Supplementary Materials: Characterization and Discrimination of Gram—Positive Bacteria Using Raman Spectroscopy with the Aid of Principal Component Analysis

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Table S1. Raman and SERS bands detected for *L. casei*/*L. monocytogenes.*

Raman Bands/cm^{-1}	SERS Bands/cm^{-1}		Tentative Assignments	Reference
	a Priori Colloid	In Situ Colloid		
603/601	657/-	656/-	phenylalanine (skeletal)	[1]
			β-D-glucose	[2]
			guanine, tyrosine	[3]
707/706	730/747	731/-	ν (adenine), purine-like molecules	[1,4–10]
		854/854	aminoacids	[2]
		959/-	ν (CN)	[6,11]
	1003/1000		phenylalanine (the symmetric ring breathing mode)	[10]
		1029/1031	β-D-glucose	[2]
	1050/1048	1050/1047	ip(CH)	[10]
			ν (adenine)	[4–9]
			ν (CO) glucose	[12]
	1080/-		amino sugars	[2]
	-/1109		ν (DNA, RNA)	[13]
	1134/1145	-/1123, 1145	ν (CN, CC) carbohydrates	[5,14]
			ν (CN, CC) lipids	[15]
			aromatic amino acids in proteins	[11]
	-/1176	-/1186	phenylalanine	[2]
1260/1262	1229/1221	1223/1221	amide III	[1,13,16,17]
	-/1291	-/1293	δ (CH) proteins ν_{sym} (COO^-)	[13,15,18]
1325/1325	1332/-	1331/-	ν (tyrosine, uracil)	[16]
			ν (adenine)	[4-9,12]
	-/1363	1376/1359	δ (CH) proteins ν_{sym} (COO^-)	[2,15]
1387/1387			ν (thymine)	[16]
	1406/-			
	-/1428	-/1427	δ (CH_2) saturated lipids	[5,6,10,15]
	1455/1449	1459/1449	ν (CC), τ (CH2), δ (CH_3, CH_2) fatty acids	[19]
	1509/1499	-/1501	ν (COH) oligosaccharides	[20]
	1539/-	-/1548	adenine-containing molecules	[2]
	1588/1585	-/1585	proteins, aminoacids ν_{asym} (COO^-), nucleic acids	[8,10]
			guanine	[12]
1659/1659			amide I band, unsaturated lipids	[2,13,21]
1700/1699 1764/1759 1764/1768			ν (C=O) ester	[13,14]

Symbols: ν—stretching; τ—twisting; δ—deformation; ip—in plane; sym—symmetric; asym—asymmetric.*

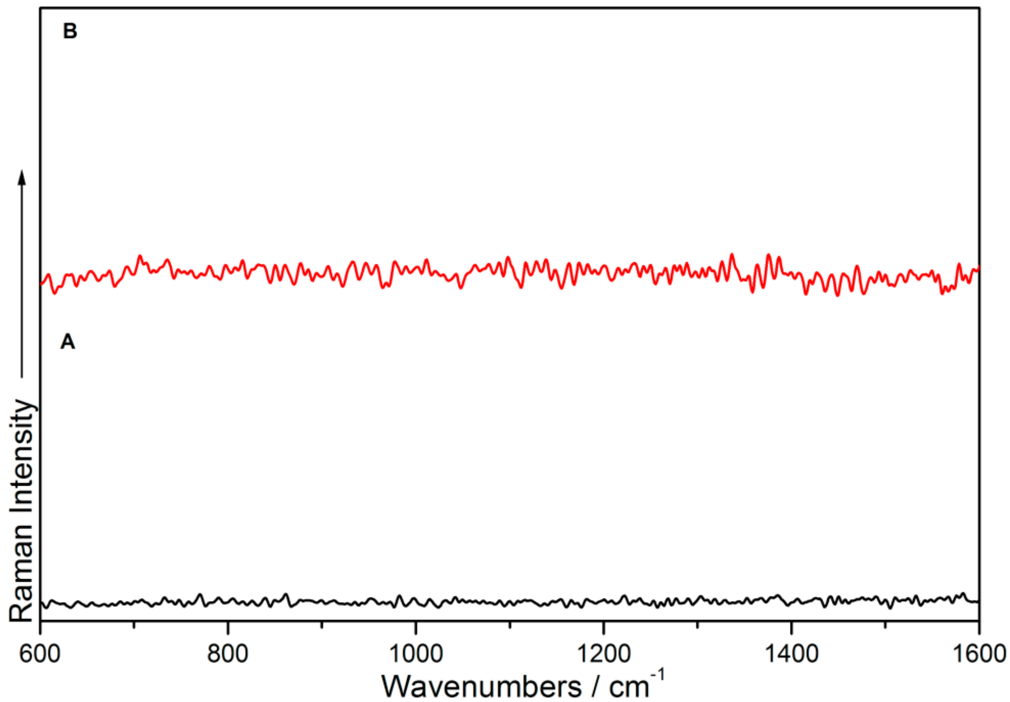


Figure S1. Raman spectra registered for the bacterial culture media used: MRS (**A**) and TSBYE (**B**).

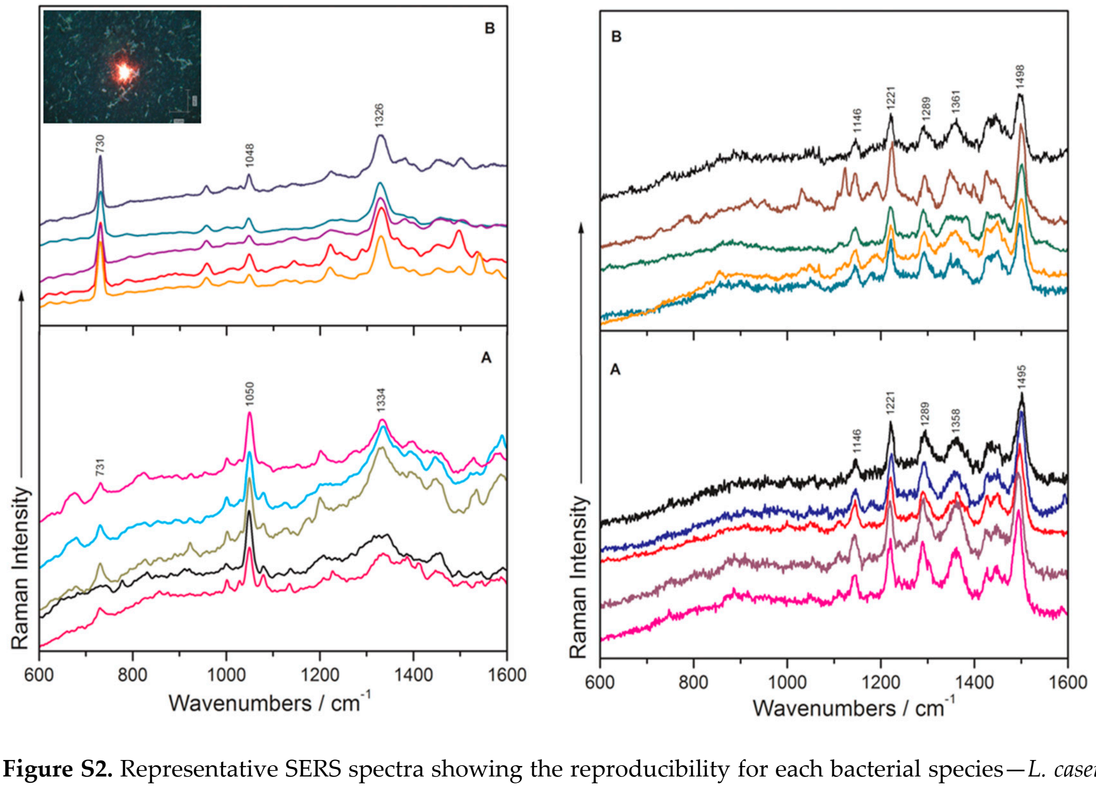


Figure S2. Representative SERS spectra showing the reproducibility for each bacterial species—*L. casei* (right) and *L. monocytogenes* (left), on clustered bacteria, in the *a priori* (**A**) and *in situ* (**B**) conditions, respectively. Inset showing the laser spotlight on a bacterial cluster.

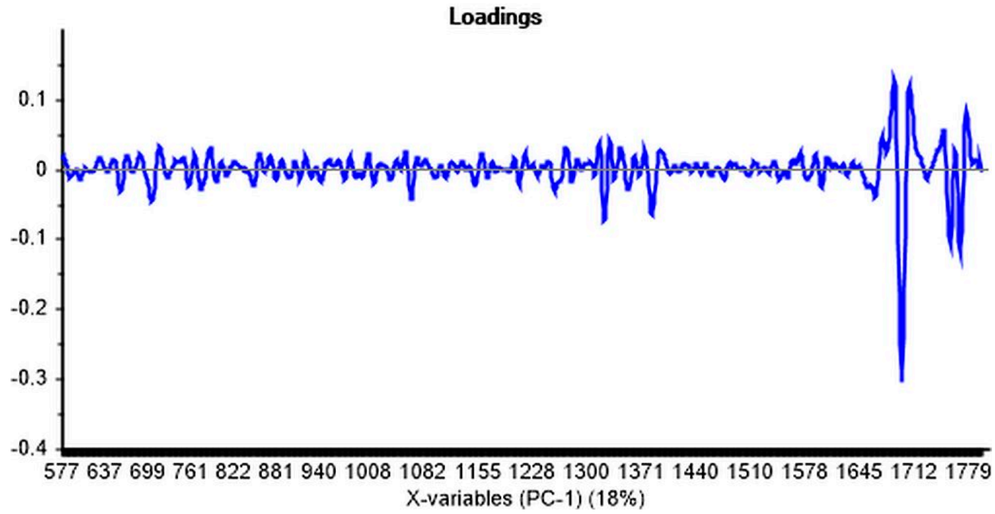
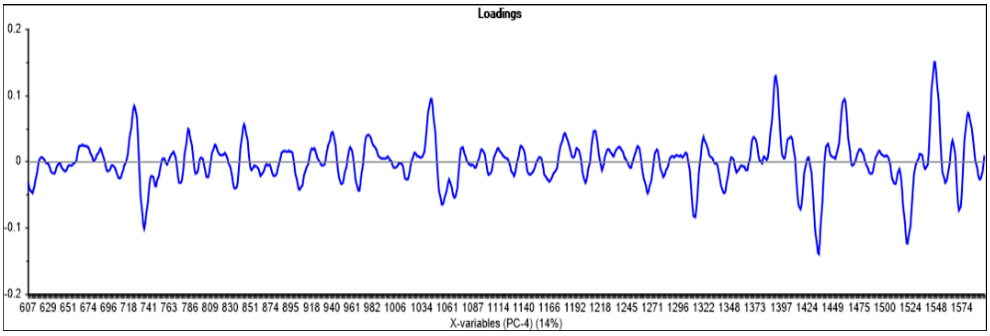
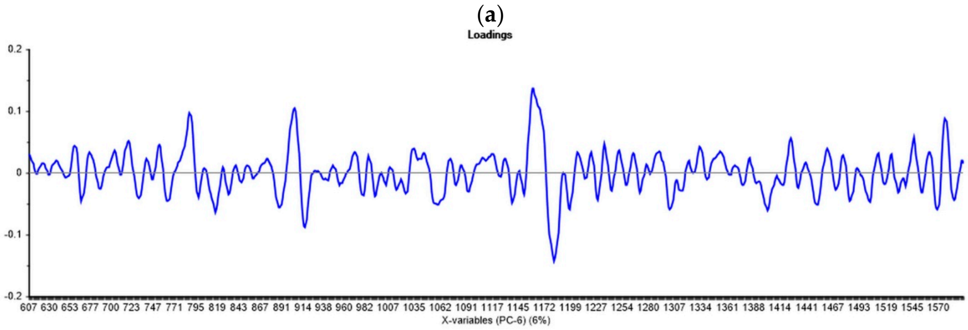


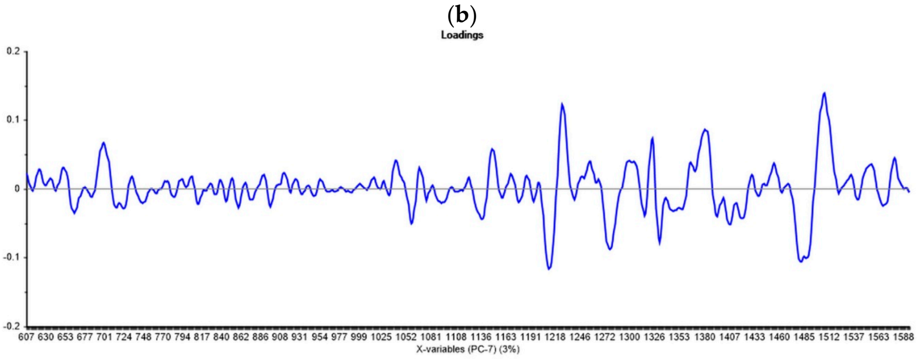
Figure S3. The PC-1 loadings plot corresponding to the PCA analysis on the Raman recorded spectra—Figure 6A.



(**a**)



(**b**)

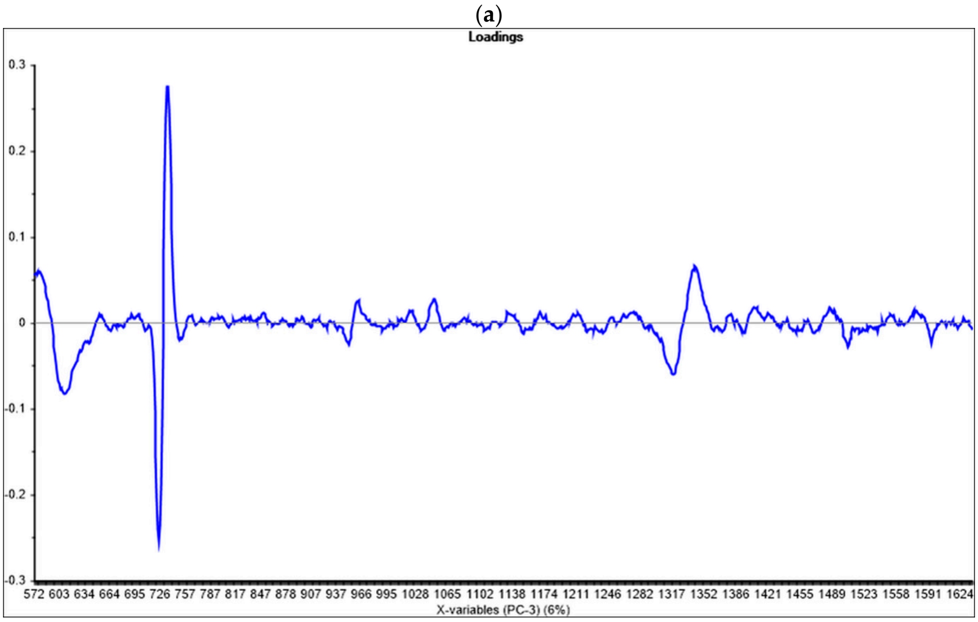


(**c**)

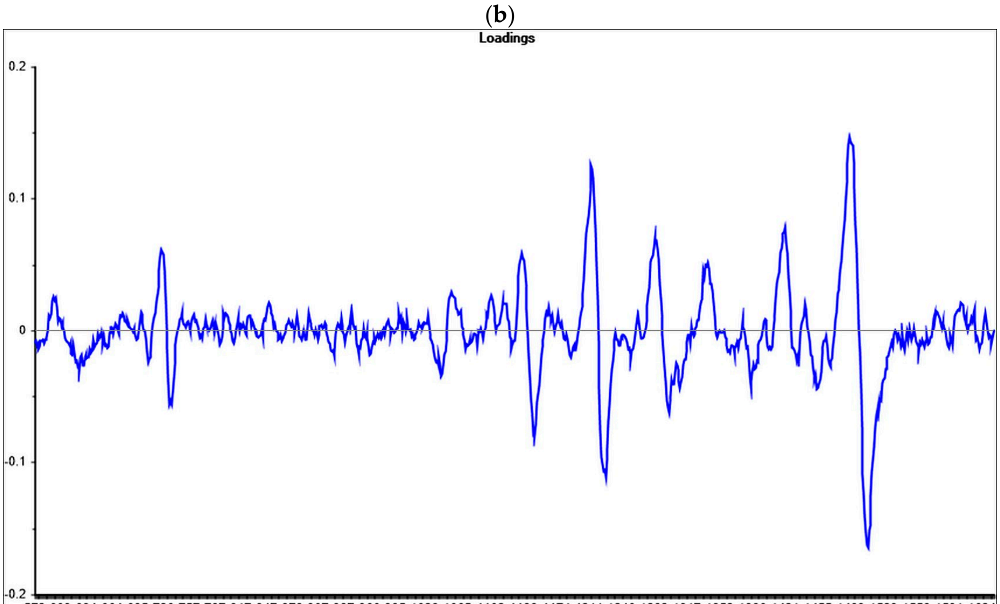
Figure S4. (**a**) The PC-4 loadings plot corresponding to the PCA analysis on the SERS *a priori* recorded spectra—Figure 6B; (**b**) The PC-6 loadings plot corresponding to the PCA analysis on the SERS *a priori* recorded spectra—Figure 6B; (**c**) The PC-7 loadings plot corresponding to the PCA analysis on the SERS *a priori* recorded spectra—Figure 6B.


Loadings
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
572 603 635 666 698 728 759 791 821 852 883 912 943 972 1006 1043 1081 1116 1154 1190 1226 1263 1298 1334 1370 1405 1440 1474 1509 1544 1578 1612
X-variables (PC-2) (20%)

(**a**)


Loadings
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
572 603 634 664 695 726 757 787 817 847 878 907 937 966 995 1028 1065 1102 1138 1174 1211 1246 1282 1317 1352 1386 1421 1455 1489 1523 1558 1591 1624
X-variables (PC-3) (6%)

(**b**)


Loadings
0.2
0.1
0
-0.1
-0.2
572 603 634 664 695 726 757 787 817 847 878 907 937 966 995 1028 1065 1102 1138 1174 1211 1246 1282 1317 1352 1386 1421 1455 1489 1523 1558 1591 1624
X-variables (PC-4) (1%)

(**c**)

Figure S5. (**a**) The PC-2 loadings plot corresponding to the PCA analysis on the SERS *in situ* recorded spectra—Figure 6C; (**b**). The PC-3 loadings plot corresponding to the PCA analysis on the SERS *in situ* recorded spectra—Figure 6C; (**c**) The PC-4 loadings plot corresponding to the PCA analysis on the SERS *in situ* recorded spectra—Figure 6C.

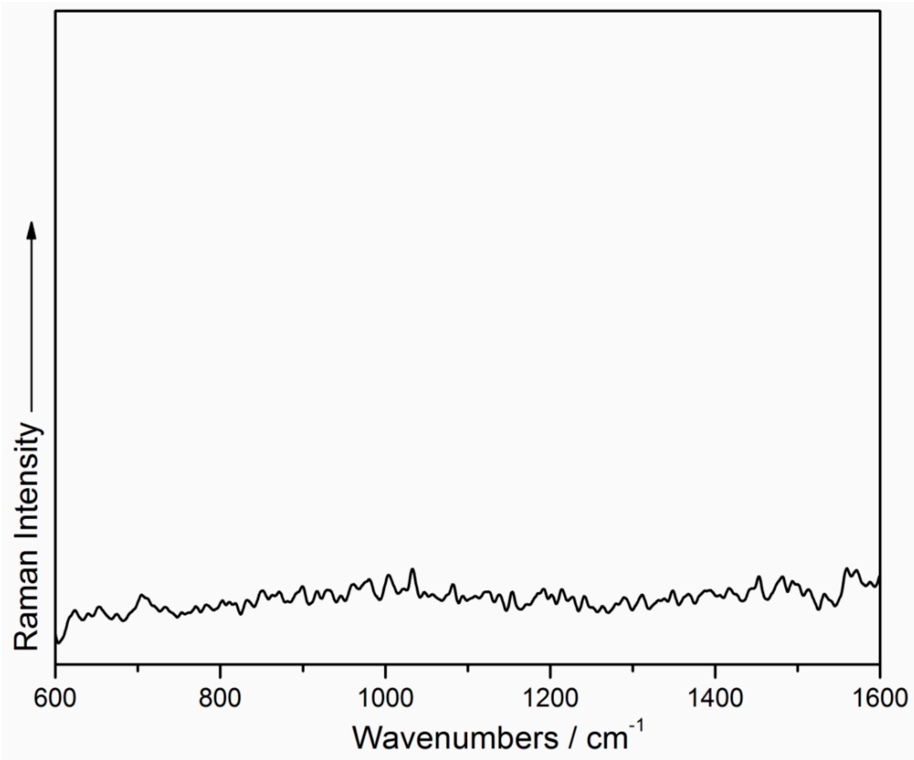


Figure S6. The 632.8 nm Raman spectrum of the Ag colloid.

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