SUPPLEMENTARY DATA

Title:

Dispersive and FT-Raman Spectroscopic Methods in Food Analysis

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Table 1S. Raman spectra of some proteins

Band position cm^{-1}	Assignment of Bonds (Molecule/Group)	Mode of Vibration	Strength of bonds	Sample / Food Matrix	Wavenumber of laser source (nm)	Type of Raman	References
1665	C=O	Stretching	-	Jack bean concanavalin A (Con A), bovine pancreas trypsin (trypsin), bovine serum albumin (BSA), bovine pancreas ribonuclease A (RNase A), horse heart cytochrome *c* (cyt *c*), human hemoglobin (Hb), horse skeletal muscle myoglobin (Mb), bovine pancreas R-chymomyosin (Chy), porcine pancreas elastase (Elas), chicken egg white lysozyme (Lyso), human erythrocyte carbonic anhydrase (Carb), porcine muscle triosephosphate isomerase (Trio), bovine pancreas insulin (Ins), tyrosine (Tyr), phenylalanine (Phe), tryptophan (Trp), histidine (His), arginine (Arg), cysteine (Cys), proline (Pro), methionine (Met), cystine / -	206.5	UV-Raman	1
	C-N	Stretching	-				
	N-H	Bending	-				
1610	Amino acid ring	Breathing	-				
	Amide (II)		-				
1555	C-N	Stretching	-				
	N-H	Bending	-				
	C-C	Stretching	-				

800-900	C-C	Stretching	-	Mineral oil and corn oil / Protein and oil interface	782	Raman microspectroscopy	2
1000-1100	C-C	Stretching	-				
1302	CH_2	Phase twist	-				
1443	CH_2	Scissoring	-				
1660	C=C	Stretch (cis)	-				
1750	C=O	Ester stretch	-				
2730	CH_2 or CH_3	Deformation	-				
2850,2870	CH_2,CH_3	Symmetric stretch	-				
3010	=CHR or $=CH_2$	=CH stretch	-				
503	S-S	Stretching vibrations (gauche-gauche-gauche)	-	Bovine Serum Albumin / Protein and oil interface	782	Raman microspectroscopy	2
750	Tryptophan	-	-				
830,850	Tyrosine doublet	-	-				
936-946	Amide III helix	-	-				
965-970	Amide III random	-	-				
980-990	amide III antiparallel β-sheet	-	-				
1003	Phenylalanine	-	-				
1338	C-H Tryptophan	Bending -	-				
1448	C-H	Bending	-				
1654	Amide I band		-				

2930	C-H	Stretching	-	Various amino acids / BSA and oil interface	782	Raman microspectroscopy	2
3076	=C-H	Stretching	-	Aromatic amino acids / BSA and oil interface			
3200	O-H	Stretching	-	Water molecules / BSA and oil interface			
497,524	Cysteine S-S	-	-	Egg albumen(unheated) / -		FT-Raman	3
761	Tryptophan	-	-				
831,852	Tyrosine doublet	-	-				
1337	C-H / Tryptophan	Bending	-				
1454	CH_2	Bending	-				
1060	C-N / C-C	Stretching	-				
933, 947, 960	Amide III'	-	-				
991	B-sheet structure	-	-				
1317	A- helix structure	-	-				
500, 511	Cysteine S-S	-	-	Whey proteins (unheated) / -		FT-Raman	3
758	Tryptophan	-	-				
831,851	Tyrosine doublet	-	-				
1350	CH Tryptophan	Bending -	-				
1418	COO-	-	-				
1450	CH_2	Bending	-				
1051	C-N / C-C	Stretching	-				
938, 951	Amide III'	-	-				
986	B-sheet structure	-	-				
1239	Amide III	-	-				
1321	α- helix structure	-	-				

1650-1660	Amide I	-	-				
1260-1300	Amide III	Weak	Weak				
850, 830	Tyrosine doublet	-	-				
2935 (2939-2950)	Native gluten	-	-				
500-550	S-S vibrational bands	-	-				
(534)	(trans-gauche-trans)rotamer	-	-				
(503)	(gauche-gauche-gauche) form	-	-				
(533)		-	-				
(514,497)	(trans-gauche-trans)	-	-	Gluten and chemically modified gluten / wheat flour or mix composed by flour and emilsifier (SSL)	1064	FT-Raman	4
1361	(gauche-gauche-gauche)	-	-				
(880,760)	Indicator of buried tryptophan residues						
	Strength of H bonding and the hydrophobicity of the enviroment	-	-				
508	S-S	Stretching	-				
540	Tryptophan	-	-				
541-576	Tryptophan	-	-				
759	Tryptophan	-	-				

761	Tryptophan	-	-				
831,856	Tyrosine Tyrosine	-	-				
832,858	Tryptophan	-	-				
883	Tryptophan	-	-				
886	Amide III' (α-	-	-				
941	helix)	-	-				
	Amide III' (α-	-	-				
947	helix)	-	-				
	Amide III'	-	-				
960	Amide III' (β-	-	-	α-lactalbumin, β-	488	Raman	5
984	sheet)	-	-	lactoglobulin / -		spectroscopy	
	Phenylalanine						
1005	Phenylalanine	-	-				
1007	Tryptophan	Shoulder	-				
1014	Phenylalanine	-	-				
1033,1034	C-N	Stretching	-				
1072,1130, 1162		-	-				
1084,1130,	C-N	Stretching	-				
1161		-	-				
(1180) 1183	Tyrosine	-	-				
(1207) 1211	Tyrosine,	-	-				
	phenylalanine	-	-				
1336, 1385	Tryptophan	-	-				
(1453) 1455	CH_2	Deformation	-				
1556	Tryptophan	-	-				
(1658) 1651	Amide I'	-	-				
		-	-				
1003	Phenylal anine (internal standard)	-	-				
1780	C=O (glutamate or aspartate*)	Stretching					
1900-1550	C=O (Carbonyl groups)	Stretching	Strong				

1800-1740	C=O (carboxylic acid monomers)	Stretching					
1732	C=O (α-carboxyl groups)		-				
1667-1673	Amide I band (predominantly β-sheet)		-				
1230-1240	Amide III band (predominantly β-sheet)	-	More intense	Soy protein isolate, whey protein isolate, egg White / -	514	Raman microspectroscopy	6
1650-1660	Amide I band (high propotion of α-helix)	-	-				
1260-1300	Amide III band (high propotion of α-helix)	-	- Weak				
1665	Amide I (high proportion of undefined or random coil)	-	-				
1245	Amide III (high proportion of undefined or random coil)	-	-				
2800-3000	Amino acid functional groups	Stretching	-				
Near 1450	Amino acid functional groups	Bending	-				
I_{850}/I_{830}	Participation of tyrosine phenolic groups Tryptophan	-	-				
757		-	-				

1003	Phenylalanine	-				
853	Tyrosine	-				
757	Tryptophan	-				
1254, 1299,1340	Amide III (α-helix)	-				
1393	Amide S ($C_\alpha H$) (α-helix)	-				
1525, 1552	Amide II(α-helix)	-				
1649, 1685	Amide I (α-helix)	(Amide I bands, mainly C=O stretching and particularly sensitive to H-bond donation to the C-O groups)	Myoglobin, Lysozyme, Cytochrome c, Concanavlin A, Concanavalin A, Ribonuclease A , Trypsin , α- Chymotrypsin, Carbonic anhydrase, Alcohol dehydrogenase , α-Lactalbumin, Conalbumin / - - / (Hemoglobin) Human blood	197, 206.5	UVRR-spectroscopy	7
1241, 1300,1363	Amide III (β-sheet)					
1399	Amide S (β-sheet)					
1537, 1562	Amide II (β-sheet)					
1630, 1670	Amide I (β-sheet)	-				
1244, 1297,1332	Amide III (β-turn)	-				
1374	Amide S (β-turn)	(Amide II and III bands, in and out of phase combinations of C-N stretching and N-H in plane bending)				
1542	Amide II (β-turn)					
1652	Amide I (β-turn)					
1253, 1279,1332	Amide III (unordered)					
1386	Amide S (unordered)	-				
1552	Amide II (unordered)	-				
1664	Amide I (unordered)	-				
1658-1650	α-helices	-				
1680-1665	β-sheets	-				
1665-1660	Random coil	-				
1309, 1273	C_α-C, C=O	Stretching, plane bending				
2938	CH_2 asymmetric,	Stretching				

	CH_3 symmetric (aliphatic residues)						
850, 830	Tyrosine doublet	-		Fish Surimi & gels	1064	FT-Raman Spectroscopy	8
(I_{850}/I_{830})		-					
3220	O-H symmetric	Stretching					
3400	O-H asymmetric	Stretching					
2500	O-D	Stretching					
937	ν(C-CN)	Stretching	-				
879	ν(C-CN)	Stretching	-				
856	ν(C-CN)	Stretching	-				
829	γ(COO)	Out of plane bending	-	Meat	1064	FT-Raman	9
		Out of plane bending	-				
480	-		-				
1265	γ(C-H),R-HC=CH-	-	-				
815,1032	R	Skeletal Vibration	-				
	C-C	Out of plane	-				
974		deformation	-	Meat	785	Raman	10
	=C-H	Anti-symmetric					
1213		stretching	-				
	-						
1654	C=O	Amide I	-				
1517	N-H, C-N	In plane bending,	-				
		Stretching	-				
1153	C-N	Stretching	-				
965	-	Amide III	-				
1450	CH_2,CH_3,CH	Bending	-	Meat	514.5	Raman	11
2930	CH_2,CH_3,CH	Bending	-				
2935	C-H	-	-				
3220	O-H	Stretching	-				
3400	O-H	Stretching	-				
1060-1080	CCC	Stretching	-				
1250-1270	=C-H	Symmetric Rock	-	Fish	785	Raman	12
1390-1440	CH_2	Scissoring	-				

1600-1660	C=C	Stretching	-				
1700-1750	C=O	Stretching	-				
870	C-N	Stretching	-				
1122	C-C	Stretching	-	Ovine	671	Raman	13
930	C-C	Stretching	-				
1655-1650	-	Amide I	-				
1340	C-H	Bending	-				
940-934	C-C	Stretching	-	Meat	785	Raman	14
1668-1663	-	Amide I	-				
1243-1237	-	Amide III	-				
1658	Amide I	-	-				
1262	Amide II	-	-				
1447	C-H	Bending	-				
1003	C-OH	-	-				
1043	C-C-1-H	Stretching, bending	-				
		Stretching, bending	-				
941-944	O-C-1-H	Stretching, bending	-				
		-	-				
848-868	O-C-1-H	-	-				
		-	-				
1331-1339	C-H	-	-	Bread	785	Raman	15
1455-1599	CH_2	-	-				
1500-1200	CH_2-C-6-O-H, C-5-C-6-H, C-O-H, C-C-H	Stretching	-				
		Bending	-				
		Bending	-				
1350	CO	Amide I	-				
	COH	-	-				
1460	CH_2		-				
1455	-		-				
1263-1255	C-1-O-H, C-6-O-H		-				
933	C-C	-					
450-550	S-S	Stretching		Gluten	1064	FT-Raman	16
2800-3100	CH	Stretching					
2934-2945	OH	-					

1582	Indole	Ring	Protein, Salt and Water	632.8	Raman	17
1360	Indole	Ring				
1014	Indole	Ring				
877	CH_2	Rock/indole ring				
757	Indole	Ring				
1268	Tyrosine	-				
1207	Tyrosine or Phenylalanine	-				
852	CCH	Aromatic Deformation				
850/830	Tyrosine	Ring				
827	CCH	Aliphatic deformation				
1605	Phenylalanine	- Ring Breathe				
1002	Phenylalanine	Stretching				
622	C-S					
530	S-S	-	Protein Extract and Winter Rye	785	Raman	18
620	Phe	-				
820	Phe	-				
1005	Phe	-				
1600	-	Amide I				
450	C-C	Stretching				
930	C-C	Stretching				
1180	Phe	-				
1200	Phe	-				
1580	Trp	-				
1280	-	Amide III				
1550	Trp	-				
1600	-	Amide I				
760,1005,1350	Trp, Phe	-				
2930	C-H	Stretching				
1600	-	Amide I				
3080-3200	OH	Stretching				
460-510	-	Stretching				
1645-1690	Amide I	-				

740-766	Tryptophan	Ring Breathing Vibration		Bread	532	Raman	19
3300-3420	OH	Stretching					
1580-1640	OH	Bending					
2800-3050	CH	Stretching					

Table 2S. Raman spectra of some carbohydrates

Band position cm^{-1}	**Assignment of Bonds (Molecule/Group)**	**Mode of Vibration**	**Strength of bonds**	**Sample / Food Matrix**	**Wavenumber of laser source (nm)**	**Type of Raman**	**References**
2725	C-H	Stretching vibration	-	Methyl group of acetyl substituent/Starchacetate	1064	FT-Raman	20
1743	C=O	Stretching vibration	-				
1338	CH_2OH	Deformation vibration	-	- / Starchacetate			
866	COC	Symmetric stretching	-	- / Starchacetate			
480	-	Skeletal mode		- / Starchacetate			
2910	C-H	Stretching vibration	-	- / Starch-	1064	FT-Raman	21
1460	CH_2	Twisting deformation	-				
	C-H	Bending	-				
1403	C-H	Deformation bending	Shoulder				
1381	C-OH	Deformation	-				
	CH	Deformation bending					
	CH_2	Scissor deformation					
1341	CH_2	Twisting deformation	-				
	C-OH	Deformation bending					
1305	C-H	Deformation	-				
1264	CH_2	Deformation	-				
	C-OH	-					
	CH_2OH	(sidechain)					
1205	C-H	relatedmode	-				
1155	C1–O–C4	Deformation	Shoulder				
1127	C-OH	Asymmetric	-				

	C-OH	stretching	-				
	C-O	Stretching vibration	-				
1110	C-C	Deformation	Shoulder				
	C-O	Stretching vibration	Shoulder				
	C-H	Related mode	Shoulder				
1084	C-OH	Related mode	-				
1053	C-OH	Related mode	-				
	C-OH	Deformation bending	-				
	C-C	Stretching vibration	-				
1003	CH_2	Deformation	-				
943	C1–O–C4	Stretching vibration	-				
910	C-OH	Related mode	Shoulder				
	CH_2	Stretching vibration	Shoulder				
	C1-H	Deformation	Shoulder				
865	C1–O–C5	Deformation	-				
	CH_2	Deformation	-				
	C-H	Stretching vibration	-				
770	C-C	Deformation	-				
721	C-C	Deformation	-				
411, 443, 480,	C-C-O	Ring mode	-				
530, 576, 618		Ring mode	-				
		Stretching vibration, pyranose ring skeletalmodes (deformation)	-				
3046	O-H	Stretching,vibration	-	Maleinated starch	1064	FT-Raman	22
2800-3000	C-H	Stretches	-	Starch			
1657	-	-	-	Amylose			
1657	C=C	Stretchingvibration	-	Maleinated starch			
1641	C=O	Stretchingvibration	-	Maleinated starch			
810-975	C-C	stretches	-	Starch			
1456	-	-	-	glucose, fructose/ sport drink	633	Micro-Raman	23
1375	-	-	-	α-anomer of glucose			
1332	-	-	-	α-anomer of glucose			

1264	-	-	-	fructose			
1128	-	-	-	β-anomer of glucose			
1065	-	-	-	β-anomer of glucose			
918	-	-	-	α-anomer of glucose			
867	-	-	-	fructose			
836	-	-	-	α-anomer of glucose			
789	-	-	-	α-anomer of glucose			
742	-	-	-	other			
710	-	-	-	sucrose			
634	-	-	-	fructose			
975	C-O-P	Asymmetric stretching	strong	Starch phosphate	1024	FT-Raman	24
3030	CH_3	Asymmetric	-	Cationicstarch / Cationic			
970	$(CH_3)_3N^+$	stretching	-	Quaternary Ammonium			
761	$(CH_3)_3N^+$	Asymmetric stretching Symmetric stretching	-	Starch	785	Dispersive Raman	25
1459	CH_2	Deformation	decreasing in intensity				
1127	C-O	Stretching	decreasing in intensity				
1127	C-O-H	Deformation	decreasing in intensity	Retrogradated starch	-	FT-IR Raman	26
856	C-C	Skeletal modes of α–glucose	decreasing in intensity				
480	Glucose	Vibration	disappearing of the band				
1607	C=O	Stretching vibration	-	Carboxymethylated non-starch polysaccharides -	514	Laser	27
415	δ(C2-C1-O1), α-glucose	Bending	- -				
437	δ(C2-C1-O1) β-glucose	Bending	- -	Glucose			

523	-	Skeletal Vibration	-				
838	ν(C-C)	-	-		785	Dispersive Raman	28
856	δ (C1-H1)	-	-				
820-950	ν(C-O)	-	-				
	ν(C-C)	-	-				
	δ (C-C-H)	-	-				
	δ(C-C-O)	-	-				
1106	δ(C-O-C)	Angle Bending	-				
314	δ(C-C-C)	Ring Vibration	-				
353	δ(C-C-C)	Ring Vibration	-				
631	-	Ring Deformation	-				
709	Fructose	Skeletal Vibration	-				
800	ν(C-C)	-	-	Fructose	785	Dispersive Raman	28
870	C-O-C	-	-				
1028	ν(C-O)	-	-				
1054	ν(C-O)	-	-				
1074	C-O-C	-	-				
419	δ(C-C-O)	Ring Vibration	-				
544	α-glycosidic bond	-	-				
744	ν(C-C)	-	-	Sucrose	785	Dispersive Raman	28
800	ν(C-C)	-	-				
1127	C-OH	Deformation	-				
3200	O-H,Water	Stretching	-				
1640	O-H,Water	Stretching	-				
2878	CH_2-CH_3,Ethanol	Stretching	-				
2929	CH_2-CH_3,Ethanol	Stretching	-				
2972	CH_2-CH_3,Ethanol	Stretching	-				
1454	CH_2-CH_3,Ethanol	Stretching	-				
1096	CH_3,Ethanol	Rocking Vibration	-	Wine	1064	FT-Raman	28
1054	C-O,Ethanol	Stretching	-				
883	C-C,Ethanol	Stretching	-				
1462	CH_2 Sugar	Bending	-				
1130	C-C,C-O, Sugar	Bending	-				
1050-1080	C-C,C-O, Sugar	Bending	-				

1449	CH_2	Bending	-	Barley and Wheat	532	Raman	29
1659	C=O	Stretching	-				
1004	-	Breathing	-				
1610	-	Stretching	-				
1095	COC	Stretching	-				
1120	COC	Stretching	-				
480	-	Skeletal Vibration	-				
901	-	Skeletal Vibration	-				
1604	-	Aromatic Ring					
1631	C=C	Streching					
3420	OH	Stretching					
858	P-OH	Stretching					
894	P-OH	Stretching					
1358	C-H	-	-	Hydroxypropyl methylcellulose	-	Raman	30
1453	C-H	-	-				
478	C-O-C, δ(C-C-O)	Skeletal Mode	-	Cereal Starch	785	Raman	31
1150	v_a(C-O-C)	Stretching	-				
944	v_s(C-O-C)	Stretching	-				
1130	v(C-OH)	Stretching and In	-				
	v(C-O)	plane bending					
	δ(C-OH)						
150	-	-	-	Mannitol	785	Raman	32
250	-	-	-				
1030	-	-	-				
1130	-	-	-				

Table 3S. Raman spectra of some lipids

Band position cm^{-1}	Assignment of Bonds (Molecule/Group)	Mode of Vibration	Strength of bonds	Sample / Food Matrix	Wavenumber of laser source (nm)	Type of Raman	References
3020	=C-H	Asymmetric stretching vibration	Medium-Strong	- / Animal fat	1064	FT-Raman	33
3007	=C-H	Symmetric stretching vibration	Medium				
2943	$-CH_2$	Asymmetric stretching vibration	Medium				
2870-2840	$-CH_2$	Symmetric stretching vibration	Strong – very strong				
1665-1630	C=C	Stretching vibration					
1480-1440	CH_2	Scissoring vibration	Medium - strong				
1296	$=CH_2$	Deformation in plane					
1269	=C-H	Symmetric rocking	Very weak Shoulder Shoulder				
1670	C=C	Stretching vibration	-	*trans*-olefin / soybean oil *cis*-olefin	1064	FT-Raman	34
1658	C=C	Stretching vibration	-	*cis*-olefin			
1266	CH=CH	Symmetric rock	-				
3015	=C-H	Stretching vibration	-	cis-olefinic group / Hake Lipid	1064	FT-Raman	35
2931	CH_2	Asymmetric stretching	-	methyl and methylene groups in aliphatic molecules			
2898	CH_3	Symmetric stretching	-	methyl and methylene groups in aliphatic molecules			
2852	CH_2	Symmetric stretching	-	methyl and methylene groups in aliphatic molecules			

1746	C=O		Strong	esters			
1658	C=C	Stretching vibration	Strong	-			
1440	CH_2	Stretching vibration	-	-			
1301	CH_2	Scissoring vibration	-	-			
1266	=CH	twisting motion	-	-			
1079	CCC	symmetric rock (cis)	-	-			
970	CCC	Asymmetric	-	-			
928	CCC	stretching	-	-			
868	CCC	Symmetric stretching	-	-			
		Symmetric stretching		-			
		Symmetric stretching					
3015	=C-H	Asymmetric stretching	-				
2970	C-H	Asymmetric stretching	-				
2940	C-H	Asymmetric stretching	-				
2900	C-H	Symmetric stretching	-				
2860	C-H	Symmetric stretching	-				
1750	C=O	Stretching vibration	-				
1670	C=C	Stretching vibration	-	Edible oil	1064	FT-Raman	36
1660	C=C	Stretching vibration	-				
1445	C-H	Deformation	-				
1310	C-H	Deformation	-				
1275	=C-H	Deformation	-				
1100-1000	C-C	Stretching vibration	-				
900-800	C-C	Stretching vibration	-				
1657	C=C	Stretching vibration	Strong	Lipid / Fish Salmon			
1440	CH_2	Scissoring vibration	Strong	Carotenoids			
1301	CH_2	Phase twist	Strong	Carotenoids			
1267	=C-H	Symmetric rock (cis)	Strong	Collagen (phenylalanine)	785	Raman	37
1076	CCC	Stretching vibration	Strong	Collagen (peptide backbone)			
1064	CCC	Stretching vibration	Strong	Collagen (proline)			

1159	-	-	Strong				
1518	-	-	Strong				
1004	-	-	Weak				
940	C-C	Stretching vibration	Weak				
857	-	-	Weak				
3060	N-H	vibration	-	Protein / Milk Powder			
2927	C-H	vibration	-	-			
2900	C-H	vibration	-	-			
2853	C-H	vibration	-	-			
1745	C=O	vibration	-	Fat			
1665	Amide I	-	-	Protein			
1654	C=C	Vibration	-	-			
1455	CH_2	Scissor deformation	-	-			
1303	CH_2	Twisting deformation	-	-			
1262	Amide III	-	-	Protein			
1121	C-C	Vibration	-	-	1024	FT-Raman	38
1082	C-C	Vibration	-	-			
1065	C-C	Vibration	-	-			
1005	Phenylalanine	Ring breathing	-	Protein			
860-920	C-C	Vibration	-	-			
	C-O	Vibration	-	-			
	CH_3	Rocking	-	-			
	Phenylalanine	Ring breathing	-	-			
445		-	-	Lactose			
355		-	-				

1618	ν (C=C)	-	-	Pulegone			
1457	-	-	-	Pulegone			
1379	-	-	-	Pulegone			
1339	-	-	-	Pulegone			
647	δ (ring)	-	-	Pulegone			
1460	-	-	-	Thymol			
1380	-	-	-	Thymol			
1261	-	-	-	Thymol			
1065	-	-	-	Thymol			
875	-	-	-	Thymol			
740	δ (ring)	-	-	Thymol			
1701	ν(nonconjugated	-	-	γ-Terpinene			
	C=C)	-	-				
1428	Methyl and	-	-	γ-Terpinene			
	isopropyl C-H	-	-		785	Dispersive Raman	39
	bending appears	-	-				
	as a double	-	-				
	broad band	-	-				
756	δ (ring)	-	-	γ-Terpinene			
1611	ν (ring)	-	-	*p*-Cymene			
1209	δ (ring)	-	-	*p*-Cymene			
804	δ (ring)	-	-	*p*-Cymene			
1460	-	-	-	Carvacrol			
1261	-	-	-	Carvacrol			
1065	-	-	-	Carvacrol			
870	-	-	-	Carvacrol			
760	δ (ring)	-	-	Carvacrol			
718	C=C-H out of	-	-	linoleic acid			
724	plane	-	-	linoleic acid			
840	νs(C-C)	-	-	linoleic acid			
908	ν(C-C)	-	-	linoleic acid			

949	ν(C-C), Cα-atom	-	-	linoleic acid			
980	-	-	-	linoleic acid			
1064	-	-	-	linoleic acid			
1078	νas(C-C)trans	-	-	linoleic acid	514.5	Raman	40
1440	ν(C-C)	-	-	linoleic acid			
2885	CH_2 scissoring	-	strong	linoleic acid			
3011	νs(CH_2) ν(=C-H)	-	-				
1265	δ(C-H)	-					
1300	C-H	Bending					
1440	δ(C-H)	Scissoring					
1650	ν(C=C)	-					
1747	ν(C=O)	-					
1008	C-CH_3	-		Carotenoid in olive oil	514.5	Raman	41
1150	C-C	Stretching					
1525	C=C	Stretching					
2850	ν(C-H)	Symmetric Stretching					
2950	ν(C-H)	Asymmetric Stretching					
3015	=C-H	Symmetric Scissoring					

Table 4S. Raman spectra of some vitamins

Band position cm^{-1}	**Assignment of Bonds (Molecule/Group)**	**Mode of Vibration**	**Strength of bonds**	**Sample / Food Matrix**	**Wavenumber of laser source (nm)**	**Type of Raman**	**References**
811	C-H bend	Ring breathing	-	Vitamin B_3/-			
811	C=C-C bend	Ring-related vibration	-	Vitamin B_3/-			
1044	C-C-C bend	Trigonal	-	Nicotinic acid/-	1064	FT-Raman	42
3087	C-H stretch	-	-	VitaminB_3/-			
2932	C-Hstretch	-	-	VitaminB_6/-			

1507	Cyanocobalamin bands	Ring vibration	strong	VitaminB_{12}/-	360	Resonance raman	43
1582/1593 2845/2865 1635/1655	Aromatic part CHstretch,(CH, polymethylene chain) C=C,C=O bend	chromanol ring - Vibrational mode of quinone group	- - strong	alfa-tocopherol/- Vitamin E/- Vitamin E/-	633	Raman	44
3000 1580/1590	C-H stretch Terminal group	- -	- -	Vitamin A/- retinol,retinal, retinoic acid/-	-	Laser-excited raman spectra	45
1113 1758 1193 1661 1323 1258 1484 984	C-O-C stretching C=O stretch C-C(=O)-O stretching C=C stretch CH bending (wagging) C-O-H bending (twisting) CH bending C-H,O-H bending	- Lactone ring - - - - - -	strong weak weak strong strong strong medium strong	Vitamin C/-	-	FT-Raman	46
3380 2916 1751 1659 1457 1257 1126	O-H stretching C-H stretching C=O stretching C=C C-H bending C-H bending(wisting) C-O-C stretching	- - - Ring stretching - - -	weak strong weak weak medium medium medium	Vitamin C/-	1064	FT-Raman	47

1034	C-O-Hbending	-	weak				
934/871/825	C-C	Ring stretching	medium				
710/633	C-C	Ring stretching	Medium				
1654	C_4=O uracil	NH_3 bending	-	Riboflavin/-	266	Red-excited raman spectrum	48
1259	C_2-N_3-C_4 stretc+N_3-H bend	vibrational vibrational	-				

Table 5S. Raman spectra of microorganisms and viruses

Band position, cm^{-1}	**Assignment of Bonds (Molecule/Group)**	**Mode of Vibration**	**Strength of bonds**	**Sample/Food Matrix**	**Wavenumber of laser source (nm)**	**Type of Raman**	**References**
~722	CH_2	Rocking		*Staphylococcus* strains/-	532	Micro-Raman	49
746		-					
~778	Cytosine, urasil ring stretching	-					
850	CC ring breathing COC 1,4 Glycosidic link	Stretching					
1001	CC aromatic ring breathing (phenylalanine)	Stretching					
1125	COC symmetric glycosidic link (C-N) and (C-C)	Stretching					
1200-1280	Amide III	-					
~1327	C-H	Deformation					
1440-1460	CH_2 scissoring	Deformation					
1575	Amide II Guanine, adenine ring stretching	-					
1650-1680	Amide I	-					
2935	CH_2 assymetric	Stretching					
3060	CH olefinic	Stretching					
856	C-C stretching	-		Bacteria, yeast and mold/-	1064	FT-Raman	50
1088	C-C	Stretching					
1304	C-H stretching	bending					
1458	C-H stretching	bending					

1658	C=C stretching	Stretching				
2931	C-H	Stretching				
3379	O-H	Stretching				
1528	C=C	Stretching	*R. mucilaginosa* - β caroten/-			
1508	C=C	Stretching	*M. luteus* - sarcinaxantin/-			
1156	C-C	Stretching	*R. mucilaginosa* - β caroten/-			
1151	C-C	Stretching	*M. luteus* - sarcinaxantin/-			
1003	C-C of the $C\text{-}CH_3$ group	Stretching	*R. mucilaginosa-β caroten*/-			
1001	C-C of the $C\text{-}CH_3$ group	Stretching	*M. luteus-sarcinaxantin*/-	633	Confocal Raman	51
1660	Amide I	-	*B. sphaericus*/-			
1445	CH_2 scissor mode	-	*B. sphaericus*/-			
1002	Aromatic ring breathing mode	-	*B. sphaericus*/-			
1449	CH_2	Deformation	*B. subtilis*/-			
3059	C=C–H aromatic	Stretching				
2975	CH_3	Stretching				
2935	C–H	Stretching				
2870–2890	CH_2	Stretching				
1735	>C=O ester	Stretching				
1650–1680	Amide I	-				
1614	Tyrosine	-				
1605–1606	Phenylalanine	-				
1582, 1593	Protein	-				
1575–1578	Guanine, adenine	ring stretching	*E. feacalis*/-	1064	FT-Raman	52
1440–1460	$C\text{–}H_2$	deformation				
1129	C-C, C-N	stretching				
1102	$> PO_2^-$	Symetric stretching				
1098	CC skeletal, and COC	stretching from glycosidic link				

1085	C–O	stretching				
1061	C–N and C–C	Stretching				
1004	Phenylalanine	-				
897	COC	stretching				
858	CC str, COC 1,4 glycosidic link	-				
852	Buried tyrosine	-				
829	Exposed tyrosine	-				
785	Cytosine, uracil	ring, stretching				
720	Adenine	-				
665	Guanine	-				
640	Tyrosine (skeletal)	-				
620	Phenylalanine (skeletal)	-				
540	COC	glycosidic ring deformation				
520–540	S–S	stretching				
1172	Tyrosine	-				
1247	Guanine, adenine, urasil	-				
1324	Guanine, adenine, tyrosine	-				
1359	Thymine, adenine	-				
1475	Guanine, adenine	-	*Bacillus* species/-	244	UV-Resonance Raman	53
1524	Cytosine	-				
1567	Guanine, adenine	-				
1607	Tyrosine, tryptophan	-				
1638	Thymine	-				
1573	C=C, N–H, and C–N str (amide II)	N–H deformation C–N streching				
1482–1487	Nucleic acids	-				
~1320	Amide III, C–H	deformation				
1220–1290	Amide III random, lipids	-				
1030-1130	Carbohydrates, –C–C– (skeletal), C–O, def(C–O–H)	C–O–H deformation	*Clostridium* species/-	633	Confocal Raman	54, 55
~1130	=C–C= (unsaturated fatty acids in lipids)	-				
810–820	Nucleic acids (C–O–P–O–C in RNA backbone)	-				
550	Range glass background	-				

481	Skeletal modes of carbohydrates (starch)	-				
407	Skeletal modes of carbohydrates (glucose)	-				
757	Tryptophan	W18				
785	Thymine, cytosine	Ring stretching				
853	Tyrosine	Ring stretching				
876	Tryptophan	W17, N1H deformation				
1010	Tryptophan	W16, CC				
1178	Tyrosine	Y9a				
1205	Tyrosine	Y7a				
1239	Tryptophan	W10				
1243	Thymine	C2N3 stretching				
1307	Adenine	C8H deformation				
1335	Adenine	N7C5 stretching, C8N7 stretching				
1372	Adenine, Guanine, Thymine	C1N9 stretching, C6N6 stretching				
1420	Adenine	C4C9 stretching, C8H deformation	*fd* virus/-	257	UVRR	56
1483	Adenine	C2H deformation, N9C8 stretching				
1507	Adenine	N7C8 stretching				
1530	Cytosine, Guanine	N3C4 stretching				
1560	Tryptophan	W3, C2C3 stretching				
1575	Guanine, Adenine, Tryptophan	C5C4, C4N3 stretching, W2				
1616	Tryptophan, Tyrosine	W1, Y8a				
1646	Thymine, Cytosine	C4=O, C5=C6 stretching				
1660	Amide I Protein	-				
1572	Guanin/adenin	Ring Stretching				

1448	CH_2	Deformation				
1240	C-C and C-N Adenin/Timin					
	Amide I	-	Natural Mineral Water	Raman		57
1003	-	Ring Breathing mode of phenylalanine				
780	O-P-O	-				
720	Adenin	-				
2975	CH_3 str	-	Protein, carbohydrate, lipids, cell wall			
2931	CH_3 and CH_2 str	-	Protein, carbohydrate, lipids, cell wall			
2870-2890	CH_2 str	-	Protein, carbohydrate, lipids, cell wall			
1735	-C=O str	-	PHB			
1669	Amide I	-	Protein			
1614	Tyr, Phe,	-	Protein			
1605	Phenylalanine (ring str),	-	Protein			
1575	Guanine, adenine (ring str)	-	DNA / RNA			
1450	CH_2 def scissoring	-	Protein, carbohydrate, lipids, cell wall	532	Raman	58
1360	Tryptophan (indole ring str)	-	Protein			
1332	Cytosine, uracil (ring str)	-	DNA / RNA			
1314	CH_2 def	-	Protein			
1236	Amide III	-	Protein			
1208	T,C,A,Tyr, Phe	-	Protein			
1175	T, G	-	DNA / RNA			
1124	C-N str, C-C str skeletal trans	-	Protein, carbohydrate, lipids, cell wall			
	Conformation	-				
1098	$>PO^-_2$ str (sym)	-	Nucleic acids and Cell wall			
	CC skeletal and COC str from glycosidic link	-				
		-				
1030	Phenylalanine, CC skeletal cis conformation	-	Protein and Cell wall			
		-				

1006	Phenylalanine, Tryptophan	-	Protein			
950	Polysaccharide, DNA backbone	-	Polysaccharide, DNA			
852	“buried” tyrosine	-	Protein			
826	“exposed” tyrosine	-	Protein			
778	Cytosine, uracil (ring stretching)	-	DNA / RNA			
745	Adenine, thymine	-	DNA / RNA			
723	Adenine	-	DNA / RNA			
695	Guanine	-	DNA / RNA			
665	Thymine, guanine	-	DNA / RNA			
640	Tyrosine (skeletal)	-	Protein			
620	Phenylalanine (skeletal)	-	Protein			
560	COC glycosidic ring def	-	Protein, carbohydrate, lipids, cell wall			
540	S-S str - disulfide conformation	-	Protein			
1656	-	Stretching				
1437	CH_2	Deformation				
1300	CH_2	Torsion	Oil	532	Micro Raman	59
1262	=CH	Deformation				
1742	C=O	Stretching				
2900	C-H	Stretching	-			
1650	-	Amide I	-			
1420	CH2	Deformation	-			
1007	-	Ring Breathing	-			
1385	C-O-C	Stretching	-	-	Micro Raman	60
1440	-	Ring	-			
1565	-	Ring	-			
1532	C=C	-	-			
1157	C-C	-	-			
1005	$C-CH_3$	Deformation	-			
2933	CH2, CH	-	-			
1659	-	Amide I	-			
1578	-	-	-			
1447	C-H	-	-			

1317,1243	-	Amide III	-	532.11	Raman	61
1094	-	-	-			
1003	Phe	-	-			
785	DNA-RNA	-	-			

Table 6S. Raman spectra of toxins and chemicals

Band position cm^{-1}	**Assignment of Bonds (Molecule/Group)**	**Mode of Vibration**	**Strength of bonds**	**Sample / Food Matrix**	**Wavenumber of laser source (nm)**	**Type of Raman**	**References**
1450 1250 1083, 1105, 1128, 1157 510, 525, 540	C-H Amide III C-N S-S	Bending - - Streching		Ricin and ricin aggluitinin/ *Ricinus communis* seeds	488	Raman Laser	62
993, 1348, 1591 624, 1003, 1065 786, 1449, 1607 1393	- - - -	- - - -		Zhibaoboshi Chongmanjue Abameclin Petroleumoil Cypermethrin /pear,grapes, apple, longan, spicy-pear, Chinese goosebeery, orange, banana etc.	1064	FT-Raman	63
1068 1220.7	B–O C–O	Symmetric streching Asymmetric streching		T-2 Toxin/-	785	Raman Microscope	64
934	Cl-O	Symmetric streching		Perchlorate /Ground waters	670	Raman	65

708 665 490 215 819 963	NH2 H2C C-O C-O CH CH2	Twisting Twisting Torsion Torsion Wagging Wagging	Weak Weak - Weak Medium Weak	Acrylamide/-	514.5-488	Raman laser	66
3066 2921 1699 1571 2983-3050 1194 96	CH CH3 C=O C-C CH2Br CH2Br CH3	Streching Asymetric strech Streching Streching Skel def Streching Deformation Torsion Skel def	Strong Medium Strong Very strong Weak Strong Very strong	6-Methyl-4-bromomethylcoumarin/-	1064	FT-Raman	67
766 399, 756, 1407 386, 745, 1386 582,1393, and 1622	- - - -	- - - -	 Strong Strong 	Naphthalene/- Anthracene/- Phenanthrene/- Pyrene/-	1064	UV resonance Raman	68
1513, 1156, 1008 1406, 1142, 407 3054, 1627, 1594, 592 1401, 394 3055, 1381 1576, 1463, 1020	ν (C C), ν (C–C), (C–CH3) C C, CH C C, CCC CH, C C C=C , =C–H	Stretching, Stretching rocking in-plane vibration, skeletal ring vibrations, bending in-plane vibration, bending stretching, in-plane vibration stretching, in-plane deformation vibration	Strong, strong medium Strong Medium Strong, medium Strong medium	Beta-carotene/- Pyrene/- Anthracene/- Napthalene/-	1064	FT-Raman	69

686	C-H	out of plane bending	-	Aflatoxin in maize	785	Raman	70
760	C-H	out of plane bending	-				
828	-	ring deformation	-				
956	*v*(C-C)	-	-				
1440	β (C-H)	ring mode	-				
1460	β (C-H)	ring mode	-				
1612	*v*(C-C)	ring mode	-				
1760	*v*(C=O)	ring mode	-				
3015	CH3	-		Metamidophos	633	Raman	71
2938	CH3	-					
2844	CH3	-					
1454	CH3	-					
1216	v(PO)2+ CH3	Stretching					
1066	CH3	-					
1036	CH3	-					
946	v(CO3)+vO3P	Stretching					
786	vSC + NH2	Stretching					
712	vO3+NH2	Stretching					
615	vPS+vNP	Stretching					
576	vCS+vPS	Stretching					
3261	N-H	Stretching					
3252	N-H	Stretching					
3265	N-H	Stretching					
3112	vC52-H+vC53-H	-					
2974	vC51-H	-					
2939	vC51-H	-					
2871	vsC-H	-					
2719	vsC-H	-					
3182	vsCH3	-					
3087	vC52(53)-H	Stretching					
3019	vC51-H	Stretching					
2982	vC52(53)-H	Stretching					
2972	vC51-H	Stretching					
2935	vC31-H+vC32-	Stretching					

	H+vC33-H					
2913	vC51-H+vC52-H+vC53-H	Stretching				
2874	C-H	Stretching				
2760	δH-C-C	Stretching				
2461	vC31-H	Stretching				
3100	vC52-H+vC51-H	Stretching				
2976	vcC52(C32)-H	Stretching				
2938	vs(C51(C31)-H	Stretching				
2877	C-H	Stretching				
2746	v(C-H)	Stretching				
2457	v(C-C)	Stretching	Atrazine, Prometryn,			72
1610	δC3-N3-H	Deformation in plane	Simetryn triazine	1064	Raman	
1599	δC5-N5-H	Deformation in plane				
1550	vC5-N6, vC3-N2	In phase, in plane				
1448	δCH3	In plane bending				
1388	δCH3	In plane bending				
1378	δC-C-H	In plane bending				
1343	vC-Cl	Stretching				
1168	δC-C-H	In plane bending				
1127	δC-C-H	In plane bending				
1084	δN-C-H	In plane bending				
993	δC-C-H	In plane bending				
1343,1310,1251, 1168	vC1-C1	Stretching				
924	vC-Cl	Stretching				
648	δN6-C1-N2, δC5-N4-C3	In plane bending				
253	C53-H, C52-H	-				
1621	δC3-N3-H	In plane bending				
1606	δC5-N5-	In plane bending				

1581	vC5-N6	Out of and in phase					
1547	vC3-N2	Out of and in phase					
1462	δCH3	In plane bending					
1350	δC-C-H	In plane bending					
1182	C-S	Stretching					
1133	C-S	Stretching					
971	-	Ring Breathing					
993	-	Ring Breathing					
<700	-	Skeletal modes of ring structure					
828	-	Ring deformation					
956	v(C-C)	-		Maize	785	Raman	73
1080	v(C-O)	-					
1400-1500	β (C-H)	Ring mode					

Table 7S. Raman spectra of food additives

Band position cm^{-1}	**Assignment of Bonds (Molecule/Group)**	**Mode of Vibration**	**Strength of bonds**	**Sample / Food Matrix**	**Wavenumber of laser source (nm)**	**Type of Raman**	**References**
-	C=C	C=C Stretching	-	Astaxanthin and Cantaxanthin/ Salmon	-	Resonance Raman	74
1600	-	Naph (**1**) ring stretching Naph (**2**) ring stretching	Strong				
1575	-	O12–H19 i. p. bend + Naph (**2**) ring stretching	Very Strong				
1515	-	Naph (**1**) ring stretching C3–O12 stretching + Naph (**2**) ring stretching	Very Strong				
1459	-	N11–N28 stretching + Naph (**2**) stretching	Strong	Amaranth/-	-	FT-Raman	75
1442	-	C2–N11 stretching +	Strong				

1365	-	CH Naph (**2**) i.p.bending CH Naph (**1**) i.p.bending + C29–N28	Very very Strong				
1300	-	stretching	Strong				
1240	-		Very Strong				
1598	-	Phenyl ring stretching	Very strong				
1502	-	Phenyl ring bending	Strong	Tartrazine/-	1064	FT-Raman	76
1357	C–N8=N9–C	Stretching	Strong				
1129	-	Out of plane C-H deformation	Strong				
1500-1700	-	-	Strong	Deuterated maltol/-	1064	FT-Raman	77
3100-3350	O-H	Stretching	Very veak	Maltol/-	1064	FT-Raman	77
2943	-	Symmetrical CH2 stretching	Very strong				
1407	COO-	Symmetrical stretching	Very strong				
1341	-	CH2 deformation	Strong	Monosodium glutamate/-	514.5	Raman micro-spectrometer	78
931	-	Completely ionized form Twisting	Strong				
180	COO-		Very very strong				
3063	CH	Symmetrical phenyl ring	Strong				
3054	CH	In plane phenyl ring bending	Strong	Aspartame/-	514.5	Raman microspectrometer	79
2955	C6H2, C5H	Symmetrical phenyl ring	Strong				
2948	C6H2	Symmetrical phenyl	Very strong				

		ring					
1005	C5C6C13	Torsion	Very very strong				
90	CH_3	Rocking	Very very strong				
61	-	Skeletal deformation	Very very strong				
57	-	Skeletal deformation	Very very strong				
42	-	C13O19, C13O18, CH_3 deformation	Very very strong				
1653	C=O	Stretching	Strong				
1585	COOH	Asymmetric stretching vibration	Weak				
1462	CH_2 and CH_3	Deformations	Very strong				
1442	CH_2 and CH_3	Deformations	Very strong				
1408	C-C	Stretching	Very strong	HMB/-	514.5	Conventional Raman	80
1306	C-H	In-plane deformation	Strong				
1258	COH	Wagging	Medium				
748	CH_2	Rocking	Very strong				
663	COOH	Wagging	Strong				
632	COH	Deformatiion bending	Medium				
1584	COOH	Asymmetrical stretching	Strong				
1463	CH_3	Deformation	Very strong				
1385	C-C	Stretching	Strong				
1245	COH	Wagging	Strong				
1195	CCO	Out of plane stretching	Strong				
		Stretching		L-carnitine/-	514.5	Conventional Raman	80
971	C-N+ $(CH_3)_3$	Asymmetrical	Strong				
948	C-N+ $(CH_3)_3$	stretching	Strong				
		Stretching					
913	C-COOH	Rocking	Strong				
772	CH2	Deformation bending	Very strong				
634	COH		Strong				

522 505 1610-1700 1225-1330	S-S S-S Amide I Amide III	- - - -	- - - -	Human Serum	Albumin	785	Raman	81
3354 3292 2892 2736 1468 1414 1379 1338 1292-1267-1241 1153-1119-1095- 1056-1036-1026- 995-972-911-898 457 437-379-352	v(OH)HB v(OH)HB v(CH2) v(CH) δ(CH)+ω(CH2)+ δ(OH) δ(CH)+ δ(OH) δ(CH2)+δ(CH)+ δ(OH)+ν(Φ) δ(CH) δ(OH...O)+ν(C- C)+ν(C-O)+ δ(CH)+ρ(CH2) ν(C-O- C)+ν(Φ)+ν(C- OH)+ν(C- CH2)+ δ(CH)+ρ(CH2) δ(COC) γ(OH)+γ(ϕ)	Stretching Stretching Stretching Stretching In plane bending+out of plane bending In-plane bending In-plane bending+Stretching In-plane bending In-plane bending+stretching Stretching+ In-plane bending In-plane bending Out of plane bending	- -	Cellulose		-	FT-Raman	82
2963 2935 2880 2719 1656 1620 1451 1415 1377	ν(CH3) ν(CH3) ν(CH2) ν(CH) ν(CO)AmI δ(NH) δ(CH)+ω(CH2)+ δ(OH) δ(CH3)+ δ(CH) δ(CH2)+	Stretching Stretching Stretching Stretching Stretching In plane bending In plane +out of plane bending In plane bending In plane	- - - - - - - - - -					

	δ(CH)+	bending+Stretching	-				
1326	δ(OH)+ν(ϕ)	In plane	-				
	ν(CN)+ δ(CH)	bending+Stretching	-				
1265+1204	δ(OH..O)+ν(C-C)+ν(C-O)+ δ(CH)+ρ(CH2)	In plane bending+Stretching	- -				
1150+1112+1057	ν(C-O-C)+ν(ϕ)+ν(C-OH)+ν(C-CH2)+ δ(CH)+ρ(CH2)+ ρ (CH3)	In plane bending+Stretching	- -	Chitin	-	FT-Raman	82
1043	ρ(CH3) +δ(CH)+ δ(OH)	In plane bending	-				
954	ν(CN)	Stretching	-				
896	ν(ϕ)+ρ(CH2)	Stretching	-				
710	ω(NH2)+ δ(ϕ)	In and out of plane bending	- -				
661+647+597	γ(OH..O)	Out of plane bending	-				
501	δ(CO-NH)+ δ(C-CH3)	In plane bending	-				
451+397+366+325	γ(OH)+γ(ϕ)	Out of plane bending	-				
253	δ(C-NH-C)+γ(OH)	In and out of plane bending	-				
3362	ν(OH)HB	Stretching	-				
2932	ν(NH2)	Stretching	-				
2885	ν(CH2)	Stretching	-				
2818	ν(NH2)	Stretching	-				
2743	ν(CH)	Stretching	-				
1654	ν(CO)	Stretching	-				
1591	δ(NH2)	In plane bending	-				
1458	δ(CH)+ω(CH2)+ δ(CH)+ δ(OH)	In and out out plane bending	- -				

1411	δ(CH3)+ δ(CH)	In plane bending	-			
1377	δ(CH2)+	In plane bending and	-			
	δ(CH)+	stretching	-			
1325	δ(OH)+ν(ϕ)	In plane bending and	-			
	ν(CN)+ δ(CH)	stretching	-	Chitosan	FT-Raman	
1263		In plane bending and	-			
	δ(OH...O)+ν(C-C)+ν(C-O)+	stretching	-			
			-			
1146+1114+1093	δ(CH)+ρ(CH2)	In plane bending and	-			
	ν(C-O-C)+ν(ϕ)+ν(C-OH)+ν(C-CH2)+ δ(CH)+	stretching	-			
			-			82
			-			
			-			
1044	ρ(CH3)+ ρ(CH2)	In plane bending and	-			
	ν(ϕ)+ δ(CH)+	stretching	-			
991	δ(OH)	In plane bending and	-			
	ν(ϕ)+ δ(CH)	stretching	-			
936		Stretching	-			
896	ν(CN)	Stretching	-			
703	ν(ϕ)+ρ(CH2)	In and out of plane	-			
	ω(NH2)+δ(ϕ)	bending	-			
566		In and out of plane	-			
	γ(NH)+	bending and stretching	-			
	ν(C=O)+ω(CH3)	In plane bending	-			
493			-			
	δ(CO-NH)+ δ(C-CH3)	In plane bending	-			
479		Out of plane bending	-			
444+424+357	δ(COC)	In and out of plane	-			
	γ(OH)+ γ(ϕ)	bending	-			
285			-			
	δ(C-NH-C)+ γ(OH)					
1151	δ(CCH), δ(C-OH)	In plane bending	-			
1250	δ(CH) of C=CH,	In plane bending and	-			

	v(CCH)	stretching	-				
1317	δ(CCH)	In plane bending	-	Curcumin	785	FT-Raman	
1430	δ(CCC),	In plane bending	-				
1600	δ(CCH), v(C=C)	Stretching	-				83
1627	v(C=C), v(C=O)	Stretching					
1528	-	-	-				
1163	-	-	-				84
1009	-	-	-	Carrot Roots	532	Raman	
958	C-H	Out of plan	-				
962	δC-N=N+v(C-N)	In plane bending, stretching					
1120	δH-N-H+v(C=O+v(C-N)	-					
1332	δH-N-H+vC-N+δN-C=O	In plane bending, stretching		Azodicarbonamide	785	Raman	85
1574	vN=N δN-H+vC=O	-					
1712	vC=O+vC-N	Stretching					
602	δN-C=O+δN-C-N+δC-N-N	In plane bending					
984	vC-N+δC-N-N	In plane bending, stretching					
1092	δNH2+vC-N+vC=O	In plane bending, stretching					
1242	vN-N vC-N+vN-N+δN-H	Stretching In plane bending, stretching		Biurea	785	Raman	85
1602	vC-N+δN-H+vC=O	In plane bending, stretching					
1676	vC-N+δN-H+vC=O	In plane bending, stretching					
508	δN-C=O+δN-H	In plane bending					
716	δC-N+δN-H	In plane bending		Semicarbazide hydrochloride	785	Raman	85
936	vC-N	Stretching					

1098	vC-N	Stretching				
1184	vC-N	Stretching				
1224	vC-N	Stretching				
1388	vC-N,δN-C=O,δN-H	In plane bending, stretching				
1538	δN-H	In plane bending				
1952	vN-H	Stretching				
1720	C=O	Stretching				
1350	HCO	-				
1200-1415	CH_2,HCC,HCO, COH	Deformation, Stretching				
1116	-	Symmetric Stretching				
1094	-	Symmetric Stretching				
1123	C=O	Stretching				
3311	N-H	-				
2885	C-H	Stretching	Chitosan	1064	FT Raman	86
2917	C-H	Stretching				
1070	O=S=O	Stretching				
1014	O=S=O	Stretching				
580	O=S=O	Deformation				
610	O=S=O	Deformation				
823	C-O-S	Stretching				
834	C-O-S	Stretching				

Table 8S. Raman spectra of raw material

Band position cm^{-1}	Assignment of Bonds (Molecule/Group)	Mode of Vibration	Strength of bonds	Sample / Food Matrix	Wavenumber of laser source (nm)	Type of Raman	References
1745	C=O	Stretching vibration	Weak	- / Marama Bean Oil	1064	FT-Raman	87
1655	cis C=C	Stretching vibration	Medium				
1442	CH_2 bend	Bending vibration	Strong				
1265	=CH	In-plane deformation	Medium				
1301	=CH	(CH_2) wagging, twisting	Medium				
1008	$HC-CH_3$	CH_3 bending	Weak	- / Oil	532	Confocal Raman	88
1156	$-(CH_2)_n-$	C-C stretching	Medium				
1267	*cis* RHC=CHR	=C-H bending	Weak				
1302	$-CH_2$	C-H bending	Medium				
1442	$-CH_2$	C-H bending	Strong				
1522	RHC=CHR	C=C stretching	Medium				
1655	*cis* RHC=CHR	C=C stretching	Strong				
1747	RC=OOR	C=O stretching	Medium				
353	Unknown carbohydrate and protein	-	Weak	- / Honey	1064	FT-Raman	89
423	Unknown carbohydrate and protein	-	Strong				
518	Unknown carbohydrate	-	Strong				
630	Unknown carbohydrate	-	Strong				
704	Unknown carbohydrate	-	Weak				
775	Unknown carbohydrate	-	Weak				
824	Unknown	-	Weak				
866	C(1)H	Bending	Weak				

915	C(1)H and COH	-	Weak				
981	Unknown	Bending	Weak				
1072	C(1)H and COH	-	Medium				
	C-N (protein or amino acids)	-					
1126	Unknown carbohydrate		Medium				
	C-N (protein or amino acids)						
1267	C(6)OH and C(1)OH	-	Medium				
	Amide III (peptide bond)	Bending	Medium				
1374	CH and OH	Bending	Medium				
1461	CH_2	-	Strong				
	COO-	Stretching	Strong				
2945	CH	Stretching	Medium				
3384	OH	Stretching	Weak				
3013	=C-H	Stretching asymmetry	Medium				
2909	C-H	Stretching asymmetry	Strong				
1750	C=O	Stretching	Weak	- / Edible Oils	1064	FT-Raman	90
1660	C=C	Streching	Medium				
1294	*cis* =C-H	Bending	Weak				
1447	C-H	Bending	Medium				
1605	Phenyl Ring	Stretching	Strong				
1630	C=C	Stretching	Strong				
1120	Cyclohexane CH, COH	Bending	Medium				
1165	Phenyl ring	Bending	Medium				
1193	Phenyl ring CH, COH	Bending	Medium				
1270	Phenyl ring	Distortion	Medium	- / Coffee	514.5	Micro Raman	91
1690	C=O	vibration	Medium				
2905	CH_2 of lipids	Stretching	Strong				
2934	CH_2 of lipids	Symmetric	Strong				
3010	Ethylenic group	Vibration Asymmetric	Weak				

		Vibration					
3008	Ethylenic group	Stretching	Medium				
2923	C-H	Stretching	Strong				
2893	C-H	Stretching	Strong				
2851	C-H	Stretching	Strong				
1750	C=O	Stretching	Medium				
1657	C=C	Stretching	Weak				
1440	CH_3	Deformation vibration	Medium	- / Coffee	1064	FT-Raman	92
1302	CH_2	Deformation vibration	Weak				
1266	CH	Deformation vibration	Weak				
879	C-C	Stretching	Strong				
1030	C-O	Stretching	Medium				
1079	CH_3	Rocking	Weak	- / Alcoholic beverage	785	Raman	93
1019	C-O	Stretching	Medium				
921	C-C	Skeletal vibration	Weak				
317	C–C–C	Deformation	-				
341	C–C–O ring mode	Deformation	-				
415-437	C2–C1–O1	Deformation bending	- -				
776	C-C	Stretching deformation	- -	Glucose / Honey	785	Raman	94
790	C1-H1	Stretching	-				
976-1028	C-O	Angel-bending	-				
1106	C-O-C	model-deformation					

314-353 419 744 800 911 933 1028 1054	C-C-C ring vibration C-C-O Ring vibration C-C C-C COH C-O C-O C-O	deformation deformation stretching stretching deformation stretching stretching stretching	- - - - - - - -	Fructose / Honey	785	Raman	94
341 434 544 842 855 1028	C-C-O Ring mode C2–C1–O1 α-glycosidic bond C-C C1-H1 C-O	Deformation Deformation Stretching Deformation Stretching vibration of glucose ring	- - - - - -	Maltose / Honey	785	Raman	94
451 520 1063	C–C–O C2–C1–O1 C–O	Deformation Deformation Stretching	- - -	Glucose / Grape Juices	785	Raman	95
629 710 821 870	CCO exo CCO C-C C-C	Deformation Deformation Stretching Stretching	- - - -	Fructose / Grape Juices	785	Raman	95
879 1030 1079	C-C C-O CH_3	Stretching Stretching Rocking	Strong Weak Weak	Ethanol / Grape Juices	785	Raman	95
891 632	C-C	Stretching	Strong weak	Acetic acid / Grape Juices	785	Raman	95

3000	C-H	Stretching	-	- / Oil	785	Raman	96
3092	=C-H	Stretching	-				
3008	C-H, C=C	Stretching	-				
1676	C=C	Stretching	-				
1500	-	Stretching	-				
1379,1293, 797	C-H,C-C	-	-				
932	C-C	Stretching	-	- / Caviar	785	Raman	97
974	=C-H	Out of plan deformation	-				
1266	=C-H	Symmetric rock	-				
1302	CH_2	Twisting	-				
1442	CH_2	Scissoring	-				
1662	C=C	Stretching	-				
1262	=C-H	Stretching	-				
1604	C=C	Stretching	-	Kahweol / Green Arabica and Robusta Coffee Beans	1064	FT-Raman	98
1630	C=C	Stretching	-				
1690	-	amide I bands of β-sheet	-				
1656	-	amide I bands of α-helix	-				
1479	-	-	-				
1567	-	-	-				
853	v(C-O-C)	Stretching	-				99
1003	v(C-CH_3)	Stretching	-				
1065	v(C-C)	Stretching	-				
1158	v(C-C)	Stretching	-				
1168	Ring δ(CH)	Deformation	-				
1267	δ(=C-H)	Deformation	-				
1303	τ(CH_2)	Twisting	-				
1439	δ(CH_2)	Deformation	-				
1521	v(C=C)	Stretching	-				
1587	Aromatic v(C-C)	Stretching	-				
1605	Aromatic Ring	-	-				
1623	C=C	Stretching	-				

1630	v(C=C)	Stretching	-			
1720	v(C=O)	Stretching	-			
2727	v(CH)	Stretching	-			
2853	$v(CH_2)$	Stretching	-			
2904	$v(CH_3)$	Stretching	-			
2921	$v(CH_2)$	Stretching	-	Organic Compounds /	514	Confocal Raman
915	C-C-C	Bending		Red and Green Tomato		
		Deformation	-			
1623	C=C	Stretching				
			-			
744	δ(N-C-C)	Deformation	-			
915	δ(C-C-C)	Deformation	-			
958	-	-				
964	-	-				
985	$\delta(CH_3)$	Deformation	-			
1325	δ(CH)	Deformation	-			
1371	$\omega(CH_2)$	Wagginh	-			
1553	v(C=C)	Stretching	-			
853	vas(C-O-C)	Stretching	-			
958	$pip(CH_3)(v4)$	In plane rocking	-			
964	$pip(CH_3)(v4)$	In plane rocking	-			
1007	$v(C\text{-}CH_3)(v3)$	Stretching	-			
1062	v(C-C)	Stretching	-			
1156	v(C-C)(v2)	Stretching	-			
1167	Ring δip(CH)	Deformation	-			
1269	V4 δip(=C-H)	Deformation	-			
1441	$\delta(CH_2)$	Deformation	-			
1518	v(C=C)(v1)	Stretching	-			
1585	v(C-C)	Stretching	-	Organic Compounds /	785	Confocal Raman
1606	Ring	-	-	Red and Green Tomato		
1720	v(C=O)	Stretching	-			
2311	2v2	Stretching	-			
2854	$v(CH_2)$	Stretching	-			
2906	$v(CH_3)$	Stretching	-			

1078, 1124 1657	C-C, C-N, C-O Amide I	- -	- -	Protein and Oil / Soybean	785	Raman	100
1241 1997 3275 3261 3300 3397-3309 1132-1207 1196	N-H O-H N-H N-H N-H O-H Amide III C-O, C-O-C, NH_2	Stretching Stretching Stretching Stretching Stretching Stretching Stretching Stretching	- - - - - - - -	- / Meat	633	Raman	101
220-200 1078 1122 1155-960 922 867	CH_2-OH C-O C-O P-OH P-O-C P-O-C	Torsial Vibration Stretching Stretching Stretching Asymmetric Stretching Symmetric Stretching	- - - - - - - -	- / Yogurt	785	Raman	102
2336 1557 4160 2925 1391	- - H-H C-H C=O	- - Stretching Stretching Stretching	- - - - -	- / Fermentation Gases	488	Raman	103

1374	-	Stretching	-	Nitrosylmyoglobin / Meat	457.9	Resonance Raman	104
1585	-	Stretching	-				
1632	-	Stretching	-				
1370	-	Stretching	-				
1380	-	Stretching	-				
1630	-	Stretching	-				
1267	cis δ(=CH)	Symmetric rock	-	Oxidation Parameters / Olive oil	785	Raman	105
1302	-	In-phase twist methylene	-				
1442	$\delta(CH_2)$	Scissoring	-				
1655	ν(C=C)	Scissoring	-				
1747	ν(C=O)	Stretching	-				
212	-	-	-	Adulterants / Dry Milk	785	Raman	106
673	-	-	-				
973	-	-	-				
1009	-	-	-				
514	ν S–S gauche–gauche–gauche conformation	-	-	Myofibrillar proteins / Pork	514.5	Raman	107
530	ν S–S gauche–gauche–trans conformation	-	-				
547	ν S–S trans–gauche–trans conformation	-	-				
630–670	ν S–S gauche conformation	-	-				
825, 852	Tyr ν-ring	-	-				
758, 882	Trp ν-ring	-	-				
932	νCC	-	-				
1003	α-helix	-	-				
1034	Phe ν-ring	-	-				
1063	Phe ν-ring	-	-				
1126	νCN, νCH νCN	-	-				
1244	Amide III (β-helix)	-	-				
1304	Amide III (α-helix)	-	-				
	δCH	-	-				

1322, 1340	νCOO− Asp, Glu	-	-				
1410	δasCH3, δCH2, and						
1450	δCH	-	-				
	Amide I	-	-				
1600–1700	νCH3, νCH2, and	-	-				
2936	νCH2						
1749	υ (C=O)	Stretching	-				
1651	ν(C=C)	Stretching	-				
1439	CH_2	Scissoring Deformation	-				
1303	CH_2	Twisting Deformation	-				
1267	δ (=C-H)	Scissoring deformation	-	Maturation Stages / Olive Oil	488	Raman	108
1009	C-CH_3	Deformation	-				
1150	ν(C-C)	-	-				
1523	ν(C=C)	-	-				
1300	CH_3	Twisting					
1500-1400	CH_2	Scissoring					
1200-1050	C-C	Stretching					
3100-2800	C-H	Stretching					
1440	CH_2	Stretching					
1643	C=O	-					
2870	C-H	Stretching					
1060-1090	ν(C-C)	Stretching					
1110-1180	δ(CH_3)	Deformation					
1400-1500	δ(CH_2)	Deformation					
1130	C-C	Stretching					
1178	C-C	Stretching					
1653-1672	C=C	Stretching					
2832-2888	CH_2	Stretching					
2090-2967	CH_3	Stretching					
3000	=C-H	Stretching					
1260	=C-H	Deformation					

1655	C=C	Stretching				
1086	C-C	Stretching				
1068	C-C	Stretching				
1120	C-C	Stretching				
1655	n(C=C)	-				
1444	n(CH_2)	-				
898	CH_2	Rocking				
912	CH_2	Rocking				
1294	CH_2	Twisting				
1433	C-H	Bending				
1409	CH_2	Bending				
1426	-	-				
3005	=C-H	Stretching				
1265	=C-H	Stretching	- / Lipids	532, 1064	Raman	109
2850	v(C-H)	Symmetric				
2890	v(C-H)	Asymmetric				
3003	=C-H	Stretching				
2923	CH_2	Stretching				
2858	CH_2	Symmetric				
2875	CH_2	Symmetric				
1064	C-C	Stretching				
1116	C-C	Stretching				
890	CH_3	Rocking				
2846	C-H in CH_2	Symmetric				
2934	C-H in CH_3	Symmetric				
1729	C=O	Stretching				
1742	C=O	Stretching				
1746	C=O	Stretching				
1440	CH_2	Scissoring				
1304	-	Twisting				
1266	=C-H	Deformation				
1269	=C-H	Deformation				
1067	C-C	Stretching				
1079	C-C	Stretching				
1114	C-C	Stretching				

1069	C-C	Stretching
1082	C-C	Stretching
1118	C-C	Stretching
3001	=C-H	Stretching
1656	C=C	Streching
1267	C-H	In plane bending
1252	-	-
1672	C=C	Stretching
3011	=C-H	Stretching
1660	C=C	Stretching
1062	C-C	Stretching
2864	CH_2	Symmetric
2930	CH_3	Symmetric
1442	CH_2	Stretching
1087	C-C	Stretching
1130	C-H	Stretching
1178	C-H	Stretching
800-1000	C-H	Backbone
701	-	In plane deformation
424	C-H	Bending
548	C-H	Bending
2846	CH_2	Stretching
2881	CH_2	Stretching
2937	CH_3	Stretching
2957	CH_3	Stretching
1739	C=O	Stretching
1668	C=C	Stretching
1298	CH_2	Twisting
2852	CH_2	Stretching
2885	CH_2	Stretching
1741	C=C	Stretching
3009	=C-H	Stretching
1670	v(C=C)	-
1659	v(C=C)	-

1306	CH_2	Stretching				
1441	CH_2	Bending				
3013	=CH	Stretching				
1662	C=C	Backbone				
1306	CH_2	Twisting				
431	C-C	-				
703	C-H	-				
2600-3200	C-H	-				
2847	CH_2	Symmetric				
2882	CH_2	-				
2959	CH_3	Asymmetric				
3007	=CH	Stretching				
1737	C=O	Stretching				
1657	C=C	Stretching				
1442	CH_2	Scissoring				
1300	CH_2	Twisting				
1267	=C-H	In plane deformation				
1090	C-C	Stretching				
719	$(CH_3)_3$	Symmetric				
876	$(CH_3)_3$	Asymmetric				
1096	P-O	Stretching				
723	$(CH_3)_3$	Symmetric				
882	$(CH_3)_3$	Asymmetric				
1655-1650	Amide I	-				
1340	CH	Bending				
940-934	C-C	Stretching	- / Meat	785	Raman	110
550-510	S-S	Stretching				
1668-1663	Amide I	-				
1230-1237	Amide III	-				

Table 9S. Raman spectra of food adulterant

Band position cm^{-1}	Assignment of Bonds (Molecule/Group)	Mode of Vibration	Strength of bonds	Sample / Food Matrix	Wavenumber of laser source (nm)	Type of Raman	References
1441	$-CH_2$	C-H bend (shear)	Strong	- / Oil	785	Portable RamTracer	111
1082	-(CH2)n-	C-C stretch	Medium				
1302	$-CH_2$	C-H bend (twist)	Medium				
1265	cis-RHC=CHR	=C-H stretch	Medium				
1657	cis-RHC=CHR	C=C stretch	Medium				
1747	RC=OOR	C=O stretch	Weak				
1082	$-(CH_2)n-$	C-C stretch	Medium	- / Oil	785	Portable	112
1265	Cis- RHC=CHR	=C-H stretch	Medium				
1300	$-CH_2$	C-H bend (twist)	Medium				
1441	$-CH_2$	C-H bend (shear)	Strong				
1742 (1747)	RC=OOR	C=O stretch	Weak				
1654 (1657)	Cis- RHC=CHR	C=C stretch	Medium				
3005	cis RHC=CHR	C–H symmetric stretching	Middle	Carotenoid / Oil	514.5	VIS Raman	113
2924	$–CH_2$	C–H asymmetric stretching	Strong				
2897	$–CH_3$	C–H symmetric stretching	Strong				
2850	$–CH_2$	C–H symmetric stretching	Strong				
1750	RC=OOR	C-O stretching	Weak				
1650	cis RHC-CHR	C-C stretching	Medium				
1525	RHC=CHR	C=C stretching	Strong				
1440	$–CH_2$	C–H bending					
1300	$–CH_2$	(scissor.)	Medium				
1265	cis RHC=CHR	C–H bending	Weak				
1150	$–(CH_2)n –$	(twisting)	Strong				

1008 968 868	$HC–CH_3$ trans RHC-CHR $–(CH_2)n –$	=C–H bending (scissor.) C–C stretching CH3 bending C-C bending C–C stretching	Weak Weak Weak				
1075 1263 1298 1440 1652 1741 2851	$-(CH_2)n-$ cis-RHC=CHR $-CH_2$ $-CH_2$ cis-RHC=CHR RC=OOR CH_2	C-C stretching =C-H bending Bending (twisting) C-H bending (scissor.) C=C stretching C=O stretching C-H stretching (sym)	Weak Medium Medium Strong Strong Weak Weak	- / Olive and Hazelnut Oils	780	Raman	114
673 982	- -	In-plane deformation Triazine ring breathing	Strong Weak	Melamine / Milk Powder	785	Conventional Raman	115
676 985 3126	C-N-C C-N-C N-H	Bending Stretching (sym) Stretching (sym) Stretching	Strong Medium Weak	Melamine / Dried Milk	785	Conventional Raman	116
3383 2924 1460 1372 1070 923 842 740	O-H C-H CH2 CH and OH C(1)H , COH C(1)H , COH C(1)H C-C, CO stretching	Stretching Stretching Bending Bending Bending Bending Bending Stretching	Strong Strong Strong Strong Medium Weak Medium Weak	- / Maple syrup	1064	FT-Raman	117
3005	cis RHC=CHR	=C–H stretching	Medium				

		(sym) C–H stretching (asym)					
2924	$–CH_2$	C–H stretching (sym)	Shoulder				
2897	$–CH_3$	C–H stretching (sym)	Strong				
2850	$–CH_2$	– C–H stretching	Strong				
2723	$–(CH_2)n$	C=O stretching	Weak				
1747	RC=OOR	C=C stretching	Weak	- / Olive oil	1064	FT-Raman	118
1651	cis RHC=CHR	C–H bending (scissoring)	Medium				
1439	$–CH_2$	C–H bending (twisting)	Strong				
1300	$–CH_2$	=C–H bending	Medium				
1265	cis RHC=CHR	C–C stretching	Shoulder				
1076	$–(CH_2)n–$	C=C bending	very weak				
968	trans RHC=CHR	C–C stretching	Weak				
868	$–(CH_2)n–$		Weak				
879	$vC_1–C_2$, CH_3 rocking,	Stretching	-				
	vC–O	Stretching	-				
1085 and	vC–C aliphatic	Stretching	-				
1304	C–C stretch	Stretching	-	- / butter	785	Raman	119
1125	v C-C	Stretching	-				
1271	δ=CH	Deformation	-				
1442	$δCH_2$	Deformation	-				
838	C-C	Stretching	-	Hazelnut / Olive and	532	Raman	120

950	C=C	Bending	-	adulterated olive oil			
1072	CH_3	Bend	-				
1264	=C-H	Scissoring	-				
1301	C-H	Scissoring	-				
1443	C-H	Twisting	-				
1656	C=C	Stretching	-				
1745	C=O	Stretching	-				
3312-3334	O-H	Stretching	-	- / Honey	532	FT-Raman Micro Raman	121
2945	C-H	Stretching	-				
2938-2944	CH_2	Asymmetric	-				
		Stretching	-				
		Stretching	-				
2900-2907	C-H	Bending	-				
1636-1642	O-H	Bending	-				
1458-1461	CH_2	Bending	-				
1372-1374	O-H, C-H	Bending	-				
1364-1369	CH_2	Wagging	-				
1349	CH_2	Stretching	-				
1265-1267	COH,Amide III	Stretching	-				
1126-1127	CN,Proteins	Stretching	-				
1077	C-O	Bending	-				
1070-1077	CH,COH,CN		-				
	Protein	Stretching	-				
1069-1064	C-O	Bending	-				
922-916	C-H,COH	Bending	-				
904	C-H	Stretching	-				
821	C-H	Bending	-				
777	C-H	Stretching	-				
707-706	CO,CCO,OCO	Ring Bending	-				
629-630	-	Skeletal Stretching	-				
590-592	-	Bending	-				
519-522	CCO,CCC	Skeletal Stretching	-				
449-450	-	Bending	-				
420-424	CCO,CCC						
680	Melamine	-	-	Melamine / Milk	-	-	122

695	Melamine	-	-				
682	Melamine	Ring Breathing Mode II and plane deformation of ring	-				
850	Amylose	-	-	Paraffin / Rice	514	Raman	123
1253	Amylose	-	-				
905	Amylopectin	-	-				
1391	Amylopectin	-	-				
1342	CH_2	Twisting	-				
1314	CH_2	Wagging	-				
1452	CH_2	Deformation	-				
1360	-	Vibration	-				
1032	-	Vibration	-				
1004	-	Ring breathing	-				
705	-	-	-	Calcium / Milk Powder	1064	FT-Raman	124
1085	Milk powder	-	-				
1300	-	-	-				
1440	-	-	-				
212	Dicyandiamide	-	-	- / Dry milk	785	Raman	125
673	Melamine	-	-				
973	Ammonium Sulphate	-	-				
1009	Urea	-	-				
1270	=C-H	Bending	-	Adipose Tissue / Meat	785	Raman	126
1660	C=C	Stretching	-				
1060-1130	C-C	Stretching	-				
1209-1305	CH_2	Twisting	-				
1655	-	Olefinic Bond	-				
1400-1500	CH_2	Scissoring	-				
1450	CH	Bending	-				
1660	-	Amide I	-				
939	C-C	Stretching	-				
1310	-	Amide III	-				
1450	CH	Bending	-				

1650	-	Amide I	-	Meat	671, 783	Raman	127
1650	-	Amide I	-				
937	C-C	Stretching	-				
1310	-	Amide III	-				
1655	-	Amide I	-				
1340	C-H	Bending	-				
899	C-C	Stretching	-				
932	C-C	Stretching	-				
1650	-	Amide I	-				
800-920	$\nu(C_1\text{-}C_2)$	Stretching	-	Meat	785	Raman	128
	$\nu(C_1\text{-}C_2)$	Rocking	-				
1070-1100	ν(C-C)	Stretching	-				
1295-1305	$\delta(CH_2)$	Twisting	-				
1400-1500	$\delta(CH_2)$	Scissor deformation	-				

1. Z. Chi, X. G. Chen, J. S. W. Holtz and S. A. Asher, *Biochemistry*, 1998, 37, 2854-2864.
2. G. T. Meng, J. C. K. Chan, D. Rousseau and E. C. Y. Li-Chan, *J Agr Food Chem*, 2005, 53, 845-852.
3. S. Ngarize, A. Adams and N. K. Howell, *Food Hydrocolloid*, 2004, 18, 49-59.
4. E. G. Ferrer, A. V. Gomez, M. C. Anon and M. C. Puppo, *Spectrochim Acta A*, 2011, 79, 278-281.
5. M. Nonaka, E. Lichan and S. Nakai, *J Agr Food Chem*, 1993, 41, 1176-1181.
6. H. W. Wong, S. M. Choi, D. L. Phillips and C. Y. Ma, *Food Chem*, 2009, 113, 363-370.
7. C. Y. Huang, G. Balakrishnan and T. G. Spiro, *J Raman Spectrosc*, 2006, 37, 277-282.
8. I. Sanchez-Gonzalez, P. Carmona, P. Moreno, J. Borderias, I. Sanchez-Alonso, A. Rodriguez-Casado and M. Careche, *Food Chem*, 2008, 106, 56-64.
9. A. Zajac, J. Hanuza and L. Dyminska, *Food Chemistry*, 2014, 156, 333-338.
10. I. H. Boyaci, H. T. Temiz, R. S. Uysal, H. M. Velioglu, R. J. Yadegari and M. M. Rishkan, *Food Chemistry*, 2014, 148, 37-41.
11. J. H. Shao, Y. F. Zou, X. L. Xu, J. Q. Wu and G. H. Zhou, *Food Res Int*, 2011, 44, 2955-2961.
12. H. M. Velioğlu, H. T. Temiz and I. H. Boyaci, *Food Chemistry*, 2015, 172, 283-290.
13. S. M. Fowler, H. Schmidt, R. van de Ven, P. Wynn and D. L. Hopkins, *Meat Sci*, 2014, 97, 597-601.
14. D. T. Berhe, S. B. Engelsen, M. S. Hviid and R. Lametsch, *Food Res Int*, 2014, 66, 123-131.
15. A. S. Sivam, D. Sun-Waterhouse, C. O. Perera and G. I. N. Waterhouse, *Food Res Int*, 2013, 50, 574-585.
16. A. V. Gomez, E. G. Ferrer, M. C. Anon and M. C. Puppo, *J Mol Struct*, 2013, 1033, 51-58.
17. N. Perisic, N. K. Afseth, R. Ofstad, S. Hassani and A. Kohler, *Food Chemistry*, 2013, 138, 679-686.

18. Z. L. Lim, N. H. Low, B. A. Moffatt and G. R. Gray, *Cryobiology*, 2013, 66, 156-166.
19. J. Huen, C. Weikusat, M. Bayer-Giraldi, I. Weikusat, L. Ringer and K. Lösche, *Journal of Cereal Science*, 2014, 60, 555-560.
20. B. Volkert, A. Lehmann, T. Greco and M. H. Nejad, *Carbohyd Polym*, 2010, 79, 571-577.
21. C. Mutungi, L. Passauer, C. Onyango, D. Jaros and H. Rohm, *Carbohyd Polym*, 2012, 87, 598-606.
22. C. K. Chong, J. Xing, D. L. Phillips and H. Corke, *J Agr Food Chem*, 2001, 49, 2702-2708.
23. I. Delfino, C. Camerlingo, M. Portaccio, B. Della Ventura, L. Mita, D. G. Mita and M. Lepore, *Food Chem*, 2011, 127, 735-742.
24. L. Passauer, H. Bender and S. Fischer, *Carbohyd Polym*, 2010, 82, 809-814.
25. E. Pigorsch, *Starch-Starke*, 2009, 61, 129-138.
26. A. Flores-Morales, M. Jimenez-Estrada and R. Mora-Escobedo, *Carbohyd Polym*, 2012, 87, 61-68.
27. S. N. Yuen, S. M. Choi, D. L. Phillips and C. Y. Ma, *Food Chem*, 2009, 114, 1091-1098.
28. K. Ilaslan, I. H. Boyaci and A. Topcu, *Food Control*, 2015, 48, 56-61.
29. A. S. Jaaskelainen, U. Holopainen-Mantila, T. Tamminen and T. Vuorinen, *Journal of Cereal Science*, 2013, 57, 543-550.
30. H. Akinosho, S. Hawkins and L. Wicker, *Carbohyd Polym*, 2013, 98, 276-281.
31. M. Labanowska, A. Weselucha-Birczynska, M. Kurdziel and P. Puch, *Carbohyd Polym*, 2013, 92, 842-848.
32. M. C. Sarraguça, T. De Beer, C. Vervaet, J.-P. Remon and J. A. Lopes, *Talanta*, 2010, 83, 130-138.
33. O. Abbas, J. A. F. Pierna, R. Codony, C. von Holst and V. Baeten, *J Mol Struct*, 2009, 924-26, 294-300.
34. G. L. Johnson, R. M. Machado, K. G. Freidl, M. L. Achenbach, P. J. Clark and S. K. Reidy, *Org Process Res Dev*, 2002, 6, 637-644.
35. I. Sanchez-Alonso, P. Carmona and M. Careche, *Food Chem*, 2012, 132, 160-167.
36. V. Baeten, P. Hourant, M. T. Morales and R. Aparicio, *J Agr Food Chem*, 1998, 46, 2638-2646.
37. B. J. Marquardt and J. P. Wold, *Lebensm-Wiss Technol*, 2004, 37, 1-8.
38. C. M. McGoverin, A. S. S. Clark, S. E. Holroyd and K. C. Gordon, *Anal Chim Acta*, 2010, 673, 26-32.
39. R. Rodríguez-Solana, D. J. Daferera, C. Mitsi, P. Trigas, M. Polissiou and P. A. Tarantilis, *Industrial Crops and Products*, 2014, 62, 22-33.
40. Y. Fan, J. Zhou and D. P. Xu, *Spectrochim Acta A*, 2014, 129, 143-147.
41. R. M. El-Abassy, P. Donfack and A. Materny, *Food Res Int*, 2010, 43, 694-700.
42. C. Cimpoiu, D. Casoni, A. Hosu, V. Miclaus, T. Hodisan and G. Damian, *J Liq Chromatogr R T*, 2005, 28, 2551-2559.
43. C. W. Tsai and M. D. Morris, *Anal Chim Acta*, 1975, 76, 193-198.
44. J. R. Beattie, C. Maguire, S. Gilchrist, L. J. Barrett, C. E. Cross, F. Possmayer, M. Ennis, J. S. Elborn, W. J. Curry, J. J. McGarvey and B. C. Schock, *Faseb J*, 2007, 21, 766-776.
45. L. Rimai, D. Gill and J. L. Parsons, *J Am Chem Soc*, 1971, 93, 1353-&.
46. C. Y. Panicker, H. T. Varghese and D. Philip, *Spectrochim Acta A*, 2006, 65, 802-804.
47. H. Yang and J. Irudayaraj, *J Pharm Pharmacol*, 2002, 54, 1247-1255.
48. M. Kim and P. R. Carey, *J Am Chem Soc*, 1993, 115, 7015-7016.
49. M. Harz, P. Rosch, K. D. Peschke, O. Ronneberger, H. Burkhardt and J. Popp, *Analyst*, 2005, 130, 1543-1550.
50. H. Yang and J. Irudayaraj, *J Mol Struct*, 2003, 646, 35-43.
51. P. Rosch, M. Schmitt, W. Kiefer and J. Popp, *J Mol Struct*, 2003, 661, 363-369.
52. K. Maquelin, C. Kirschner, L. P. Choo-Smith, N. van den Braak, H. P. Endtz, D. Naumann and G. J. Puppels, *J Microbiol Meth*, 2002, 51, 255-271.

53. E. C. Lopez-Diez and R. Goodacre, *Anal Chem*, 2004, 76, 585-591.
54. K. C. Schuster, I. Reese, E. Urlaub, J. R. Gapes and B. Lendl, *Anal Chem*, 2000, 72, 5529-5534.
55. K. C. Schuster, E. Urlaub and J. R. Gapes, *J Microbiol Meth*, 2000, 42, 29-38.
56. Z. Q. Wen, S. A. Overman and G. J. Thomas, *Biochemistry-Us*, 1997, 36, 7810-7820.
57. A. Silge, W. Schumacher, P. Rosch, P. A. Da Costa, C. Gerard and J. Popp, *Syst Appl Microbiol*, 2014, 37, 360-367.
58. D. Kusic, B. Kampe, P. Rosch and J. Popp, *Water Res*, 2014, 48, 179-189.
59. U. Munchberg, L. Wagner, E. T. Spielberg, K. Voigt, P. Rosch and J. Popp, *Bba-Mol Cell Biol L*, 2013, 1831, 341-349.
60. P. Rosch, M. Harz, M. Schmitt, K. D. Peschke, O. Ronneberger, H. Burkhardt, H. W. Motzkus, M. Lankers, S. Hofer, H. Thiele and J. Popp, *Appl Environ Microb*, 2005, 71, 1626-1637.
61. U. Munchberg, P. Rosch, M. Bauer and J. Popp, *Anal Bioanal Chem*, 2014, 406, 3041-3050.
62. N. N. Brandt, A. Y. Chikishev, A. I. Sotnikov, Y. A. Savochkina, I. I. Agapov and A. G. Tonevitsky, *J Mol Struct*, 2005, 735–736, 293-298.
63. P. X. Zhang, Z. Xiaofang, Y. S. C. Andrew and F. Yan, *Journal of Physics: Conference Series*, 2006, 28, 7.
64. G. Gupta, A. S. B. Bhaskar, B. K. Tripathi, P. Pandey, M. Boopathi, P. V. L. Rao, B. Singh and R. Vijayaraghavan, *Biosensors and Bioelectronics*, 2011, 26, 2534-2540.
65. T. G. Levitskaia, S. I. Sinkov and S. A. Bryan, *Vibrational Spectroscopy*, 2007, 44, 316-323.
66. N. Sundaraganesan, N. Puviarasan and S. Mohan, *Talanta*, 2001, 54, 233-241.
67. V. Sortur, J. Yenagi, J. Tonannavar, V. B. Jadhav and M. V. Kulkarni, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2006, 64, 301-307.
68. S. A. Asher, *Anal Chem*, 1984, 56, 720-724.
69. A. I. Alajtal, H. G. M. Edwards and I. J. Scowen, *J Raman Spectrosc*, 2011, 42, 179-185.
70. K. M. Lee, T. J. Herrman and U. Yun, *Journal of Cereal Science*, 2014, 59, 70-78.
71. G. D. Fleming, J. Villagrán and R. Koch, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2013, 114, 120-128.
72. S. Bonora, E. Benassi, A. Maris, V. Tugnoli, S. Ottani and M. Di Foggia, *J Mol Struct*, 2013, 1040, 139-148.
73. K.-M. Lee, J. Davis, T. J. Herrman, S. C. Murray and Y. Deng, *Food Chemistry*, 2015, 173, 629-639.
74. I. V. Ermakov, M. R. Ermakova and W. Gellermann, *P Soc Photo-Opt Ins*, 2006, 6078, 7835-7835.
75. M. Snehalatha, C. Ravikumar, N. Sekar, V. S. Jayakumar and I. H. Joe, *J Raman Spectrosc*, 2008, 39, 928-936.
76. N. Peica, I. Pavel, S. C. Pinzaru, V. K. Rastogi and W. Kiefer, *J Raman Spectrosc*, 2005, 36, 657-666.
77. K. Zborowski, R. Grybos and L. M. Proniewicz, *Vibrational Spectroscopy*, 2005, 37, 233-236.
78. N. Peica, C. Lehene, N. Leopold, S. Schlucker and W. Kiefer, *Spectrochim Acta A*, 2007, 66, 604-615.
79. N. Peica, *J Raman Spectrosc*, 2009, 40, 2144-2154.
80. E. Podstawka, M. Swiatlowska, E. Borowiec and L. M. Proniewicz, *J Raman Spectrosc*, 2007, 38, 356-363.
81. D. Wu, J. Yan, J. Wang, Q. Wang and H. Li, *Food Chemistry*, 2015, 170, 423-429.
82. A. Zając, J. Hanuza, M. Wandas and L. Dymińska, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2015, 134, 114-120.
83. C. S. Mangolim, C. Moriwaki, A. C. Nogueira, F. Sato, M. L. Baesso, A. M. Neto and G. Matioli, *Food Chemistry*, 2014, 153, 361-370.
84. A. G. Gonzalvez, D. Martin, K. Slowing and A. Gonzalez Ureña, *Food Structure*, DOI: http://dx.doi.org/10.1016/j.foostr.2014.09.001.
85. Y. Xie, P. Li, J. Zhang, H. Wang, H. Qian and W. Yao, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2013, 114, 80-84.
86. K. Zhang, J. Helm, D. Peschel, M. Gruner, T. Groth and S. Fischer, *Polymer*, 2010, 51, 4698-4705.
87. M. Holse, F. H. Larsen, A. Hansen and S. B. Engelsen, *Food Res Int*, 2011, 44, 373-384.

88. R. Korifi, Y. Le Dreau, J. Molinet, J. Artaud and N. Dupuy, *J Raman Spectrosc*, 2011, 42, 1540-1547.
89. M. M. Paradkar and J. Irudayaraj, *Food Chem*, 2002, 76, 231-239.
90. H. Yang, J. Irudayaraj and M. M. Paradkar, *Food Chem*, 2005, 93, 25-32.
91. R. M. El-Abassy, P. Donfack and A. Materny, *Food Chem*, 2011, 126, 1443-1448.
92. A. B. Rubayiza and M. Meurens, *J Agr Food Chem*, 2005, 53, 4654-4659.
93. I. H. Boyaci, H. E. Genis, B. Guven, U. Tamer and N. Alper, *J Raman Spectrosc*, 2012, 43, 1171-1176.
94. B. Özbalci, I. H. Boyaci, A. Topcu, C. Kadılar and U. Tamer, *Food Chem*, 2013, 136, 1444-1452.
95. R. S. Uysal, E. A. Soykut, I. H. Boyaci and A. Topcu, *Food Chemistry*, 2013, 141, 4333-4343.
96. M. R. Almeida, C. H. V. Fidelis, L. E. S. Barata and R. J. Poppi, *Talanta*, 2013, 117, 305-311.
97. H. M. Monavar, N. K. Afseth, J. Lozano, R. Alimardani, M. Omid and J. P. Wold, *Talanta*, 2013, 111, 98-104.
98. A. Keidel, D. von Stetten, C. Rodrigues, C. Máguas and P. Hildebrandt, *Journal of Agricultural and Food Chemistry*, 2010, 58, 11187-11192.
99. J. Trebolazabala, M. Maguregui, H. Morillas, A. de Diego and J. M. Madariaga, *Spectrochim Acta A*, 2013, 105, 391-399.
100. H. Lee, B. K. Cho, M. S. Kim, W. H. Lee, J. Tewari, H. Bae, S. I. Sohn and H. Y. Chi, *Sensor Actuat B-Chem*, 2013, 185, 694-700.
101. A. A. Argyri, R. M. Jarvis, D. Wedge, Y. Xu, E. Z. Panagou, R. Goodacre and G. J. E. Nychas, *Food Control*, 2013, 29, 461-470.
102. R. Rodriguez, S. Vargas, M. Estevez, F. Quintanilla, A. Trejo-Lopez and A. R. Hernandez-Martinez, *Vib Spectrosc*, 2013, 68, 133-140.
103. Y. Numata, Y. Shinohara, T. Kitayama and H. Tanaka, *Process Biochem*, 2013, 48, 569-574.
104. P. J. Li, B. H. Kong, Q. Chen, D. M. Zheng and N. Liu, *Meat Sci*, 2013, 93, 67-72.
105. E. Guzmán, V. Baeten, J. A. Fernández Pierna and J. A. García-Mesa, *Food Control*, 2011, 22, 2036-2040.
106. J. Qin, K. Chao and M. S. Kim, *Journal of Food Engineering*, 2011, 107, 277-288.
107. X.-L. Xu, M.-Y. Han, Y. Fei and G.-H. Zhou, *Meat Sci*, 2011, 87, 159-164.
108. I. Gouvinhas, N. Machado, T. Carvalho, J. M. M. M. de Almeida and A. I. R. N. A. Barros, *Talanta*, 2015, 132, 829-835.
109. K. Czamara, K. Majzner, M. Z. Pacia, K. Kochan, A. Kaczor and M. Baranska, *Journal of Raman Spectroscopy*, 2014, DOI: 10.1002/jrs.4607, n/a-n/a.
110. D. T. Berhe, A. J. Lawaetz, S. B. Engelsen, M. S. Hviid and R. Lametsch, *Food Control*, 2015, 52, 119-125.
111. M. Q. Zou, X. F. Zhang, X. H. Qi, H. L. Ma, Y. Dong, C. W. Liu, X. Guo and H. Wang, *J Agr Food Chem*, 2009, 57, 6001-6006.
112. X. F. Zhang, X. H. Qi, M. Q. Zou and F. Liu, *Anal Lett*, 2011, 44, 2209-2220.
113. R. M. El-Abassy, P. Donfack and A. Materny, *J Raman Spectrosc*, 2009, 40, 1284-1289.
114. E. C. Lopez-Diez, G. Bianchi and R. Goodacre, *J Agr Food Chem*, 2003, 51, 6145-6150.
115. Y. Cheng, Y. Y. Dong, J. H. Wu, X. R. Yang, H. Bai, H. Y. Zheng, D. M. Ren, Y. D. Zou and M. Li, *J Food Compos Anal*, 2010, 23, 199-202.
116. S. Okazaki, M. Hiramatsu, K. Gonmori, O. Suzuki and A. T. Tu, *Forensic Toxicol*, 2009, 27, 94-97.
117. M. M. Paradkar, S. Sakhamuri and J. Irudayaraj, *J Food Sci*, 2002, 67, 2009-2015.
118. H. Yang and J. Irudayaraj, *J Am Oil Chem Soc*, 2001, 78, 889-895.
119. R. S. Uysal, I. H. Boyaci, H. E. Genis and U. Tamer, *Food Chemistry*, 2013, 141, 4397-4403.
120. D. I. Ellis, V. L. Brewster, W. B. Dunn, J. W. Allwood, A. P. Golovanov and R. Goodacre, *Chem Soc Rev*, 2012, 41, 5706-5727.
121. F. Corvucci, L. Nobili, D. Melucci and F.-V. Grillenzoni, *Food Chemistry*, 2015, 169, 297-304.
122. E. Domingo, A. A. Tirelli, C. A. Nunes, M. C. Guerreiro and S. M. Pinto, *Food Res Int*, 2014, 60, 131-139.
123. X. W. Feng, Q. H. Zhang, P. S. Cong and Z. L. Zhu, *Talanta*, 2013, 115, 548-555.

124. G. P. S. Smith, K. C. Gordon and S. E. Holroyd, *Vib Spectrosc*, 2013, 67, 87-91.
125. J. W. Qin, K. L. Chao and M. S. Kim, *Food Chemistry*, 2013, 138, 998-1007.
126. J. R. Beattie, S. E. J. Bell, C. Borggaard, A. M. Fearon and B. W. Moss, *Lipids*, 2007, 42, 679-685.
127. K. Sowoidnich and H. D. Kronfeldt, *Appl Phys B-Lasers O*, 2012, 108, 975-982.
128. I. H. Boyaci, R. S. Uysal, T. Temiz, E. G. Shendi, R. J. Yadegari, M. M. Rishkan, H. M. Velioglu, U. Tamer, D. S. Ozay and H. Vural, *Eur Food Res Technol*, 2014, 238, 845-852.