

Supplementary Material to the article “Analysis of skin neoplasms’ Raman spectra using the Lorentz approximation method: pilot studies”

Table S1. The description of analyzed samples, including histological analysis, the type of sample storage medium, and gender and age of patients from whom tumors were removed.

Sample, #	Histological analysis	Storage medium	Gender	Age
1	Normal skin	NaCl solution 0,9 %	f	37
2	Normal skin	NaCl solution 0,9 %	m	55
3	Normal skin	NaCl solution 0,9 %	f	48
4	Normal skin	NaCl solution 0,9 %	m	39
5	Normal skin	NaCl solution 0,9 %	f	43
6	Ulcerated basal cell cancer with adnexal (adenoid and piloid) differentiation, growing into the reticular layer of the dermis	NaCl solution 0,9 %	m	55
7	Superficial spreading and nodular basal cell carcinoma with ulceration, with invasion into the reticular layer of the dermis (R1); LV0 Pn0; pT2. 2.	NaCl solution 0,9 %	f	59
8	Superficial spreading and nodular basal cell carcinoma with ulceration, with invasion into the reticular layer of the dermis, without reliable signs of lymphovascular and perineural invasion (R1); LV0 Pn0; pT1.	NaCl solution 0,9 %	m	58
9	Nodular basal cell carcinoma, extended, with ulceration, with invasion into the reticular layer of the dermis and subcutaneous fat layer, without reliable signs of lymphovascular and perineural invasion (LV0, Pn0).	NaCl solution 0,9 %	m	55
10	Ulcerated nodular basal cell cancer growing into the reticular layer of the dermis without convincing signs of lymphovascular and perineural invasion.	NaCl solution 0,9 %	m	39

11	Multicentric superficially spreading basal cell cancer with adnexal (piloid) differentiation, growing into the reticular layer of the dermis.	NaCl solution 0,9 %	f	60
12	Superficial spreading and nodular basal cell carcinoma, with ulceration, with invasion into the reticular layer of the dermis, without reliable signs of lymphovascular and perineural invasion (R1); LV0 Pn0; pT1.	NaCl solution 0,9 %	f	70
13	Squamous cell keratinizing carcinoma	NaCl solution 0,9 %	f	62
14	Ulcerated well-differentiated squamous cell keratinizing carcinoma	NaCl solution 0,9 %	m	50
15	Squamous cell keratinizing carcinoma	NaCl solution 0,9 %	f	54
16	Ulcerated, highly differentiated squamous cell keratinizing carcinoma with invasion into the dermis, without reliable signs of angiolymphatic and perineural invasion. pT1 LV0 Pn0; R0.	NaCl solution 0,9 %	m	51
17	Non-keratinizing squamous cell carcinoma	NaCl solution 0,9 %	f	49
18	Invasive squamous cell weakly keratinizing carcinoma, G2 with severe squamous intraepithelial neoplasia high grade SIN III.	NaCl solution 0,9 %	m	50
19	Papilloma	NaCl solution 0,9 %	m	67
20	Papilloma	NaCl solution 0,9 %	f	73
21	Papilloma	NaCl solution 0,9 %	m	69

Table S2. Parameters of Raman spectral bands of healthy skin, BCC, SCC and papilloma for spectra obtained upon excitation at wavelengths of 532 nm and 785 nm. Each cell contains up to three rows corresponding to the spectral position of the peak, its width, and the area under the curve.

Wavenumber, cm^{-1}
Width, cm^{-1}

Spectral bands' assignment	Area, arb. units							
	Laser excitaion wavelength 785 nm				Laser excitaion wavelength 532 nm			
	Normal skin	BCC	SCC	Papilloma	Normal skin	BCC	SCC	Papilloma
α -helices in proteins	–	959.39 39.42±3.56 7.92±0.86	960.42 53.71±5.65 10.98±1.61	958.40 36.28±1.42 5.59±0.26	–	961.48 22.02±5.59 1.61±0.34	963.92 13.18±12.27 0.15±0.11	967.58 15.44±4.74 0.23±0.12
Proteins	972.01	–	–	–	971.23	–	–	–
β -sheets in proteins	–	–	–	–	–	983.41	984.63	983.41
CH, Tyr, Phe	1030.34 18.68±1.00 5.68±0.59	1030.35 14.55±1.54 4.33±0.93	1031.39 18.59±0.87 6.64±0.73	1031.31 18.82±1.96 4.97±1.36	1031.95 20.27±1.66 3.70±0.37	1031.95 18.07±2.54 3.14±0.56	1033.16 14.14±2.42 3.28±1.05	1034.37 31.07±4.45 9.05±2.65
C–C in lipids	1061.44 15.72±1.09 3.88±0.46	1061.46 23.15±2.03 7.07±1.33	1062.50 30.52±3.64 6.74±1.41	1061.44 30.05±5.78 5.56±2.65	1063.36 33.26±3.91 5.63±0.90	1063.36 41.13±5.70 8.69±1.58	–	–
–PO ₂ in nucleic acids	–	1104.23	1103.32	1100.33	–	1099.45	1103.85	1101.85
Lipids	1127.55	1127.56	1127.63	1127.55	1127.04	1128.24	1127.04	1128.24
C–N, C–C phospholipids	14.34±0.79 4.29±0.29	14.42±1.07 5.14±0.58	14.92±0.95 4.52±0.44	14.64±0.90 4.52±0.43	21.95±1.71 4.46±0.49	14.46±1.05 4.76±0.40	17.01±1.92 5.90±1.09	19.67±1.41 10.94±1.21
C–C ₆ H ₅ , tryptophan, Phe (proteins)	1207.26	1206.30	1207.34	1207.26	1204.51	1208.07	1205.70±0	1208.07
Amide III β -sheets in proteins	1238.37	1236.44	–	–	–	–	–	–
CH ₂ , CN, Amide III in disordered state RNA, C, T	–	–	1244.28	1244.28	–	1248.31 26.24±5.04 4.43±0.78	1243.58 42.36±2.78 13.01±0.86	1241.22 44.18±2.07 20.44±1.38
Amide III in disordered state	–	1252.97	–	1251.01	–	1252.41	–	–
Amide III β -sheets in proteins	1263.65	1268.52	1268.58	1267.53	1264.82	1264.82	1266.00	1270.71
CH ₂ in saturated lipids	1297.67 23.56±3.24 10.50±2.02	1298.66 27.17±4.45 10.82±2.80	1299.69 40.33±1.40 16.38±1.06	1299.61 39.39±4.76 17.94±4.09	1301.28 30.22±1.14 20.20±0.75	1298.93 43.29±2.12 29.06±1.31	1309.49 40.32±1.60 24.03±1.01	1308.31 31.94±1.11 21.37±1.29
A, G in nucleic acids; CH in proteins	1342.39 9.67±5.37 0.94±0.51	1342.40 11.25±3.40 1.65±0.54	1342.46 30.34±0.70 13.13±0.49	1341.42 33.38±2.14 18.41±1.99	1344.59 35.10±6.96 3.53±0.61	1341.08 24.07±3.39 4.95±0.70	1339.91 19.9±1.26 6.13±0.44	1339.91 38.42±1.52 24.40±1.33
Ceramide III	1416.27	1417.82	1419.26	1419.18	1412.25	1414.28	1416.21	1416.82
CH ₂ in lipids, in proteins	1439.60 26.69±1.14 32.89±1.45	1440.58 28.84±0.70 36.43±0.89	1447.45 30.36±0.21 33.03±0.28	1444.46 29.73±0.42 33.02±0.52	1438.60 21.51±0.76 28.06±0.93	1439.80 21.64±0.83 25.12±0.93	1447.88 31.33±0.49 26.31±0.53	1444.42 30.55±0.43 34.01±0.53
CH ₂ in lipids, in proteins	1462.93 25.11±1.65 17.66±1.46	1461.00 24.49±1.08 19.55±0.89	1464.95 23.68±0.33 11.12±0.18	1462.93 25.26±0.66 14.89±0.48	1459.41 21.38±1.36 15.73±0.94	1459.41 21.27±1.17 17.44±0.92	1461.72 21.11±2.12 4.57±0.51	1461.98 23.60±0.79 12.54±0.46
Amide I α - helices in proteins	1655.41 33.35±0.89 43.00±2.08	1651.53 30.39±1.05 34.69±2.28	1652.56 41.60±0.37 58.62±0.80	1658.33 40.96±0.92 63.13±1.97	1654.20 29.11±0.52 36.65±0.73	1653.07 31.58±1.30 29.40±1.79	1650.82 40.47±1.23 55.73±1.66	1658.70 50.13±0.38 79.72±0.87
C=O esters	–	–	–	–	–	1740.47	1734.90	1732.67
C=O esters in triglycerides	1745.82 47.53±5.48 15.06±3.39	1745.83 59.09±7.56 16.12±4.28	1749.78 80.28±2.74 16.16±0.59	1740.96 64.79±9.38 13.88±3.90	1744.93	–	–	–
	–	–	–	–	–	1757.18	1751.61	1763.45

Table S3. Parameters of Raman spectral bands of healthy skin, BCC, SCC and papilloma for spectra obtained upon excitation at wavelengths of 532 nm and 785 nm. Each cell contains up to three rows corresponding to the spectral position of the peak, its width, and the area under the curve.

Spectral bands' assignment	Wavenumber, cm ⁻¹							
	Width, cm ⁻¹							
	Area, arb. units							
	785 nm				532 nm			
Normal skin	BCC	SCC	Papilloma	Normal skin	BCC	SCC	Papilloma	
CH ₃ , C-C, α -helices (proteins),	936.04 40.14±1.73 13.18±0.78	935.08 22.76±1.08 7.80±0.35	936.12 23.06±1.33 6.54±0.36	936.04 33.28±0.82 7.90±0.22	937.05 17.87±1.43 0.75±0.04	934.60 18.96±2.50 2.65±0.30	935.82 20.21±1.02 3.57±0.14	932.15 26.01±1.09 2.03±0.19

amino acids, collagen								
CH ₂ , C–C, α- helices in proteins	– 44.73±5.57 5.20±0.71	959.39 39.42±3.56 7.92±0.86	960.42 53.71±5.65 10.98±1.61	958.40 36.28±1.42 5.59±0.26	– 12.87±0.99 0.66±0.03	961.48 22.02±5.59 1.61±0.34	963.92 13.18±12.27 0.15±0.11	967.58 15.44±4.74 0.23±0.12
Proteins	972.01 44.73±5.57 5.20±0.71	–	–	–	971.23 12.87±0.99 0.66±0.03	–	–	–
β-sheets in proteins	987.94	986.29	987.55	986.29	–	983.41	984.63	983.41
Phe ring, C–C in proteins	1003.12 15.83±0.72 8.20±0.57	1003.13 16.98±0.63 12.06±0.73	1003.20 17.52±0.49 12.48±0.57	1003.12 18.24±0.45 17.96±0.80	1004.07 32.20±2.01 11.15±1.23	1004.07 22.75±1.19 10.75±0.79	1004.07 23.27±1.33 12.92±1.16	1005.29±0 23.70±0.86 24.21±1.83
CH, Tyr, Phe	1030.34 18.68±1.00 5.68±0.59	1030.35 14.55±1.54 4.33±0.93	1031.39 18.59±0.87 6.64±0.73	1031.31 18.82±1.96 4.97±1.36	1031.95 20.27±1.66 3.70±0.37	1031.95 18.07±2.54 3.14±0.56	1033.16 14.14±2.42 3.28±1.05	1034.37 31.07±4.45 9.05±2.65
PO ₄ (HA) C–CH ₃ in lactic acid	1045.89 25.94±5.76 4.11±1.22	1046.88 30.79±7.75 7.49±2.74	1046.94 29.25±3.70 9.44±1.76	1047.83 35.87±12.81 6.76±4.11	–	–	1050.09 36.63±7.89 13.43±5.05	–
C–C in lipids	1061.44 15.72±1.09 3.88±0.46	1061.46 23.15±2.03 7.07±1.33	1062.50 30.52±3.64 6.74±1.41	1061.44 30.05±5.78 5.56±2.65	1063.36 33.26±3.91 5.63±0.90	1063.36 41.13±5.70 8.69±1.58	–	–
PO ₂ , C–C, C–O in nucleic acids, in lipids	1083.80 56.74±2.07 28.47±1.97	1081.87 28.93±2.30 9.65±1.39	1082.91 28.85±2.42 7.30±1.07	1082.83 37.00±6.04 10.44±3.09	1085.04 49.65±2.21 20.64±1.44	1087.44 66.34±6.94 18.52±2.86	1082.63 43.72±23.78 7.44±6.98	1085.04 84.62±6.19 65.85±11.01
–PO ₂ in nucleic acids	–	1104.23 38.56±6.79 7.74±1.95	1103.32 37.99±3.43 10.31±1.29	1100.33 47.82±4.71 15.07±1.88	–	–	–	–
Lipids C–N, C–C phospholipids	1127.55 14.34±0.79 4.29±0.29	1127.56 14.42±1.07 5.14±0.58	1127.63 14.92±0.95 4.52±0.44	1127.55 14.64±0.90 4.52±0.43	1127.04 21.95±1.71 4.46±0.49	1128.24 14.46±1.05 4.76±0.40	1127.04 17.01±1.92 5.90±1.09	1128.24 19.67±1.41 10.94±1.21
CC, COH C–C, C–N in proteins (also carotenoids), glycogen	1156.71 5.85±1.47 0.43±0.10	1156.73 11.89±1.41 1.72±0.23	1155.82 10.42±1.27 1.13±0.16	1155.74 15.14±0.35 7.533±0.24	1155.73 10.89±0 0.27±0	1156.92 12.45±0 0.52±0	1155.73 13.19±2.73 1.60±0.36	1155.73 23.33±1.01 14.60±0.83
C–C C, G	1174.21 34.11±3.41 8.52±1.39	1175.20 33.64±3.51 9.18±1.50	1175.26 35.56±2.98 9.32±1.25	1176.15 47.27±4.18 13.92±2.15	1175.99 36.84±5.41 4.98±1.38	1177.18 23.57±4.31 3.31±0.87	1173.61 18.51±3.74 2.88±0.81	1177.18 47.79±8.04 23.83±8.11
C–C ₆ H ₅ , Tryptophan, Phe (proteins)	1207.26 28.36±5.60 5.73±1.24	1206.30 23.89±3.05 6.55±0.98	1207.34 16.84±0.70 3.13±0.16	1207.26 37.20±1.60 12.04±0.73	1204.51	1208.07	1205.70	1208.07

tyrosine								
Amide III β - sheets in proteins CH ₂ , CN, Amide III in disordered state RNA, C, T	1238.37 21.95 \pm 5.77 3.89 \pm 1.42	1236.44 25.00 \pm 4.70 5.52 \pm 1.81	1244.28 42.75 \pm 0.80 16.25 \pm 0.48	1237.40 23.89 \pm 1.33 6.62 \pm 0.64	—	1248.31 26.24 \pm 5.04 4.43 \pm 0.78	1243.58 42.36 \pm 2.78 13.01 \pm 0.86	1241.22 44.18 \pm 2.07 20.44 \pm 1.38
Amide III in disordered state (?)	—	1252.97 26.45 \pm 10.58 5.80 \pm 3.22	—	1251.01 23.27 \pm 3.04 5.08 \pm 1.18	—	—	—	—
Amide III β - sheets in proteins	1263.65 41.43 \pm 5.56 20.95 \pm 3.48	1268.52 38.24 \pm 8.66 12.61 \pm 4.10	1268.58 42.31 \pm 2.03 13.74 \pm 1.07	1267.53 40.11 \pm 4.00 22.63 \pm 3.97	1264.82 48.29 \pm 2.19 18.72 \pm 0.78	1264.82 6.32 \pm 5.17 0.40 \pm 0.30	1266.00 23.20 \pm 6.96 1.93 \pm 0.65	—
CH ₂ in saturated lipids	1297.67 23.56 \pm 3.24 10.50 \pm 2.02	1298.66 27.17 \pm 4.45 10.82 \pm 2.80	1299.69 40.33 \pm 1.40 16.38 \pm 1.06	1299.61 39.39 \pm 4.76 17.94 \pm 4.09	1301.28 30.22 \pm 1.14 20.20 \pm 0.75	1298.93 43.29 \pm 2.12 29.06 \pm 1.31	1309.49 40.32 \pm 1.60 24.03 \pm 1.01	1308.31 31.94 \pm 1.11 21.37 \pm 1.29
	1320.03 97.39 \pm 5.02 68.30 \pm 5.53	1319.07 72.45 \pm 3.05 59.37 \pm 3.94	1318.16 37.20 \pm 1.14 17.09 \pm 0.85	1318.08 33.16 \pm 3.21 11.60 \pm 2.50	—	—	—	—
A, G in nucleic acids; CH in proteins	1342.39 9.67 \pm 5.37 0.94 \pm 0.51	1342.40 11.25 \pm 3.40 1.65 \pm 0.54	1342.46 30.34 \pm 0.70 13.13 \pm 0.49	1341.42 33.38 \pm 2.14 18.41 \pm 1.99	1344.59 35.10 \pm 6.96 3.53 \pm 0.61	1341.08 24.07 \pm 3.39 4.95 \pm 0.70	1339.91 19.9 \pm 1.26 6.13 \pm 0.44	1339.91 38.42 \pm 1.52 24.40 \pm 1.33
Tryptophan	—	—	1366.76 14.22 \pm 3.71 0.50 \pm 0.16	1358.91 16.24 \pm 6.52 0.85 \pm 0.60	1370.24	1370.24	—	1364.41
	—	—	—	1374.47 32.44 \pm 8.05 3.20 \pm 1.12	—	—	—	—
CH ₃ in lipids	—	—	1398.84 35.51 \pm 1.32 7.66 \pm 0.33	1397.80 32.82 \pm 3.63 5.94 \pm 0.96	1398.13	1395.81	1393.49	1396.97
	1416.27 9.95 \pm 3.73 1.43 \pm 0.55	—	1419.26 11.06 \pm 1.31 0.74 \pm 0.10	1419.18 7.02 \pm 3.32 0.30 \pm 0.15	—	—	—	—
CH ₂ in lipids, in proteins	1439.60 26.69 \pm 1.14 32.89 \pm 1.45	1440.58 28.84 \pm 0.70 36.43 \pm 0.89	1447.45 30.36 \pm 0.21 33.03 \pm 0.28	1444.46 29.73 \pm 0.42 33.02 \pm 0.52	1438.6 21.51 \pm 0.76 28.06 \pm 0.93	1439.80 21.64 \pm 0.83 25.12 \pm 0.93	1447.88 31.33 \pm 0.49 26.31 \pm 0.53	1444.42 30.55 \pm 0.43 34.01 \pm 0.53
CH ₂ in lipids, in proteins	1462.93 25.11 \pm 1.65 17.66 \pm 1.46	1461.00 24.49 \pm 1.08 19.55 \pm 0.89	1464.95 23.68 \pm 0.33 11.12 \pm 0.18	1462.93 25.26 \pm 0.66 14.89 \pm 0.48	1459.41 21.38 \pm 1.36 15.73 \pm 0.94	1459.41 21.27 \pm 1.17 17.44 \pm 0.92	1461.72 21.11 \pm 2.12 4.57 \pm 0.51	1461.98 23.60 \pm 0.79 12.54 \pm 0.46

A, G	—	—	1493.14 11.06±1.91 0.52±0.10	—	—	—	1490.47 6.24±2.76 0.39±0.13	—
C = C carotenoids Cytosine β-carotene	—	—	—	—	1513.40	1513.40	1514.54	1514.54
	—	1520.30 54.21±11.13 9.38±3.77	—	1522.23 24.20±2.30 9.73±1.49	—	—	—	—
Amide II C=O, N-H	1527.09 58.74±12.17 10.24±4.21	—	—	—	1537.41	1536.26	1536.26	—
NH, CN Amide II tryptophan	1555.28 26.45±4.23 3.25±0.59	1553.35 26.09±2.54 5.17±0.75	1554.38 18.66±1.12 1.96±0.16	1553.34 16.97±2.64 2.87±0.57	1553.37 22.77±4.55 2.82±0.57	1553.37 26.62±4.79 2.99±0.66	1553.37 21.67±3.85 4.18±0.65	1552.23 29.96±0.93 10.80±0.39
C=C C-C in Phe	1579.58 19.038.25 1.25±0.87	1582.51 28.85±4.57 5.02±1.48	1584.52 43.01±2.48 6.94±0.48	1582.50 34.67±6.10 7.02±1.85	1582.95 18.97±6.17 1.41±0.51	1584.09 12.45±6.72 0.67±0.45	1582.95 20.38±4.59 4.17±0.99	1582.95 25.33±0.51 15.31±0.38
Phe	1604.86 9.17±4.78 0.43±0.25	1603.90 23.80±2.52 5.32±1.06	1604.93 10.15±1.13 0.71±0.11	1604.86 14.26±2.42 2.72±0.75	1605.64 50.31±6.65 8.90±1.31	1605.64 52.84±8.01 13.60±2.52	1604.50 26.41±5.13 6.41±1.41	1609.03 33.60±1.17 9.96±0.36
Tyrosine	1615.55 62.89±3.96 37.89±3.85	1614.59 25.73±3.71 7.42±1.99	1616.60 31.76±1.51 7.45±0.57	1619.44 21.31±3.67 6.51±1.39	1609.30	1609.43	1605.43	1609.30
	—	1631.12 30.64±5.27 6.82±2.36	—	1633.05 8.07±4.78 0.57±0.46	—	—	—	—
Amide I α- helices in proteins, C-C in lipids, C-O elastin in proteins	1655.41 33.35±0.89 43.00±2.08	1651.53 30.39±1.05 34.69±2.28	1652.56 41.60±0.37 58.62±0.80	1658.33 40.96±0.92 63.13±1.97	1654.20 29.11±0.52 36.65±0.73	1653.07 31.58±1.30 29.40±1.79	1650.82 40.47±1.23 55.73±1.66	1658.70 50.13±0.38 79.72±0.87
	1672.91 24.28±2.61 7.17±0.99	1670.00 30.18±1.25 24.14±1.59	1673.95 28.08±0.97 7.61±0.47	—	—	1669.09	—	—
Amide I	1690.41 15.72±3.10 2.17±0.66	1689.45 13.18±3.36 1.36±0.52	1685.62 26.48±0.99 4.68±0.30	1684.57 22.32±2.87 3.98±0.73	—	—	—	—
C=O-OH (amino acids, aspartic and	—	—	1723.53 1.21±8.29 0.00209±0.01	—	—	—	—	—

glutamic acids)			434					
C=O esters	–	–	–	–	–	1740.47	1734.90	1732.90
C=O esters in triglycerides	1745.82 47.53±5.48 15.06±3.39	1745.83 59.09±7.56 16.12±4.28	1749.78 80.28±2.74 16.16±0.59	1740.96 64.79±9.38 13.88±3.90	1744.93	–	–	–
	–	–	–	–	–	1757.18	1751.61	1763
C=O esters in triglycerides	–	–	–	–	1779.40	1779.40	–	–
	1745.82 47.53±5.48 15.06±3.39	1745.83 59.09±7.56 16.12±4.28	1749.78 80.28±2.74 16.16±0.59	1740.96 64.79±9.38 13.88±3.90	–	1804.88	–	–
	–	–	–	–	–	1892.92	–	–