

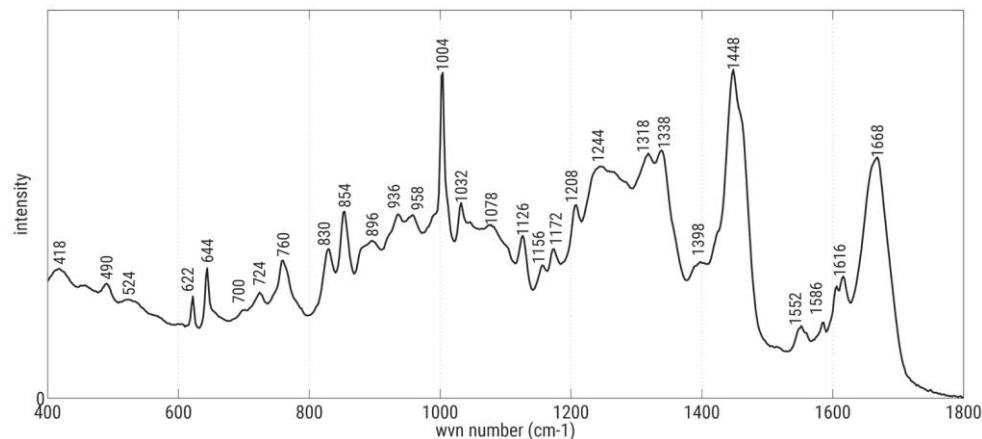
PURE-COMPOUND REFERENCE SPECTRA

A complete overview of the specifications (name, CAS-number, chemical class, firm, product number, purity, source, instrument, measured condition (dry/dissolved), solvent, concentration, pH, acquisition time, accumulations, spectral corrections and S/N ratio), as well as the peak positions of all pure- compound measurements are given.

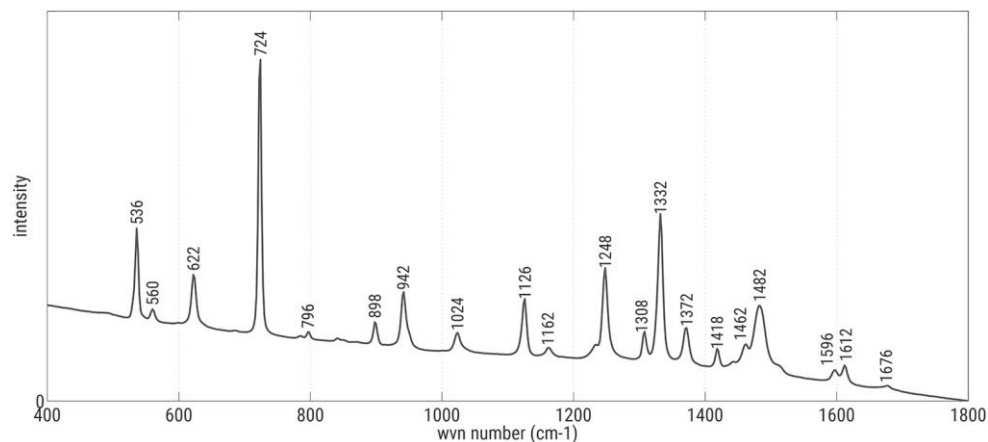
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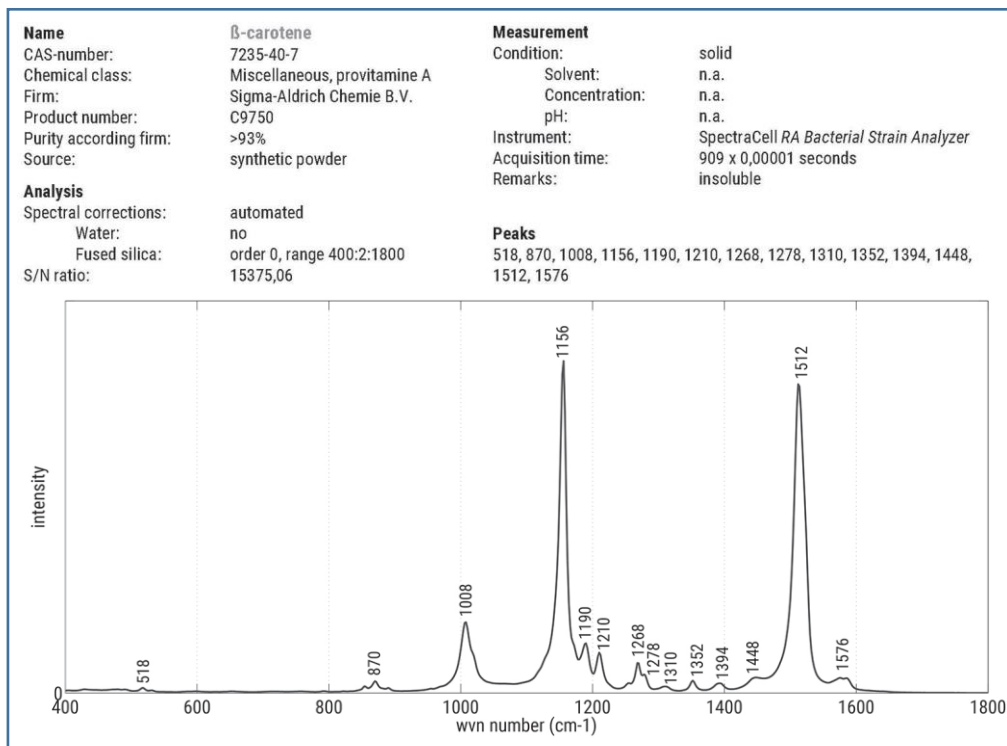
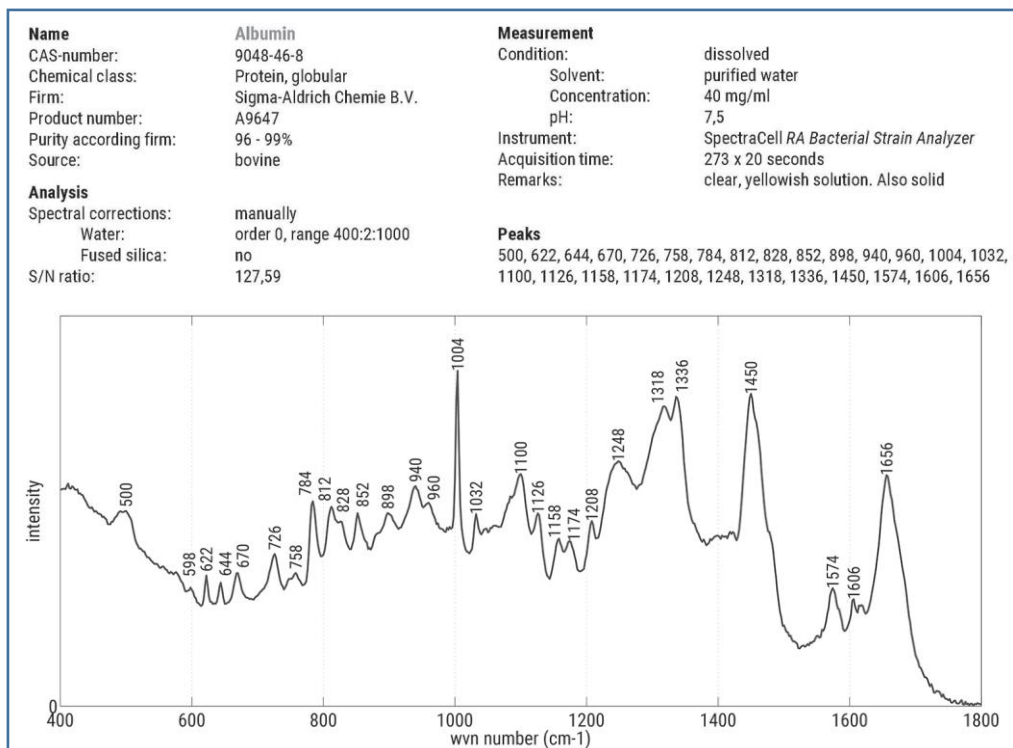
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Name	Actin	Measurement	
CAS-number:	51005-14-2	Condition:	solid
Chemical class:	Protein, globular	Solvent:	n.a.
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	n.a.
Product number:	A3653	pH:	n.a.
Purity according to firm:	99%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	bovine muscle	Acquisition time:	635 x 5 seconds
		Remarks:	soluble in H ₂ O, but in different solutions only water bands
Analysis		Peaks	
Spectral corrections:	automated		418, 490, 524, 622, 644, 700, 724, 760, 830, 854, 896, 936, 958, 1004, 1032, 1078, 1126, 1156, 1172, 1208, 1244, 1318, 1338, 1398, 1448, 1552, 1586, 1616, 1668
Water:	no		
Fused silica:	order 1, range 400:2:1800		
S/N ratio:	318,50		

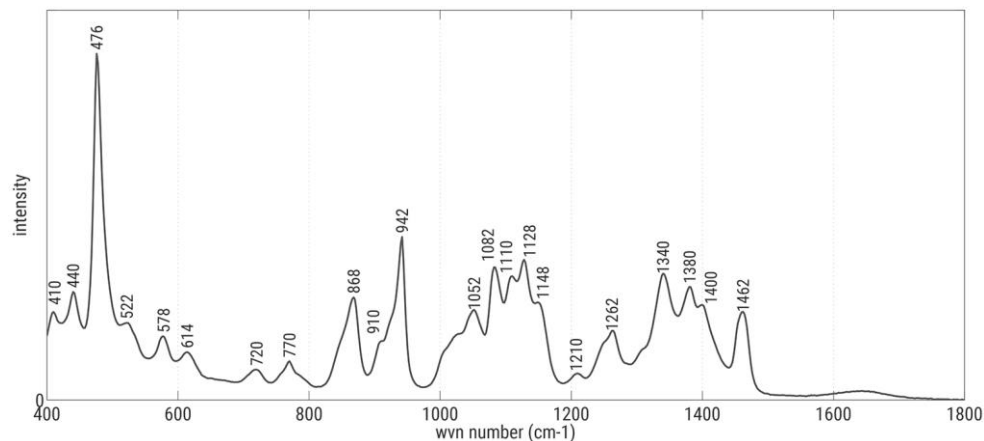


Name	Adenine	Measurement	
CAS-number:	73-24-5	Condition:	solid
Chemical class:	Nucleotide, purine	Solvent:	n.a.
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	n.a.
Product number:	A8626	pH:	n.a.
Purity according to firm:	>99%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	not mentioned	Acquisition time:	433 x 1 seconds
		Remarks:	soluble in NaOH 1M
Analysis		Peaks	
Spectral corrections:	automated		536, 560, 622, 724, 796, 796, 898, 942, 1024, 1126, 1162, 1248, 1308, 1332, 1372, 1418, 1462, 1482, 1596, 1612, 1612, 1676
Water:	no		
Fused silica:	order 1, range 400:2:1800		
S/N ratio:	2982,38		

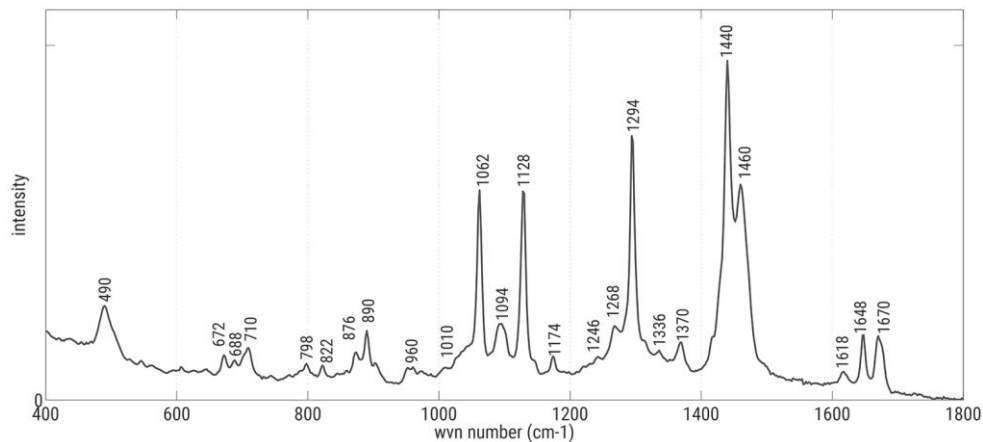




Name	Amylopectin	Measurement	
CAS-number:	9037-22-3	Condition:	dissolved
Chemical class:	Carbohydrate, polysaccharide	Solvent:	purified water
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	25 mg/ml
Product number:	10120	pH:	7,0
Purity according firm:	not mentioned	Instrument:	Skin Analyzer
Source:	maize	Acquisition time:	500 x 5 seconds
		Remarks:	heated, clear solution
Analysis		Peaks	
Spectral corrections:	automated		410, 440, 476, 522, 578, 614, 720, 770, 868, 910, 942, 1052, 1082, 1110, 1128, 1148, 1210, 1262, 1340, 1380, 1400, 1462
Water:	no		
Fused silica:	no		
S/N ratio:	1019,69		



Name	Ceramide	Measurement	
CAS-number:	3102-57-6	Condition:	solid
Chemical class:	Lipid, saturated fatty acid	Solvent:	n.a.
Firm:	Enzo Life Sciences, Inc	Concentration:	n.a.
Product number:	ALX303001	pH:	n.a.
Purity according firm:	>98%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	bovine brain	Acquisition time:	1191 x 5 seconds
		Remarks:	insoluble
Analysis		Peaks	
Spectral corrections:	automated		490, 672, 688, 710, 798, 822, 876, 890, 960, 1010, 1062, 1094, 1128, 1174, 1268, 1294, 1336, 1370, 1440, 1460, 1618, 1648, 1670
Water:	no		
Fused silica:	no		
S/N ratio:	280,54		

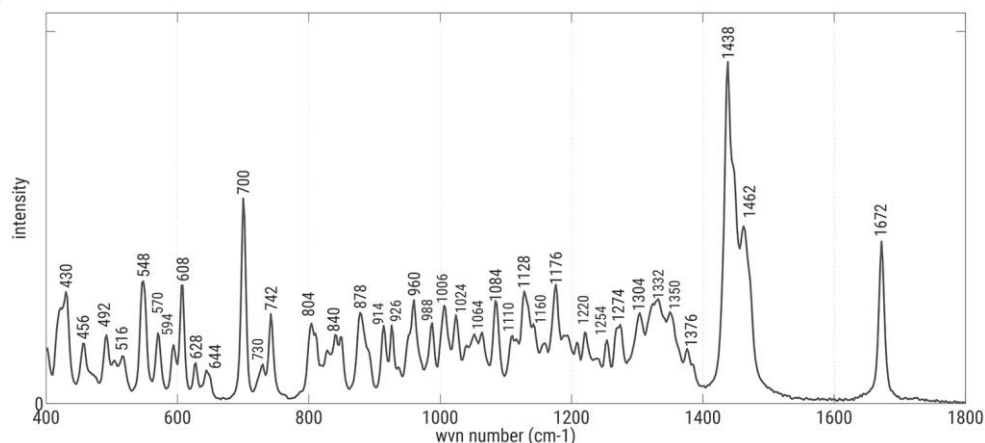


Name Cholesterol
CAS-number: 57-88-5
Chemical class: Lipid, sterol
Firm: Sigma-Aldrich Chemie B.V.
Product number: C8667
Purity according firm: 99%
Source: not mentioned

Measurement
Condition: solid
Solvent: n.a.
Concentration: n.a.
pH: n.a.
Instrument: SpectraCell RA Bacterial Strain Analyzer
Acquisition time: 3000 x 4 seconds
Remarks: insoluble

Analysis
Spectral corrections: automated
Water: no
Fused silica: order 0, range 400:2:1800
S/N ratio: 273,41

Peaks
 422, 430, 456, 492, 504, 516, 548, 570, 594, 608, 628, 644, 700, 730, 742, 804, 828, 840, 850, 878, 914, 926, 936, 960, 988, 1006, 1024, 1040, 1052, 1064, 1084, 1110, 1128, 1142, 1160, 1176, 1194, 1208, 1220, 1238, 1254, 1274, 1304, 1332, 1350, 1376, 1438, 1462, 1672

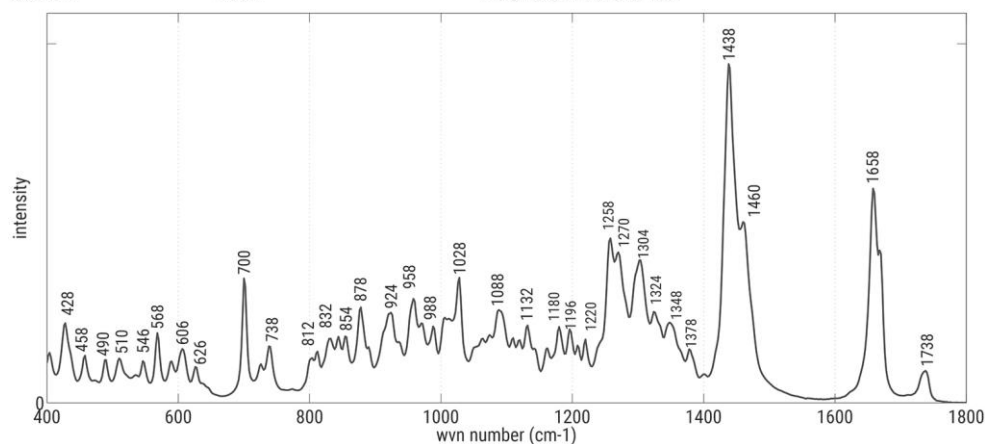


Name Cholesteryl linoleate
CAS-number: 604-33-1
Chemical class: Lipid, lipoprotein
Firm: Sigma-Aldrich Chemie B.V.
Product number: C0289
Purity according firm: >98%
Source: not mentioned

Measurement
Condition: solid
Solvent: n.a.
Concentration: n.a.
pH: n.a.
Instrument: SpectraCell RA Bacterial Strain Analyzer
Acquisition time: 270 x 15 seconds
Remarks: insoluble

Analysis
Spectral corrections: automated
Water: no
Fused silica: order 1, range 400:2:1800
S/N ratio: 960,58

Peaks
 404, 428, 458, 490, 510, 546, 568, 590, 606, 626, 700, 726, 738, 802, 812, 832, 844, 854, 878, 924, 958, 970, 988, 1006, 1028, 1064, 1074, 1088, 1110, 1120, 1132, 1162, 1180, 1196, 1208, 1220, 1258, 1270, 1304, 1324, 1348, 1378, 1438, 1460, 1658, 1738

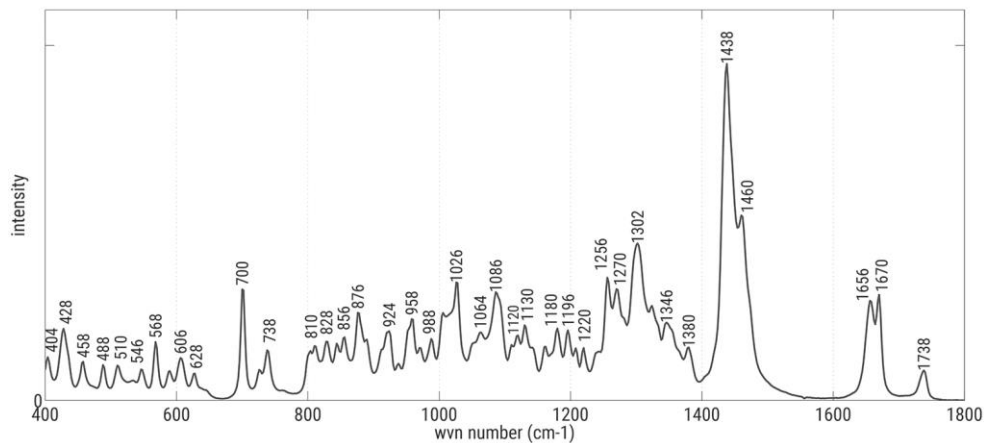


Name Cholesteryl oleate
CAS-number: 303-43-5
Chemical class: Lipid, lipoprotein
Firm: Sigma-Aldrich Chemie B.V.
Product number: C9253
Purity according firm: >98%
Source: not mentioned

Measurement
Condition: solid
Solvent: n.a.
Concentration: n.a.
pH: n.a.
Instrument: SpectraCell RA Bacterial Strain Analyzer
Acquisition time: 647 x 10 seconds
Remarks: insoluble

Analysis
Spectral corrections: automated
Water: no
Fused silica: order 1, range 400:2:1800
S/N ratio: 1381,33

Peaks
 404, 428, 458, 488, 510, 546, 568, 590, 606, 628, 700, 726, 738, 810, 828, 844, 856, 876, 890, 924, 938, 958, 970, 988, 1006, 1026, 1064, 1086, 1120, 1130, 1162, 1180, 1196, 1208, 1220, 1244, 1256, 1270, 1302, 1324, 1346, 1380, 1438, 1460, 1656, 1670, 1738

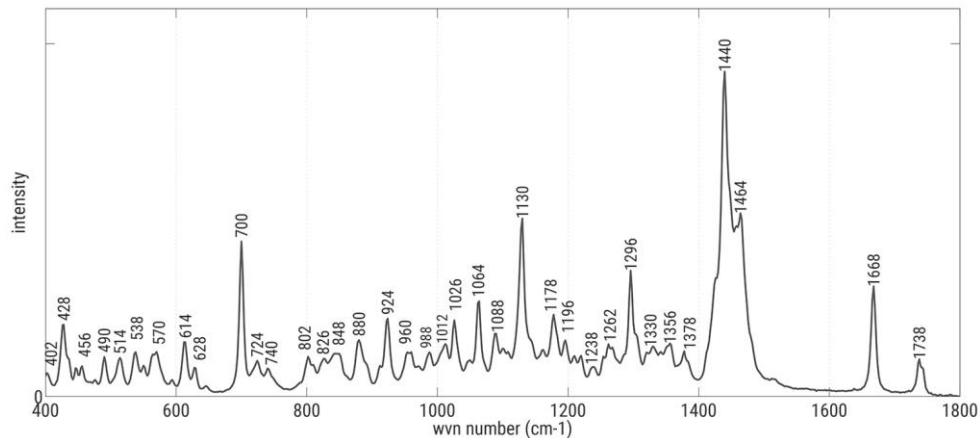


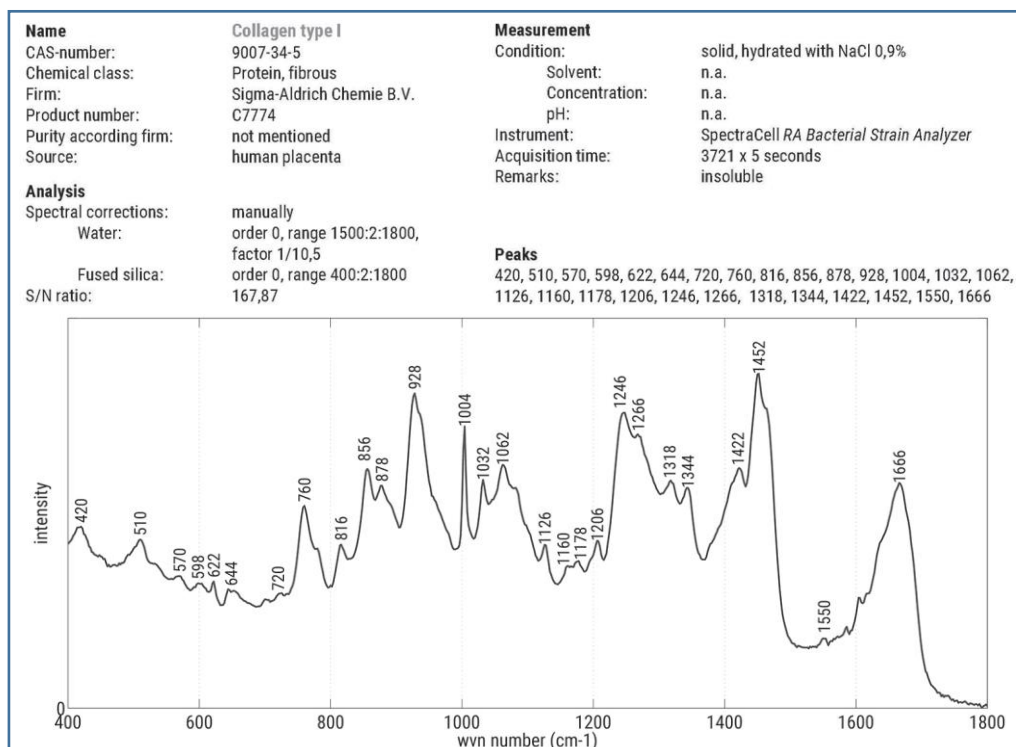
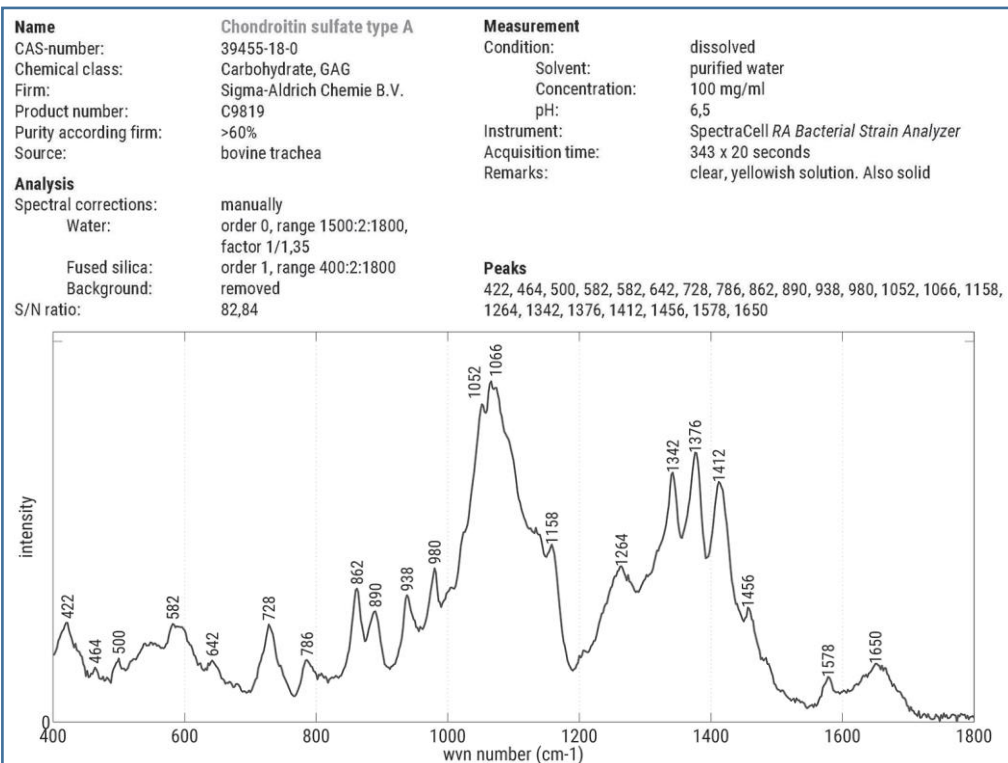
Name Cholesteryl palmitate
CAS-number: 601-34-3
Chemical class: Lipid, lipoprotein
Firm: Sigma-Aldrich Chemie B.V.
Product number: C6072
Purity according firm: >98%
Source: not mentioned

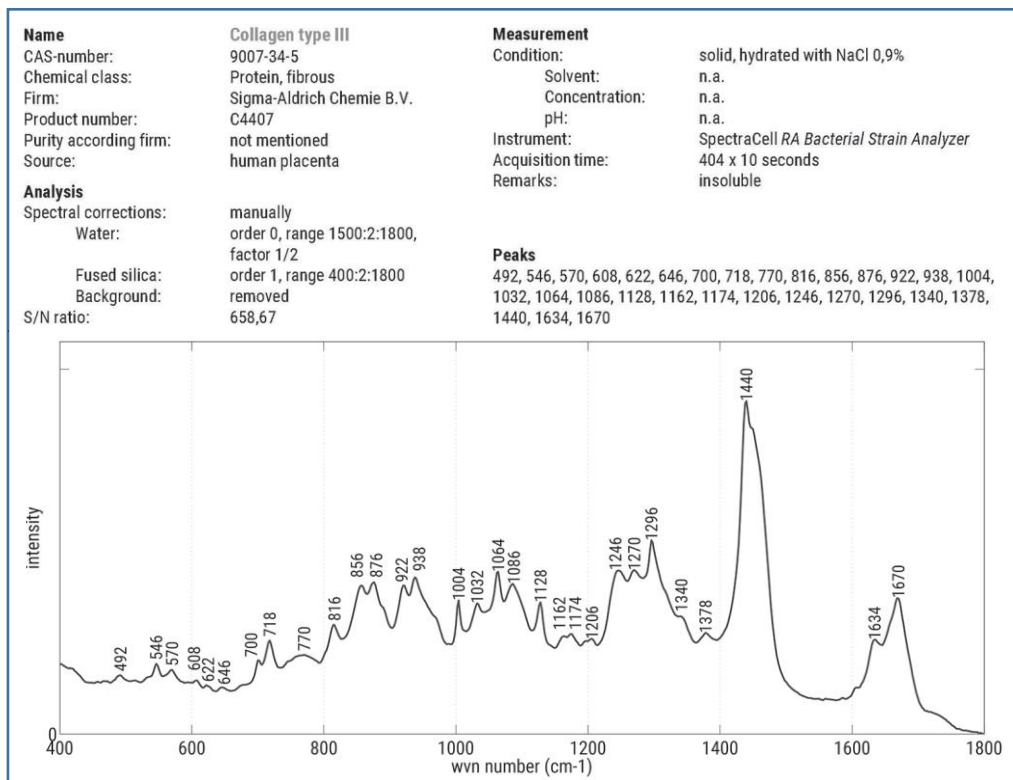
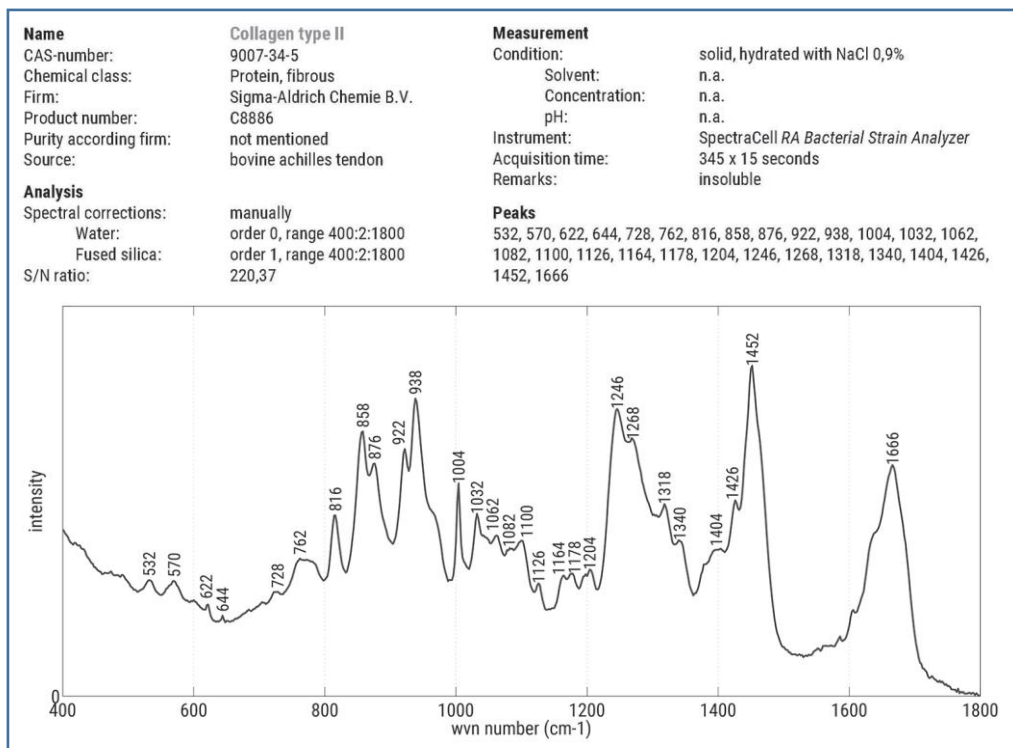
Measurement
Condition: solid
Solvent: n.a.
Concentration: n.a.
pH: n.a.
Instrument: SpectraCell RA Bacterial Strain Analyzer
Acquisition time: 1584 x 5 seconds
Remarks: insoluble

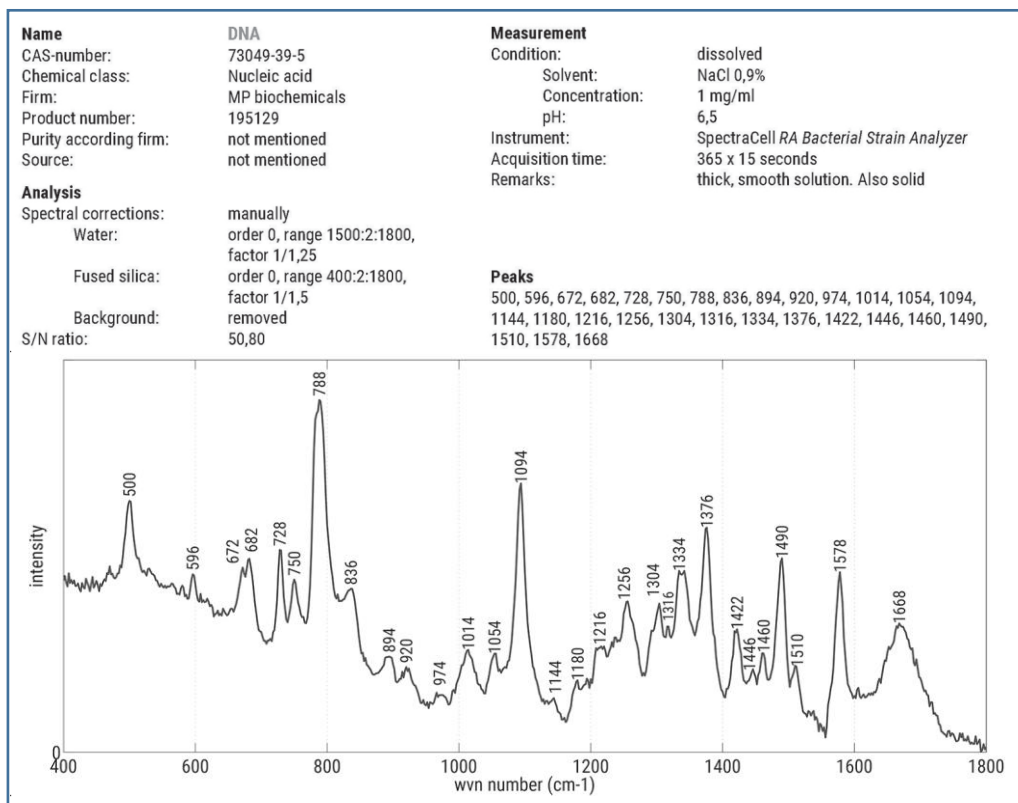
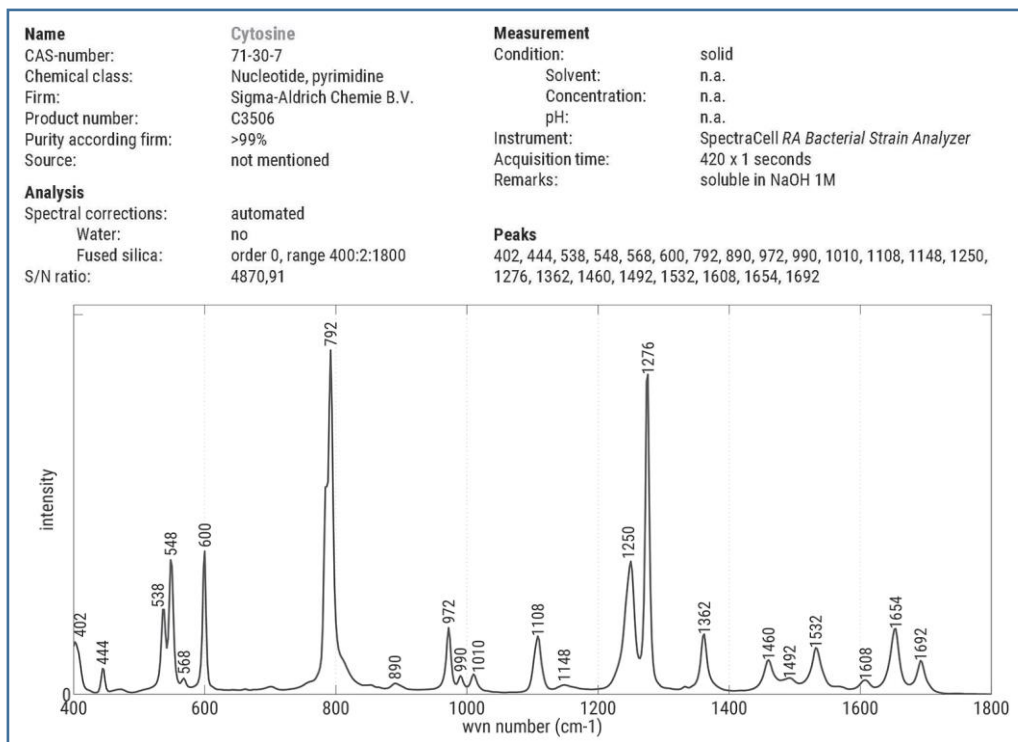
Analysis
Spectral corrections: manually
Water: no
Fused silica: order 1, range 400:2:1800
Background: removed
S/N ratio: 347,12

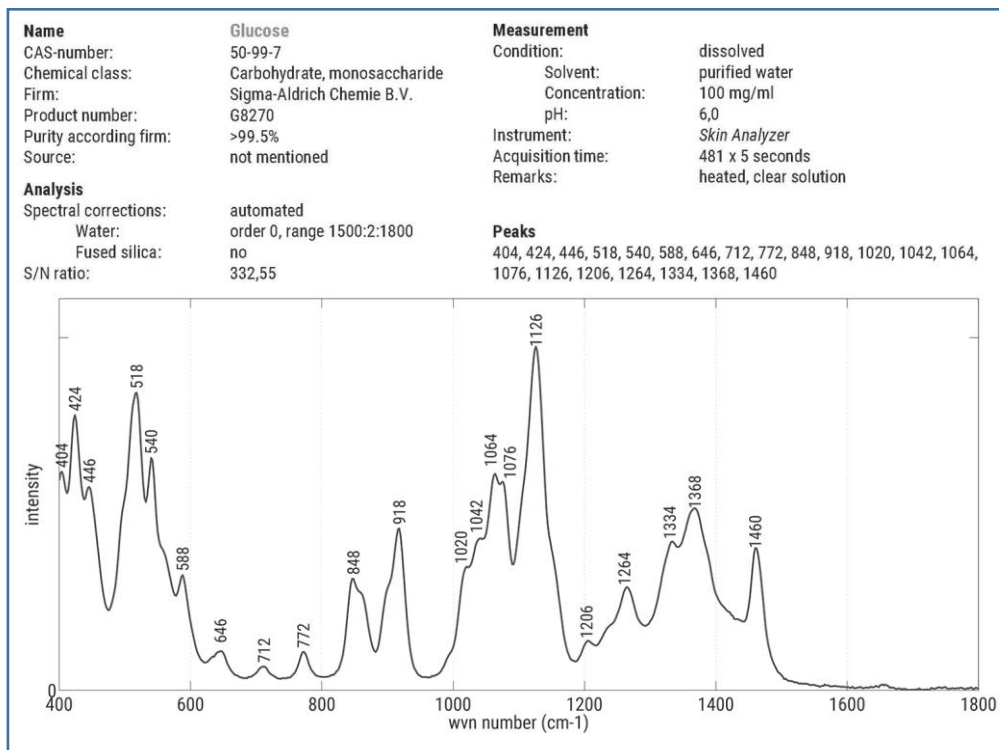
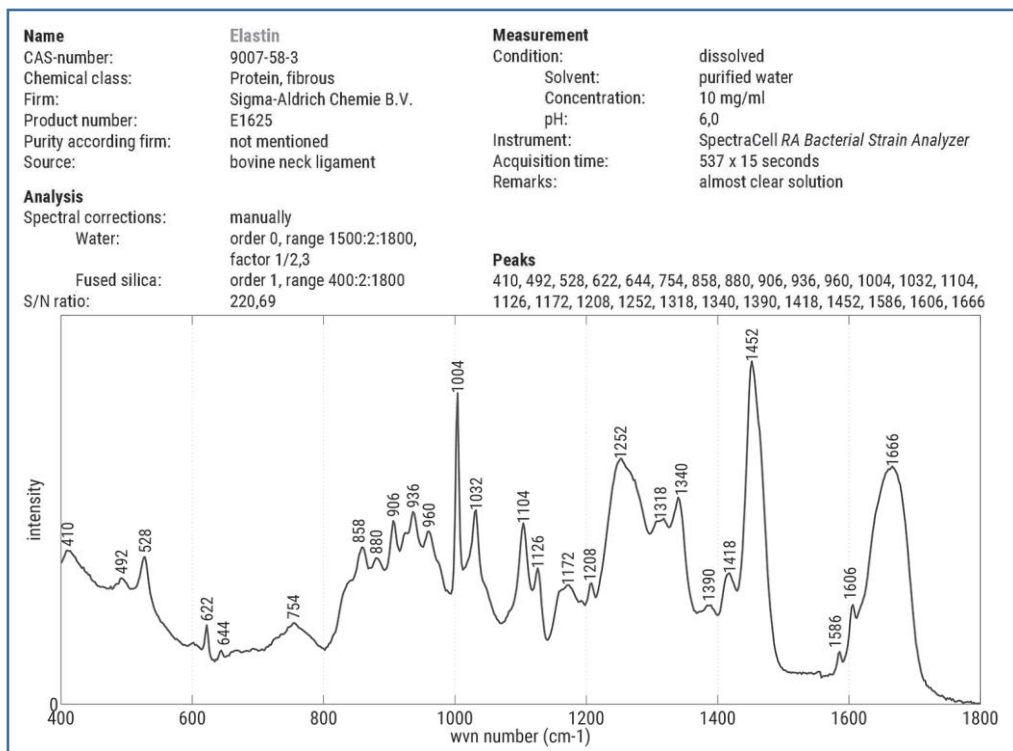
Peaks
 402, 428, 446, 456, 476, 490, 514, 538, 550, 570, 594, 614, 628, 646, 700, 724, 740, 802, 826, 848, 880, 924, 960, 972, 988, 1012, 1026, 1050, 1064, 1088, 1100, 1130, 1162, 1178, 1196, 1210, 1220, 1238, 1262, 1296, 1330, 1356, 1378, 1440, 1464, 1668, 1738

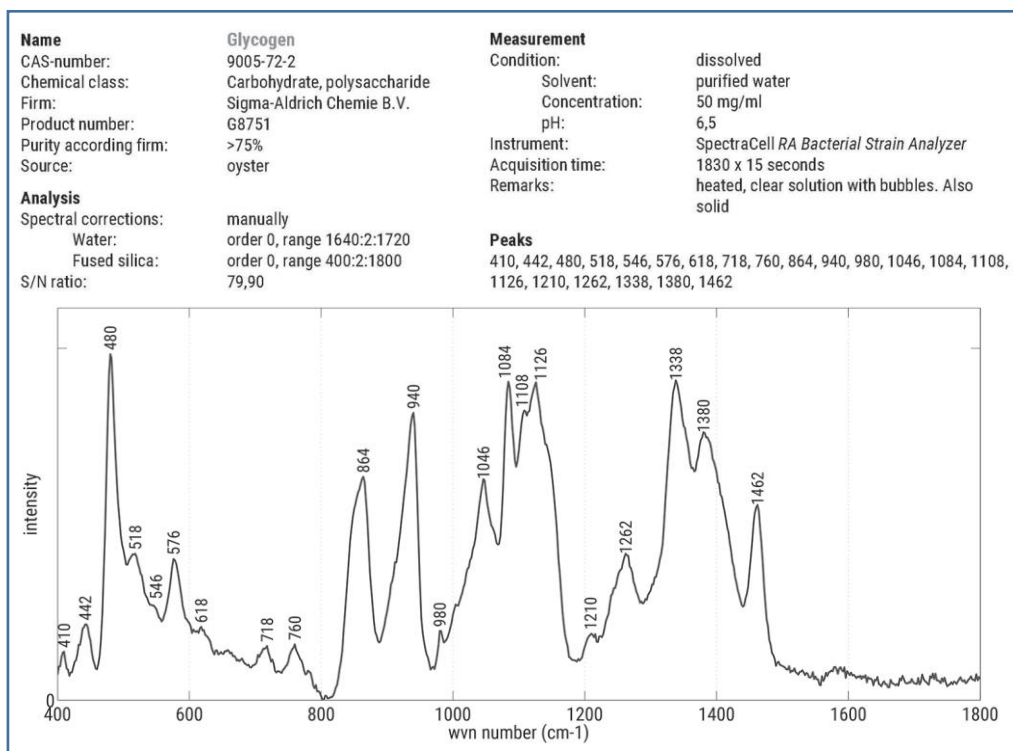
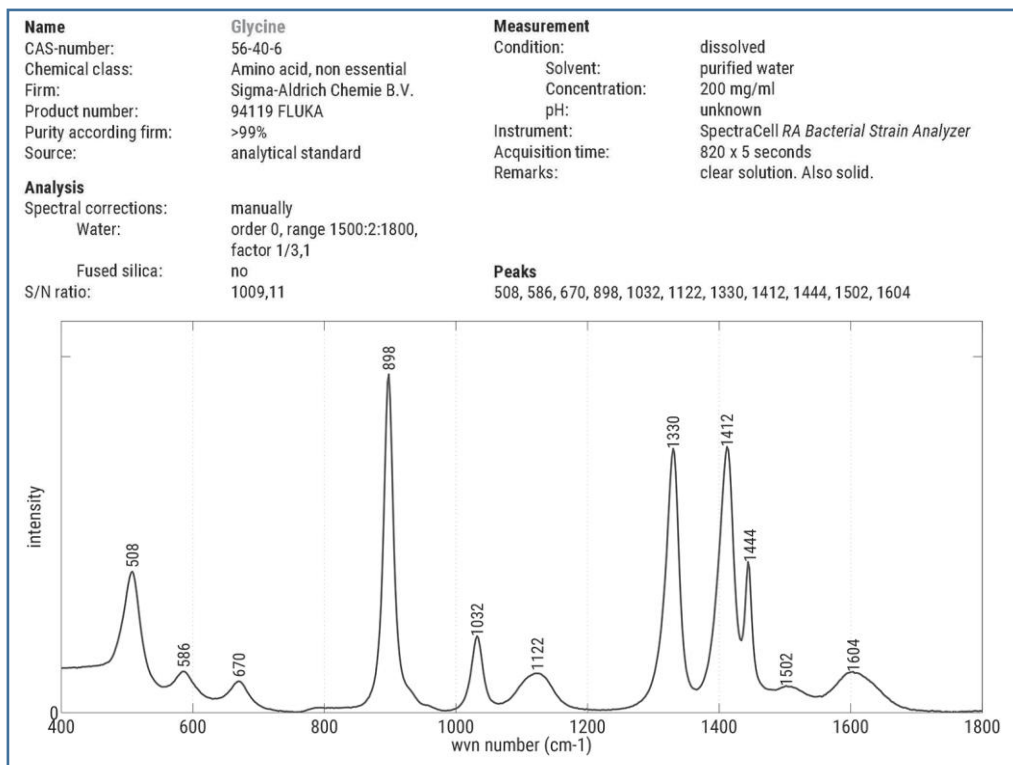






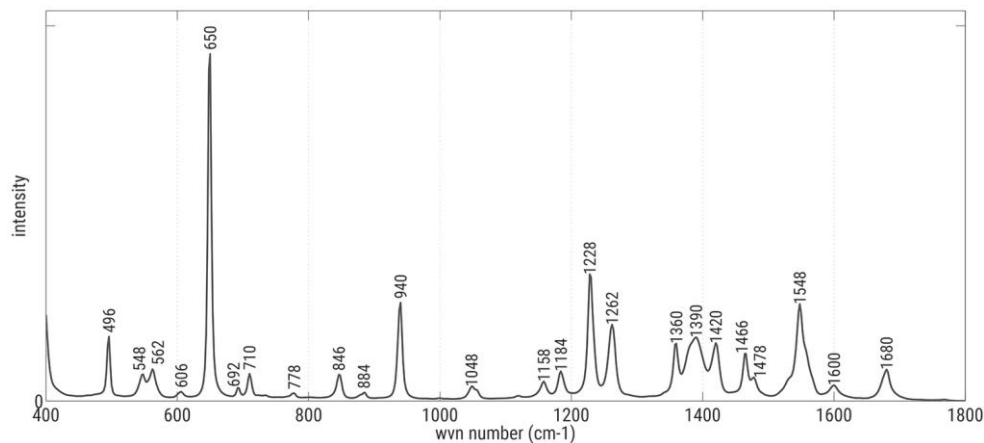






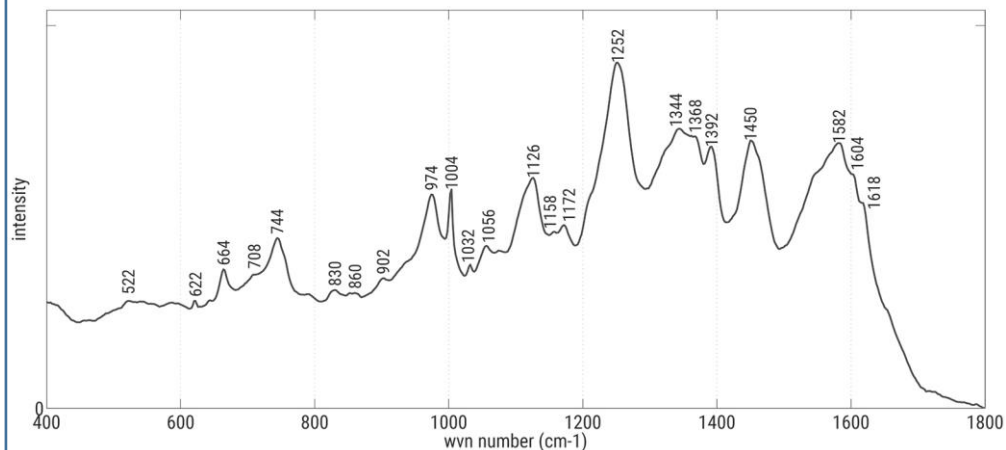
Name	Guanine	Measurement	
CAS-number:	73-40-5	Condition:	solid
Chemical class:	Nucleotide, purine	Solvent:	n.a.
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	n.a.
Product number:	G11950	pH:	n.a.
Purity according firm:	98%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	not mentioned	Acquisition time:	1199 x 1 seconds
		Remarks:	soluble in NaOH 1M

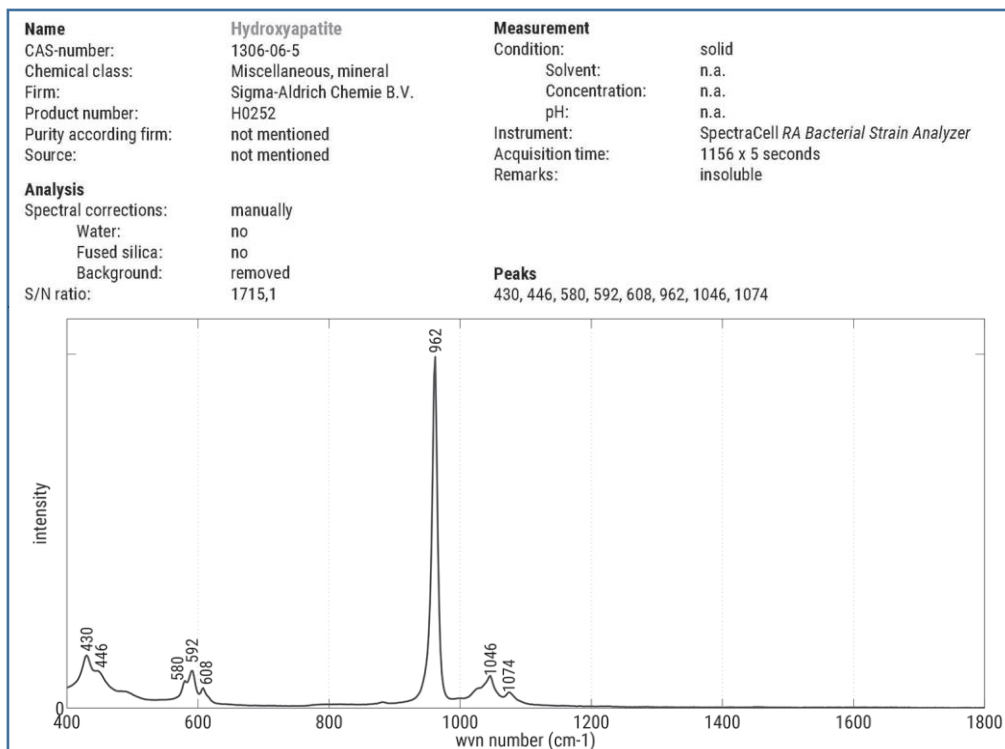
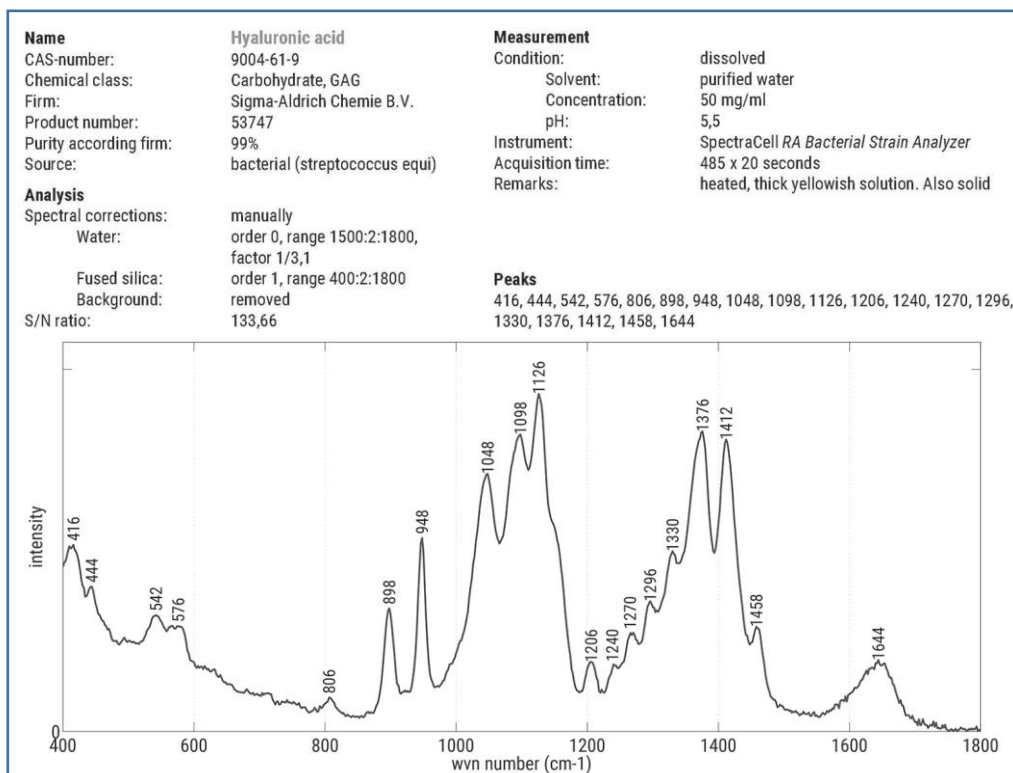
Analysis		Peaks
Spectral corrections:	automated	496, 548, 562, 606, 650, 692, 710, 778, 846, 884, 940, 1048, 1158, 1184, 1228, 1262, 1360, 1390, 1420, 1466, 1478, 1548, 1600, 1680
Water:	no	
Fused silica:	order 0, range 400:2:1800	
S/N ratio:	1155,32	

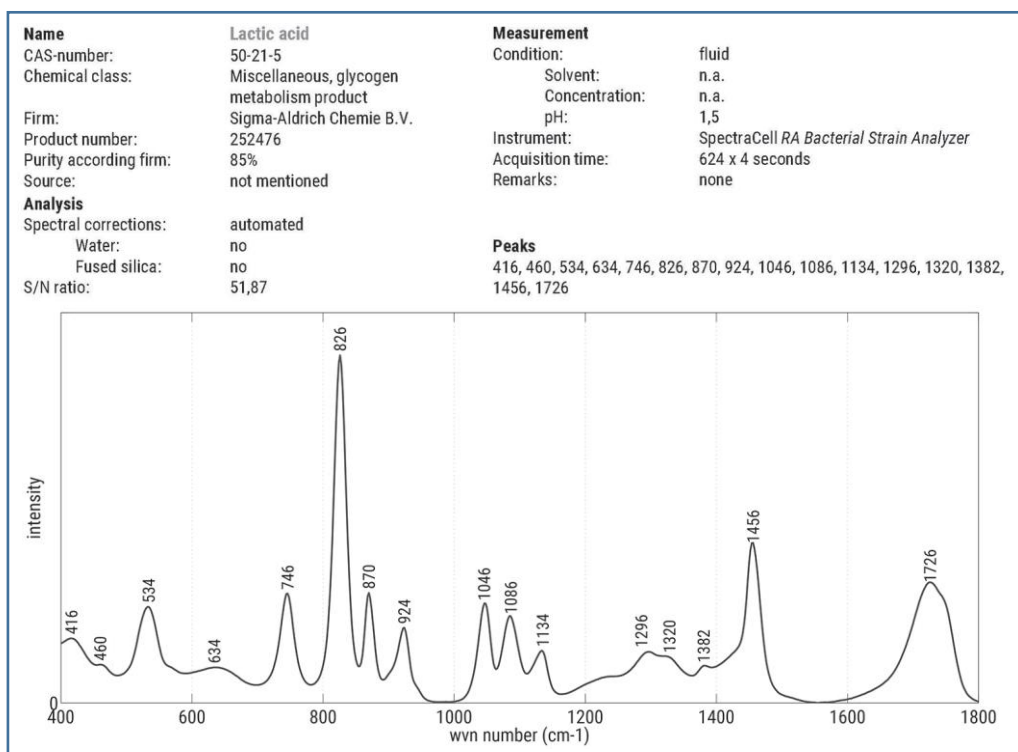
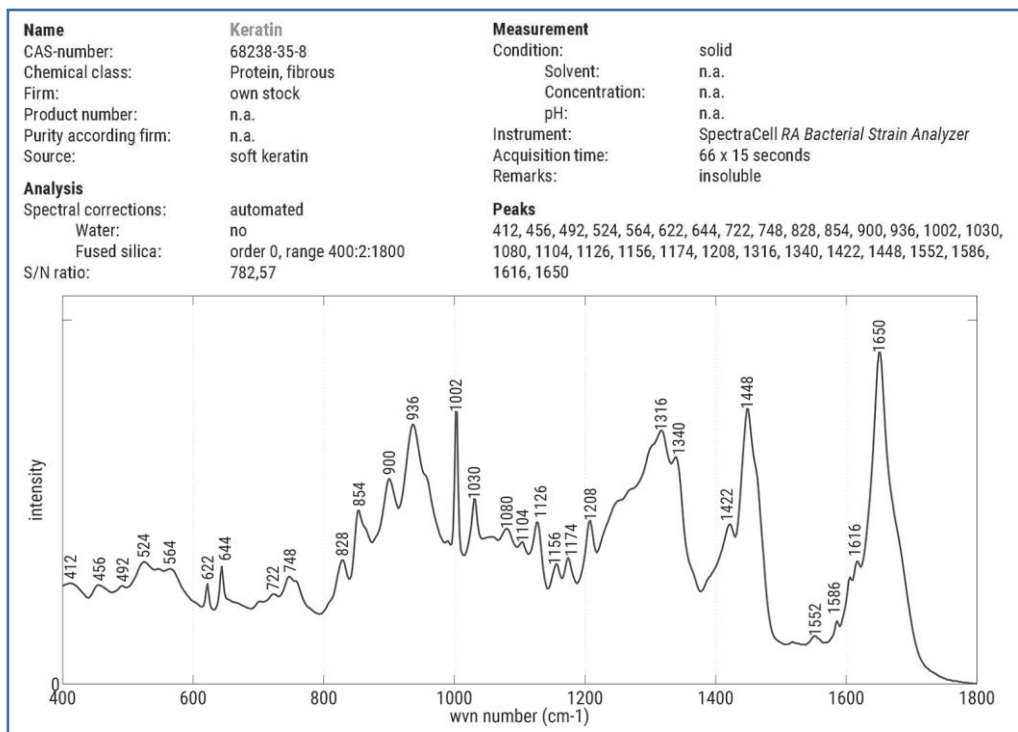


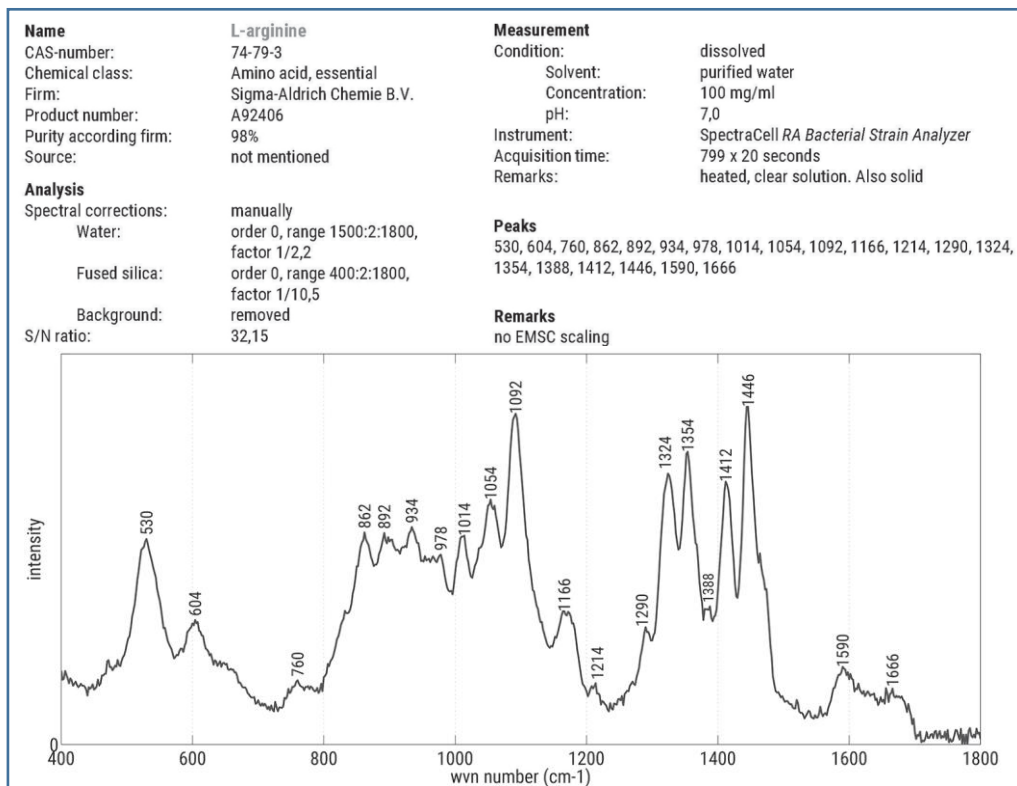
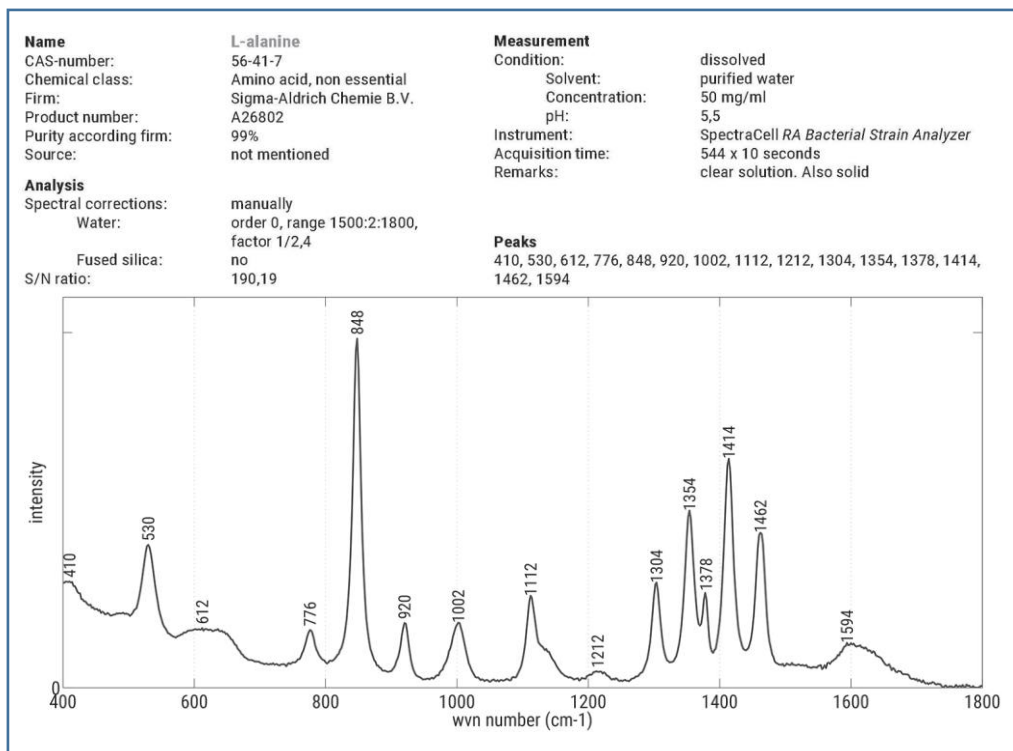
Name	Hemoglobin	Measurement	
CAS-number:	9008-02-0	Condition:	dissolved
Chemical class:	Protein, globular	Solvent:	purified water
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	unknown
Product number:	H0267	pH:	6,5
Purity according firm:	>90%	Instrument:	Skin Analyzer
Source:	human	Acquisition time:	108 x 1 seconds
		Remarks:	clear reddish solution

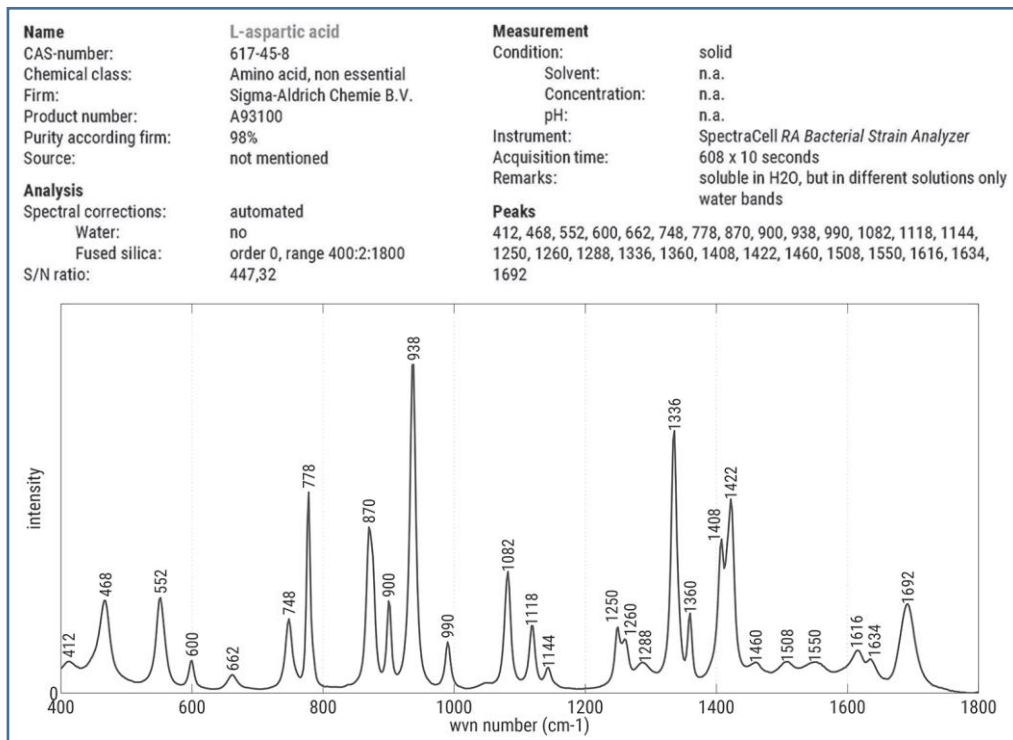
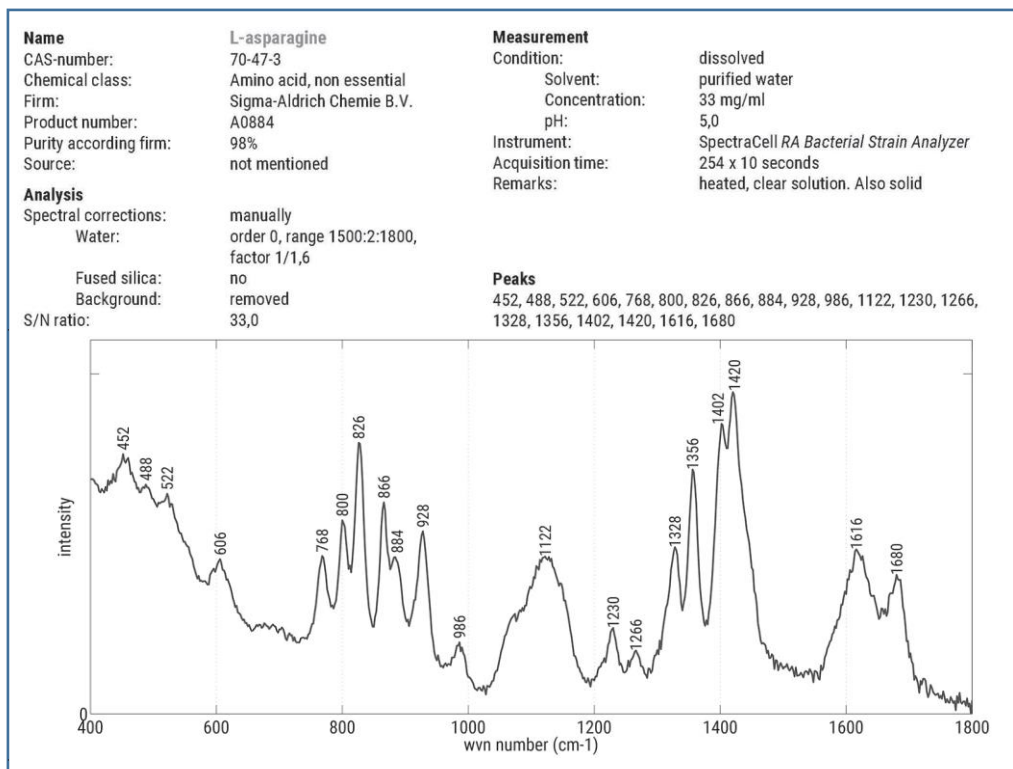
Analysis		Peaks
Spectral corrections:	manually	522, 622, 664, 708, 744, 830, 860, 902, 974, 1004, 1032, 1056, 1126, 1158, 1172, 1252, 1344, 1368, 1392, 1450, 1582, 1604, 1618
Water:	order 1, range 400:2:1800	
Fused silica:	no	
S/N ratio:	292,85	

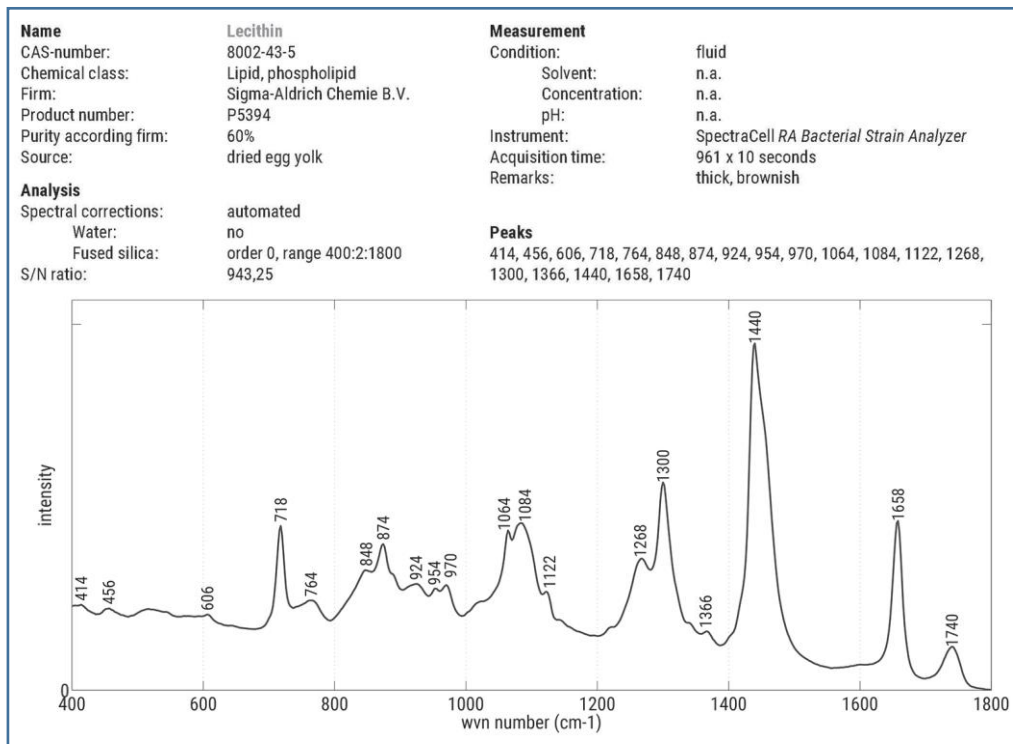
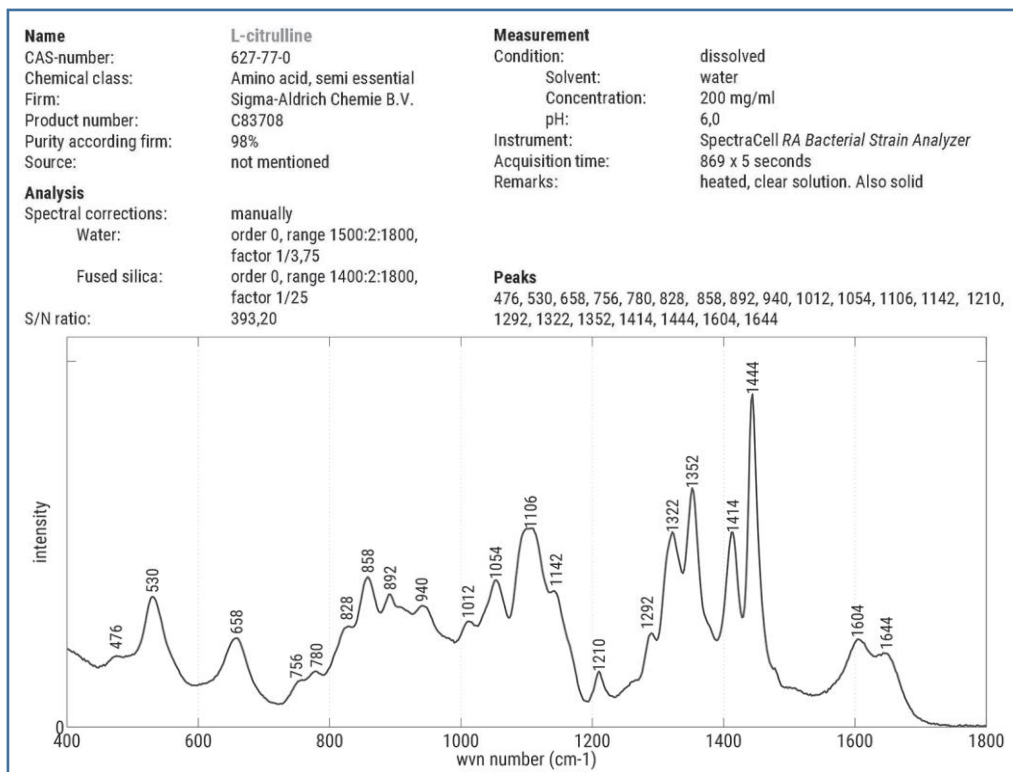


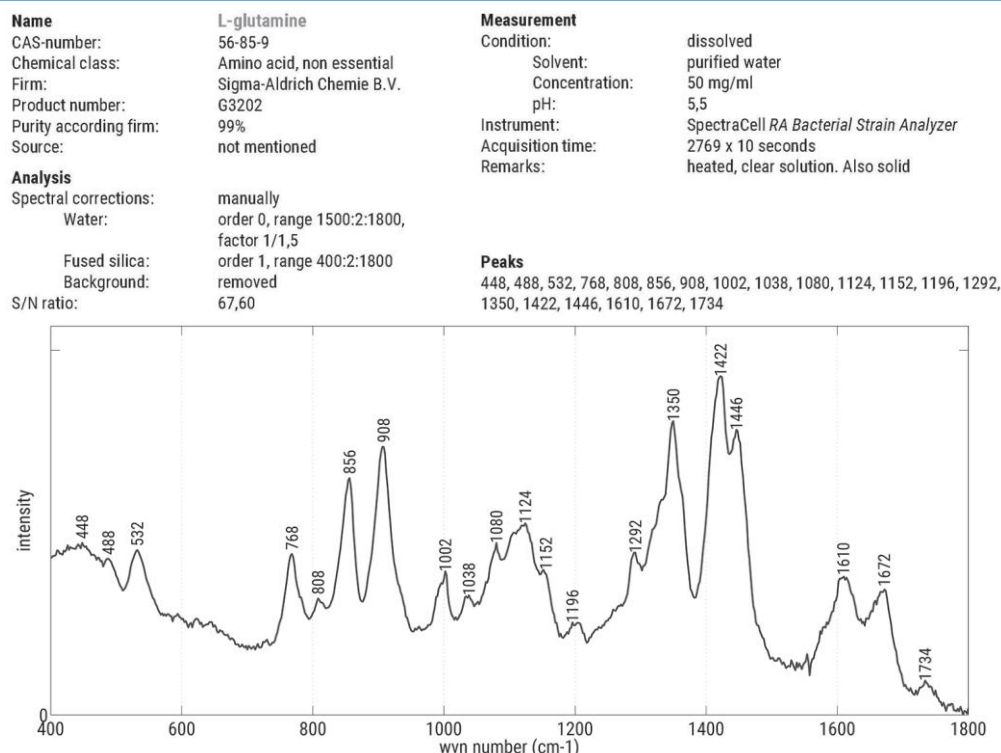
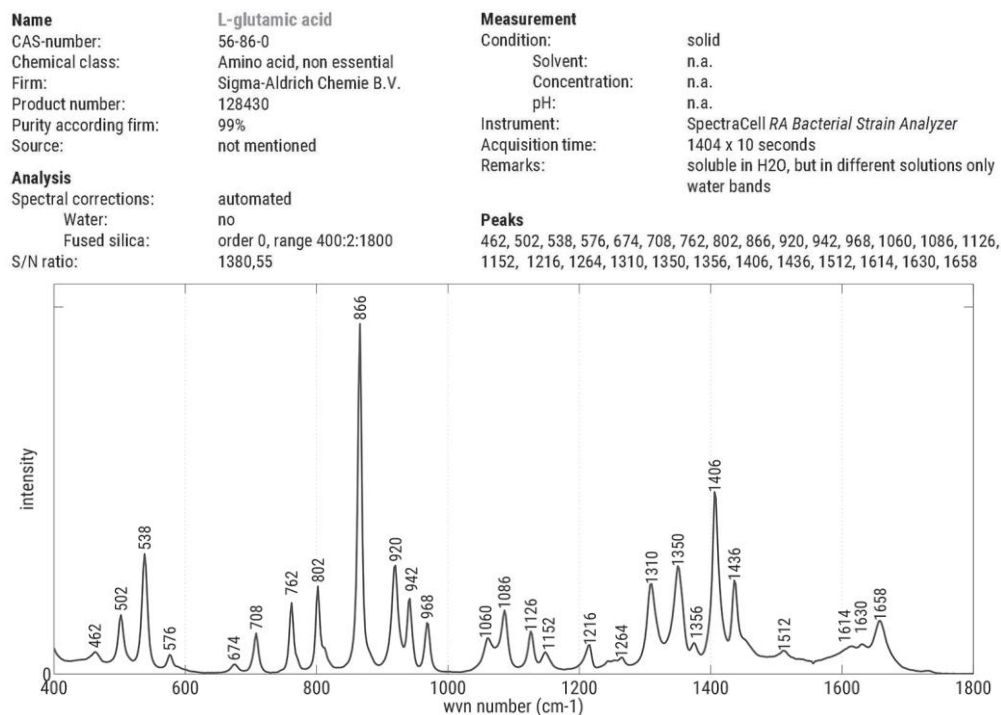


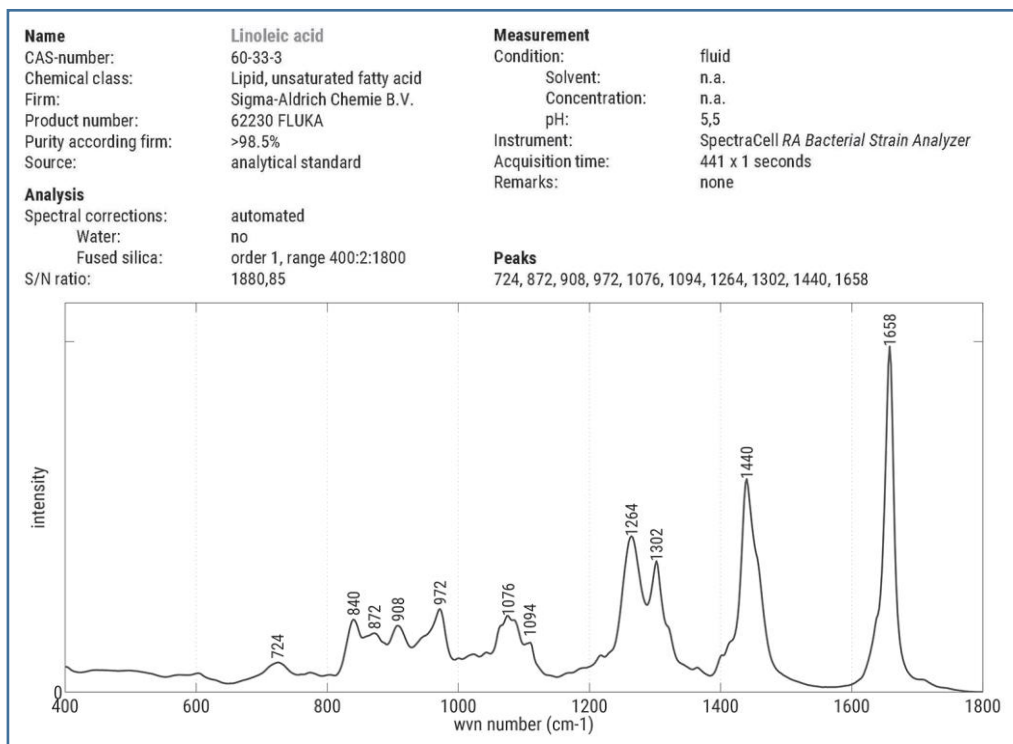
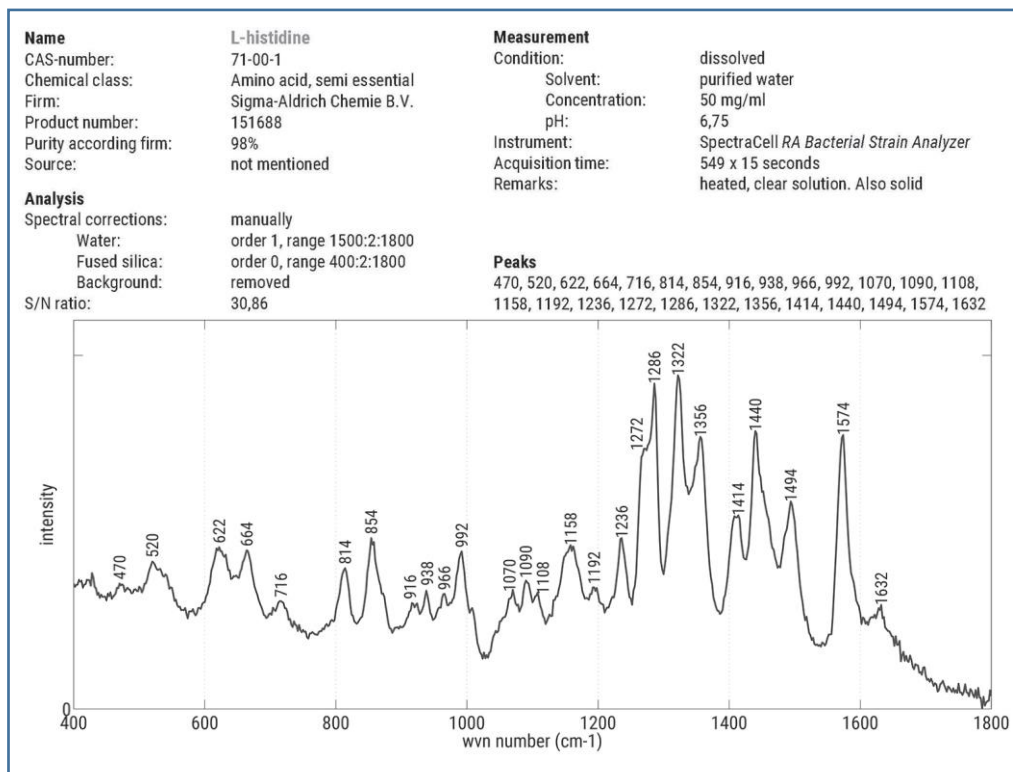






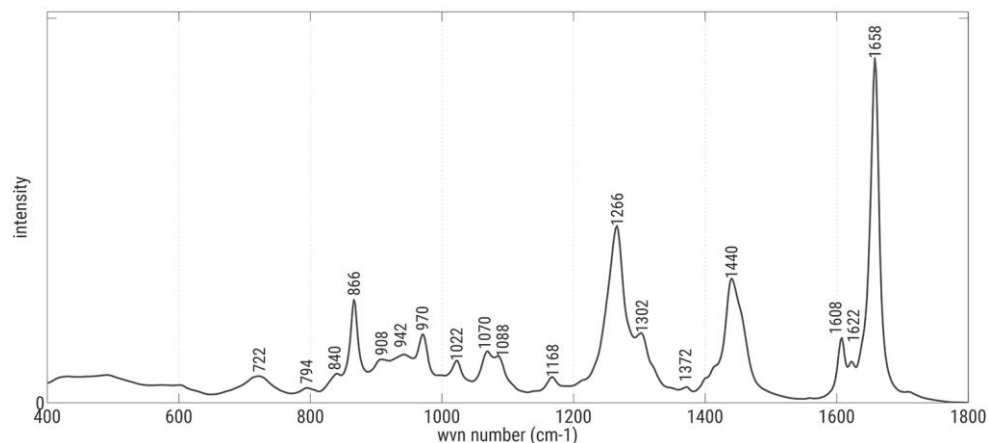






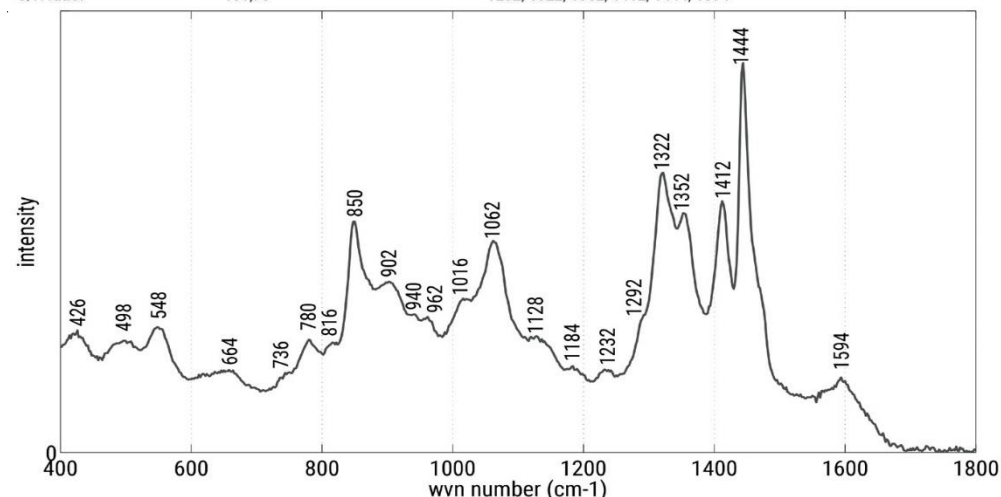
Name	Linolenic acid	Measurement	
CAS-number:	463-40-1	Condition:	fluid
Chemical class:	Lipid, unsaturated fatty acid	Solvent:	n.a.
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	n.a.
Product number:	62160 FLUKA	pH:	5,5
Purity according firm:	>98.5%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	analytical standard	Acquisition time:	441 x 1 seconds
		Remarks:	none

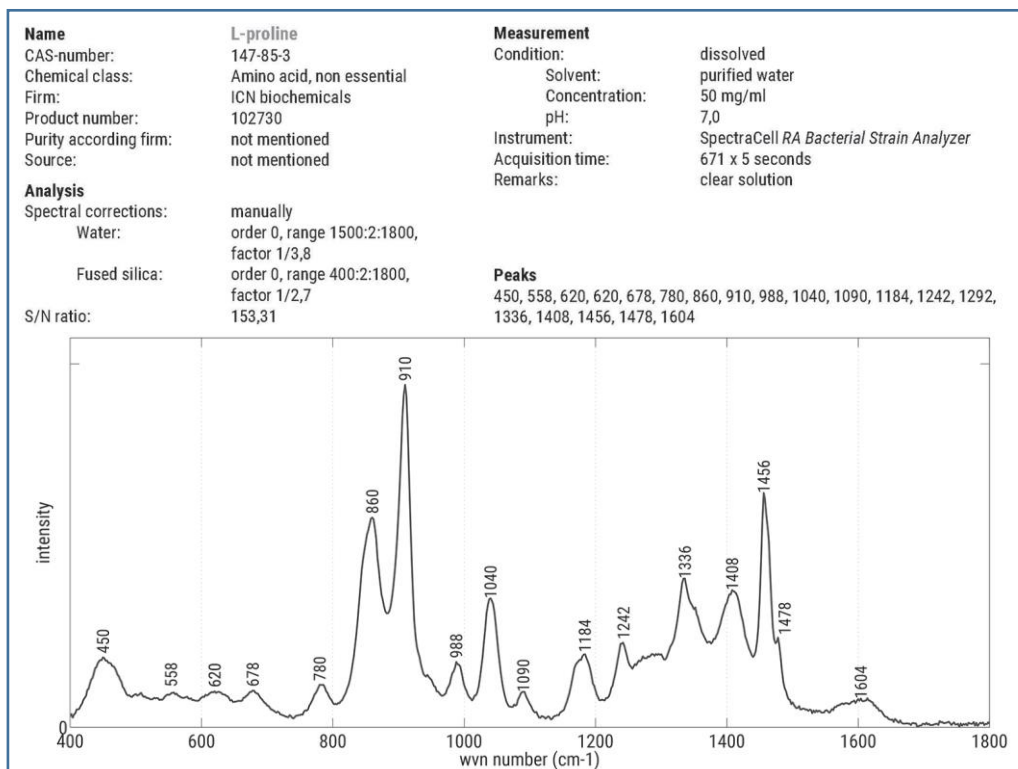
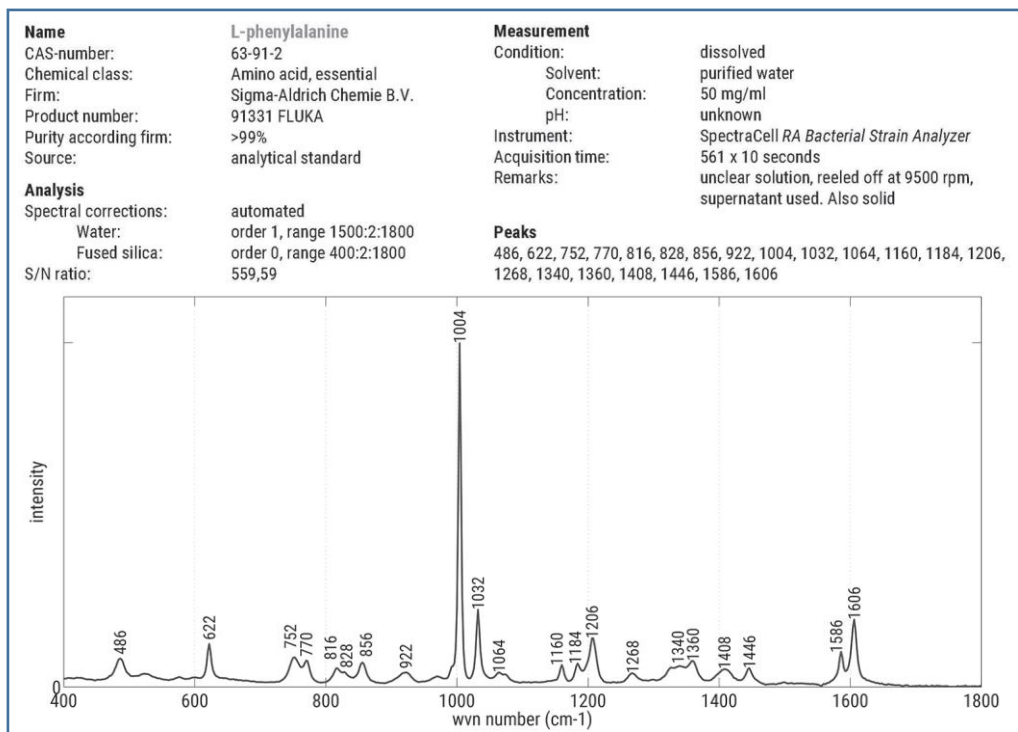
Analysis		Peaks
Spectral corrections:	automated	722, 794, 840, 866, 908, 942, 970, 1022, 1070, 1088, 1168, 1266, 1302, 1372, 1440, 1608, 1622, 1658
Water:	no	
Fused silica:	order 1, range 400:2:1800	
S/N ratio:	3549,36	

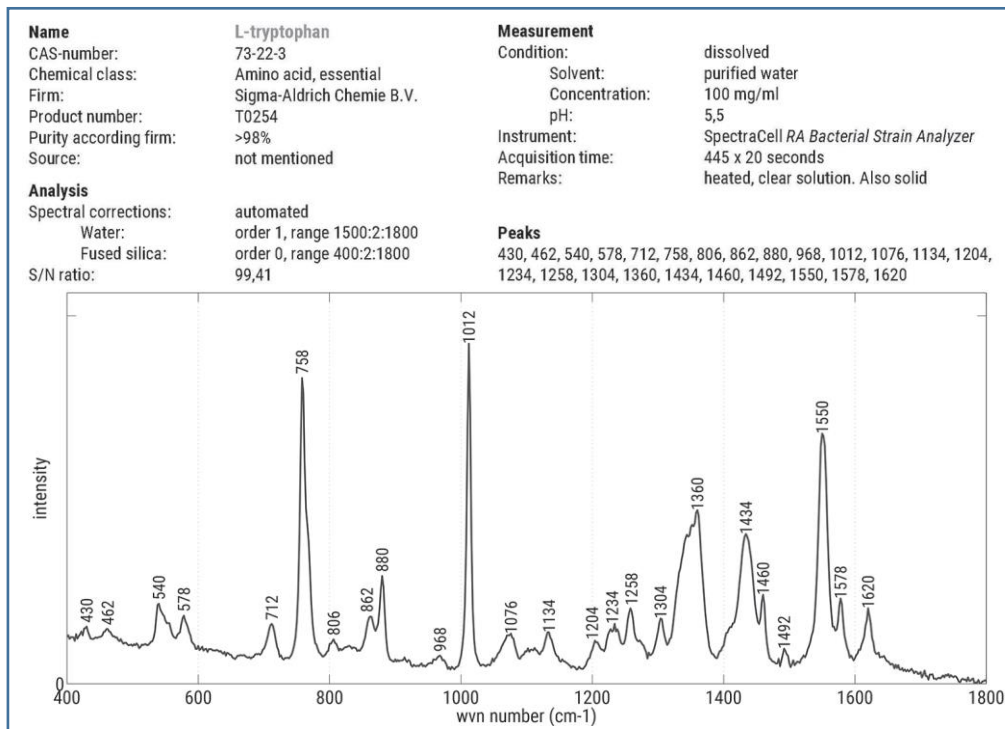
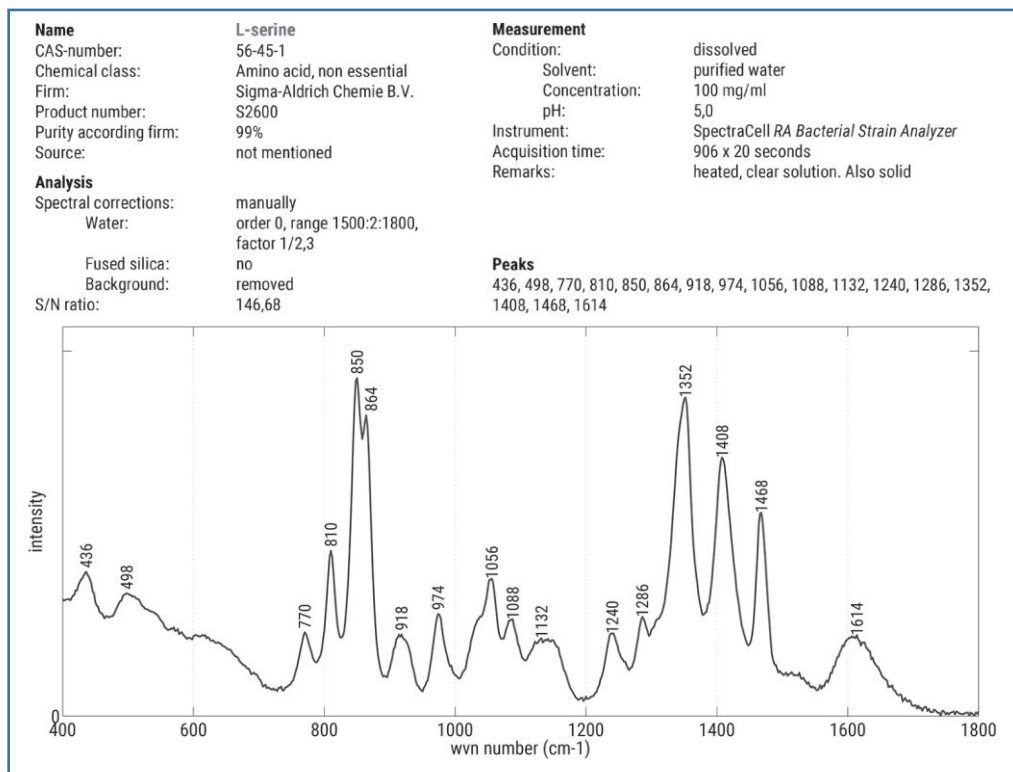


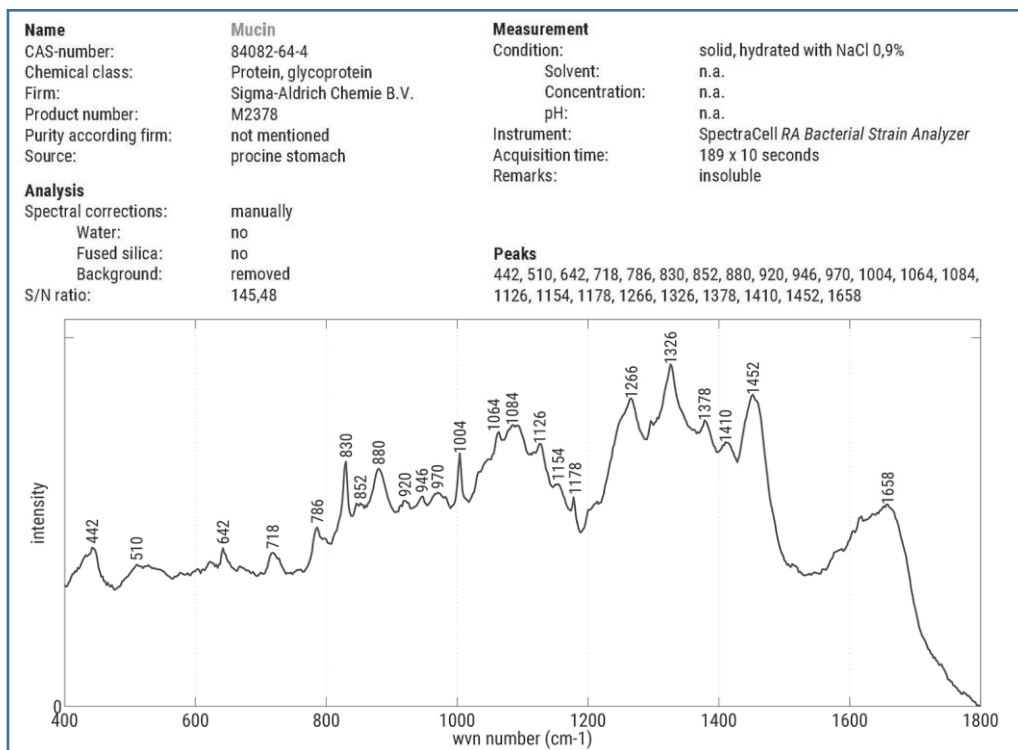
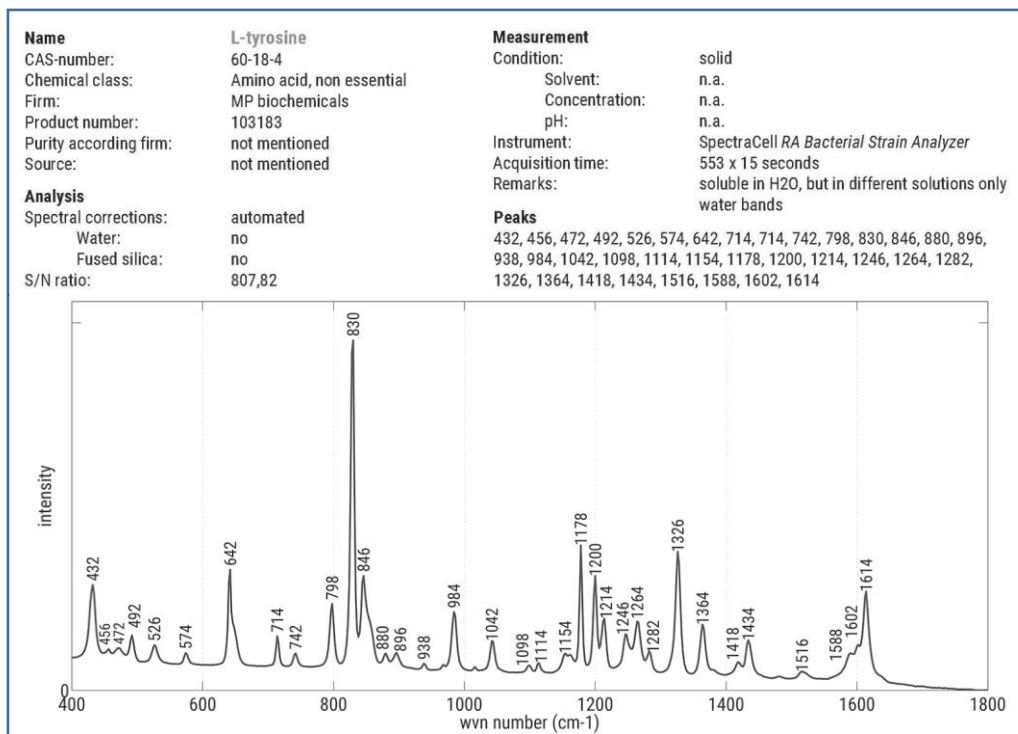
Name	L-lysine	Measurement	
CAS-number:	56-87-1	Condition:	dissolved
Chemical class:	Amino acid, essential	Solvent:	purified water
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	100 mg/ml
Product number:	62840	pH:	9,0
Purity according firm:	>98%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	not mentioned	Acquisition time:	533 x 10 seconds
		Remarks:	clear solution. Also solid

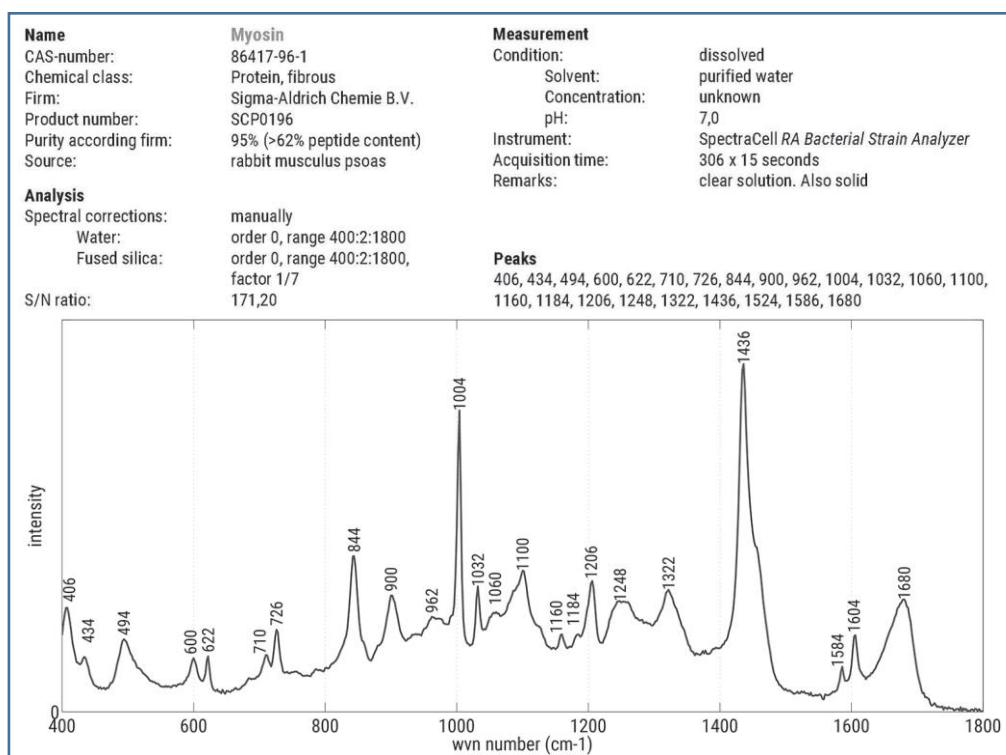
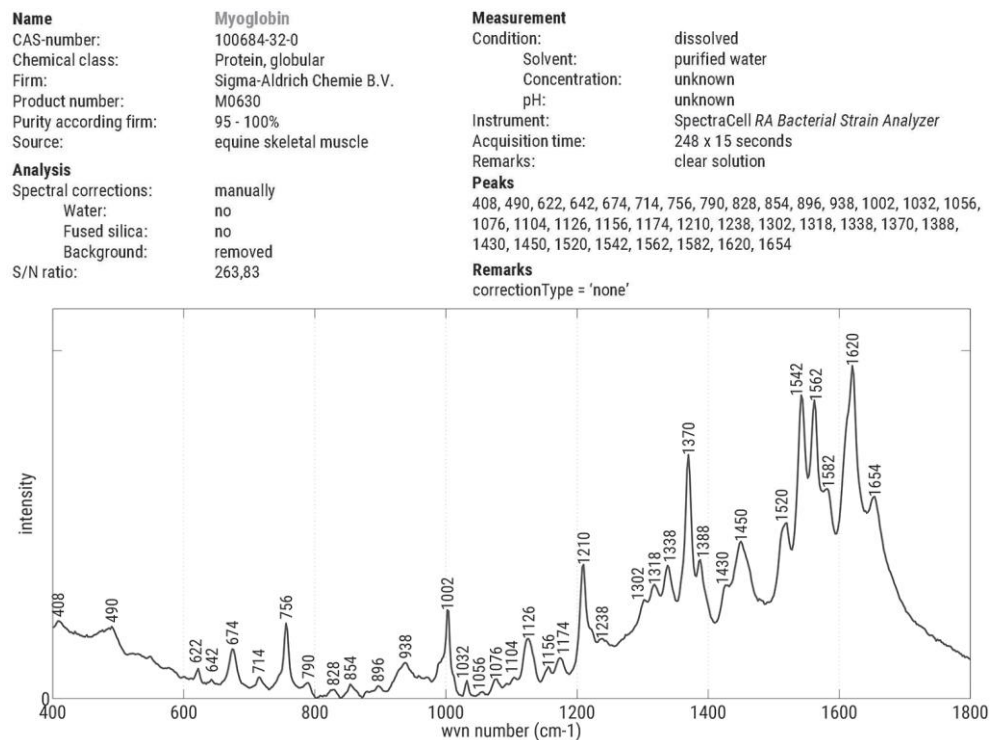
Analysis		Peaks
Spectral corrections:	automated	426, 496, 548, 658, 780, 822, 850, 902, 942, 962, 1016, 1062, 1128, 1184, 1232, 1322, 1352, 1412, 1444, 1594
Water:	order 1, range 1500:2:1800	
Fused silica:	order 0, range 400:2:1800	
S/N ratio:	131,73	

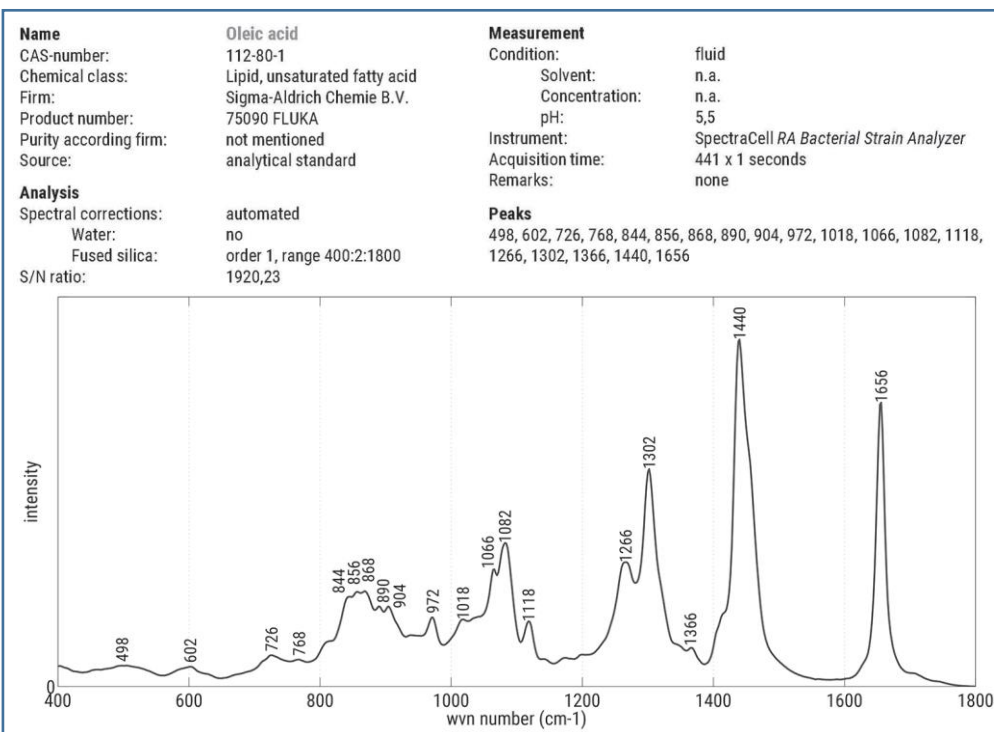
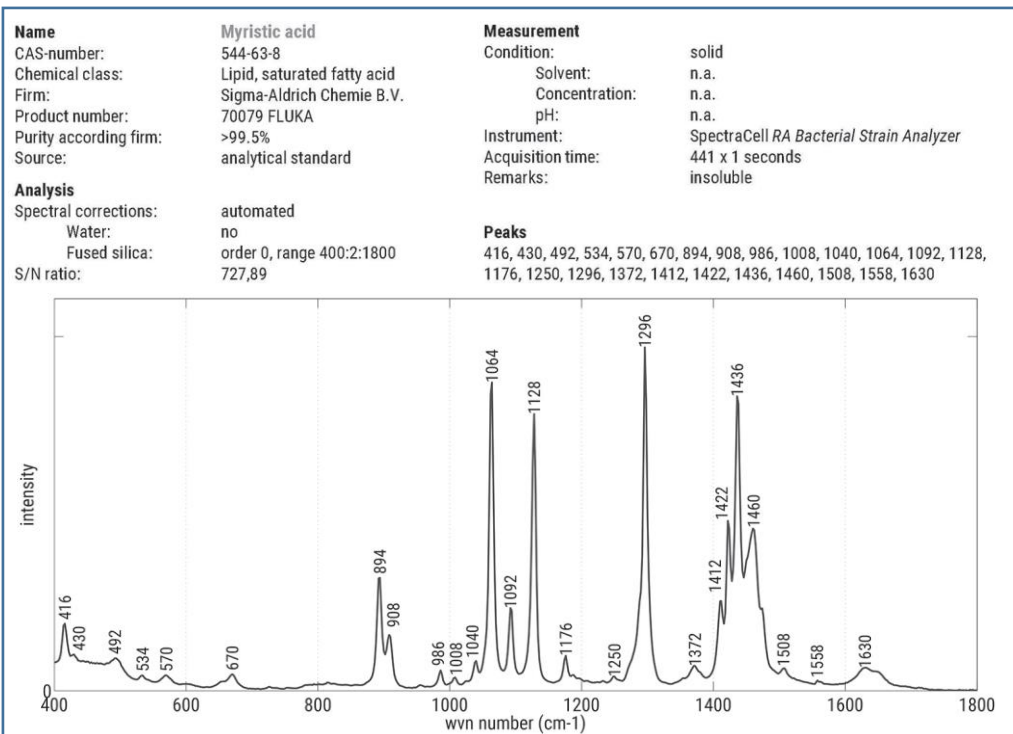


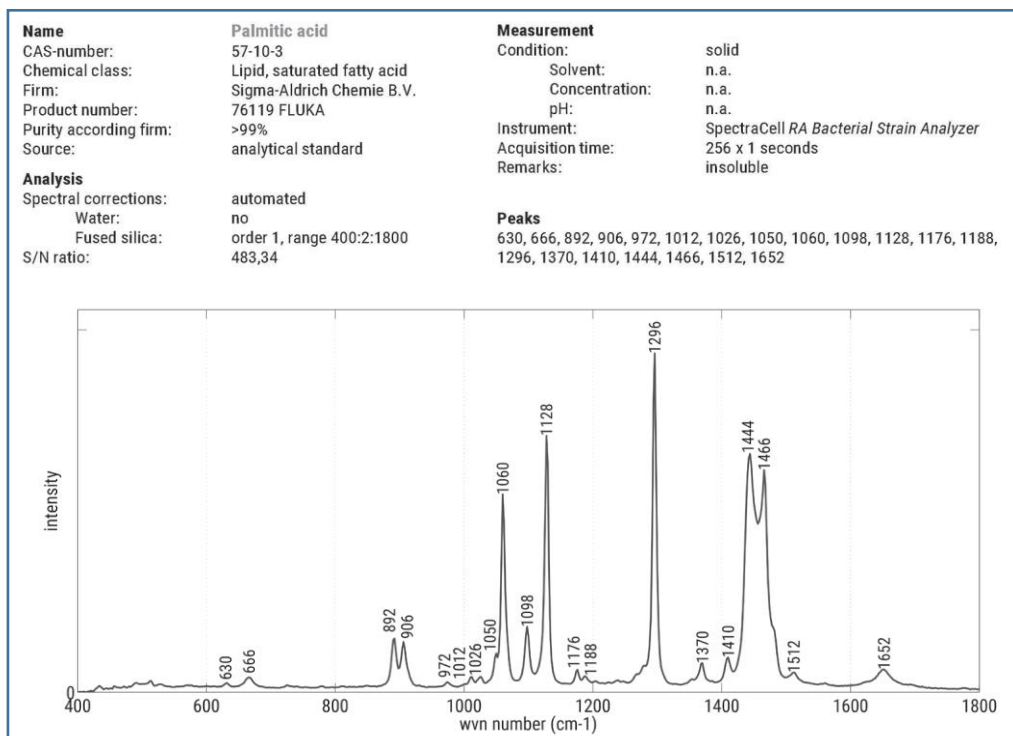
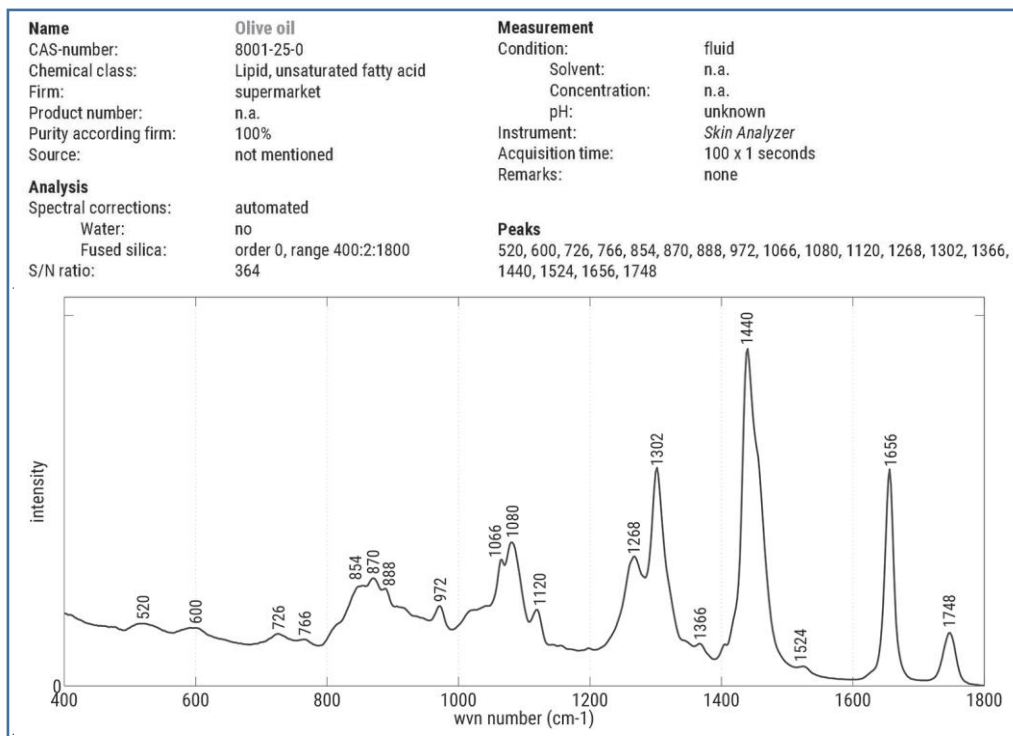


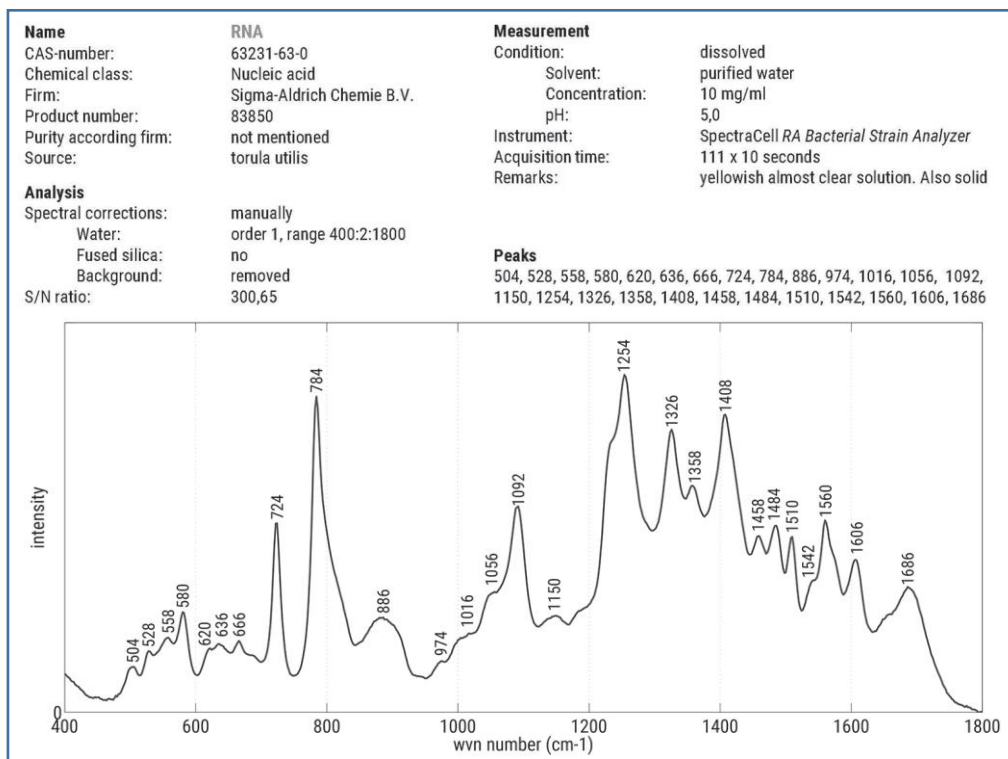
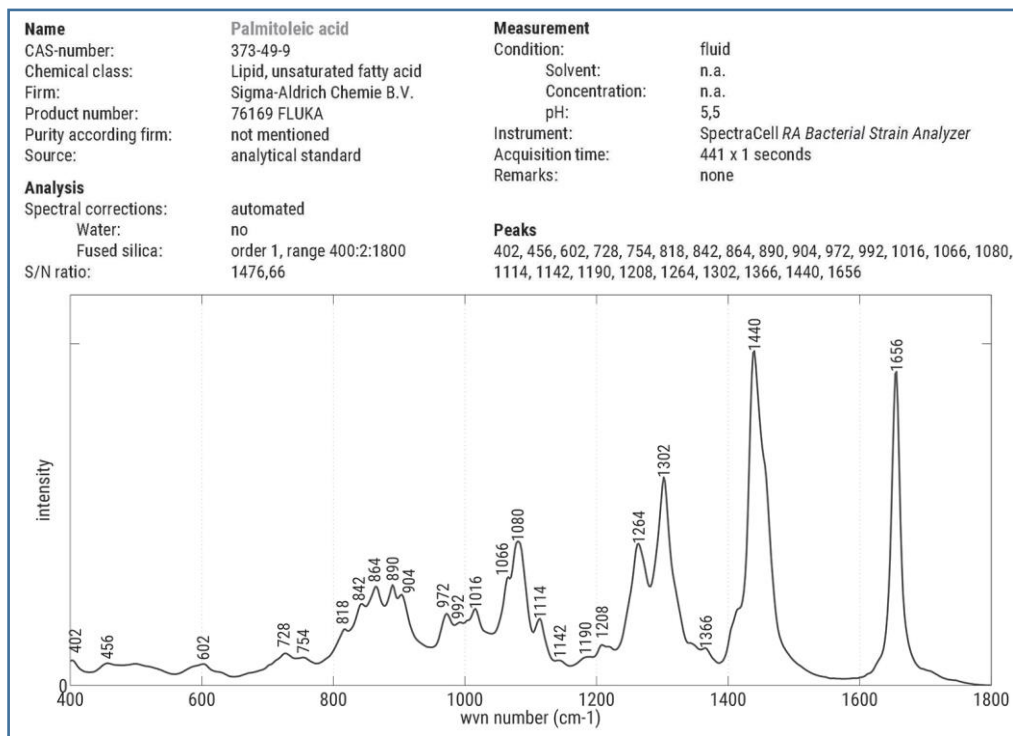


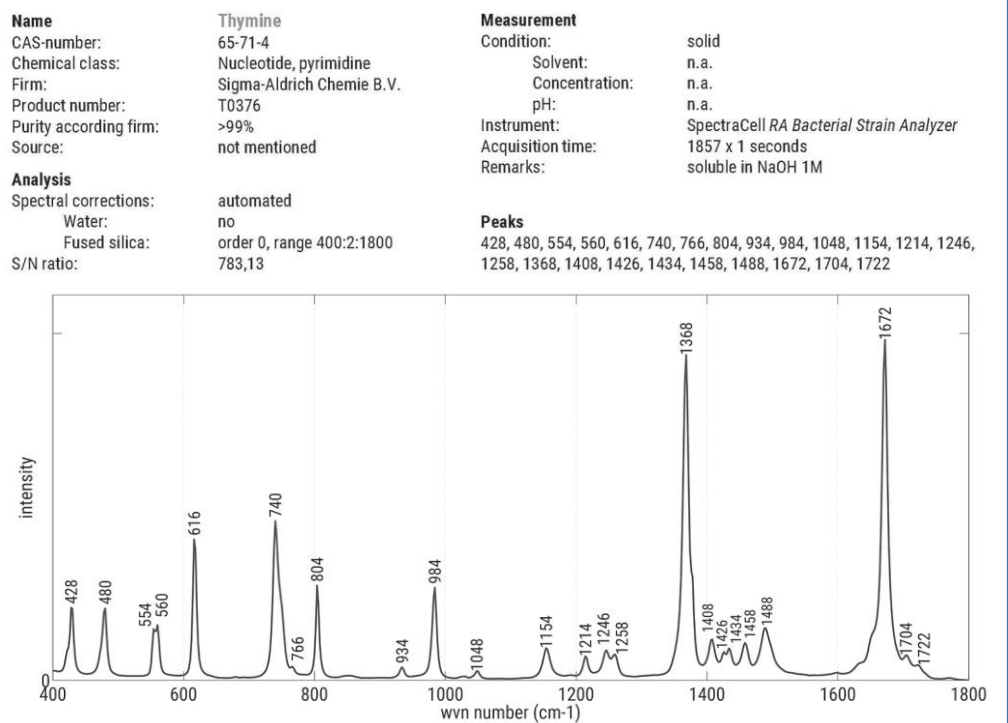
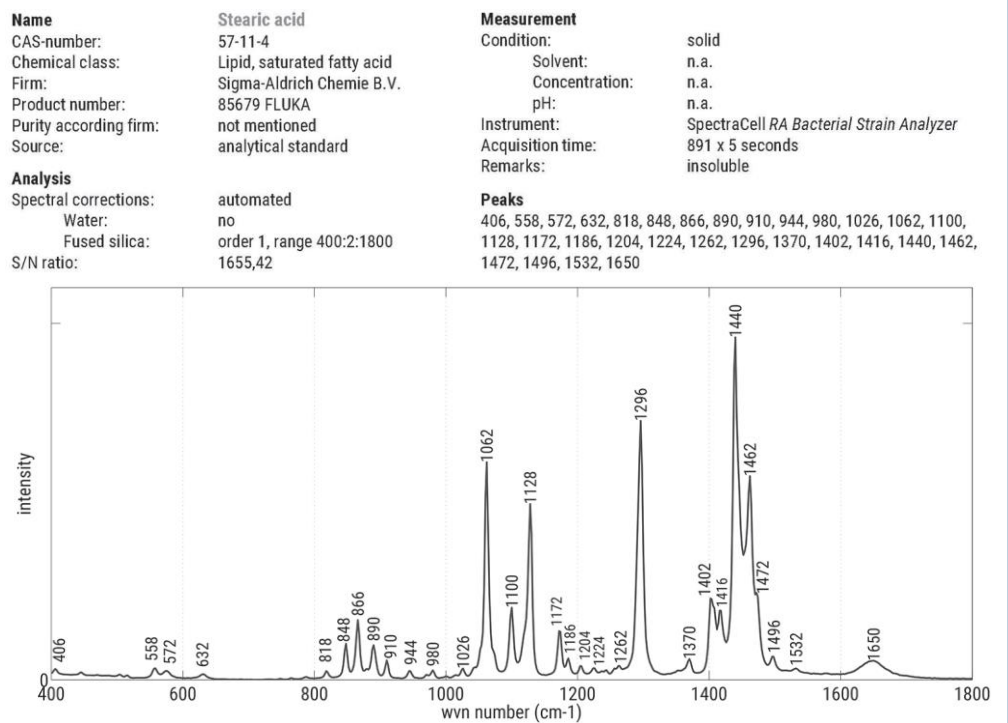












Name	Uracil	Measurement	
CAS-number:	66-22-8	Condition:	solid
Chemical class:	Nucleotide, pyrimidine	Solvent:	n.a.
Firm:	Sigma-Aldrich Chemie B.V.	Concentration:	n.a.
Product number:	U0750	pH:	n.a.
Purity according firm:	>99%	Instrument:	SpectraCell RA Bacterial Strain Analyzer
Source:	not mentioned	Acquisition time:	1792 x 1 seconds
		Remarks:	soluble in NaOH 1M

Analysis		Peaks
Spectral corrections:	automated	430, 530, 538, 556, 578, 790, 826, 984, 994, 1010, 1100, 1162, 1236, 1254, 1394, 1418, 1454, 1504, 1610, 1646, 1714
Water:	no	
Fused silica:	order 0, range 400:2:1800	
S/N ratio:	1715,25	

