

Table S1: Peak assignments from PCA loading for *S. aureus* and *P. aeruginosa*

Bacterial species	PC	Regions	Wavenumber (cm ⁻¹)	Assignment	References
<i>S. aureus</i>	+1	Lipid	2924	(C–H) from methylene (–CH ₂) groups of lipids	1, 2
			2852	(C–H) from acyl chains and aliphatic alkanes of the lipids (phospholipid) Symmetric CH ₂ stretch	1-3
		Amide I	1658	Stretching C=C	2
			1185	CH ₂	2
		Polysaccharides	1117	C–O stretching vibration of C–OH group of ribose (RNA)	2, 3
			1035	Skeletal trans conformation (CC) of DNA ν(CO), ν(CC), ν(CCO), (polysaccharides-cellulose)	2, 4
		Lipid	2945	ν _{as} (C–H) of the CH ₂ groups in the lipids	2
			2838	Stretching C–H in lipid	2
		Amide I	1638	Protein structure: antiparallel β-sheet ν(C=O) of carboxylate and ν(C=C) of aromatic compounds	1, 2, 4
	-1	Amide II	1570	Protein structure: N–H, C–N	2
			1550	Protein structure: perpendicular modes of the α-helix and antiparallel β-sheet N–H bending and C–N stretching	1, 2
		Polysaccharides	1164	ν(CC), ν(COH), ν(CO) stretching Hydrogen-bonded stretching mode of C–OH groups	2
	+2	Lipid	2924	(C–H) from methylene (–CH ₂) groups of lipids	1, 2
			2852	(C–H) from acyl chains and aliphatic alkanes of the lipids (phospholipid) Symmetric stretching vibration of CH ₂ of acyl chains (lipids)	1-4
		Amide I	1665	Amide I (disordered structure-solvated)	2
		Amide II	1164	C–O stretching	2
		Polysaccharides	1060	Stretching C–O deoxyribose ν(CO), ν(CC), δ(OCH) (polysaccharides-cellulose)	2
		Lipid	2838	Stretching C–H in lipid	2
		Amide I	1650	Protein: the C=O stretching vibration, stretching C=C uracil, NH ₂ guanine Peptide amide I	2, 4
		Amide II	1540	Protein absorption- predominately β-sheet N–H, C–N	2, 4
			1180	Amide III band region	2
		Polysaccharides	1117	C–O stretching vibration of C–OH group of ribose (RNA)	2

<i>P. aeruginosa</i>		1040	Symmetric PO ₂ ⁻ stretching in RNA and DNA	2, 4
			vs CH ₃	
	Lipid	2870	Stretching C-H, N-H Symmetric stretching vibration of CH ₃ of acyl chains (lipids)	1, 2
	Amide I	1671	Protein structure: anti-parallel β-sheet)	1, 2, 5
	Amide II	1589	Ring C-C stretch of phenyl	2
	Polysaccharides	1155	C-O stretching vibration	2
		1071	Phosphate I band for two different C-O vibrations of Deoxyribose in DNA in disordering structure	2
		1045	-CH ₂ OH groups and the C-O stretching vibration coupled with C-O bending of the C-OH groups of carbohydrates	2, 4
	Lipid	2926	C-H stretching bands ν _{as} CH ₂ lipids	1-3
		2852	ν _s (C-H) from methylene (-CH ₂) groups of lipids	1, 2
	Amide I	1646	Amide I C=O, stretching C=C uracil, NH ₂ guanine	2, 4
	Amide II	1545	Protein structure: δN-H, νC-N) Peptide amide II	2
	Polysaccharides	1117	C-O stretching vibration of C-OH group of ribose (RNA)	2, 4
		2925	ν _{as} (C-H) from methylene (-CH ₂) groups of lipids	1-3
	Lipid	2852	(C-H) from acyl chains and aliphatic alkanes of the lipids Symmetric stretching vibration of CH ₂ of acyl chains (lipids)	1-3
	Amide I	1665	Amide I (disordered structure-solvated)	2
	Lipid	2945	C-H stretching in the lipids	2
		2838	Stretching C-H in lipid	2
	Amide II	1514	Protein structure: parallel mode of the α-helix ν(C=C)-diagnostic for the presence of a carotenoid structure, most likely a cellular pigment	1, 2
		1185	CH ₂	2
	Polysaccharides	1071	Phosphate I band for two different C-O vibrations of Deoxyribose in DNA in disordering structure	2
		1040	Symmetric PO ₂ ⁻ stretching in RNA and DNA	2, 4

References

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