

S1. Table of the Molecular Vibrational Frequencies and Mode Assignments

Frequency values (cm ⁻¹)	Assignments
418-429	cholesterol, cholesterol ester
702	cholesterol, cholesterol ester
719-725	sphingomyelin, C-N (membrane phospholipid head), symmetric stretch vibration of choline group, characteristic for phospholipids
763	ethanolamine group, phosphatidylethanolamine
782-791	cytosine/uracil ring breathing (nucleotide), phosphodiester bands in DNA, uracil, thymine, DNA: O P O, cytosine, pyrimidine
876	C-C-N+ symmetric stretching (lipids)
1007, 1022, 1033	phenylalanine (symmetric ring breathing), phenylalanine mode
1064-1069	skeletal C-C stretch of lipids, triglycerides (fatty acids)
1104	vibration (C-C), lipids, fatty acids
1090	phospholipids acyl chains
1131	fatty acid
1203-1263	amide III (β sheet) arising from coupling of C-N stretching and N-H
1267	C-H lipid, =C-H phospholipids
1272, 1286	unsaturated fatty acids, scissoring (=CH)
1295-1299	ceramide, palmitic acid, fatty acids, CH ₂ deformation (lipid)
1302	fatty acid, phospholipids
1344	nucleic acid modes (DNA and RNA)
1384, 1427	unassigned mode
1428	lipid band, cholesteryl palmitate
1437	CH ₂ deformation (lipid)
1446	CH ₂ bending mode of proteins and lipids
1453	CH ₂ deformation, protein band
1464	fatty acids, cholesterol, cholesterol ester
1494	DNA
1583	pyrimidine ring (nucleic acids)
1610-1614	cytosine (NH ₂), Tyrosine, Phenylalanine
1660	amide I (C=O stretching) α -helix structure; (C-C) <i>cis</i> , lipids, fatty acids, C-C groups in unsaturated fatty acids
1670-1675	amide I (C=O stretching) β -sheet structure; cholesterol and its esters, (C-C) <i>trans</i> , lipids, fatty acids, ceramide
1681	glutamate, DNA unassigned mode
2727	C-H stretches
2843, 2850	CH ₂ symmetric stretching of lipids (total lipids)
2880	CH ₂ asymmetric stretching of lipids and proteins
2930-2935	CH ₃ symmetric stretching of lipids and proteins
2947	C-H vibrations in lipids and proteins, asymmetric vibration CH ₂ , lipids, fatty acids
2952	CH ₃ asymmetric stretching
2968	asymmetric vibration CH ₂ , lipids, fatty acids, cholesterol and cholesterol ester
2972	fatty acids
3016	CH ₂ of lipids
070	amide B (NH stretching, resonant with amide II in β sheet), Fermi resonance