Experimental Data			Shewanella and heme lines							Flagella and Flagellin						Comment		
SERS HS Raman			Porfirine[1] MtrC[2]		OmcA[2] CS[2]			2]	CS II	[3]	Flagell	a[4]	Flagellin[4]					
		170	w															No comment
		216	VW															Histidine
232	VS	238	W															
202	V3	268	1/14/															No comment
		200	VVV															No comment
		204	VVV															No comment
		552	VVV									246						No comment
												340	vv					
386	m	394	m									394	VS					E_{c}^{II} in low spin state[6]
113	m	113	1/14/									117	m					
443		443	VVV									447	m					
407												400						No comment
407	vv											500	~					No comment
500	VW	E10										500	m					
505		518	vs															
525	W											50.4						No comment
= 10												534	m					
543	S																	Substrate
579	S	571	w															No comment
615	m																	No comment
630	m	638	m									630	VS					No comment
666	w	668	vw															No comment
												675	m					No comment
690	vw	690	w	692	m													Heme
												712	w					No comment
738	m	735	m															No comment
				752	S									750	w			No comment
777	VW	778	w									768	m					No comment
802	w											808	w					No comment
832	S	827	S															CCH (aliphatic)[7]
860	w											864	S					No comment
														903	m	903	w	Flagellin(no match)
														940	m	945	w	Flagellin(no match)
1000	vw											998	VS	1005	w	1003	w	No comment
1026	m	1018	w															No comment
1045	m	1036	w									1036	m					No comment
												1068	S					No comment
1081	S																	No comment
		1112	S															No comment
																		Due to low intensities and
																		possible line shit[8] there is
1129	m			1129	S							1127	m	1127	m	1127	w	no prove of flagellin
																		presence
1146	m	1147	w															No comment
																		Rocking of Hs on C_{β}
1174	vw	1185	m	1174	m													atoms[1] and $C_{\beta} - C_{\phi}$
																		bond stretching[9]
1007		1004		1000		1007		1004		1004		1000						Rocking of Hs on N
1227	m	1224	m	1230	m	1227	W	1234	W	1224	S	1238	S					atoms[1]

Table S1. Tabulated Raman Spectroscopy data and comparison with published materials

Ex	perime	ental Data	a	Shewanella and heme lines										Flag	jella ar	nd Flagell	in	Comment
SERS HS Raman		Porfirir	ne[1]	MtrC	[<mark>2</mark>]	Omc	OmcA[2]		CS[2]		CS II[3]		Flagella[4]		in[4]			
1250	w	1243	w			1252	w	1254	w	1246	S			1248	s	1246	S	3° amide [7]. Although there is a match with both flagella and flagellin, lines are indistinguishable with pure decaheme lines. Intensities diff. too much
1275	m					1279	vw	1271	vw			1269	S					
								1287	vw	1288	vw							No comment
1307	S	1303	S	1312	S	1316	VS	1314	vs	1306	vs	1307	vs					$N - C_{\alpha} - C_{\beta}$ or $HN - C_{\alpha'} - C_{\beta'}$ assym. stretching[1] and ν_{21} ImH [5]
														1327	m	1322	m	Flagellin (no match)
1341	VS	1336	w															Peak in multiple wide line
1356	vs	1357	vw	1362	s	1373	m	1368	m	1362	S							ν_4 ImH[5]. Also indicates six-coordinated Fe^{II} in low-spin state[6]
1398	vs	1407	w	1399	vs	1399	S	1399	s	1398	vs							$C_{\alpha} - N(H) - C_{\alpha}$ sym. stretching[1] and ν_{29} ImH[5]
1432	m	1435	m			1430	m					1425	m					Match with spectra and flavine (semiquinone)[9]
1445	m	1459	m			1458	vw	1446	w	1448	m			1452	vs	1453	vs	CH_2 scissoring[7]. Although there is a match with both flagella and flagellin, lines are indistinguishable with pure decaheme lines. Intensities diff. too much
1463	w	1467	m							1466	S							No comment
1514	m	1503	vw	1483	s	1500	vw	1500	s	1494	w							$C_{\alpha} - NH - C_{\alpha}$ sym. stretching[1] Also indicates Intermediate-Spin Fe^{II} [10]
1541	vs	1547	w	1548	vs			1536	m	1528	m							ν_{11} ImH[5]. Also indicates six-coordinated Fe^{II} in low-spin state[6]
1569	m	1561	w			1564	vs		m									ν_{38} ImH[5] Also indicates Intermediate-Spin Fe^{II} [10]
1589	m	1605	VS	1584	vs	1588	VS	1588	vs	1594	vs	1583	vs					$ u_{37} \text{ and } u_2 \text{ ImH[5] Also} $ indicates Intermediate-Spin Fe^{II} [10]
1621	s	1617	m	1620	vs					1617	vs							ν_{10} ImH[5] also may be a trace of semiquinone[9]
1642	m					1639	VS	1641	S			1660	m	1652	VS	1662	VS	MtrC and OmcA match. ν_{10} ImH[5]. Also indicates Intermediate-Spin Fe^{II} [10] Flagellin in aerobic cells
Intensit	ies: v	w - very	weak.	w - wea	ak, m	- mediu	m, s -	strong,	vs - v	ery stron	ig. Ot	ner: Im	H - Ir	nidazole	comp	lex of cy	tochro	ome. γ_i or ν_i - lines

numbering according to given citations. Numbers in **bold** indicate the most important lines in spectra.

References

- 1. Aydin M (2013) DFT and Raman spectroscopy of porphyrin derivatives: Tetraphenylporphine (TPP). Vibrational Spectroscopy 68:141–152.
- 2. Wang Y et al. (2013) Single-cell imaging and spectroscopic analyses of Cr(VI) reduction on the surface of bacterial cells. Langmuir : the ACS journal of surfaces and colloids 29(3):950-6.
- 3. Ravindranath SP, Henne KL, Thompson DK, Irudayaraj J (2011) Surface-enhanced Raman imaging of intracellular bioreduction of chromate in Shewanella oneidensis. PLoS ONE 6(2):1-10.
- 4. Uchiyama T et al. (2008) Raman optical activity of flagellar filaments of Salmonella: Unusually intense ROA from L-type self-assembled protein filaments and their possible higher level chiral organization. *Vibrational Spectroscopy* 48(1):65–68.
- 5. Othman S, Le Lirzin A, Desbois A (1994) Resonance Raman investigation of imidazole and imidazolate complexes of microperoxidase: Characterization of the bis(histidine) axial ligation in c- type cytochromes. *Biochemistry* 33(51):15437–15448.
- Linard JE, Shriver DF, Basolo F (1980) Structure-sensitive resonance Raman bands of capped tetraphenylporphyrinatoiron complexes. *Proc.Natl.Acad.Sci.U.S.A* 77(0027-8424 (Print)):1741–1744.
 Preciado-Flores S et al. (2011) SERS spectroscopy and SERS imaging of Shewanella oneidensis using silver nanoparticles and nanowires. *Chemical communications (Cambridge, England)*
- 47(14):4129–4131.
 8. Ghosh C, Mukherjee S, Dey SG (2013) Direct electron transfer between Cyt c and heme-Aβ relevant to Alzheimer's disease. *Chemical communications (Cambridge, England)* 49(51):5754–6.
- Tripathi GNR (1981) Resonance Raman scattering of semiquinone radical anions. *The Journal of Chemical Physics* 74(11):6044–6049.
- 10. Spiro TG, Burke JM (1976) Protein control of porphyrin conformation. Comparison of resonance Raman spectra of heme proteins with mesoporphyrin IX analogues. Journal of the American Chemical Society 98(18):5482-9.