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Supplementary material for Article

Biogenic Selenium Nanoparticles: A Fine Characterization to Unveil Their Thermodynamic Stability

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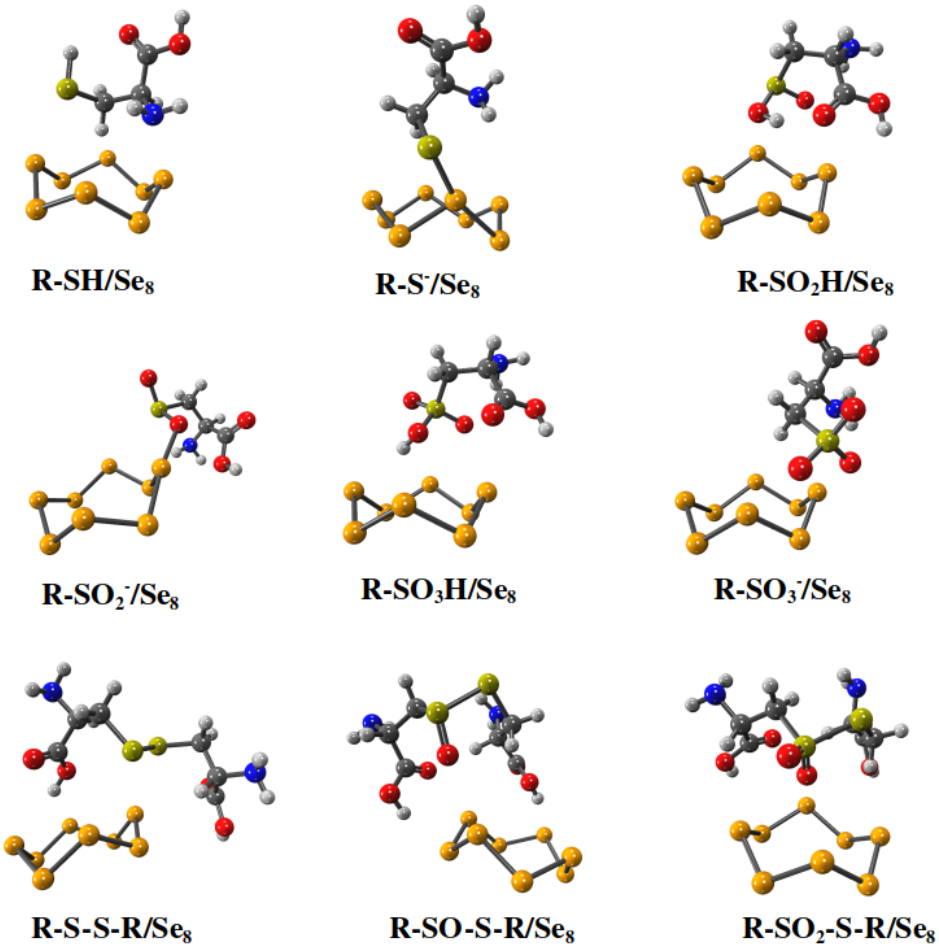

Figure S1: Thiol (RSH)-containing and deriving species on which Density Functional Theory (DFT) calculations were performed, either as isolated molecules or interacting with a Se_8 unit, where R-S^-, R-SO_2H, R-SO_2^-, R-SO_3H, R-SO_3^-, R-S-S-R, R-SO-S-R, and R-SO_2-S-R represent thiolate, sulfinic acid, sulfinate, sulfonic acid, sulfonate, disulfide, disulfide monoxide, and disulfide dioxide moieties, respectively.

Table S1. Density Functional Theory (DFT) calculations for IR vibrations performed considering free RSH-containing molecules (*i.e.,* L-cysteine and its derivatives) and their adsorption on Se_8 nuclei.

Vibrational modes	$\tilde{\nu}$ **(cm^{-1})**											
	R-SH	**R-SH/Se$_8$**	**R-S$^-$**	**R-S$^-$/Se$_8$**	**R-SO$_2$H**	**R-SO$_2$H/Se$_8$**	**R-SO$_2^-$**	**R-SO$_2^-$/Se$_8$**	**R-SO$_3$H**	**R-SO$_3$H/Se$_8$**	**R-SO$_3^-$**	**R-SO$_3^-$/Se$_8$**
ν (S)OH					3449	3485				3555		
ν (NH$_2$)	3456	3456	3495	3534	3543	3545	3485	3515	3547	3548	3521	3533
			3253	3447	3462	3461	3379	3446	3473	3473	3240	3423
ν (CH$_2$)	3149	3161	3011	3119	3148	3149	3127	3137	3183	3182	3140	3112
	3086	3099	2950	3058	3077	3077	3036	3059	3102		3068	3081
ν (CH)	2986	2984	2927	2988	2997	2994	2949	2993	3015	3012	2952	2991
ν (CO)	1816	1819	1801	1817	1780	1778	1805	1823	1831	1819	1814	1821
δ (NH$_2$)	1664	1638	1635	1646	1654	1652	1665	1667	1669	1662	1672	1655
	958	962	1270	1151	963	961	1124	987	947	953	1400	1398
	934	933	1014	973	400		1021		892		1230	994
				950			788				1002	965
				880							971	
δ (CH$_2$)	1423	1423	1430	1419	1423	1421	1419	1406	1410	1409	1412	1417
	1297	1300	1139	1286	1267	1270	1247	1263	1301	1307	1290	1301
	1257	1257	1121	1233	1238	1153	1203	1216	1236	1284	1191	1240
	1164	1163	892	1132	1130	1131	1106	1135	1142	1234	1167	1126
		1142	814	809	992	992	955	1115	1007	1175	1108	1067
					864	865	851	967	823	1007	892	897
					853	833		881		823	827	827
								819				
δ (CH)	1389	1389	1322	1374	1396	1395	1390	1375	1394	1392	1332	1321
						1303	1298	1312		1292	1137	1169
								456				
δ (OH)	1373	1373	1349	1358	1391	1389	1354	1361	1378	1376	1363	1367
	1309	1308	1204	1183	1188	1189	1161	1184	1187	1188	1187	1194
	1179	1175	1178	747	755	755	735	756	753	752	758	1177
	741	743	742	675	663	671	609	647	685	676	577	760

	668	670	670	632		592	435	561	636	630	520	626
	634	633	613	560				516			516	579
	551	554						433				535
		546										
δ (S)OH					1273	1249			1317	1144		
					691	1221			1175	1132		
						639			1152	1083		
						578			1091			
ν (SO)					1063	1050	1047	1074	756	759	953	939
							915	792				
ν SO(H)					733	730						
ν (CS)											684	692
δ (SH)	1040	1038										
	851	852										
	779	777										
	371	370										
	334	337										
		315										
		274										
δ (NH_2)	305		373	270	356	355	421	321	360	360	350	361
								296	319	328		
						322		278				
backbone	265	418	325	522	534	533	560	572	580	576	474	517
			277	443	455	456	518	377	522	523	409	476
				346	415	415	514	262	506	504	357	369
				305	324	390	462		451	453	299	302
				258	292		318		416	425	269	
							261		397	418		
									293	268		
δ (SO_3)											468	474
δ OH (HSO_3)									282	341		
Se_8		262-257		281-251		264-258		266-251		265-253		

Where ν and δ indicate stretching and bending vibrations.

Table S2. Density Functional Theory (DFT) calculations for IR vibrations performed considering cystine (RSSR) and its derivatives and their adsorption on Se_8 nuclei.

Vibrational modes	$\tilde{\nu}$ (cm^{-1})					
	R-S-S-R	**R-S-S-R/Se$_8$**	**R-SO-S-R**	**R-SO-S-R/Se$_8$**	**R-SO$_2$-S-R**	**R-SO$_2$-S-R/Se$_8$**
ν (NH_2)	3540	3540	3566	3570	3573	3573
	3538	3536	3518	3523	3533	3535
	3460	3459	3481	3482	3486	3485
	3454	3454	3444	3444	3450	3451
ν (CH_2)	3124	3132	3141	3147	3166	3166
	3103	3109	3111	3144	3162	3161
	3061	3065	3059	3073	3084	3088
	3034	3038	3022	3068	3068	3067
ν (CH)	3088	3084	3069	3071	3091	3074
	2965	2968	2914	2983	2987	2980
ν (CO)	1845	1842	1835	1814	1837	1838
	1831	1816	1834	1781	1812	1812
δ (NH_2)	1642	1642	1655	1647	1645	1647
	1627	1627	1617	1610	1614	1614
	951	953	903	1257	1267	1408
	883	880	863	951	1020	1266
				926	921	1173
				897	884	1020
				862	855	921
						883
						852
δ (CH_2)	1420	1416	1433	1432	1432	1432
	1414	1405	1408	1422	1421	1422
	1244	1253	1265	140	1406	1259
	1110	1242	1198	1400	1256	1208
	1099	1225	1191	1140	1136	1194
	787	1192	1145	1133	1130	1110
	768	936	1007	1005	1106	1007
		895	837	813	1007	961
		629	761	638	958	828
		622			826	822
		582			819	
δ (CH)	1436	1459	1425	1371	1420	1405
	1370	1441	1359	1322	1370	1401
	1356	1374	1248	1276	1285	1375
	1325	1362	1136	1191	1207	1290
	1254	1149	1020	1189	1195	
	1224	1112	953	1108		
	1148	1097	921	1017		
δ (OH)	1321	1328	1398	1437	1343	1331
	1263	1319	1381	1352	1312	1314
	1190	1262	1335	1285	1273	1273
	1169	1174	1306	1210	1185	1175
	801	1145	1273	1204	1176	1141
	640	802	1178	830	771	1126

	626	788	1164	780	754	758
	622	770	1120	758	681	749
	576	756	803	720	644	679
		682	756	666	636	639
		496	690	591	615	635
			648	506	581	591
			636	480	569	575
			594			569
			569			511
			486			
			483			
ν (SO)			1049	1037	1068	1069
ν (CS)	710	715	704	712	725	720
	708	710		694		
	397					
	370					
backbone	1049	1046			509	481
	1034	1029			482	
	936					
	896					
	755					
	710					
	503					
	287					
ν (SS)	485	487				
	476	480				
δ (NH_2)	356	404	342	418	352	354
	294	337	328	338	336	336
	274	317	316	325	313	319
	270	279	295	285	306	295
	259	269	282	270	293	278
		268	265	263	273	257
				256	251	254
δ (CH_2)	321	317	449	412	421	421
		288	421	352	382	384
			391	303		
δ (SO)			251	450		
δ (SO_2)					467	470
Se_8		259-258		263-254		263

Where ν and δ indicate stretching and bending vibrations.

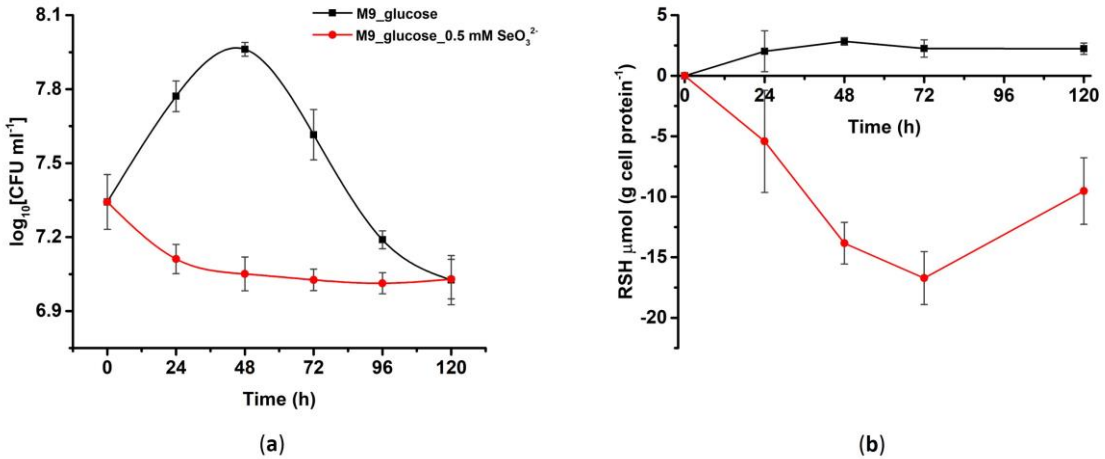

Figure S2: (**a**) Growth profile and (**b**) RSH depletion of *Micrococcus* sp. cells in M9 medium supplied with either glucose or glucose and SeO_3^{2-}

Table S3. ATR-FTIR absorption bands and identification of *Micrococcus* sp. unchallenged cells or exposed to SeO_3^{2-}.

$\tilde{\nu}$ (cm^{-1})						Vibrational modes	Identification
M9_24h	**M9_72h**	**M9_120h**	**M9_0.5 mM SeO_3^{2-}_24h**	**M9_0.5 mM SeO_3^{2-}_72h**	**M9_0.5 mM SeO_3^{2-}_120h**		
3286	3284	3286	3285	3282	3284	ν (NH)	Proteins (Amide A) [1]
3070	3068	3068	3069	3062	3067	ν_s (NH^{3+})	Proteins (Amide B) [2]
2955	2953	2962	2960	2958	2962	ν_{as} (CH_3)	Fatty acids [1-3]
2923	2921	2924	2925	2926	2928	ν_{as} (CH_2)	Fatty acids [1-3]
2869	2876	2872	2875	2872	2873	ν_s (CH)	Amino acids in fatty acids [3]
2856	2850	2852	2854	2853	2855	ν_s (CH_2)	Fatty acids [1-3]
1742	1739	1740	1736	1740	1739	ν (CO)	Ester moieties of lipids and polysaccha-

							rides [1-3]
1652	1650	1651(s)				ν (CO)	α-helix proteins (Amide I) [1-3]
1642(s)	1643(s)	1643	1646	1644	1645	ν_{as} (COO^-); β (NH_2); δ (NH)	β-sheet proteins [1]
			1559(s)	1561(s)	1558(s)	δ (NH); ν (CN)	α-helix proteins (Amide II) [1-3]
1545	1544	1539	1541	1542	1539	δ (NH); ν (CN)	α-helix proteins (Amide II) [1-3]
			1515(s)	1514(s)	1515(s)	δ_s (NH_3^+); δ (NH); ν (CN)	Amino acid residues [2]; RSH-containing molecules
1467(s)	1469(s)	1468(s)	1467(s)	1468(s)	1468(s)	δ (CH_2); δ (CH_3); β (CH_2)	Lipids and proteins [3]
1450	1452	1450	1448	1450	1451	δ_{sciss} (CH_2); δ (OH); ν CC(O); ν_s (COO^-)	Polysaccharides [4]; aliphatic groups of proteins [5]; R-SO_2H-containing molecules adsorbed on SeNP
1395	1394	1393	1395	1394	1395	ν_s (COO^-)	Amino acid side chains; free fatty acids [3]; peptides [5]
1385(s)	1384(s)	1385(s)				δ (CH); δ (COH); β (CH_3); ν CC(O); ν_s (COO^-); δ (NH_2); ν (CN)	Aldehydes; carboxylic acids; peptides [5]; aromatic amines [6]
			1373(s)	1377(s)	1373(s)	β (CH_3); δ (CH); δ (OH);	Lipids and proteins [3]; RSH-, RSO_3H-, RSSR-, and RSO_2SR-containing molecules; RSH-, RS^--, RSO_2^--, RSO_3H-, RSSR-, RSOSR-, and RSO_2SR-containing molecules adsorbed on SeNP
1301	1299	1299	1298	1300	1300	ω (CH_2); ν (CN); δ (NH_2); $\varrho_{as(oph)}$ (CH); ν (COC); ν (CCO); δ (OH); δ (CH)	Ester moieties [1]; proteins [3]; RSH-, RSO_2^--, RSO_3H-, RSSR-, RSOSR-containing molecules; RSH-and RSO_2H-, RSO_3H-, RSO_3^--containing molecules adsorbed on SeNP;
1249	1246	1243	1244	1243	1243	ν (CN); δ (NH_2)	Proteins (Amide III) [1]
1149	1146	1147	1149	1150	1151	ν_{as} (COC); δ (CH_2); δ (CH); δ (NH_2); δ (OH); δ (S)OH; ν (CO)	Nucleic acids; $\alpha_{(1,4)}$ glycosidic bonds [7]; polysaccharide ring [8]; amino acids [9]; RSH-containing molecules

1102(s)	1099(s)	1101(s)	1099(s)	1102(s)	1101(s)	ν_{as} (COC); ν (CC); ν (CO); δ (COH); ν $P(OH)_2$	$\beta_{(1,4)}$ glycosidic bonds [7]; amino acids [9]; polysaccharides [4,8]
1075	1076	1070(s)	1073	1074(s)	1071(s)	ν (CO); ν (CC); ν (COH); δ (COC); ϱ (NH_3^+); ν (SO)	Polysaccharides, proteins, and polyesters [10]; amino acid residues [11]; RSO_2^--containing molecules adsorbed on SeNP
1062	1063					ν (CO); ϱ (CO); ν_s (PO_2^-); ν (CC); ν (C)OH; ν (COH); δ (COC)	Nucleic acids [4]; phospholipids [4]; $\beta_{(1,3)}$ glycosidic bonds [7]; polysaccharides [1]
1049(s)	1050(s)		1055	1054	1055	ν (CC); ν (CO); δ (COH); ν (SO)	Polysaccharides [9]; RSO_2H-containing molecules adsorbed on SeNP
1037	1037	1035	1038	1036	1038	ν (PO); ν (SH); ν (SO); backbone vibration	Polysaccharides and nucleic acids [1-4]; RSSR-containing molecules; RSH- and RSOSR-containing molecules adsorbed on SeNP
990	988	985(s)	990	982(s)	982(s)	δ (NH_2); δ (HNCC); ν (CO); ν_s (PO_3^{2-}); δ (COH); ν (CC)	Amino acids [9,12]; $\beta_{(1,3)}$ glycosidic bonds [7]; nucleic acids [11]; polysaccharides [8]; RS^--containing molecules adsorbed on SeNP
922	921	922	920	921	922	δ (=CH); τ (CH_2); ν_s (PO_4^{3-}); δ (SH); ν (SO); δ (NH_2); δ (CH_2)	Alkyl halides, carboxylic acids; amines; $\alpha_{(1,3)}$ glycosidic bonds [7]; amino acid residues [9]; nucleic acids [4]; RSH-, RSSR-, RSO_2SR-containing molecules; RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
860	857	860	863	862	863	δ (NH_2); ν (CC); ν (CN)	Amino acid residues [9]; RSO_2H-containing molecules adsorbed on SeNP
802	803	802	802	800(s)	796(s)	ν SO(H); δ (OH) δ_{op} (HOCC); ν (PO)	Amino acids [9]; nucleic acids [13]; RSH-, RS^--, RSSR-containing molecules; RS^--, RSOSR-containing molecules ad-

							sorbed on SeNP
779	779	779	778	777	777	ν C(COOH); δ (NH_2); ϱ (CH_2); δ (HNC); δ (CCH); δ (OH)	Amino acids [9]; RSH-, RSSR-, RSOSR-, RSO_2SR-containing molecules; RSO_3^--containing molecules adsorbed on SeNP
				754	755		
			739	738	738	δ (NH_2)C(COOH); ϱ (CH_2); δ (OH)	Amino acids [9]; RSH-, RS^--, RSO_2H-, RSO_2^--, RSO_2SR-containing molecules adsorbed on SeNP
722	724	723	722	721	722	β_{op} *cis* (CH); ν (CN); ϱ (CH_2); ν (CS)	Amino acids [9]; fatty acid chains [3]; RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
700	700	701	701	699	700	ω (CO); δ (=CH); ν (CS)	Alkyl halides, carboxylic acids, and amines [2-4]
			670	671	673	δ (OH); δ (CCC); δ (COO)	Amino acid residues [9]; RSO_2^--containing molecules adsorbed on SeNP
631(s)	630(s)	629(s)				ν (CS); δ (OH); δ (S)OH	RSH-containing molecules; RSH-, RS^--, RSO_3^--, RSSR-containing molecules adsorbed on SeNP
			534	532	533	δ (OH); ϱ (COO^-); backbone vibrations	RSH-, RSO_2H-, RSSR-containing molecules; RSO_2H-, RSO_3^--containing molecules adsorbed on SeNP
527	527	528	527	528	525	δ (OH); δ (COO^-); backbone vibrations	Amino acid residues [9]; RSO_3H-, RSO_3^--containing molecules; RS^--, RSO_3H-containing molecules adsorbed on SeNP
520	521	520	519	518	519	δ_{op} (OH); δ (COO^-); ω (OH)	Amino acid residues [9]; polysaccharides [14]; RSO_3H-containing molecules adsorbed on SeNP
	469	470	470	471(s)	471(s)	δ (OH); τ (NH_2)	Amino acid residues [9]; RSO_2^--, RSO_3^--RSO_2SR-containing molecules; RSO_2SR-containing molecules adsorbed on SeNP

409(s)	408(s)	410(s)	412	415	411	δ (OH); δ (SO_3)	Amino acid residues [9]; RSO_2H-containing molecules; RSO_2H-, RSO_3^--, RSSR-containing molecules adsorbed on SeNP

Where ν, δ, β, ϱ, τ, and ω indicate stretching, bending, deformation, rocking, twisting, and wagging, respectively; sciss, oph, as, s, and ip stand for scissoring, out of phase, asymmetric, symmetric, and in plane vibrations.

Table S4. ATR-FTIR absorption bands and identification of biogenic samples (Bio SeNP extract, OM, and Bio SeNP extract_w).

$\tilde{\nu}$ (cm^{-1})			Vibrational modes	Identification
Bio SeNP extract	**OM**	**Bio SeNP extract_w**		
		3438(s)	ν (OH)	H-bonded water impurities [15]
		3387(s)	ν (OH); ν_{as} (NH)	Proteins [16]
		3349(s)	ν (OH); ν_s (NH)	Proteins [16]
		3303	ν (OH); ν (NH)	Water; proteins (Amide A) [10]
3289	3285		ν (NH)	Proteins (Amide A) [1]
3200(s)		3220(s)	ν (CH); ν (NH)	Free amino acid residues [17]
		3145(s)	ν (CH); ν_{as} (NH^{3+})	Proteins or amino acid residues [11]; RS^--containing molecules adsorbed on SeNP
		3092	ν_s (NH^{3+}); ν (CH)	Microbial proteins (Amide A) [10]; S^- and SO_2^- adsorbed on SeNP
3070	3073	3065	ν_s (NH^{3+})	Proteins (Amide B) [2]
		3030	ν (CH); ν_s (NH^{3+})	Amino acid residues [9]; RSH- and RSO_2^--containing molecules adsorbed on SeNP
2950	2960	2956	ν_{as} (CH_3)	Fatty acids [1-3]
2923	2923	2925	ν_{as} (CH_2)	Fatty acids [1-3]
2877	2873	2872	ν_s (CH)	Amino acids in fatty acids [3]
2857	2851	2856	ν_s (CH_2)	Fatty acids [1-3]
		2476	ν ($-NH^+$)	Free amino acids [17]
		2410	ν ($-NH^+$)	Free amino acids [17]
1740	1739	1737	ν (CO)	Ester moieties of lipids and polysaccharides [1-3]
1649	1651	1652	ν (CO); ν *cis* (HC=CH)	*α*-helix proteins [1-3]

1634(s)	1629(s)	1634(s)	ν_{as} (COO^-); β (NH_2); δ (NH)	β-sheet proteins [1,10]
1538	1538	1548(s)	δ (NH); ν (CN)	α-helix proteins (Amide II) [1-3]
1517(s)	1511(s)		δ_s (NH_3^+)	Proteins [2]; RSH-containing molecules
1458	1457		β scissoring (CH_2); $\varrho_{as(oph)}$ (CH); δ_{as} (CH_3); δ (OH); ν CC(O)	Lipids, proteins and polyesters ([1,3]
		1440	δ_{sciss} (CH_2); δ (OH); ν CC(O); ν_s (COO^-)	Polysaccharides [4]; aliphatic groups of proteins [5]; RSO_2H-containing molecules adsorbed on SeNP
1385	1384	1385(s)	δ (CH); δ (COH); β (CH_3); ν CC(O); ν_s (COO^-); δ (NH_2); ν (CN)	Aldehydes; carboxylic acids; peptides [5]; aromatic amines [6]
		1329	δ (CH); ϱ (CH_2); δ (OH); β C(OH)	Polysaccahrides [3-4]; RSH-containing molecules; RS^--containing molecules adsorbed on SeNP
1303	1301	1304	ω (CH_2); ν (CN); δ (NH_2); δ (OH); δ (CH); $\varrho_{as(oph)}$ (CH); ν (COC); ν (CCO)	Ester moieties [1]; proteins (Amide III) [1-3]; RSH-, RSO_2^--, RSO_3H-, RSSR-, RSOSR-containing molecules; RSH-and RSO_2H-, RSO_3H-, RSO_3^--containing molecules adsorbed on SeNP;
1256	1253(s)	1246	ν (CN); δ (NH_2)	Proteins (Amide III) [1-3]
1229	1231		ν CO(H); δ (COH); ν (CO); ν_{as} (PO_2^-); ν (CN)	Nucleic acids [15]; amino acids [12]
1173(s)	1169		ν (CN); ϱ (NH); $\varrho_{as(oph)}$ (CH); ν (CO); δ (CH); δ (S)OH; ν (CC); δ (OH)	Triglyceride ester linkage; $\beta_{(1,3)}$ glycosidic bonds [7]; amino acids [9]; RS^--, RSSR-containing molecules; RSH-containing molecules adsorbed on SeNP
1151(s)	1149	1158(s)	ν_{as} (COC); δ (CH_2); δ (CH); δ (NH_2); δ (OH); δ (S)OH; ν (CO)	Nucleic acids; $\alpha_{(1,4)}$ glycosidic bonds [7]; polysaccharide ring [8]; amino acids [9]; RSH-containing molecules
1098	1100		ν_{as} (COC); ν (CC); ν (CO); δ (COH); ν $P(OH)_2$	$\beta_{(1,4)}$ glycosidic bonds [7]; amino acids [9]; polysaccharides [4,8]
		1070	ν (CO); ν (CC); ν (COH); δ (COC);	Polysaccharides, proteins, and polyesters [10]; amino acid residues [11]; RSO_2^--containing

			ϱ (NH_3^+); ν (SO)	molecules adsorbed on SeNP
1057	1059	1052(s)	ν (CO); ϱ (CO); ν_s (PO_2^-); ν (CC); ν (C)OH; ν (COH); δ (COC)	Nucleic acids, phospholipids, and polysaccharides [1-4]
981	980		δ (NH_2); δ (HNCC); ν (CO); ν_s (PO_3^{2-}); ν (CO); ν (CC)	Amino acids [9,12]; $\beta_{(1,3)}$ glycosidic bonds [7]; nucleic acids [10]; RS^--containing molecules adsorbed on SeNP
		969(s)	δ (NH_2); δ (HNCC)	Amino acid residues [9]; RSH-containing molecules adsorbed on SeNP
932	926	931	δ (=CH); τ (CH_2); ν_s (PO_4^{3-}); δ (SH); ν (SO); δ (NH_2); δ (CH_2)	Alkyl halides, carboxylic acids; amines; $\alpha_{(1,3)}$ glycosidic bonds [7]; amino acid residues [9]; nucleic acids [4]; RSH-, RSSR-, RSO_2SR-containing molecules; RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
899	894	897	δ (NH_2); ν (COC); ν (CC); ν (CN); δ (CH_2)	$\beta_{(1,4)}$ glycosidic bonds [7]; amino acid residues [9]; RSO_3H-, RSO_3^--containing molecules; RS^--, RSO_3^--, RSSR-, RSOSR-containing molecules adsorbed on SeNP
		857(s)	δ (NH_2); ν (CC); ν (CN)	Amino acid residues [9]; RSO_2H-containing molecules adsorbed on SeNP
824(s)			δ (NH_2); ω (COO^-); δ (CH_2); δ (OH)	RSH-, RSO_3H-, RSO_3^--, RSSR-, RSO_2SR-containing molecules; RSH-, RSO_2H-, RSO_2^--, RSO_3H-, RSO_3^--, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
806	811		ν SO(H); δ (OH) δ_{op} (HOCC); ν (PO)	Amino acids [9]; nucleic acids [13]; RSH-, RS^--, RSSR-containing molecules; RS^--, RSOSR-containing molecules adsorbed on SeNP
		790	ν SO(H); ϱ (CH_2)	RSH-containing molecules; RSO_2H-containing molecules adsorbed on SeNP
769		768	ν C(COOH); δ (NH_2); ϱ (CH_2); δ (HNC); δ (CCH); δ (OH)	Amino acids [9]; RSH-, RSSR-, RSOSR-, RSO_2SR-containing molecules; RSO_3^--containing molecules adsorbed on SeNP
740	738		δ (NH_2)C(COOH);	Amino acids [9]; RSH-, RS^--, RSO_2H-, RSO_2^--,

			ϱ (CH_2); δ (OH)	RSO_2SR-containing molecules adsorbed on SeNP
714(s)	717	718(s)	β_{op} *cis* (CH); ν (CN); ϱ (CH_2); ν (CS)	Amino acids [9]; fatty acid chains [3]; RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
700	700	697	ω (CO); δ (=CH); ν (CS)	Alkyl halides, carboxylic acids and amines [1-4]
		672	δ (OH); δ (CCC); δ (COO)	Amino acid residues [9]; RSO_2^--containing molecules adsorbed on SeNP
659	660	652(s)	δ (OH); δ_{op} (HOCC)	Amino acid residues [9]; RSO_2H-, RSOSR-containing molecules adsorbed on SeNP
		641	δ (OH); δ_{op} (HOCC)	Amino acid residues [9]; RS^--, RSO_2^--, and RSO_3H-containing molecules adsorbed on SeNP
625		626	ν (CS); δ (OH); δ (S)OH	RSH-containing molecules; RSH-, RS^--, RSO_3^--, RSSR-containing molecules adsorbed on SeNP
604		604	δ (OH); δ_{op} (NH_2)	Amino acid residues [9]; RSO_2^--containing molecules
		595	δ (OH)	RSO_2^-- and RSO_3H-containing molecules adsorbed on SeNP
		588	δ (NH_2); δ (COO^-)	Amino acid residues [9]; RSO_3^-- containing molecules adsorbed on SeNP
		577	δ (COO^-); δ_{op} (OH)	Amino acid residues [9]; RSO_2^-- containing molecules adsorbed on SeNP
566			δ (OH); δ (NH_2); δ (OCOH); backbone vibrations	Amino acid residues [9]; RSOSR-containing molecules; RS^--, RSO_2^--, RSO_2SR-containing molecules adsorbed on SeNP
		555	δ (OH); δ (NH_2); δ (OCOH)	Amino acid residues [9]; RSH-containing molecules adsorbed on SeNP
	534	536	δ (OH); ϱ (COO^-); backbone vibrations	RSH-, RSO_2H-, RSSR-containing molecules; RSO_2H-, RSO_3^--containing molecules adsorbed on SeNP
524		524(s)	δ (OH); δ (COO^-); backbone vibrations	Amino acid residues [9]; RSO_3H-, RSO_3^--containing molecules; RS^--, RSO_3H-containing molecules adsorbed on SeNP
		514	δ_{op} (OH); ω (OH); δ (COO^-)	Amino acid residues [9]; RSO_3H-containing

				molecules adsorbed on SeNP
		500(s)	δ (SO_2)	RSO_3^--containing molecules adsorbed on SeNP
		473	δ (SO_2); δ (OH)	RSO_2H- and RSO_3H-containing molecules adsorbed on SeNP
464	464	464	δ (OH); τ (NH_2)	Amino acid residues [9]; RSO_2^--, RSO_3^--RSO_2SR-containing molecules; RSO_2SR-containing molecules adsorbed on SeNP
		456	δ (CNN)	RSH-containing molecules
		435(s)	δ SO(OH)	RSO_3H-containing molecules adsorbed on SeNP
408		409	δ (OH); δ (SO_3)	Amino acid residues [9]; RSO_2H-containing molecules; RSO_2H-, RSO_3^--, RSSR-containing molecules adsorbed on SeNP
		400(s)	δ (SO_2)	RSO_2H- containing molecules adsorbed on SeNP
		386		
375		369	δ (NCC); δ (CCCO); δ (SH); δ (CCN); τ (NH_3); δ (NH_2); backbone vibrations	Amino acid residues [9]; RSH-, and RS^--, RSSR-containing molecules; RSO_2^--containing molecules adsorbed on SeNP
		358	δ (NCC); δ (CCCO); δ (SH)	Amino acid residues [9]; RSO_2^--containing molecules adsorbed on SeNP
		347	δ (NH_2)	RSO_2^--containing molecules adsorbed on SeNP
337		337	δ (NH_2); δ (OH); δ_{ip} (CCC)	Amino acid residues [9]; RSOSR-, RSO_2SR-containing molecules; RSH-, RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
		325	δ (NH_2); τ (COO^-); backbone vibrations	Amino acid residues [9]; RSO_3H-, RSOSR-, RSO_2SR-containing molecules; RSH-, RSO_2^--, RSSR-, RSO_2SR-containing molecules adsorbed on SeNP
316		316	δ (NH_2); τ (COO^-); β (CN); δ (SH)	Amino acid residues [9]; RSO_3H-, RSOSR-, RSO_2SR-containing molecules; RSH-, RSO_2^--, RSSR-, RSO_2SR-containing molecules adsorbed

			on SeNP
	305	δ (SH); τ (COO^-)	Amino acid residues [9]; RSH-containing molecules adsorbed on SeNP
294	290	ν (S)OH; δ (NH_2); δ (CCC); backbone vibrations	Amino acid residues [9]; RSH-, RSO_2^--, RSO_3H-, RSO_3^--, RSOSR-, RSO_2SR-containing molecules; RSO_2^-- and RSO_2SR-containing molecules adsorbed on SeNP
	280	δ (NH_2); τ (NH_2)	Amino acid residues [9]; RS^--containing molecules adsorbed on SeNP
	272	δ_{ip} (CCN); δ (SH); backbone vibrations; δ (NH_2)	RSH-, RS^--, RSO_3^--, RSSR-, RSOSR-, RSO_2SR-containing molecules; RSH-, RSO_2^--, RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
265	266	τ (NH_2); Se_8 vibration; backbone vibrations	RSH-, RS^--, RSO_2H-, RSO_2^--, RSO_3H-, RSO_3^--, RSSR-, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP
	260	Se_8 vibration	RSH-, RSO_2H-, RSO_2^--, RSO_3H-, RSO_3^--, RSSR-, RSOSR-, RSO_2SR-containing molecules
249	249	Se_8 vibration	RS^--, RSO_2^--, RSO_3H-, RSO_3^--, RSOSR-, RSO_2SR-containing molecules adsorbed on SeNP

Where ν, δ, β, ϱ, τ, and ω indicate stretching, bending, deformation, rocking, twisting, and wagging, respectively; sciss, oph, as, s, and ip stand for scissoring, out of phase, asymmetric, symmetric, and in plane vibrations.

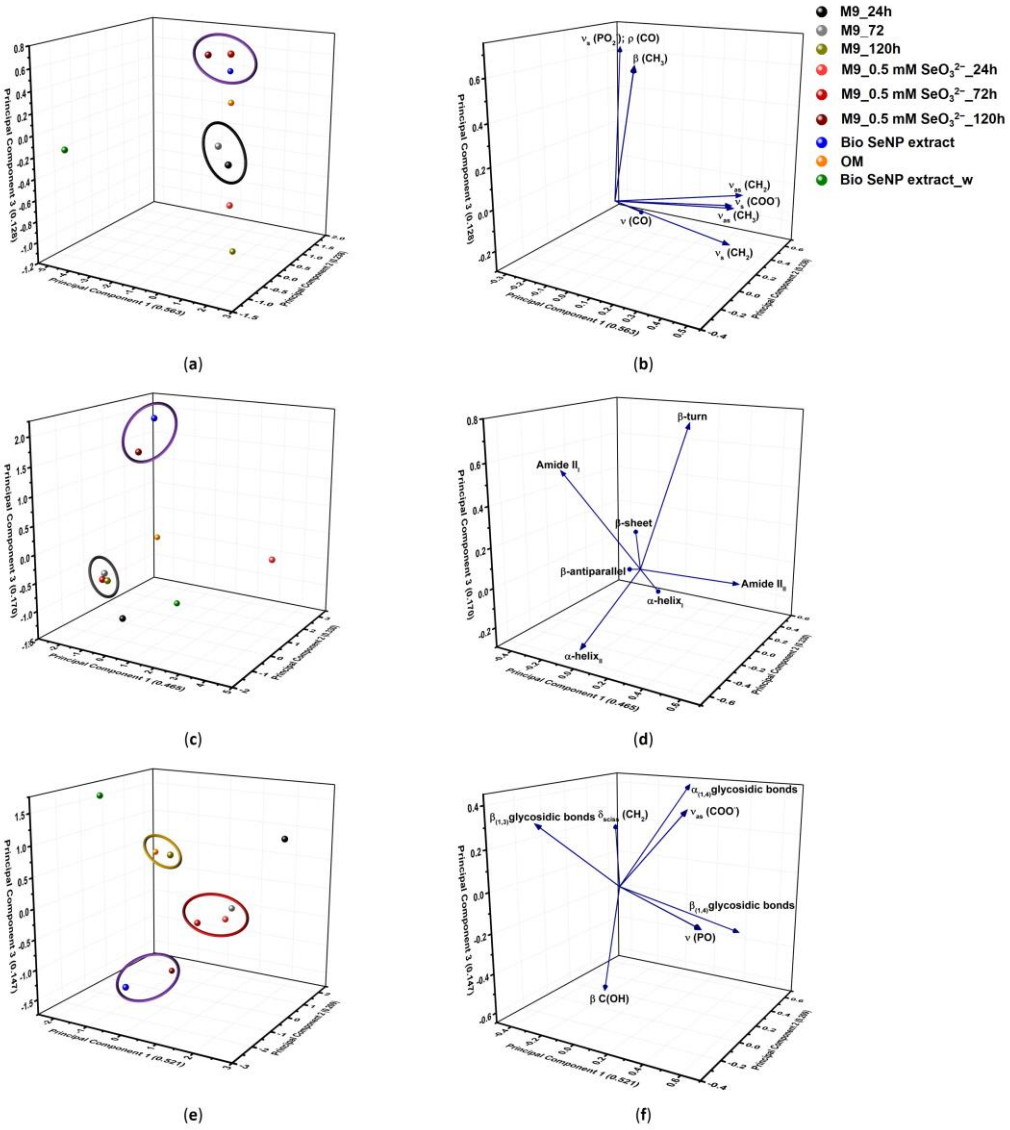

Figure S3. Representation of (**a, c,** and **e**) score and (**b, d,** and **f**) loading plots obtained by performing PCA on IR contributions referring to (**a-b**) lipids, (**c-d**) proteins, and (**e-f**) polysaccharides of *Micrococcus* sp. cells incubated in the presence/absence of SeO_3^{2-} and the derived Bio SeNP extracts, alongside OM.

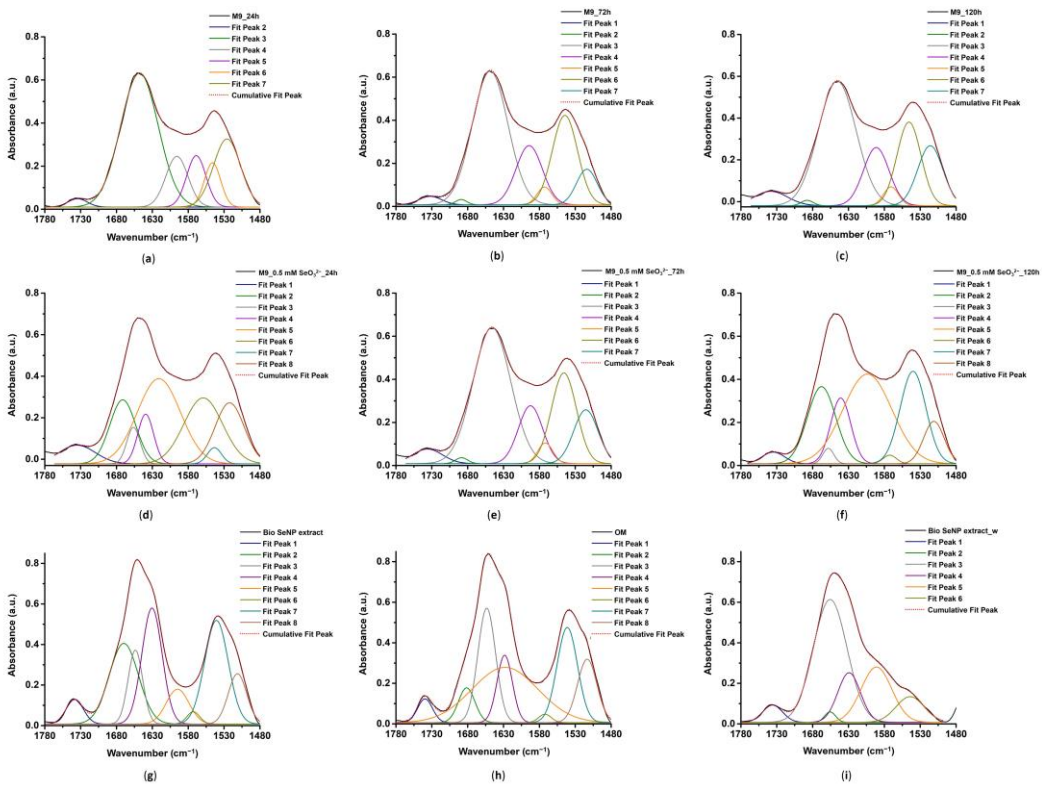

Figure S4. ATR-FTIR spectral deconvolution performed on the 1780-1480 cm^{-1} region for *Micrococcus* sp. cells incubated for (**a, d**) 24h, (**b, e**) 72h, and (**c, f**) 120h with either (**a-c**) glucose or (**d-f**) glucose and SeO_3^{2-}, (**g**) Bio SeNP extract, (**h**) OM, and (**i**) Bio SeNP extract_w.

Table S5. Deconvolution of ATR-FTIR spectra of *Micrococcus* sp. unchallenged cells in the 1780-1480 cm^{-1} region.

M9_24h	w	A	M9_72h	w	A	M9-120h	w	A	Vibrational mode
1734	26.74	1.293	1732	31.42	1.554	1738	46.56	4.008	ν (CO)
			1670	15.72	0.484	1675	16.73	0.536	δ (NH); ν (CO)
1648	52.25	40.86	1649	49.49	38.51	1645	52.54	39.27	ν (CO)
1596	30.34	9.116	1594	36.71	12.65	1591	35.72	12.46	δ_{as} (NH_3^+)
1569	26.88	8.031	1572	20.61	2.137	1570	20.84	2.352	ν_{as} (COO^-)
1546	22.75	5.852	1544	35.25	18.34	1545	33.39	16.74	δ_s (NH); ν (CN)
1526	37.85	14.98							
			1514	28.94	5.983	1516	35.08	12.63	δ_s (NH_3^+)

Where ν, δ, as, and s indicates stretching, bending, asymmetric, and symmetric vibrations, respectively.

Table S6. Deconvolution of ATR-FTIR spectra of *Micrococcus* sp. cells incubated with SeO_3^{2-} in the 1780-1480 cm^{-1} region.

M9_0.5 mM SeO_3^{2-}_24h	w	A	M9_0.5 mM SeO_3^{2-}_72h	w	A	M9_0.5 mM SeO_3^{2-}_120h	w	A	Vibrational mode
1734	50.54	5.681	1736	41.63	3.533	1735	31.25	2.116	ν (CO)
			1689	16.91	0.581				
1671	36.16	13.96				1668	39.56	17.73	δ (NH); ν (CO)

1656	18.63	4.094				1658	15.35	1.373	ν (CO)
			1646	52.45	41.53				ν (CO)
1639	22.09	6.615				1640	28.11	10.74	ν (CO); δ (NH)
1621	60.29	30.97							ν (CO); δ (NH)
			1592	33.90	11.40	1603	68.29	35.61	δ_{as} (NH_3^+)
			1572	21.00	2.524	1572	18.70	0.933	ν_{as} (COO^-)
1559	53.90	21.44							δ_s (NH); ν (CN)
1543	19.64	1.915	1546	34.88	18.39	1540	35.92	19.32	δ_s (NH); ν (CN)
1522	40.69	14.98							δ_s (NH); ν (CN)
			1515	34.07	10.659	1511	28.69	7.073	δ_s (NH_3^+); δ_s (NH); ν (CN)

Where ν, δ, as, and s indicates stretching, bending, asymmetric, and symmetric vibrations, respectively.

Table S7. Deconvolution of ATR-FTIR spectra of biogenic SeNP extracts and OM in the 1780-1480 cm^{-1} region.

Bio SeNP extract	**w**	**A**	**OM**	**w**	**A**	**Bio SeNP extract_w**	**w**	**A**	**Vibrational mode**
1738	24.22	3.675	1739	20.72	3.033	1735	27.61	2.950	ν (CO)
1670	40.74	20.29	1681	22.95	4.924				δ (NH); ν (CO)
1654	20.36	9.292	1653	24.74	17.49	1655	15.22	0.985	ν (CO)
						1650	47.01	35.70	ν (CO)
1630	28.19	20.21	1628	21.40	8.90	1629	31.53	9.670	ν (CO); δ (NH)
			1625	91.94	31.37				ν (CO); δ (NH)
1595	31.53	6.782				1590	42.53	14.54	δ_{as} (NH_3^+)
1573	17.79	1.354	1572	17.60	0.909				ν_{as} (COO^-)
1540	32.89	21.06	1541	28.49	16.75	1544	39.31	6.246	δ_s (NH); ν (CN)
1511	25.76	8.000	1513	27.07	10.61				δ_s (NH_3^+)

Where ν, δ, as, and s indicates stretching, bending, asymmetric, and symmetric vibrations, respectively.

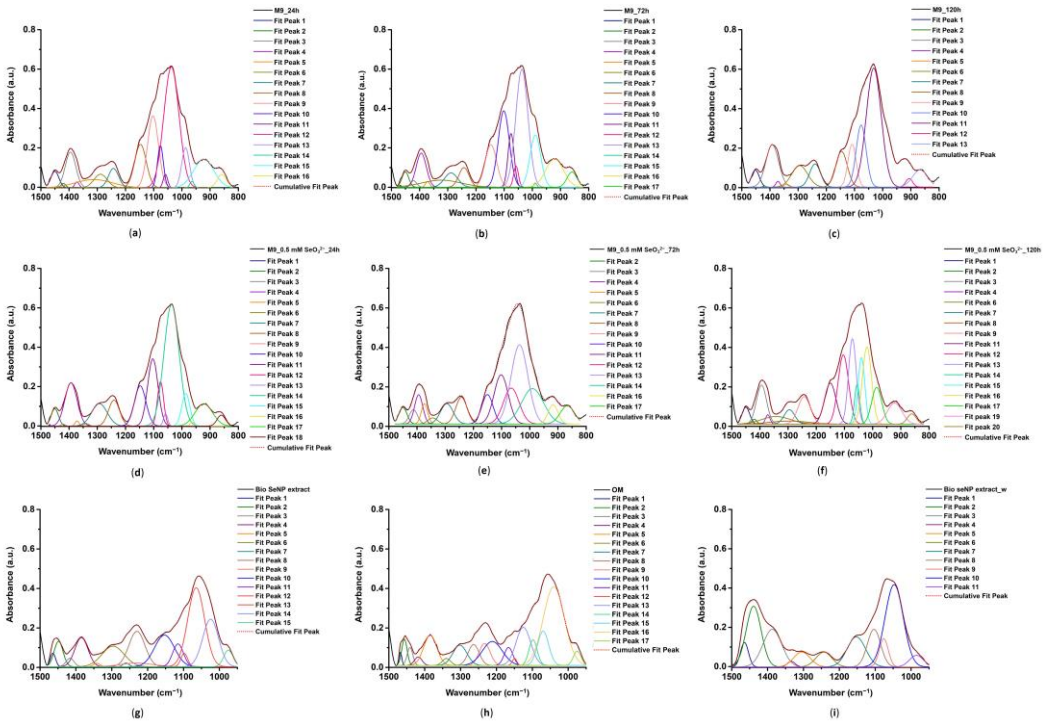

Figure S5. ATR-FTIR spectral deconvolution performed on the 1500-800 cm^{-1} region for *Micrococcus* sp. cells incubated for (**a, d**) 24h, (**b, e**) 72h, and (**c, f**) 120h with either (**a-c**) glucose or (**d-f**) glucose and SeO_3^{2-}, (**g**) Bio SeNP extract, (**h**) OM, and (**i**) Bio SeNP extract_w.

Table S8. Deconvolution of ATR-FTIR spectra of *Micrococcus* sp. unchallenged cells in the 1500-800 cm^{-1} region.

M9_24h	w	A	M9_72h	w	A	M9_120h	w	A	Vibrational mode
			1468	5.852	0.073				δ (CH_2); δ (CH_3)
1450	28.48	2.977	1450	24.19	2.377	1451	28.14	3.032	δ_{sciss} (CH_2); δ (OH); ν CC(O); ν_s (COO^-)
1420	16.65	0.455	1421	22.14	0.927	1420	10.16	0.067	ν_s (COO^-)
1395	37.14	8.421	1394	35.58	7.734	1392	45.15	12.13	δ (CH); δ (OH); δ (COH); β (CH_3); ν (CN)
1371	15.11	0.558	1371	14.90	0.549	1371	14.62	0.539	β (CH_3)
						1340	18.93	0.337	β C(OH); δ (OH); δ (CH)
1312	130.1	6.811	1322	1318.8	6.297				
1292	46.68	4.016	1288	47.22	4.319	1294	56.32	7.672	ω (CH_2), $\varrho_{as(oph)}$ (CH); ν (COC); ν (CCO); δ (OH)
1242	36.05	4.437	1242	36.21	4.536	1240	38.43	5.642	β (NH); ν_{as} (PO_2^-)
1146	41.14	11.37	1147	40.83	11.11	1146	40.53	9.179	ν_{as} (COC); δ (CH_2); δ (CH); δ (NH_2)
1102	38.27	17.52	1101	39.47	19.21	1108	29.06	7.899	ν_{as} (COC); ν (CC); ν (CO); δ (COH); ν $P(OH)_2$
1076	20.93	5.60	1075	21.75	7.435	1076	34.98	13.76	ν (CO); ν (CC); ν (COH); δ (COC); ϱ (NH_3^+)
1058	15.53	1.319	1058	17.02	2.304				ν (CC); ν (CO); δ (COH); ν_s (PO_2^-)
1037	53.58	41.26	1037	43.41	32.61	1032	52.90	39.65	ν (PO); ν (SH); ν (SO)
987	27.15	6.935	989	10.20	0.283				δ (NH_2); δ (HNCC); ν (CO); ν_s (PO_2^-); ν (CO); ν (CC)
			985	37.81	12.57				δ (NH_2); δ (HNCC); ν (CO); ν_s (PO_2^-); ν (CO); ν (CC)
964	15.47	0.610							δ (NH_2); δ (HNCC)
922	71.42	12.96	920	62.20	11.31				δ (=CH); τ (CH_2); ν_s (PO_4^{3-}); δ (NH_2); δ (CH_2)
						906	24.13	1.3	
858	33.04	2.797	859	35.32	3.427	867	54.04	5.896	δ (NH_2); ν (CC); ν (CN)

Where ν, δ, β, ϱ, and ω indicate stretching, bending, deformation, rocking, and wagging, respectively; sciss, oph, as, s, and ip stand for scissoring, out of phase, asymmetric, symmetric, and in plane vibrations.

Table S9. Deconvolution of ATR-FTIR spectra of *Micrococcus* sp. cells incubated with SeO_3^{2-} in the 1500-800 cm^{-1} region.

M9_0.5 mM SeO_3^{2-}_24h	w	A	M9_0.5 mM SeO_3^{2-}_72h	w	A	M9_0.5 mM SeO_3^{2-}_120h	w	A	Vibrational mode
1469	4.836	0.053							δ (CH_2); δ (CH_3)
1451	26.25	2.894	1450	28.95	3.056	1450	26.70	2.896	δ_{sciss} (CH_2); δ (OH); ν CC(O); ν_s (COO^-)
1421	13.07	0.170							ν_s (COO^-)
			1413	29.19	2.643	1415	17.65	0.570	ν_s (COO^-)
1393	43.29	11.93	1394	28.92	11.368	1390	35.80	8.879	δ (CH); δ (OH); δ (COH); β (CH_3); ν (CN)
1371	14.04	0.461	1373	22.64	2.917	1372	15.90	0.952	β (CH_3); δ (CH); δ (OH)
1339	18.35	0.308	1344	33.63	1.301	1342	103.3	5.042	β C(OH); δ (OH); δ (CH)
1292	55.53	7.941	1294	44.83	5.786	1303	39.41	4.330	ω (CH_2); $\varrho_{as(oph)}$ (CH); ν (COC); ν (CCO); δ (OH)
						1276	136.2	2.765	ν (CO); δ (S)OH; δ (NH_2); δ (CH_2); δ (OH); ν_{as} (PO_2^-)
1241	38.92	6.445	1242	39.86	6.772	1243	43.60	7.644	β (NH); ν_{as} (PO_2^-)
			1220	0.023	232.2	1223	0.202	3.300	ν CO(H) δ (COH); ν (CO); ν_{as} (PO_2^-); ν (CN); δ (S)OH; δ (CH_2)
1206	11.12	0.078							ν (CO); δ (CH_2); δ (CH); δ (OH)
1148	40.86	10.46	1150	40.06	7.479	1150	41.20	10.74	ν_{as} (COC); δ (CH_2); δ (CH); δ (NH_2)
1102	36.70	15.72	1101	50.11	15.68	1104	37.30	16.43	ν_{as} (COC); ν (CC); ν (CO); δ (COH); ν $P(OH)_2$
1075	21.97	6.195	1066	55.63	12.69	1072	27.65	14.99	ν (CO); ν (CC); ν (COH); δ (COC); ϱ (NH_3^+); ν (SO)
1058	15.22	1.191				1055	18.59	4.663	ν (CC); ν (CO); δ (COH); ν (SO); ν_s (PO_2^-)
1037	53.65	41.51	1036	59.66	29.99	1040	23.48	9.951	ν (PO); ν (SH); ν (SO)
						1020	32.36	15.89	ν (POC); δ (NH_2)
986	28.81	5.980	990	77.64	17.44	985	35.91	8.389	δ (NH_2); δ (HNCC); ν (CO); ν_s (PO_2^-); ν (CO); ν (CC)
963	13.96	0.381							δ (NH_2); δ (HNCC)
						940	240.6	3.169	
922	62.24	8.829	917	34.48	4.227	921	51.53	6.940	δ (=CH); τ (CH_2); ν_s (PO_4^{3-}); δ (SH); ν (SO); δ (NH_2); δ (CH_2)
860	29.97	2.098	866	50.34	5.842	861	31.44	2.060	δ (NH_2); ν (CC); ν (CN)

Where ν, δ, β, ϱ, and ω indicate stretching, bending, deformation, rocking, and wagging, respectively; sciss, oph, as, s, and ip stand for scissoring, out of phase, asymmetric, symmetric, and in plane vibrations.

Table S10. Deconvolution of ATR-FTIR spectra of biogenic SeNP extracts and OM in the 1500-950 cm^{-1} region.

Bio SeNP extract	w	A	OM	w	A	Bio SeNP extract_w	w	A	Vibrational mode
1464	14.59	1.263	1468	7.498	0.624	1464	21.87	3.420	δ (CH_2); δ (CH_3)
			1457	14.99	2.491				β_{sciss} (CH_2); δ_{as} (CH_3); $\varrho_{as(oph)}$ (CH); δ (OH); ν CC(O)
1448	24.84	4.015	1441	15.65	1.778	1438	41.79	16.19	δ (OH); ν CC(O)
1416	22.36	1.205	1418	21.19	1.140				ν_s (COO^-)
1385	36.38	6.738	1385	36.40	6.969	1386	52.58	12.55	δ (CH); δ (OH); δ (COH); β (CH_3); ν (CN)
1342	18.11	0.402	1339	23.07	1.023	1333	21.58	0.777	β C(OH); δ (OH); δ (CH)
1296	61.55	8.045	1302	38.94	5.022	1304	46.08	4.393	ω (CH_2); $\varrho_{as(oph)}$ (CH); ν (COC); ν (CCO); δ (OH)
1260	16.38	0.395	1264	30.58	4.070				ν (CO); δ (S)OH
						1242	44.49	4.208	β (NH); ν_{as} (PO_2^-)
1229	44.80	10.08	1233	30.75	4.293				ν CO(H) δ (COH); ν (CO); ν_{as} (PO_2^-); ν (CN); δ (S)OH; δ (CH_2)
1226	60.58	2.126							ν CO(H) δ (COH); ν (CO); ν_{as} (PO_2^-); ν (CN); δ (S)OH; δ (CH_2)
			1211	55.61	8.460				ν (CO); δ (CH_2); δ (CH); δ (OH)
			1166	24.27	2.758				ν (CN); $\varrho_{as(oph)}$ (CH); ϱ (NH); ν (CO); δ (S)OH; δ (CH); ν (CC)
1153	55.17	11.09	1150	12.71	0.564	1152	51.15	9.825	ν_{as} (COC); δ (CH_2); δ (CH); δ (NH_2)
			1125	40.63	9.824				δ_{ip} (OH)
1115	30.06	4.358							ϱ (CNH_3); ω (CH_2); ν_{as} (PO_2^-)
1098	18.85	1.602	1098	22.96	3.732	1103	37.22	8.934	ν_{as} (COC); ν (CC); ν (CO); δ (COH); ν $P(OH)_2$
1065	49.97	23.56	1069	31.27	6.810	1076	25.31	4.550	ν (CO); ν (CC); ν (COH); δ (COC); ϱ (NH_3^+); ν (SO); ν_s (PO_2^-)
			1040	58.44	29.24	1047	50.59	26.58	ν (PO); ν (SH); ν (SO)
1024	44.07	13.31							ν (POC)
975	26.12	2.751	974	21.58	1.949	984	39.18	2.902	δ (NH_2); δ (HNCC); ν (CO); ν_s (PO_2^-); ν (CO); ν (CC)

Where ν, δ, β, ϱ, and ω indicate stretching, bending, deformation, rocking, and wagging, respectively; sciss, oph, as, s, and ip stand for scissoring, out of phase, asymmetric, symmetric, and in plane vibrations.

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