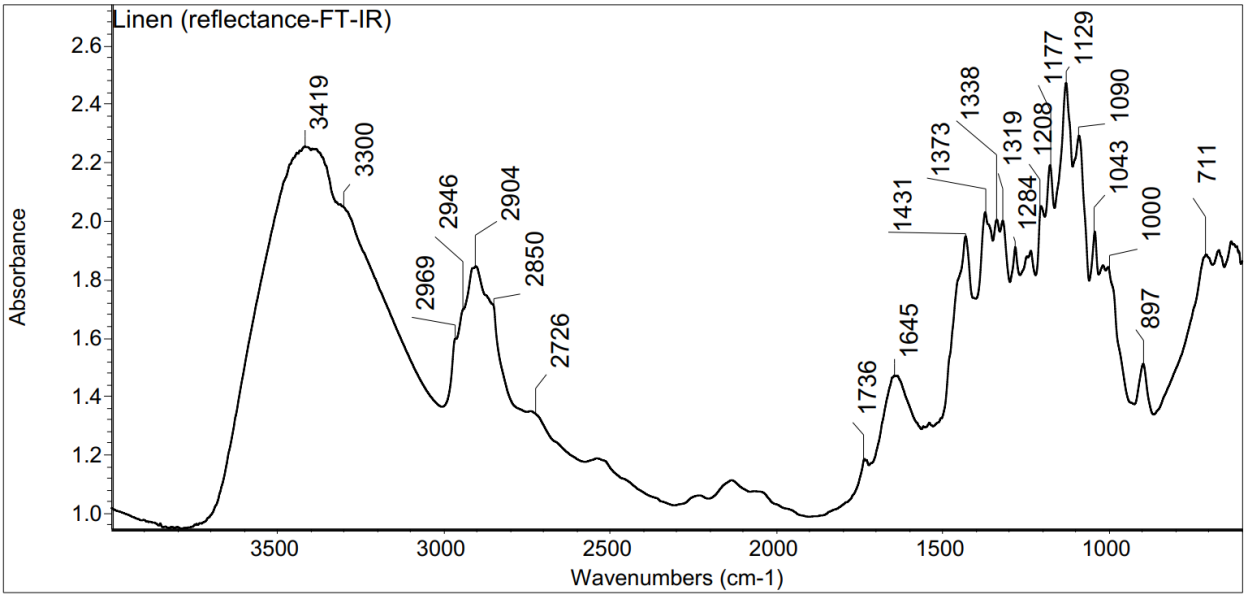


Figure S4. r-FT-IR spectrum of linen fiber

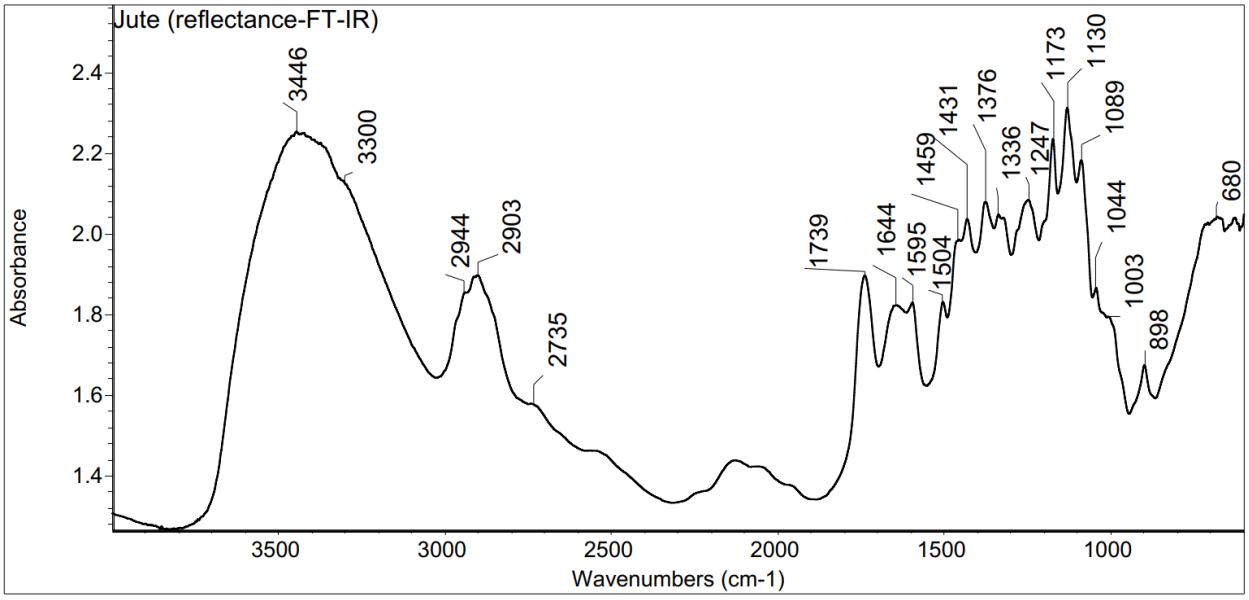


Figure S5. r-FT-IR spectrum of jute fiber

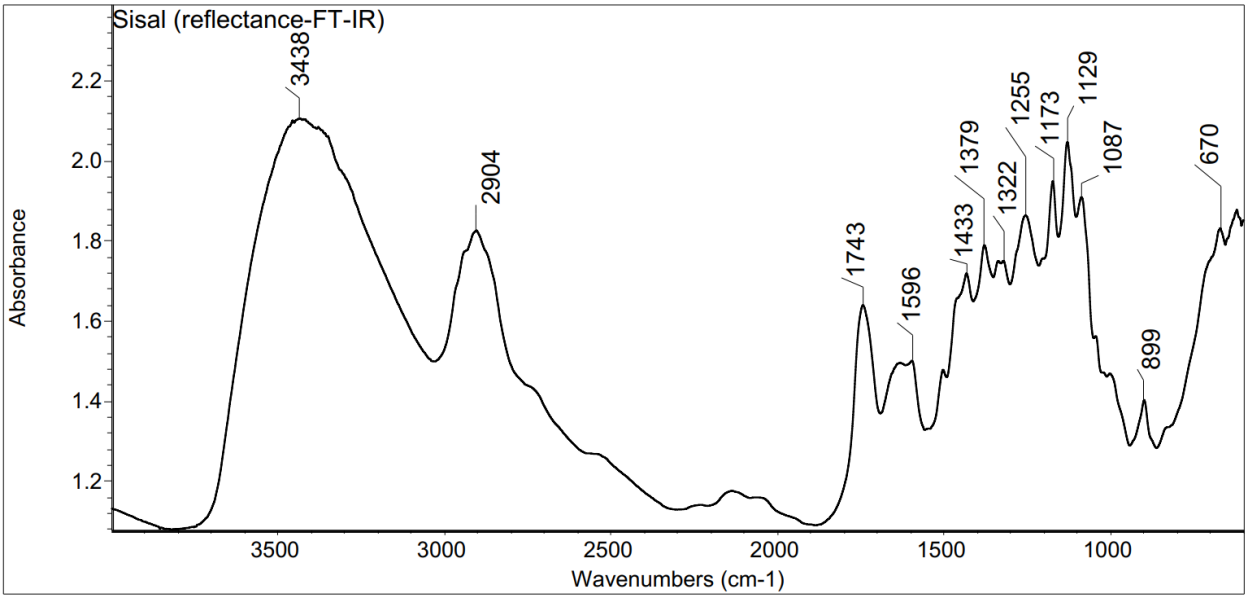


Figure S6. r-FT-IR spectrum of sisal fiber

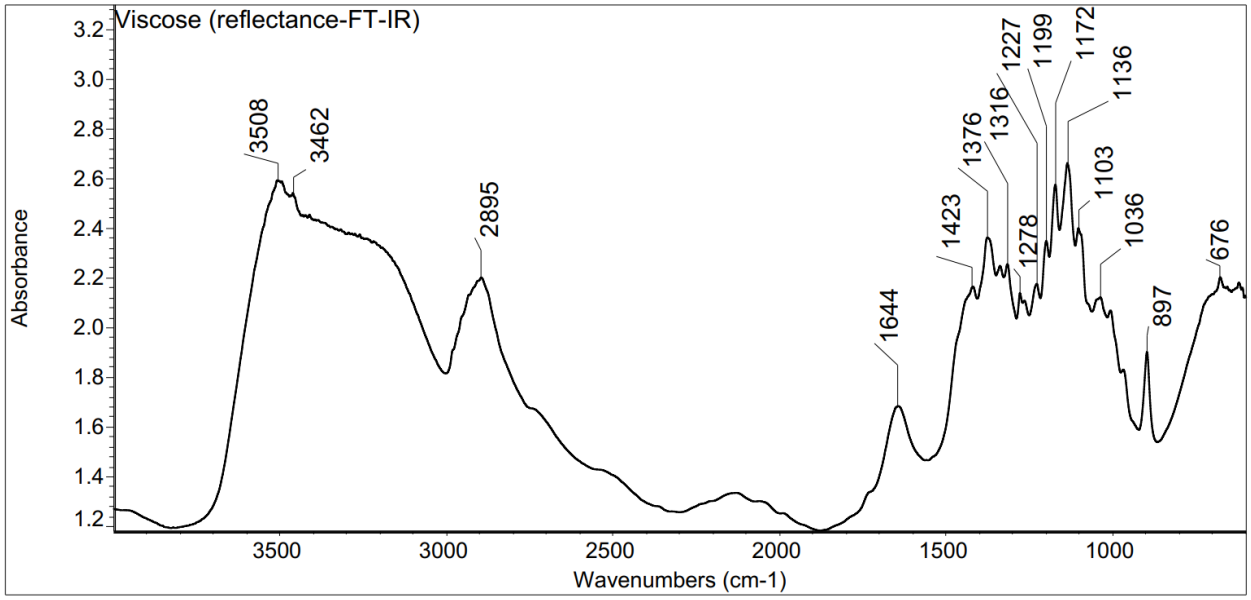


Figure S7. r-FT-IR spectrum of viscose fiber

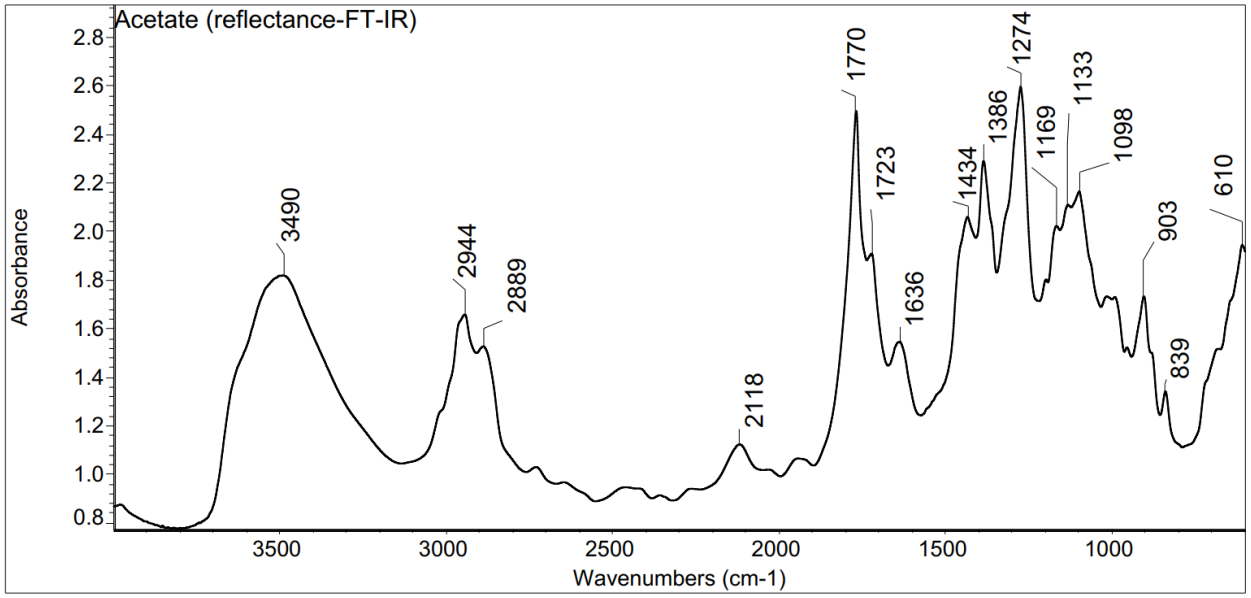


Figure S8. r-FT-IR spectrum of cellulose acetate fiber

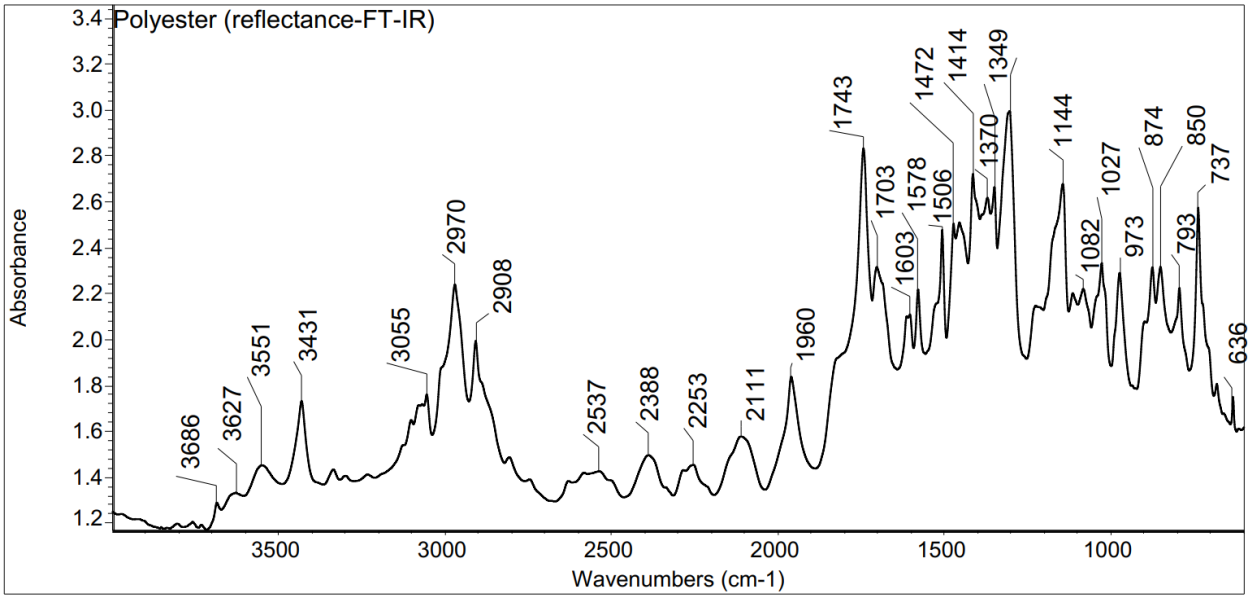


Figure S9. r-FT-IR spectrum of polyester fiber

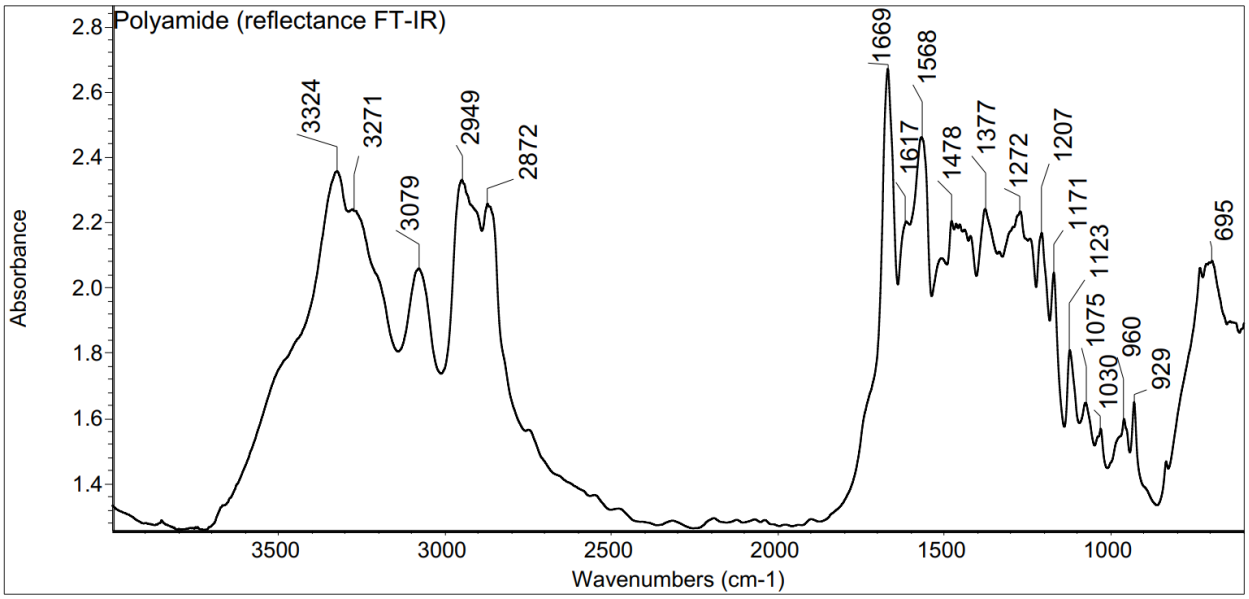


Figure S10. r-FT-IR spectrum of polyamide fiber

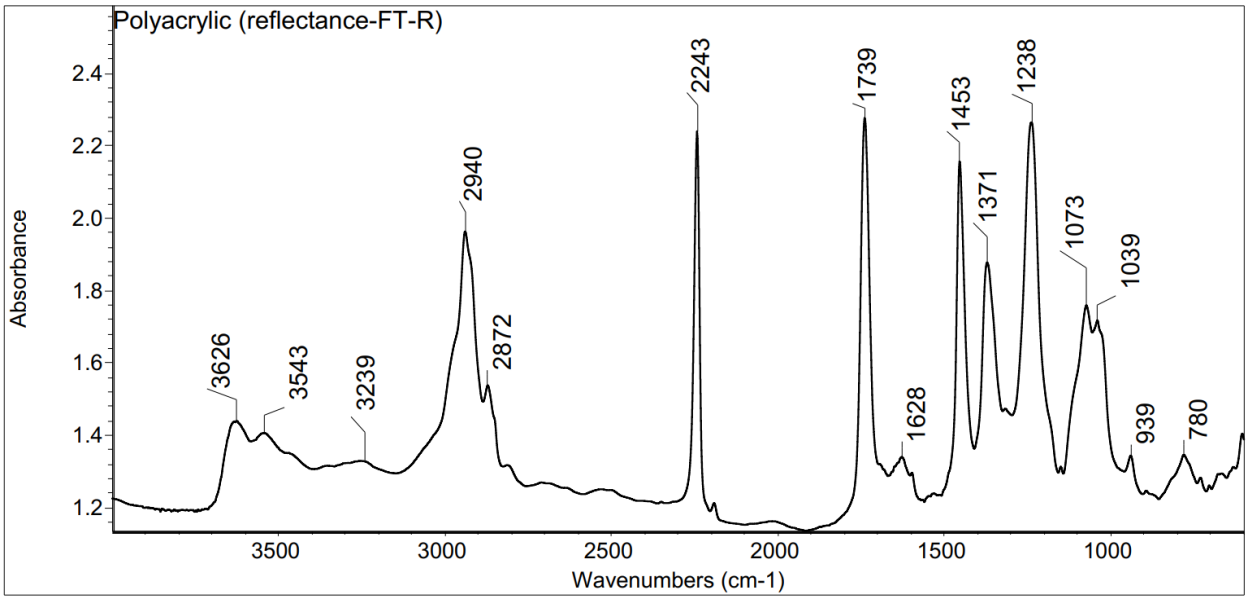


Figure S11. r-FT-IR spectrum of polyacrylic fiber

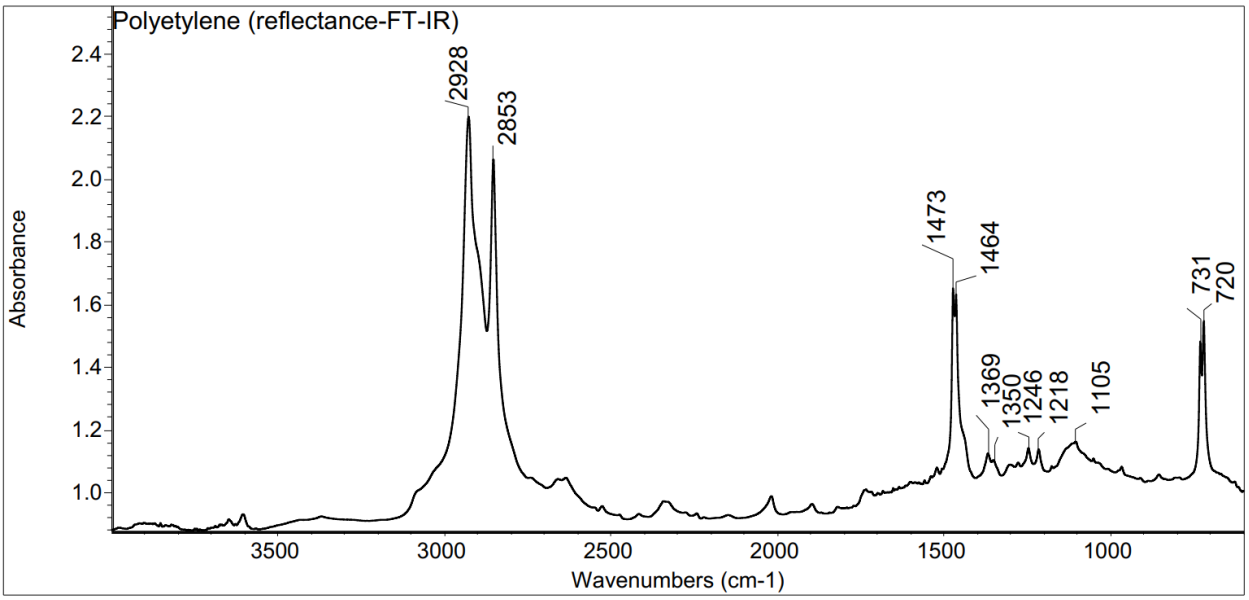


Figure S12. r-FT-IR spectrum of polyethylene fiber

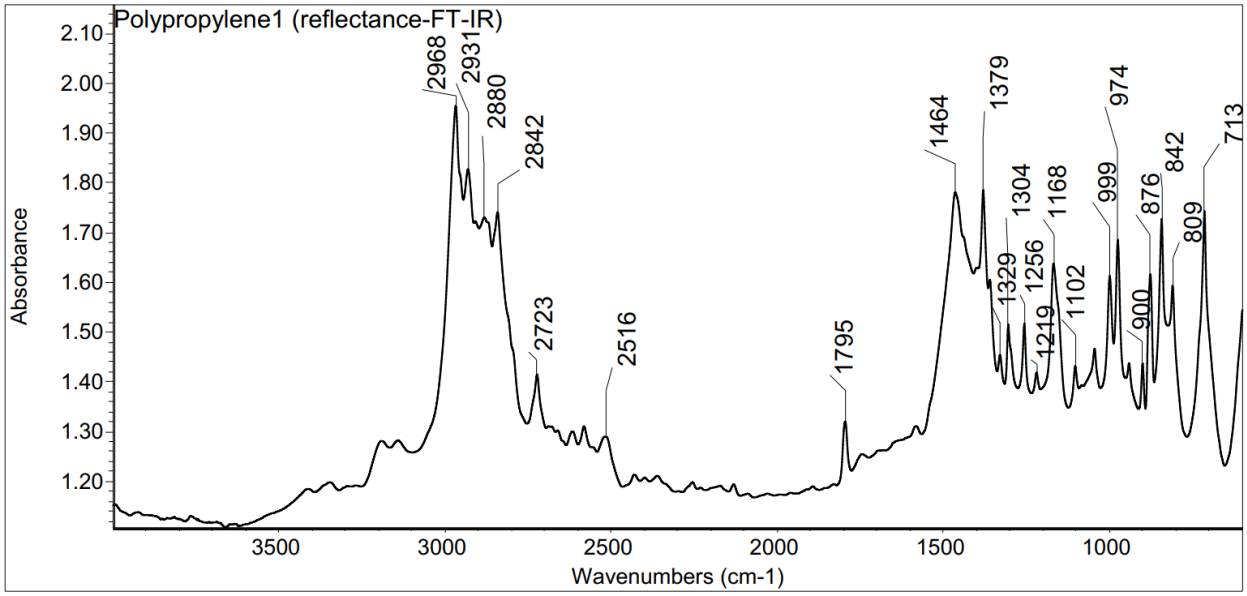


Figure S13. r-FT-IR spectrum of polypropylene fiber

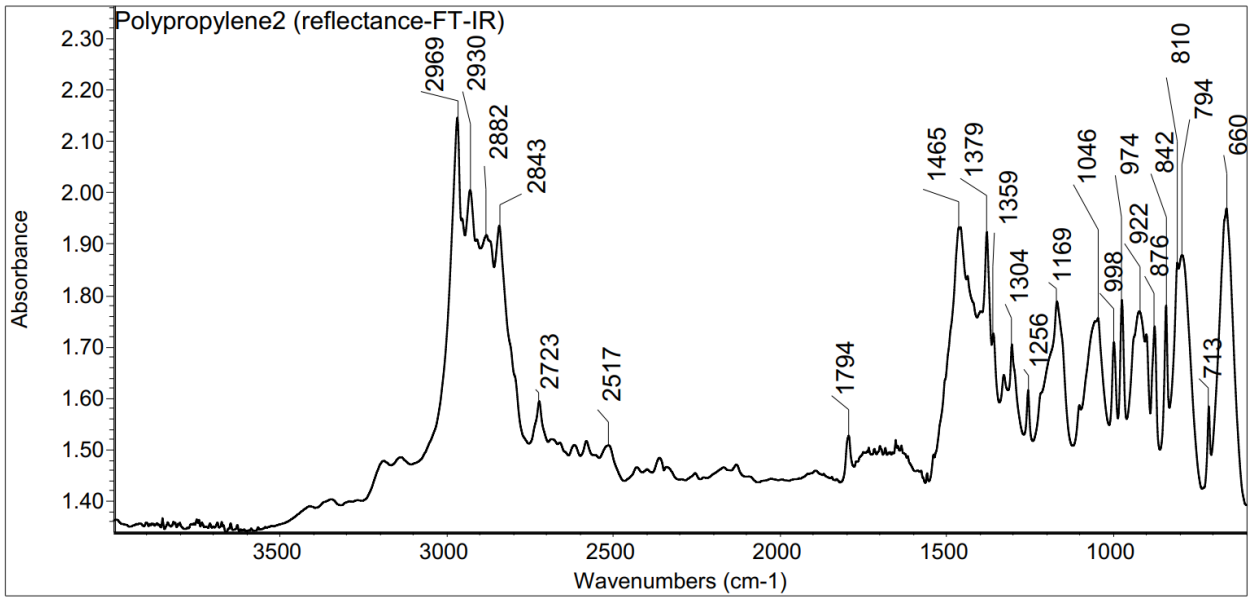


Figure S14. r-FT-IR spectrum of polypropylene fiber

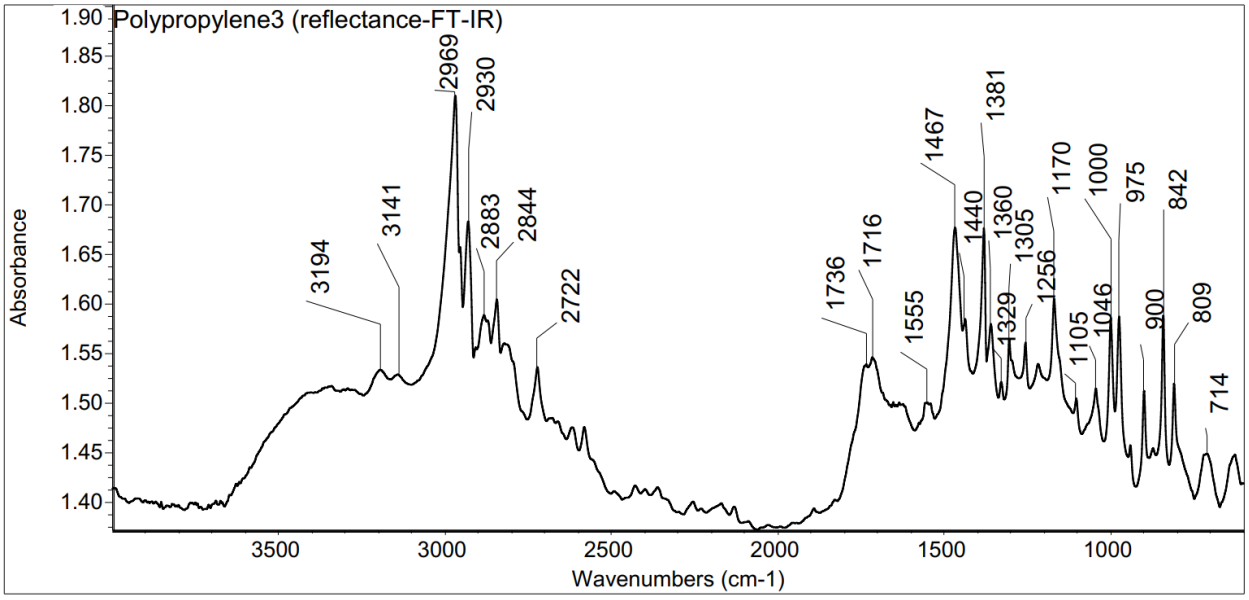


Figure S15. r-FT-IR spectrum of polypropylene fiber

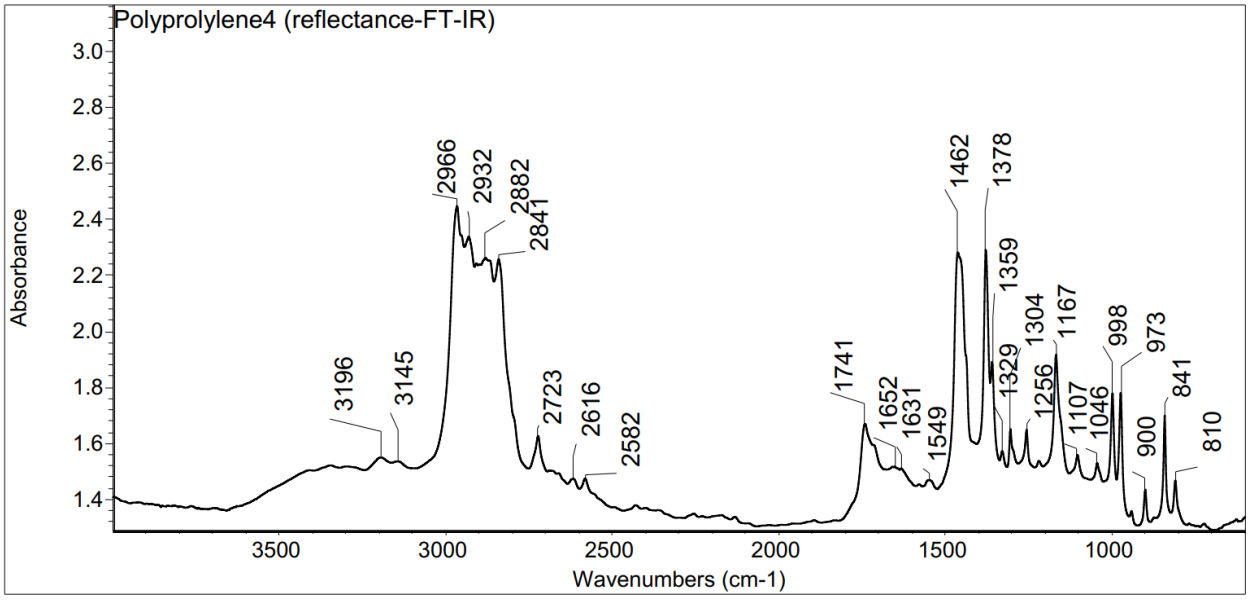


Figure S16. r-FT-IR spectrum of polypropylene fiber

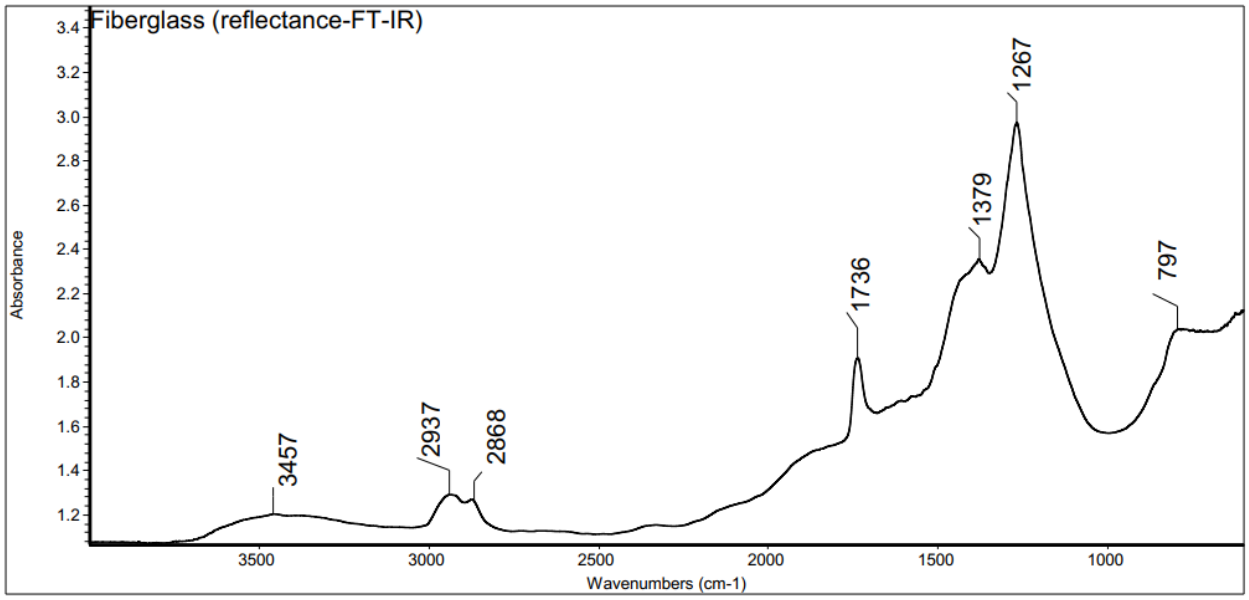


Figure S17. r-FT-IR spectrum of fiberglass

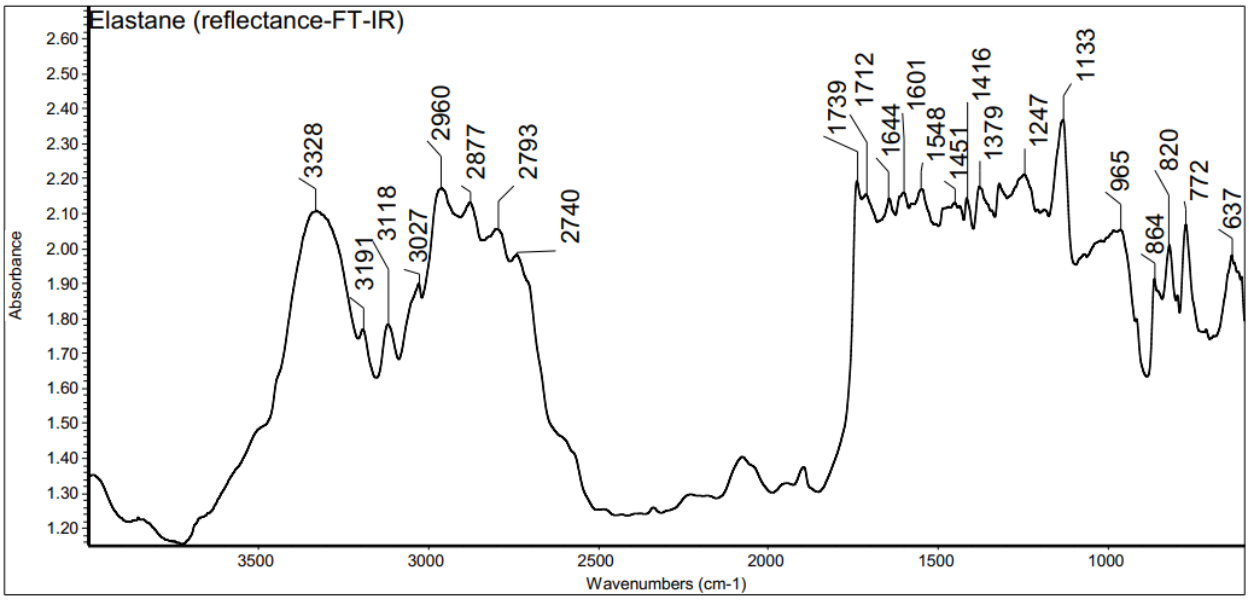


Figure S18. r-FT-IR spectrum of elastane fiber (deformed due to small fiber diameter)

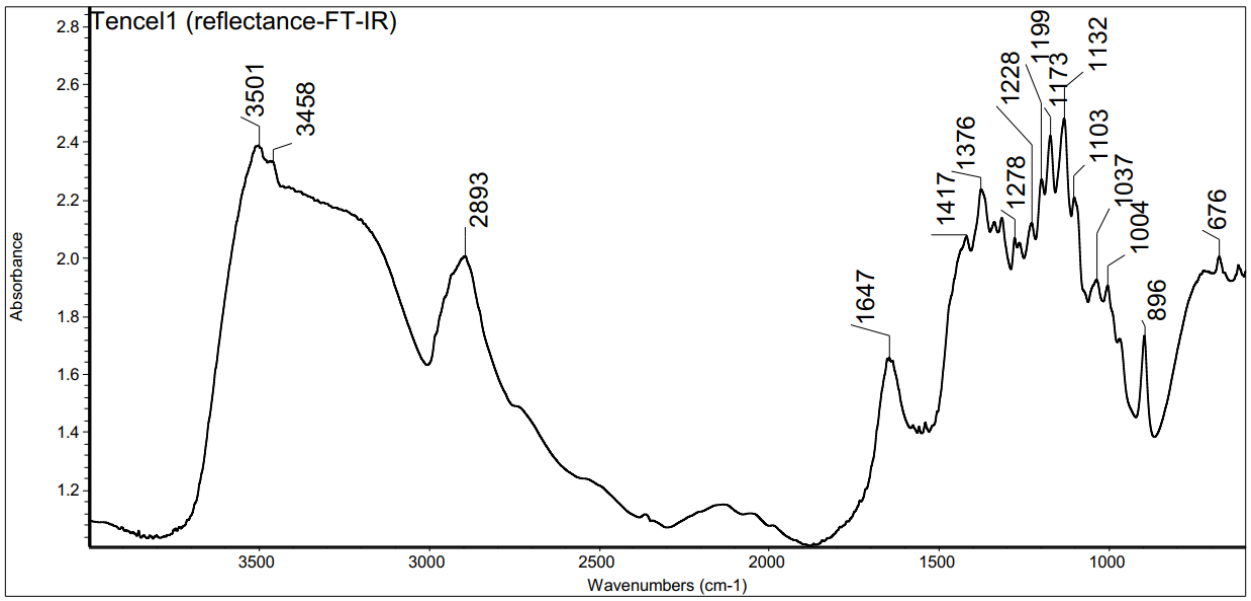


Figure S19. r-FT-IR spectrum of Tencel

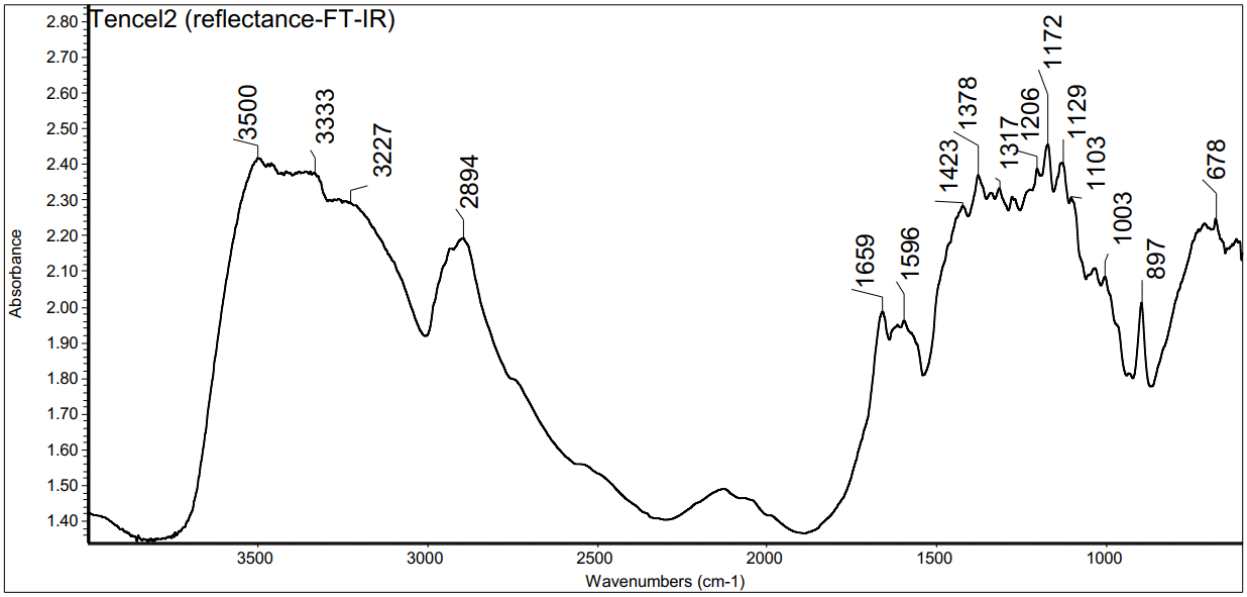


Figure S20. r-FT-IR spectrum of Tencel

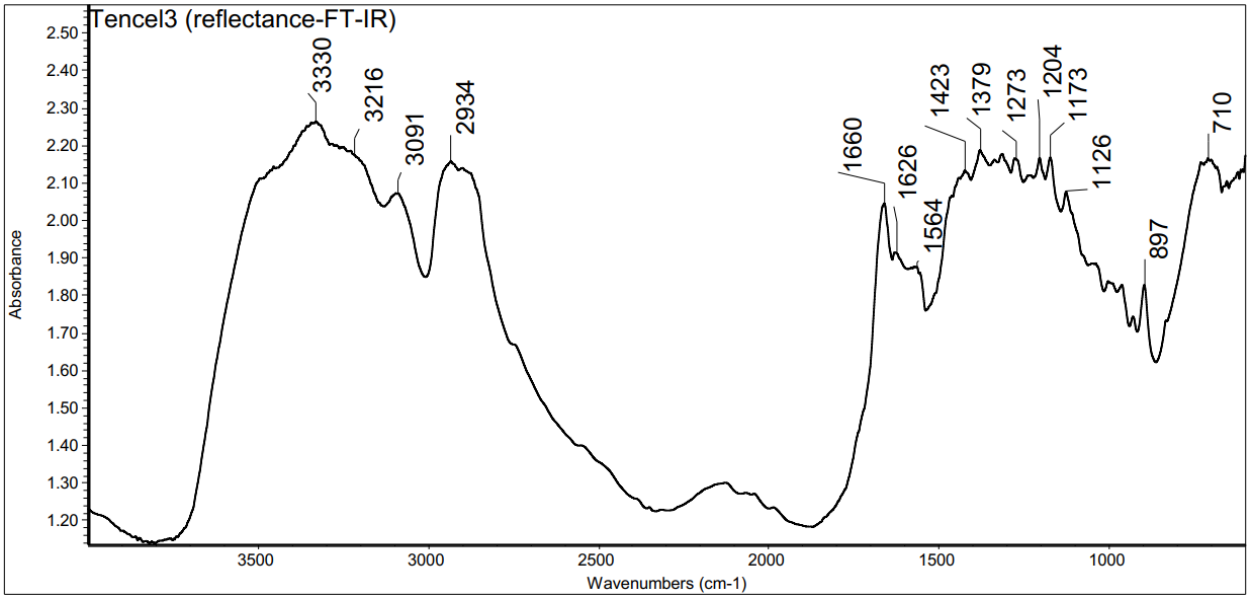


Figure S21. r-FT-IR spectrum of Tencel

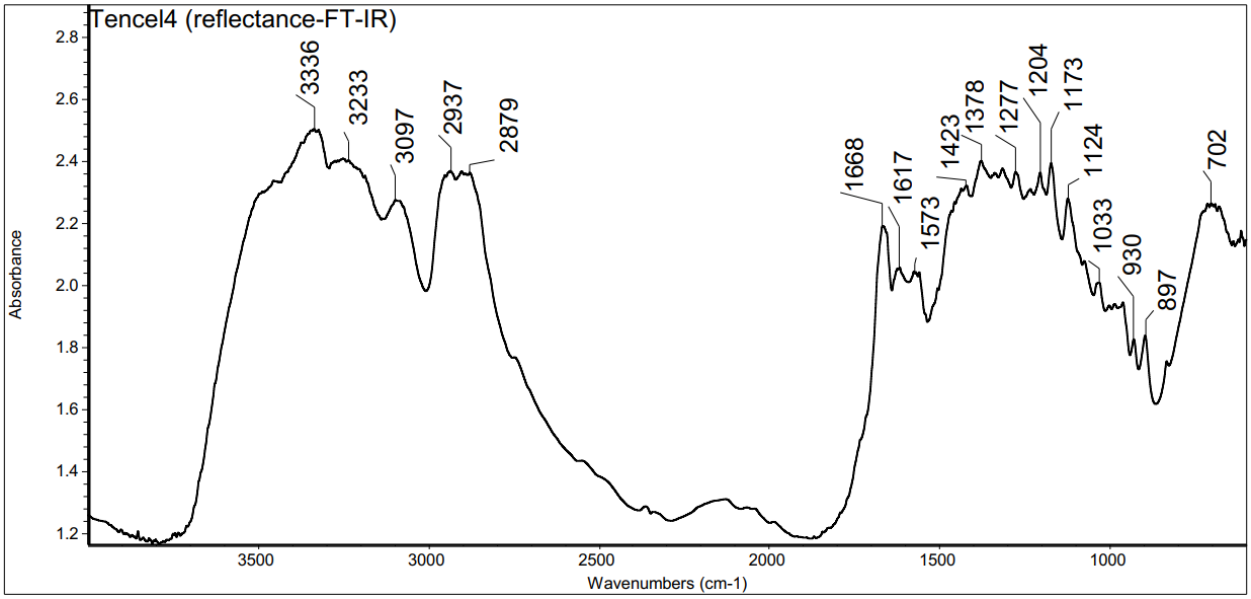
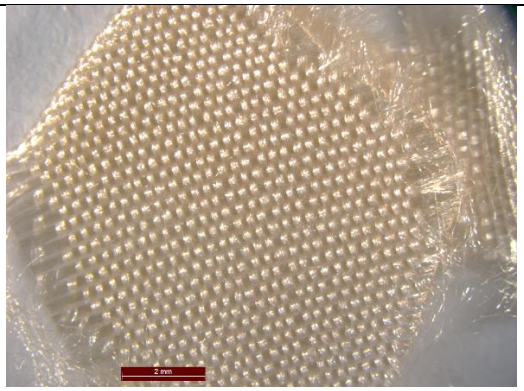
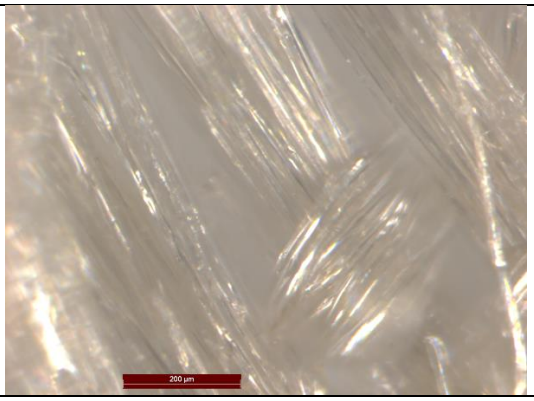
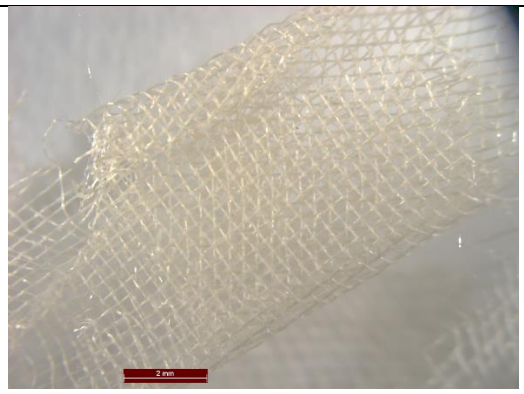
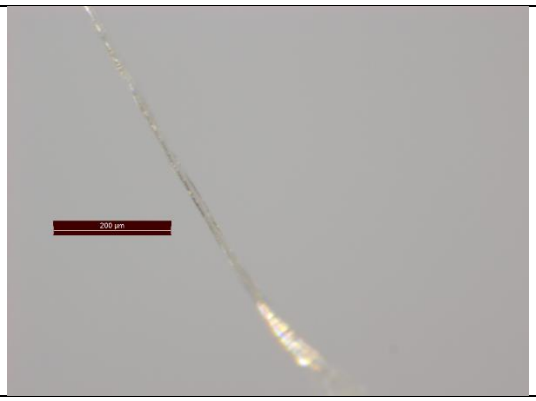
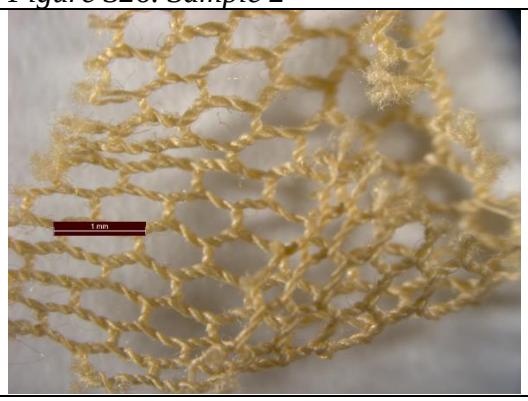
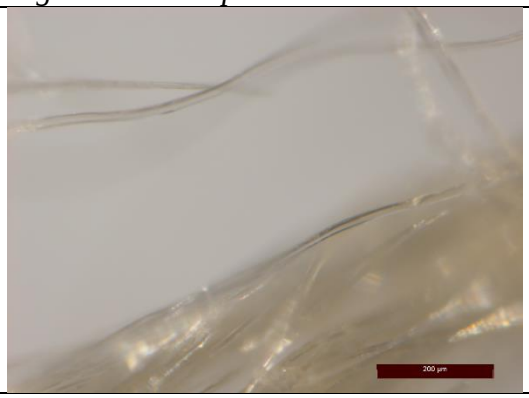
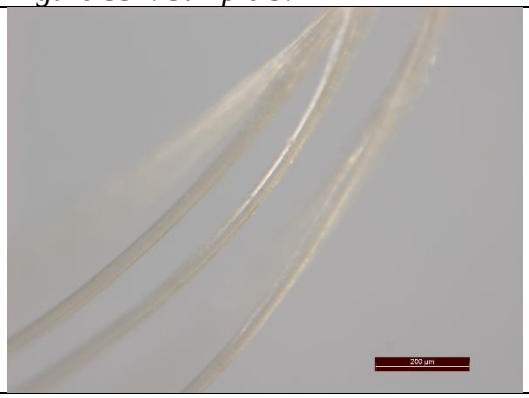


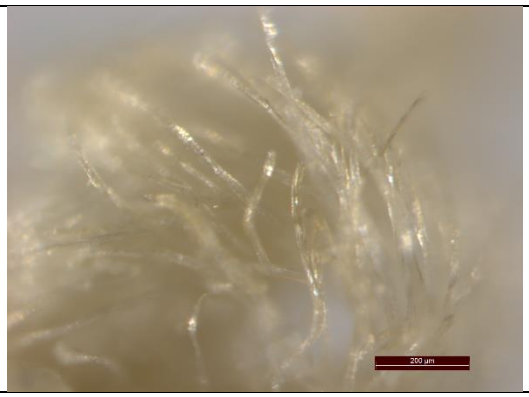
Figure S22. r-FT-IR spectrum of Tencel

Case-study: Scarf from 20th century

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*

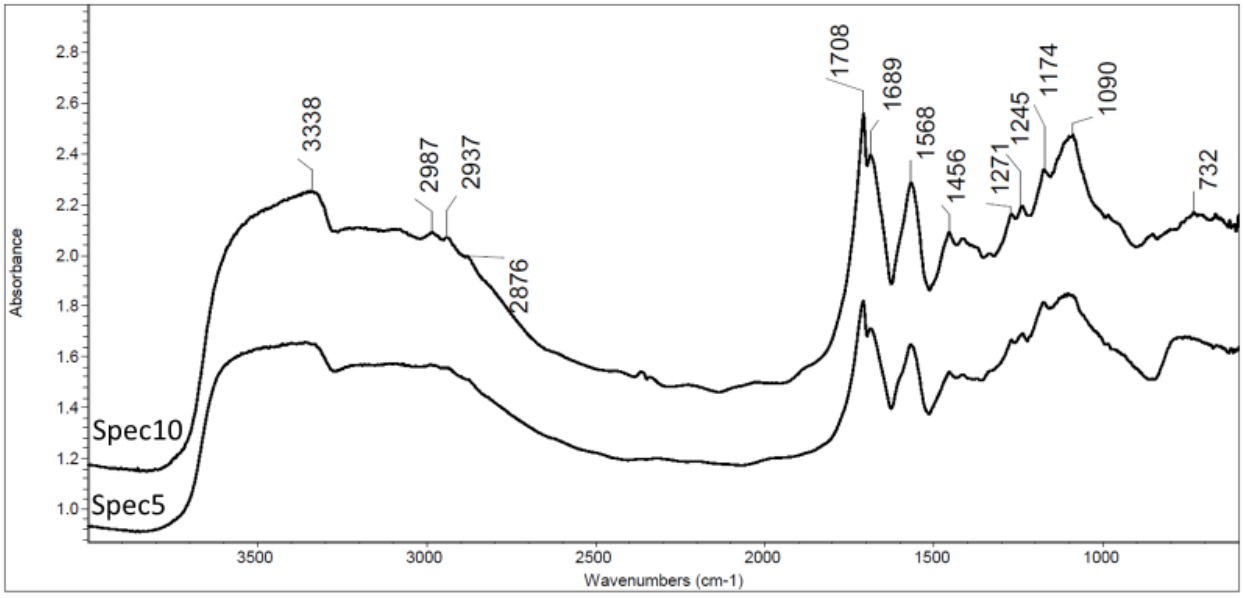


Figure S38. Examples of r-FT-IR spectra of sample 1. Two spectra are presented to show the spectral differences within the sample.

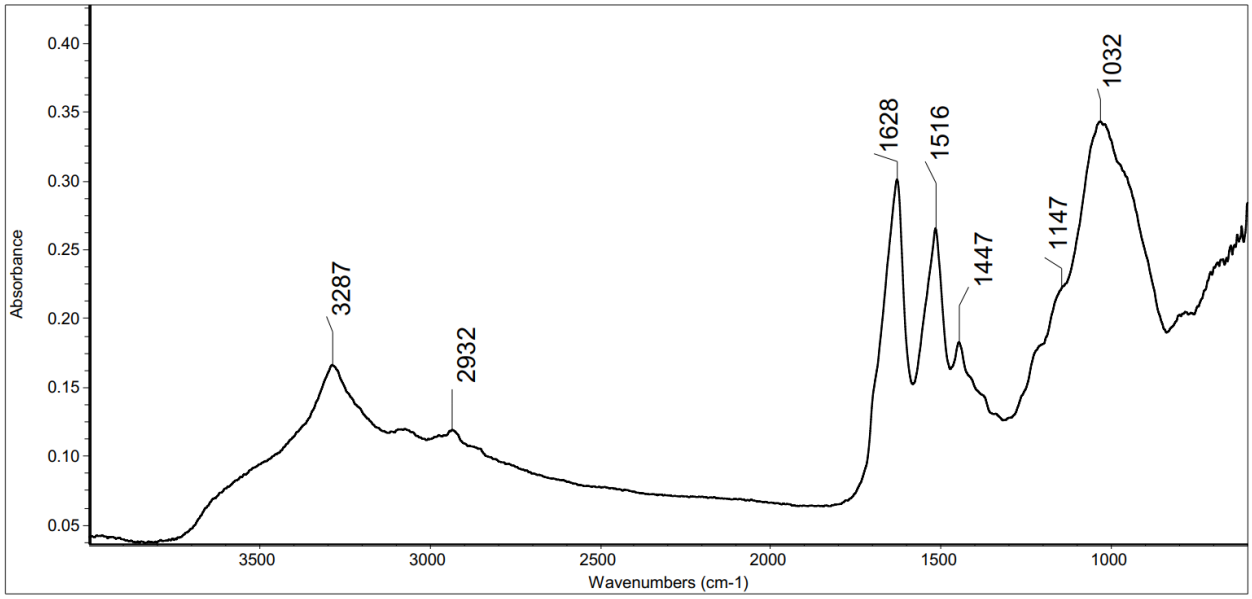


Figure S39. Example of mATR-FT-IR spectrum of sample 1

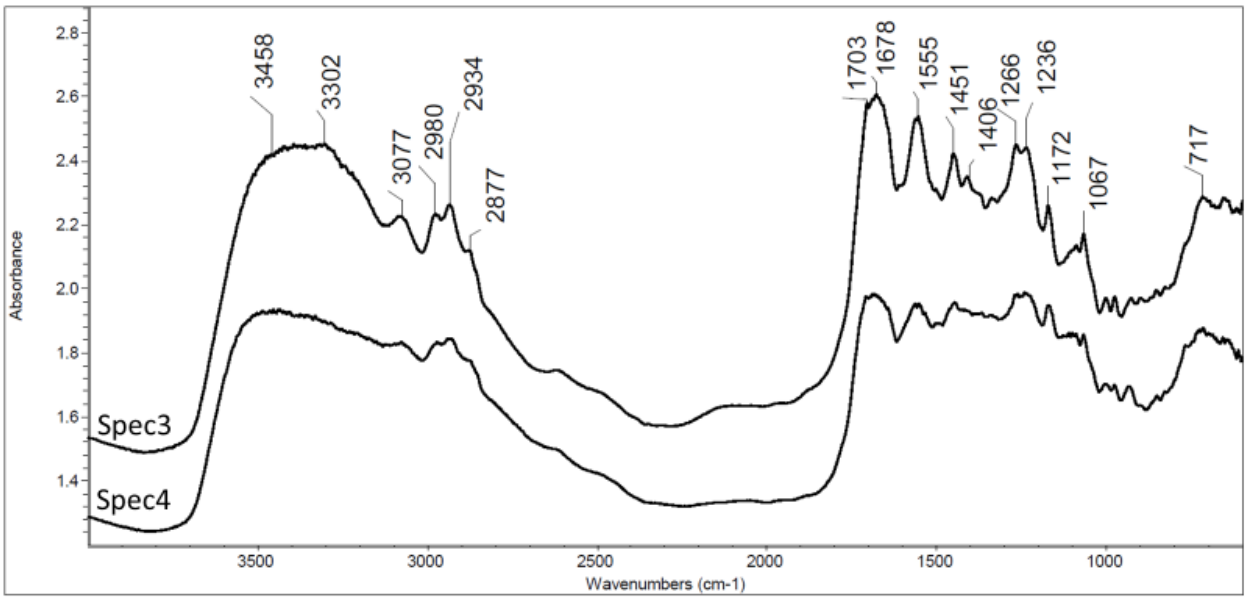


Figure S40. Examples of r-FT-IR spectra of sample 2. Two spectra are presented to show the spectral differences within the sample.

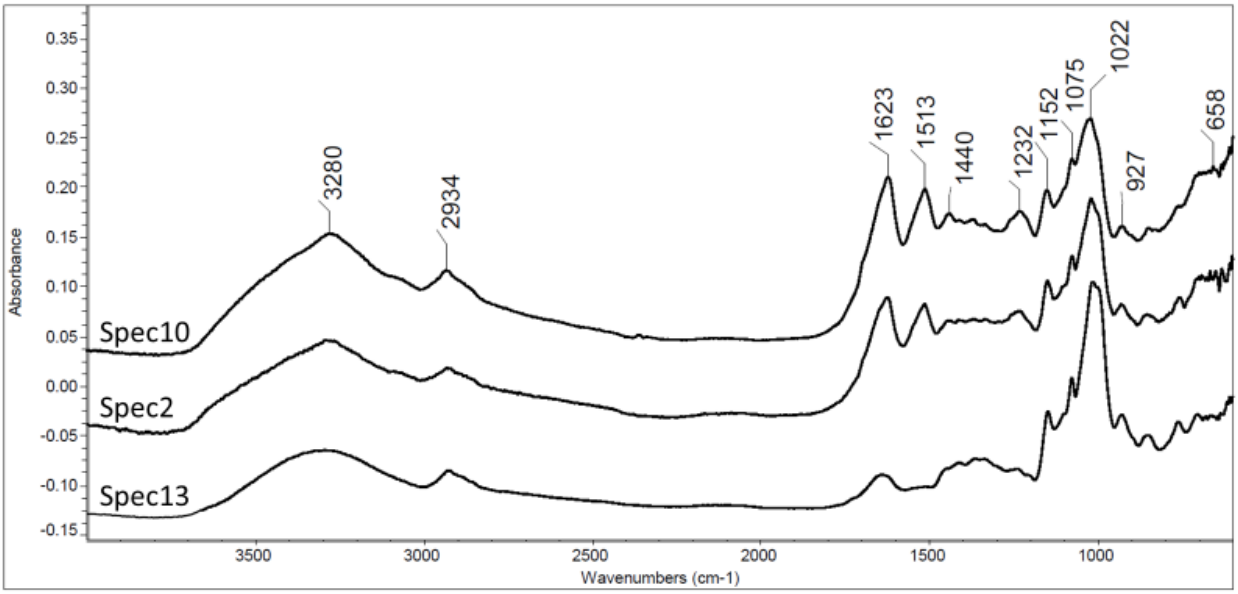


Figure S41. Examples of mATR-FT-IR spectra of sample 2. Three spectra are presented to show the spectral differences within the sample

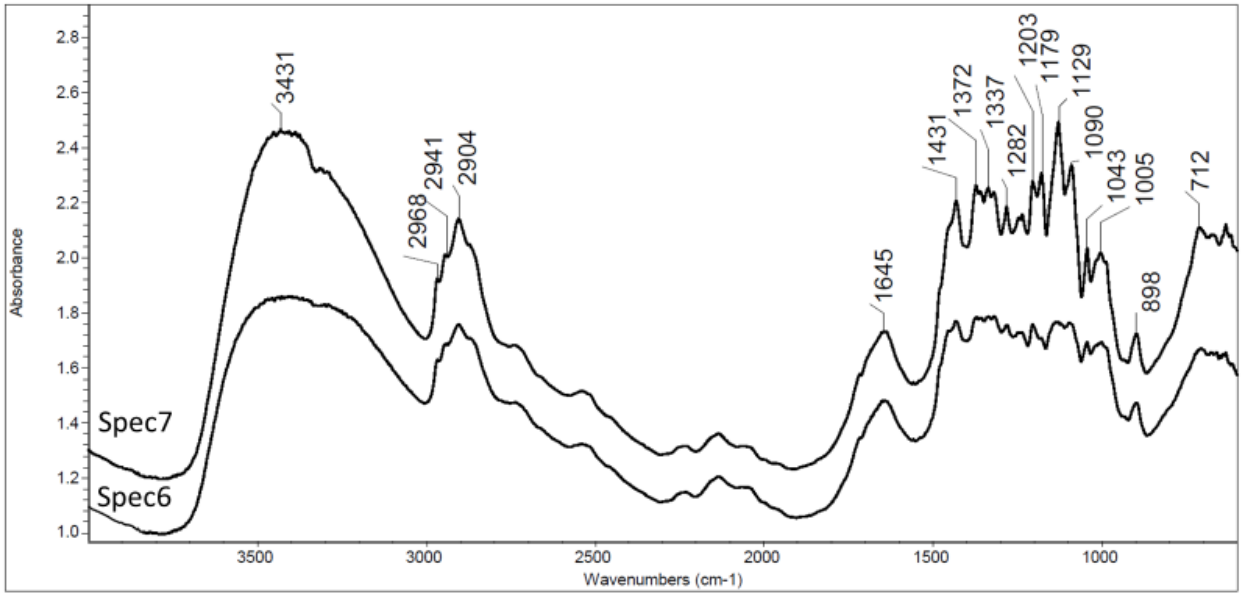


Figure S42. Examples of r-FT-IR spectra of sample 3.1. Two spectra are presented to show the spectral differences within the sample

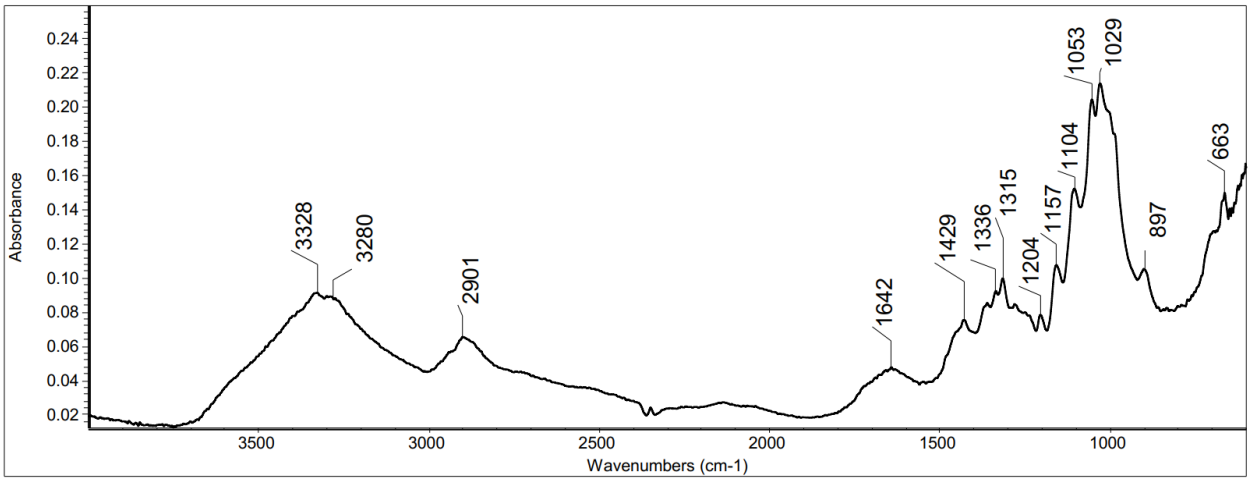


Figure S43. Examples of mATR-FT-IR spectra of sample 3.1.

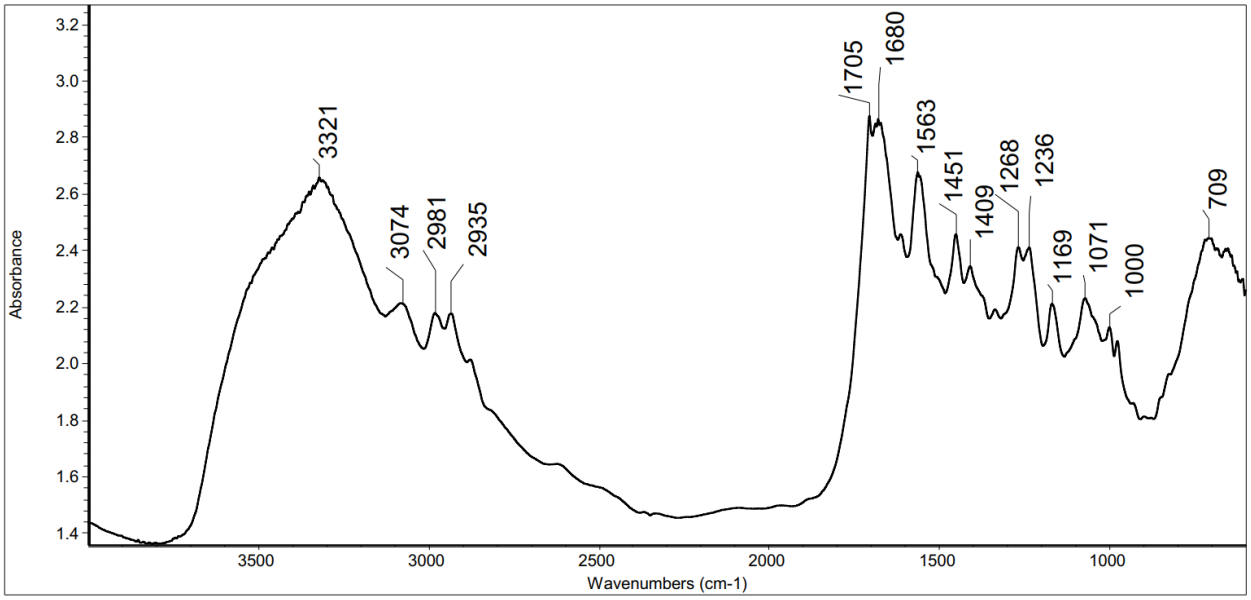


Figure S44. Example of r-FT-IR spectrum of sample 3.2

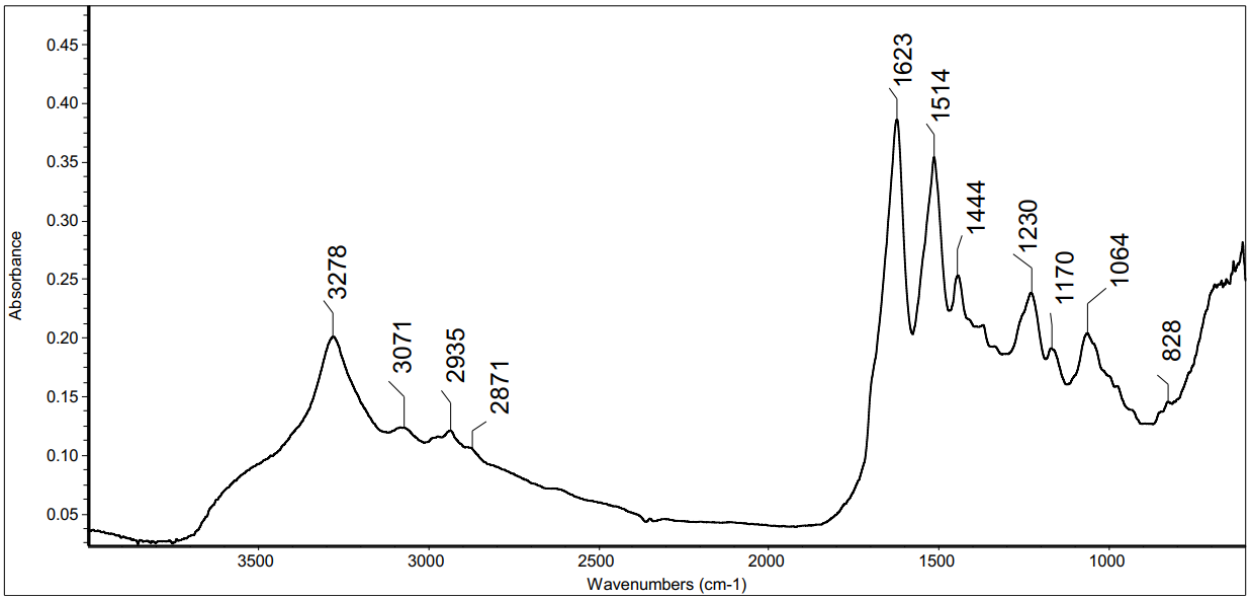


Figure S45. Examples of mATR-FT-IR spectra of sample 3.2

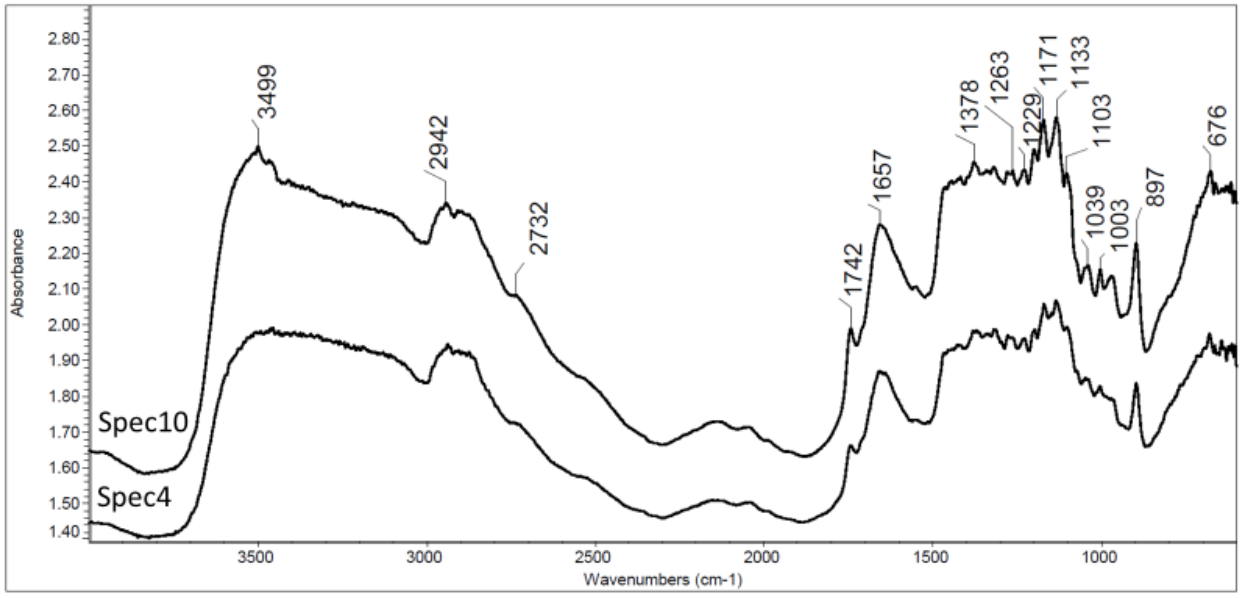


Figure S46. Examples of r-FT-IR spectra of sample 4. Two spectra are presented to show the spectral differences within the sample.

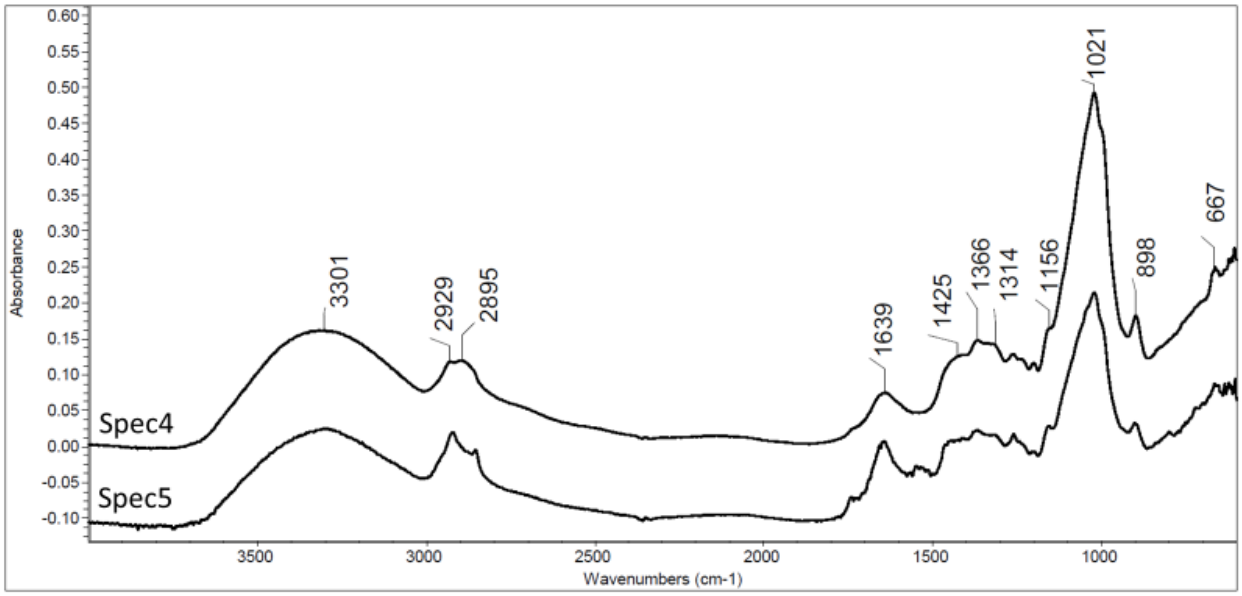


Figure S47. Examples of mATR-FT-IR spectra of sample 4. Two spectra are presented to show the spectral differences within the sample.

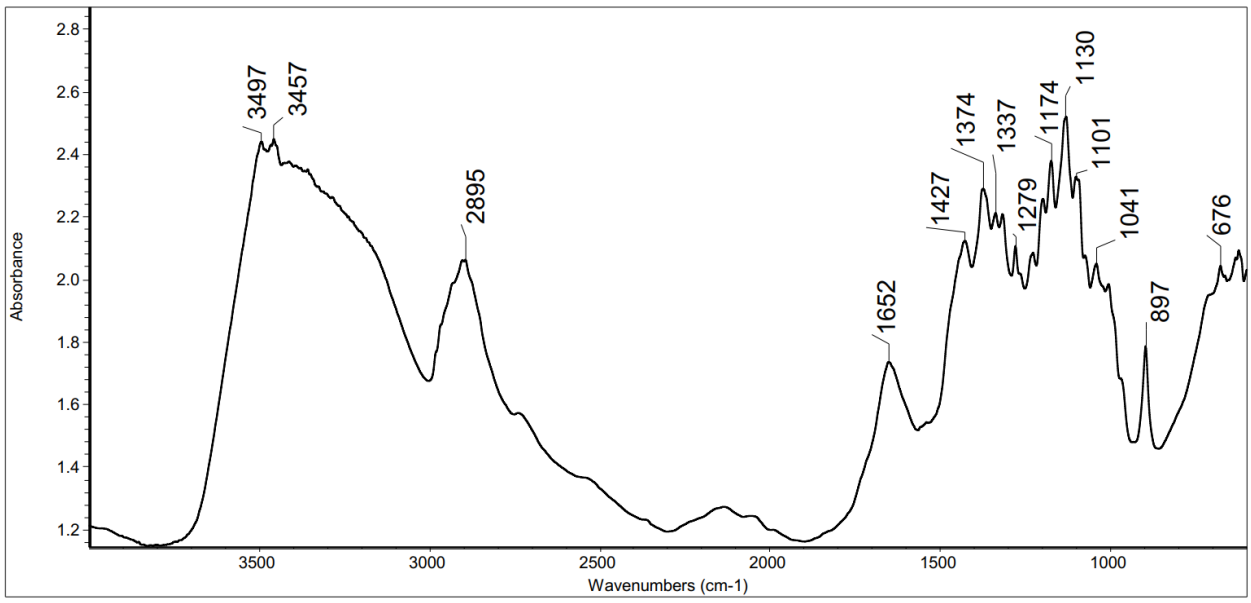


Figure S48. Example of r-FT-IR spectrum of sample 5.1

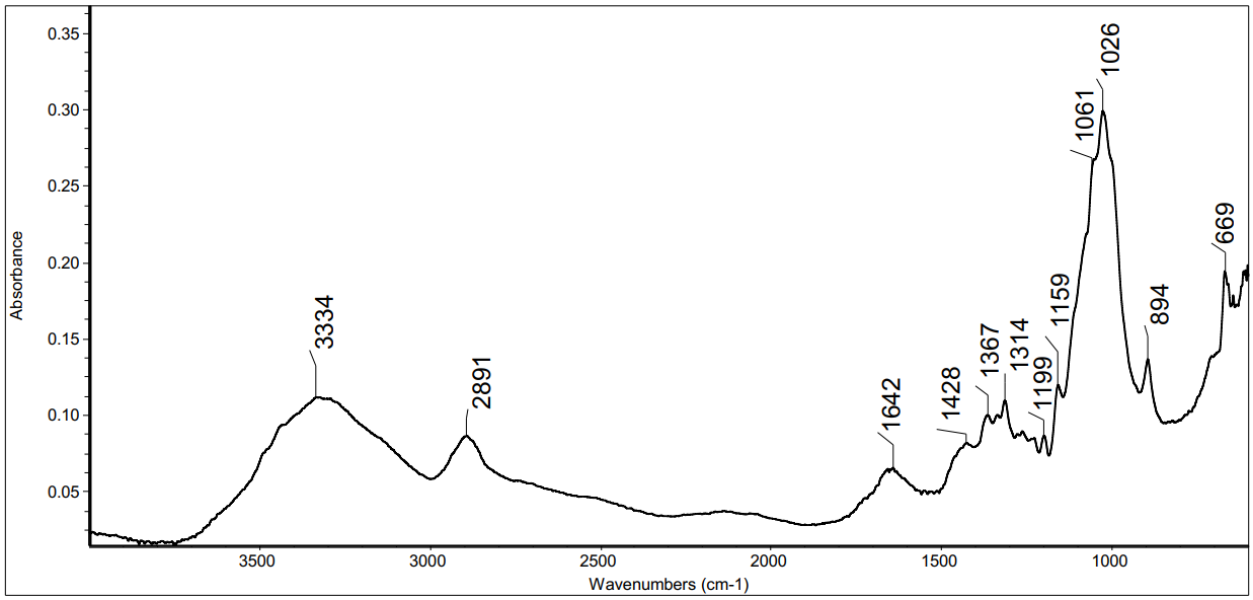


Figure S49. Examples of mATR-FT-IR spectra of sample 5.1

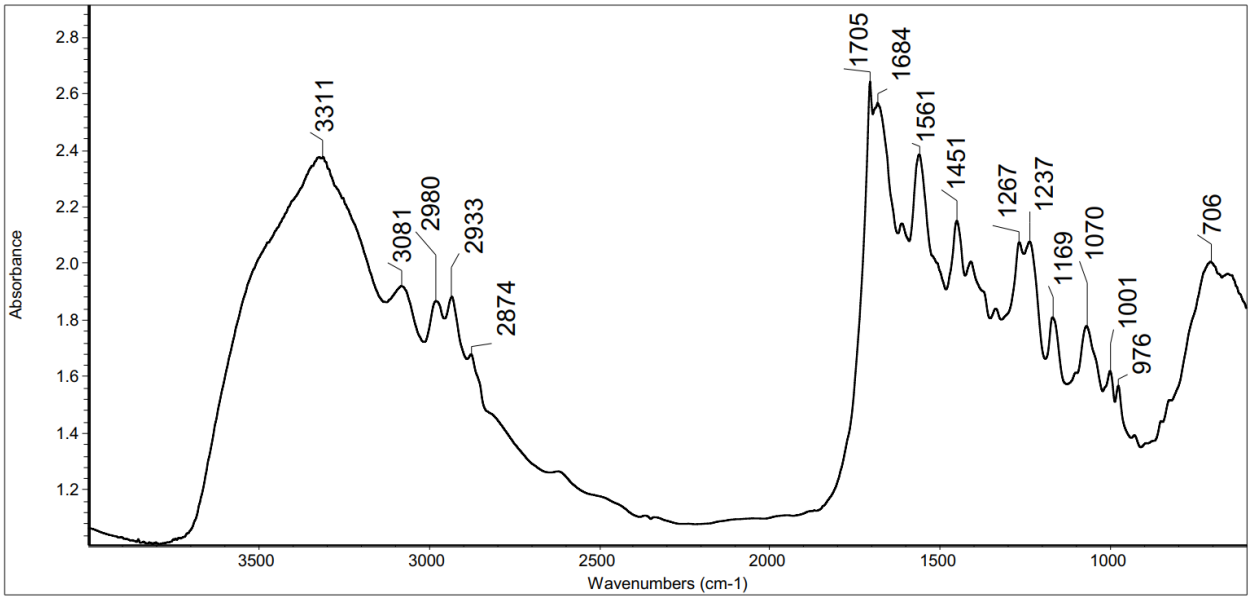


Figure S50. Example of r-FT-IR spectrum of sample 5.2

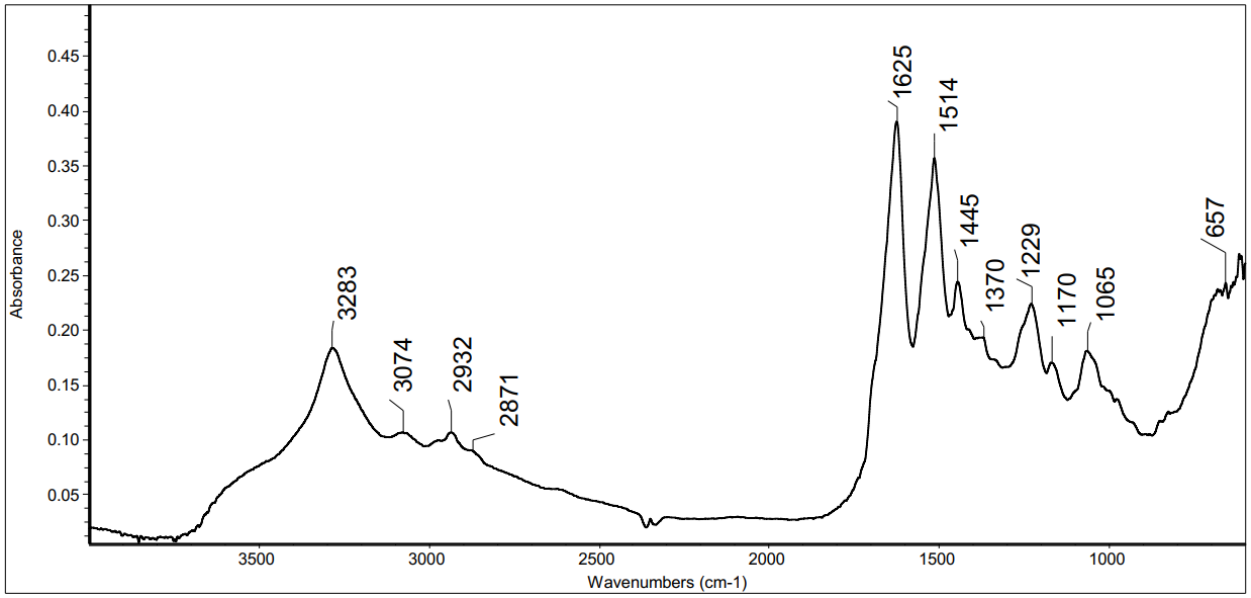


Figure S51. Examples of mATR-FT-IR spectra of sample 5.2

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).

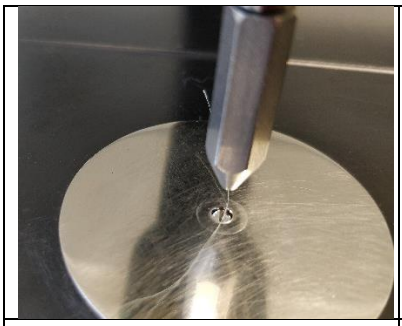


Figure S53. Picture of the analyzed fiber on ATR diamond crystal.

Figure S54. Microscope picture of the fibers

Figure S55. Microscope picture of the fibers

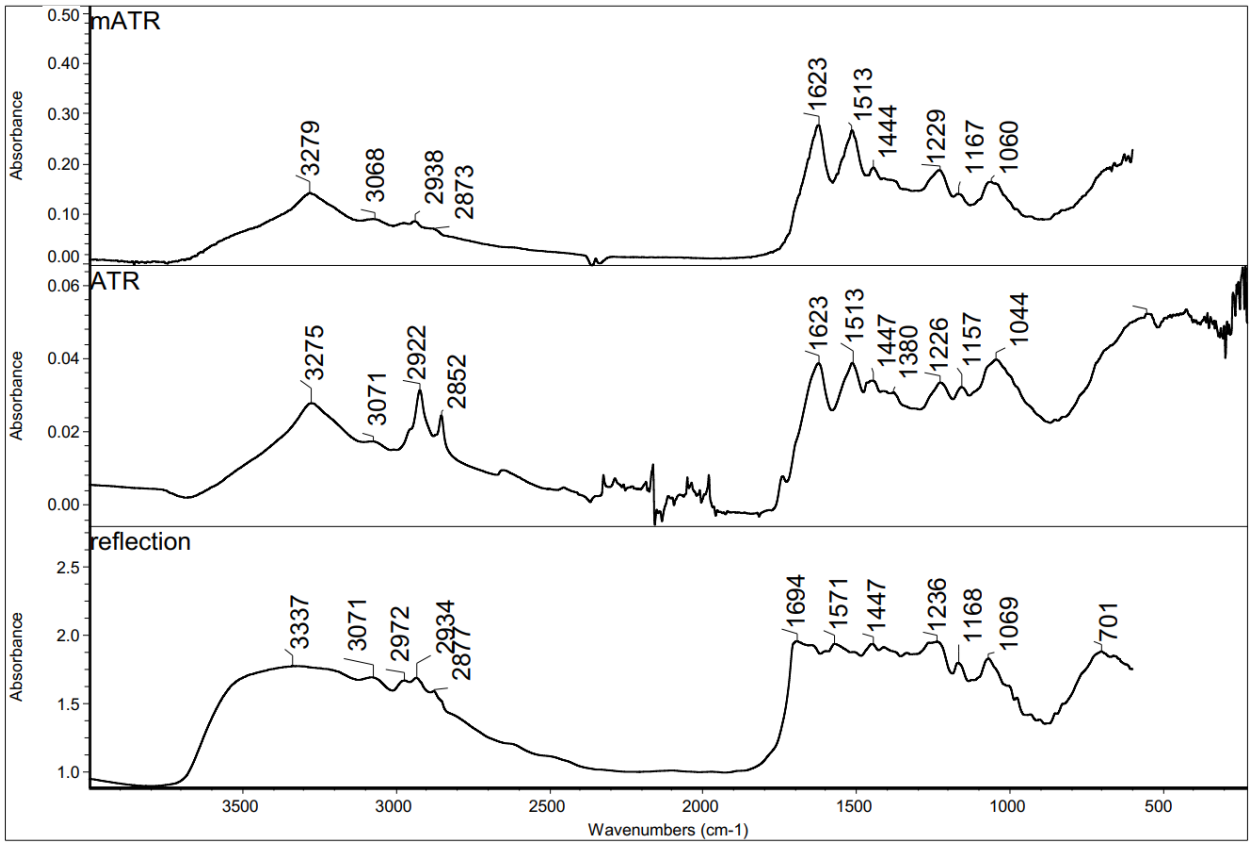


Figure S56. FT-IR spectra of analyzed paint fiber. Spectra are recorded using FT-IR microspectrometer in ATR mode, ATR-FT-IR spectrometer and FT-IR microspectrometer in reflectance mode.

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