

Supplemental Information S1

Review - TIBTECH

Cardiac multiscale bioimaging: from nano- through micro- to mesoscales

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Table 1. Potential Raman bands associated with molecular vibrations in biological probes based on a reference database.

Wavenumber (cm ⁻¹)	Assignment of vibrational modes	Possible Functions	References
520–530, 545, 555	S–S stretching	cystine or cysteine amino acids	[1]
625	C–C twisting mode	phenylalanine	[1]
643, 691	cytochrome c	mitochondrial functions	[2]
750	cytochrome c, c1 and b, b ₅ distribution	responsible for the mitochondrial functions i.e. changes in mitochondria respiration	[3] [4]
758	symmetric ring breathing		[5]
770	ring breathing	tryptophan	[1]
785-788 775-808	O-P-O stretching and ring breathing modes of uracil, thymine and cytosine	DNA/RNA, nucleic acids (nucleus/nucleoli)	[6] [7]
854	ring breathing	-	[5]
939	C-C stretching, C–O–S or C–O–S vibrations	-	[5]
1003-1004 (1000-1020)	phenylalanine aromatic ring-breathing modes, C-C skeletal mode	phenylalanine/proteins	[6] [7]
1032	C-H plane bending	-	[5]
1096-97	Symmetric PO ₂ stretching	DNA backbone	[6]
1100	C-C stretching	lipids	[1]
1124	C-N stretching	-	[5]
1127-1330	cytochromes c and b distribution	responsible for the mitochondrial functions i.e. changes in mitochondria respiration	[3] [4]
1130	C-C stretching mode	lipid droplets	[6]
1158	C-N stretching	carotenoids (antioxidant)	[5]
1125	cytochromes b	-	[3] [4]
1186	C-H mode of tyrosine and phenylalanine	protein contest	[6]
1208, 1236, 1240	Amide III (β-sheet)	protein contest	[6] [5]
1262-67, 1275	C=H bending modes	lipid droplets	[6] [7]
1300, 1305	CH ₂ -twisting, C-H bending modes	lipids, lipid droplets, collagen and phospholipids	[6] [7] [1]
1310	CH ₃ vibrational modes	lipid droplets	[6]
1313-14	cytochrome c	mitochondrial functions	[3] [2]
1317, 1336		guanine	[1]
1337	cytochrome b	mitochondrial functions	[3]
1344	phenylalanine	e.g. glucose	[1]
1379	ring breathing mode in thymine, adenine, guanine	DNA/RNA	[6]
1381	nucleic bases	-	[7]
1432	DNA conformation	-	[1]
1420-1460	C-H bending modes	lipids	[6]
1442	CH ₂ bending mode	fatty acids	[1]
1447-1448	CH ₂ and CH ₃ bending modes	lipids, lipid droplets and amino acids side chains	[7] [5]
1452	bending modes of methyl groups	collagen	[1]

1458	CH ₂ vibrational modes	lipid droplets	[6]
1461	δ CH ₂	disaccharides	[1]
1471	C=N stretching	-	[1]
1481	amide II-side chains	-	[1]
1488	ring breathing mode in adenine und guanine	-	[6]
1520	C=C vibrations	carotenoids (antioxidant)	[5]
1552	amide II, indol ring mode in tryptophan	protein contest	[6] [1]
1558	tryptophan	tryptophan	[1]
1572, 1576	C=C, ring breathing modes in adenine and guanine	DNA/RNA	[8] [6]
1585, 1587, 1589	oMb and reduced cytochromes c, c1 and b ₅	mitochondrial functions, hemoglobin level	[3] [6] [9] [2]
1586	ring breathing mode in adenine und guanine	adenine und guanin detection	[6]
1606	NH ₂	cytosine	[1]
1610	tyrosine, tryptophane, phenylalanine bands	protein contest	[6]
1616	C=C	tyrosine or tryptophan	[1]
1625	tryptophan	tryptophan	[1]
1640	oMb, reduced form of cytochromes b	level of oMb in mitochondria in CM	[3] [9]
1645, 1650	amide I	α -helix, proteins	[1]
1650	C=O bonds	DNA	[8]
1654	Amide I	α -helix of collagen	[1]
1658, 1660, 1666-1670	C=C stretching modes	lipids	[6] [7]
1659	amide I	protein contest	[5]
1662-64	amide I	collagen/proteins	[6] [1]
1674	amide I (β -sheet)	protein contest	[5]
1686	amide I	protein contest	[6]
1799	C=O	lipids	[1]
2830-2900	2850	alkane groups	protein contest
	2855	C-H stretching	lipid contest
	2885	alkane groups	proteins
2934-35	CH ₂ symmentric stretching (alkane groups)	protein contest	[5]
3013	C=H	lipid droplets	[7]
3003-3027	e.g. C-N, =CH	unsaturated lipids	[6]

Supplemental references for S1

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