

Supporting Information

Array-based specific classification of bacterial species via hydrophilic/hydrophobic biosensors

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1. Chemical structure of ligands

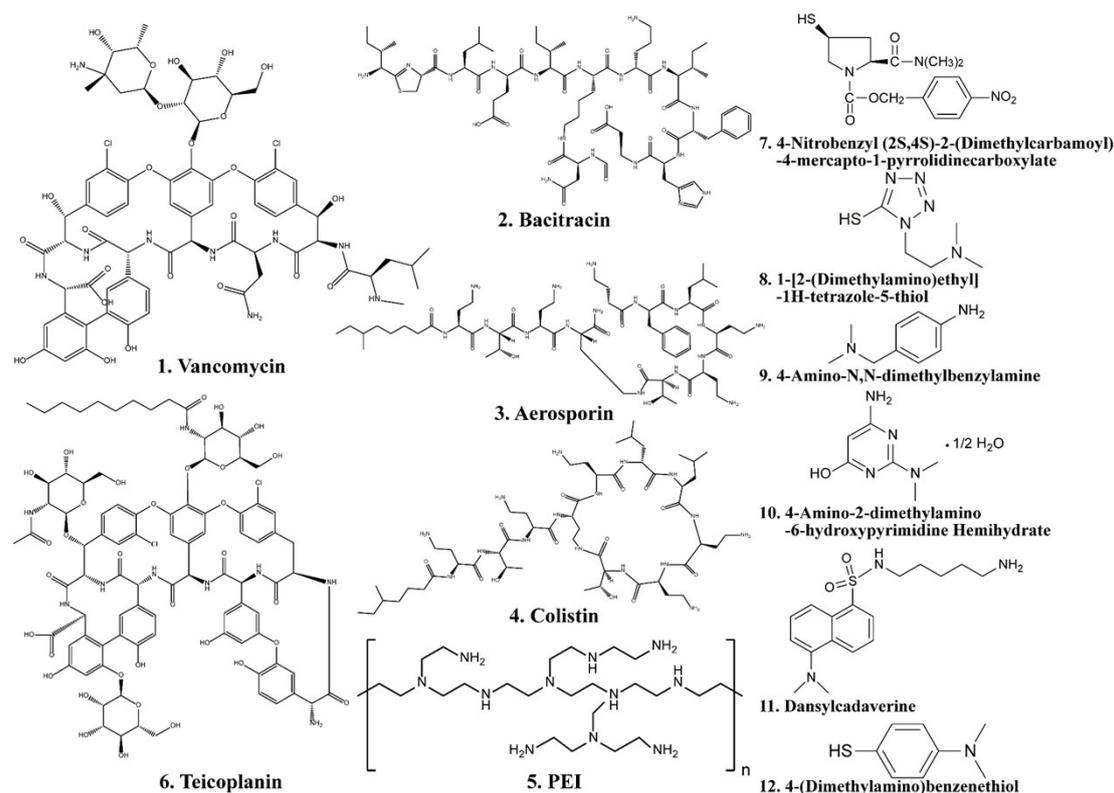


Figure S1. Chemical structure of the 12 ligands.

2. Detailed information of the ligands

Table S1. Detailed chemical information of the 12 ligands.

No	Compound	CAS number	Molecular mass	Molecular formula	logP*	Name of synthesized AuNCs [#]
1	Vancomycin	1404-93-9	1485.71	C ₆₆ H ₇₆ Cl ₃ N ₉ O ₂₄	-1.44	Vanco@AuNCs
2	Bacitracin	1405-87-4	1422.69	C ₆₆ H ₁₀₃ N ₁₇ O ₁₆ S	-2.21	Bacit@AuNCs
3	Aerosporin (Polymyxin B)	1405-20-5	1301.6	C ₅₆ H ₁₀₀ N ₁₆ O ₁₇ S	-3.4	Acros@AuNCs
4	Colistin (Polymyxin E)	1264-72-8	1155.43	C ₅₂ H ₉₈ N ₁₆ O ₁₃	-3.68	Colistin@AuNCs
5	PEI (Polyethylenimine)	9002-98-6	~1800	(CH ₂ CH ₂ NH) _n	-5.41	PEI@AuNCs
6	Teicoplanin	61036-62-2	1709.39	C ₈₈ H ₉₇ Cl ₂ N ₉ O ₃₃	0.4	Teico@AuNCs
7	4-Nitrobenzyl (2S,4S)-2-(Dimethylcarbamoyl)-4-mercapto-1-pyrrolidinecarboxylate	96034-64-9	353.39	C ₁₅ H ₁₉ N ₃ O ₅ S	0.5	DMC-P@AuNCs
8	1-[2-(Dimethylamino)ethyl]-1H-tetrazole-5-thiol	61607-68-9	173.24	C ₅ H ₁₁ N ₃ S	0.28	DMAE-T@AuNCs
9	4-Amino-N,N-dimethylbenzylamine	6406-74-2	150.2	C ₉ H ₁₄ N ₂	0.7	DMA-BA@AuNCs
10	4-Amino-2-dimethylamino-6-hydroxypyrimidine Hemihydrate	76750-84-0	154.17	C ₆ H ₁₀ N ₄ O	-1.54	DMA-HP@AuNCs
11	Dansylcadaverine (N-(Dimethyl-amino-naphthalene-sulfonyl)-1,5-pentane-diamine)	10121-91-2	335.46	C ₁₇ H ₂₅ N ₃ O ₂ S	2.83	DMA-N@AuNCs
12	4-(Dimethylamino)benzenethiol	4946-22-9	153.24	C ₈ H ₁₁ NS	2.63	DMA-BT@AuNCs

*Predicted data is generated using the ACD/Labs Percepta Platform-PhysChem Module.

[#]The hydrophilic ligands were designated by a few letters or abbreviations of the chemical name; the hydrophobic ligands were denoted by utilizing the abbreviation for the dimethylamino group attached to the chemical scaffold.

3. Detailed information of the bacteria

Table S2. Detailed information of the 17 kinds of bacteria.

No	Name of bacteria	Abbreviation	Gram species	Strains	Zeta potential
1	<i>Staphylococcus aureus</i> 1	<i>S. aureus</i> 1	positive		-28.34±0.79
2	<i>Staphylococcus aureus</i> 2	<i>S. aureus</i> 2	positive		-33.30±0.73
3	<i>Staphylococcus aureus</i> 3	<i>S. aureus</i> 3	positive		-29.67±0.52
4	Methicillin-resistant <i>Staphylococcus aureus</i>	MRSA	positive		-28.58±1.21
5	<i>Listeria monocytogenes</i>	<i>L. monocytogenes</i>	positive		-30.74±0.78
6	<i>Enterococcus faecalis</i>	<i>E. faecalis</i>	positive		-33.76±0.50
7	<i>Bacillus subtilis</i>	<i>B. subtilis</i>	positive		-28.84±1.56
8	<i>Streptococcus mutans</i>	<i>S. mutans</i>	positive		-30.16±1.41
9	<i>Escherichia coli</i>	<i>E. coli</i>	negative		-31.50±1.75
10	<i>Escherichia coli</i>	<i>E. coli</i> 1	negative	CMCC(B)44102	-35.00±1.02
11	<i>Escherichia coli</i> BL21	<i>E. coli</i> BL21	negative	BL21	-27.99±0.86
12	<i>Pseudomonas aeruginosa</i>	<i>P. aeruginosa</i>	negative		-30.33±0.70
13	<i>Pseudomonas fluorescens</i>	<i>P. fluorescens</i>	negative		-30.32±0.97
14	<i>Salmonella paratyphi</i> B	<i>S. paratyphi</i> B	negative		-9.38±0.57
15	<i>Shigella flexneri</i>	<i>Sh. flexneri</i>	negative		-19.10±0.32
16	<i>Enterobacter sakazakii</i>	<i>E. sakazakii</i>	negative		-22.80±1.73
17	<i>Enterobacter cloacae</i>	<i>E. cloacae</i>	negative		-24.67±1.33

4. The dosage of various ligands in the synthesis process of AuNCs

Table S3. Detailed dosage of each compound

Compound	Volume (μL)	Concentration
HAuCl ₄ solution	435	24 mM
GSH aqueous solution	150	100 mM
Ultrapure water	4415	-
Vancomycin	200	1% w/w
Bacitracin	200	1% w/w
Aerosporin (Polymyxin B)	200	1% w/w
Colistin (Polymyxin E)	200	1% w/w
PEI (Polyethyleneimine)	100	1% w/w
4-Nitrobenzyl (2S,4S)-2-(Dimethylcarbamoyl)-4-mercapto-1-pyrrolidinecarboxylate	30	100 mM
1-[2-(Dimethylamino)ethyl]-1H-tetrazole-5-thiol	15	100 mM
4-Amino-N,N-dimethylbenzylamine	30	100 mM
4-Amino-2-dimethylamino-6-hydroxypyrimidine Hemihydrate	30	100 mM
Dansylcadaverine (N-(Dimethyl-amino-naphthalene-sulfonyl)-1,5-pentane-diamine)	75	100 mM
4-(Dimethylamino)benzenethiol	10	100 mM

5. Characterization of AuNCs

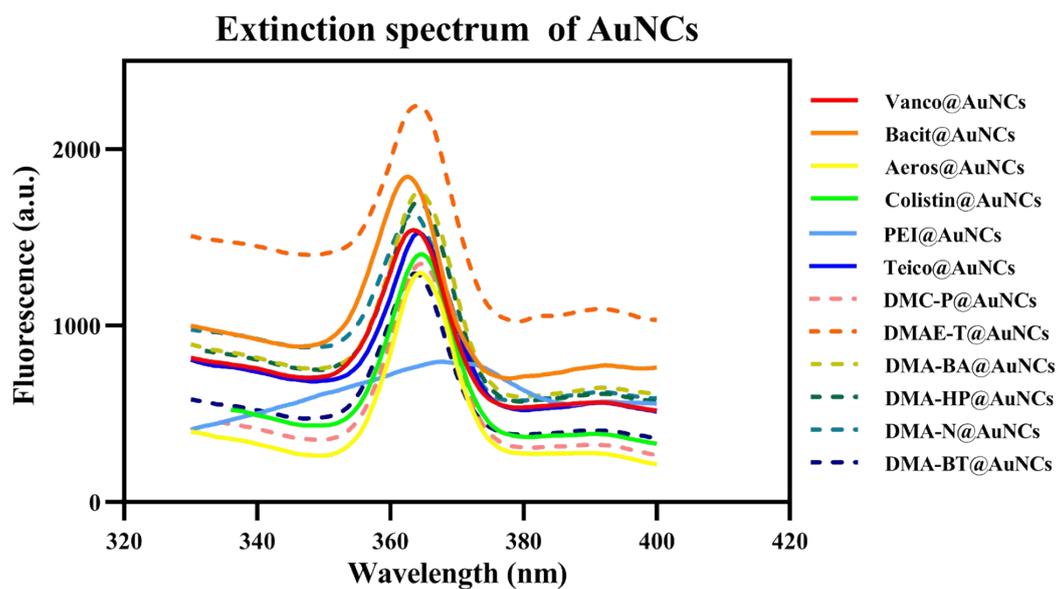


Figure S2. Extinction spectrum of AuNCs with hydrophilic and hydrophobic ligands, respectively.

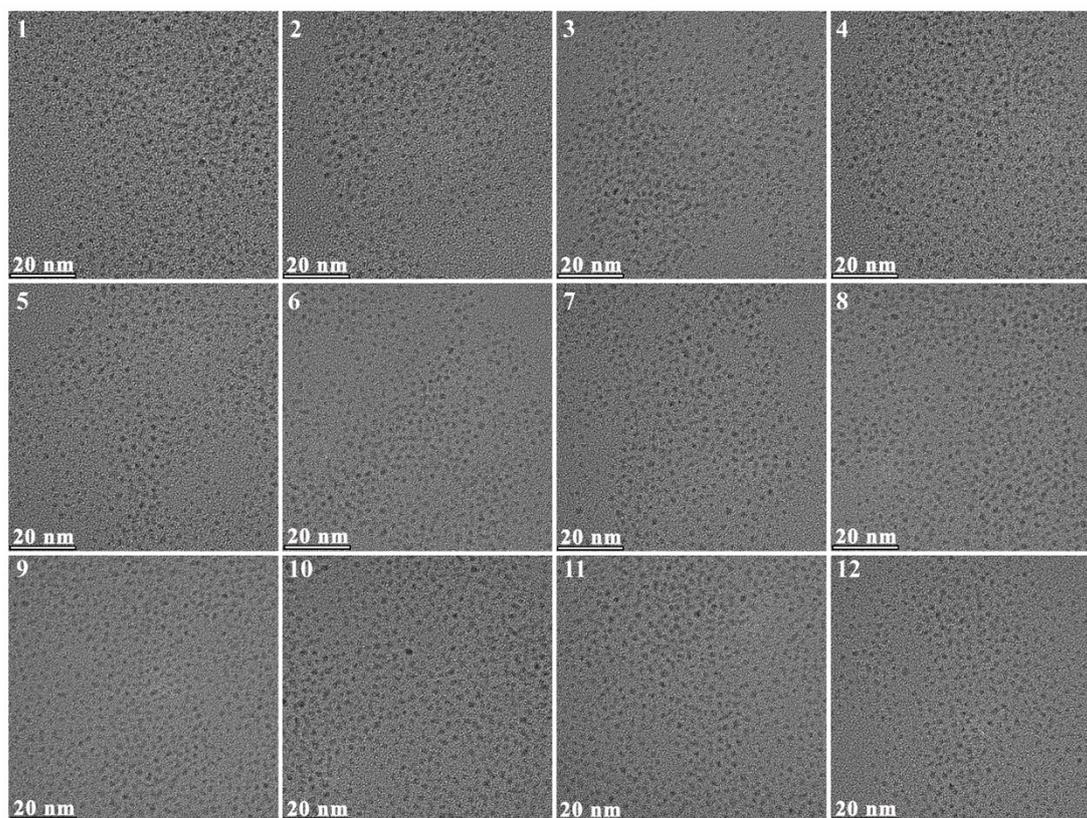


Figure S3. TEM imaging of the synthesized AuNCs

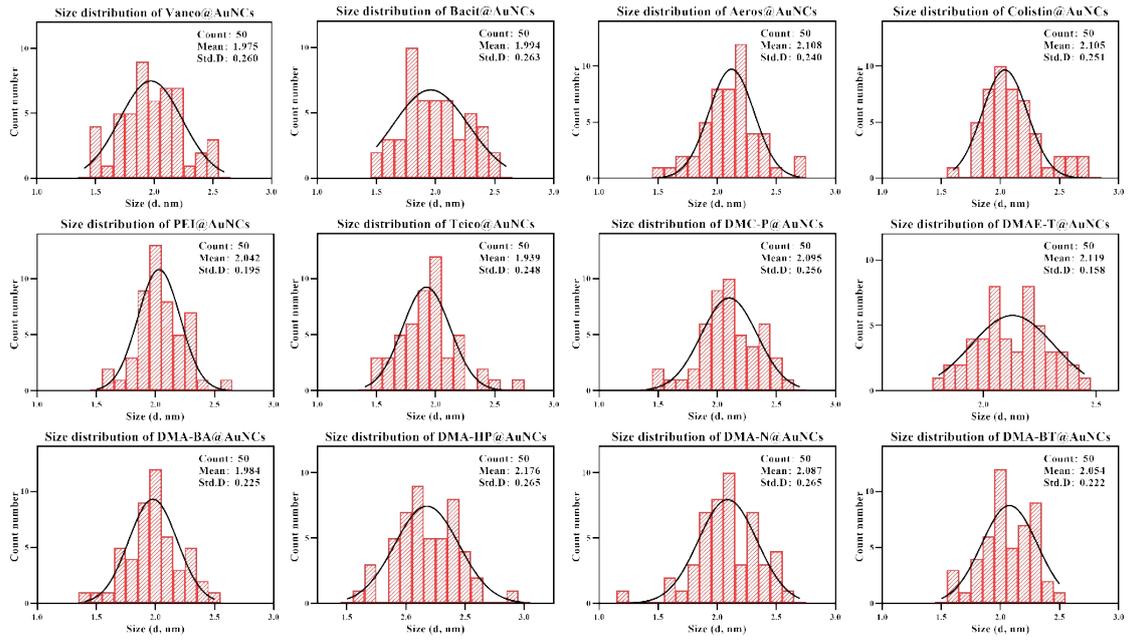


Figure S4. Size distribution of the AuNCs.

6. Fluorescent response patterns

Table S4. Fluorescent response patterns of training set in the detection of bacterial samples in water.

	Vanco@AuNCs	Bacitr@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Teico@AuNCs	DMC-P@AuNCs	DMAL-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
<i>S. aureus</i> 1	2.588	-2.037	-1.217	-11.076	-1.609	3.958	18.047	-7.400	-9.582	-1.552	-17.292	1.575
<i>S. aureus</i> 1	2.475	-0.895	-2.089	-7.574	-2.992	2.703	17.473	7.878	-14.038	10.870	-8.568	-2.731
<i>S. aureus</i> 1	2.129	-1.441	-2.868	-11.364	-1.710	1.601	17.892	-4.211	-11.244	-3.959	-13.827	-0.528
<i>S. aureus</i> 1	2.661	-1.590	-2.268	-10.453	-1.769	2.727	18.648	2.029	-7.556	-0.423	-12.038	0.611
<i>S. aureus</i> 1	1.164	-0.543	-1.992	-10.107	-0.835	2.432	17.456	3.583	0.838	10.645	-6.864	0.409
<i>S. aureus</i> 1	1.904	-3.744	-2.432	-11.499	-0.173	2.243	17.715	5.542	-10.077	-2.093	-9.425	-1.380
<i>S. aureus</i> 2	2.484	-1.353	-2.093	-5.477	-3.340	4.580	-6.424	2.515	3.310	1.126	2.417	-4.697
<i>S. aureus</i> 2	2.174	-2.290	-5.019	-7.201	-4.841	3.677	-10.628	-7.551	-12.011	-8.398	-4.870	-10.797
<i>S. aureus</i> 2	1.948	-2.390	-4.764	-6.198	-3.929	4.402	-7.839	7.982	2.782	0.497	3.243	-11.250
<i>S. aureus</i> 2	3.160	-2.763	-3.879	-4.724	-1.601	5.067	-3.000	0.608	-0.465	0.241	9.193	-2.255
<i>S. aureus</i> 2	1.358	-3.189	-5.135	-7.714	-3.587	3.794	-6.997	-6.720	-6.512	-6.174	-0.713	0.307
<i>S. aureus</i> 2	1.638	-2.347	-3.961	-7.544	-2.189	4.397	-6.122	6.840	5.471	5.726	4.977	-2.286
<i>S. aureus</i> 3	-7.198	-3.670	-4.917	-15.351	-2.174	2.817	3.359	-3.869	-7.542	-35.229	2.707	-9.833
<i>S. aureus</i> 3	-5.865	-4.626	-4.217	-13.109	-3.224	2.555	4.731	4.263	10.096	-24.083	4.519	-7.387
<i>S. aureus</i> 3	-7.636	-3.414	-5.580	-16.476	-3.339	2.460	2.001	-4.236	-6.604	-43.923	-2.720	-10.639
<i>S. aureus</i> 3	-7.543	-5.174	-5.403	-13.903	-2.492	3.774	1.412	-2.156	-2.684	-28.690	3.233	-2.985
<i>S. aureus</i> 3	-4.125	-4.443	-5.724	-12.500	-3.087	3.177	3.707	2.865	1.992	-14.535	6.166	-3.355
<i>S. aureus</i> 3	-7.730	-4.711	-5.604	-15.124	-2.918	2.174	0.170	-6.397	-4.887	-31.653	-0.842	1.665
MRSA	-0.158	-8.271	-6.727	-12.405	-6.392	2.081	1.818	8.144	-11.273	-0.086	-7.120	0.140
MRSA	0.267	-12.552	-5.718	-17.112	-7.229	2.071	0.231	0.857	-10.571	-20.304	-7.634	-7.077
MRSA	0.977	-9.866	-5.290	-12.102	-5.587	2.090	-0.662	8.482	-11.435	-4.430	-2.292	-0.705
MRSA	0.380	-10.219	-3.726	-10.840	-7.970	2.658	2.321	6.091	4.492	-6.197	-0.524	-1.081
MRSA	-0.937	-12.406	-6.834	-16.520	-7.043	2.418	-2.455	1.482	-5.085	-22.096	-0.425	0.477
MRSA	-0.382	-9.180	-6.623	-12.052	-5.749	2.253	-0.652	3.842	-4.460	-7.302	-1.095	-1.926
<i>L. monocytogenes</i>	-0.157	-18.178	-7.341	-9.585	-6.692	1.433	-5.668	4.655	-11.912	-12.298	-12.148	0.211
<i>L. monocytogenes</i>	-0.880	-15.425	-8.720	-8.859	-8.552	0.279	-2.064	11.326	-5.372	2.782	-5.277	-3.705
<i>L. monocytogenes</i>	-0.566	-20.152	-9.612	-9.490	-9.718	1.529	-5.658	-1.034	-16.224	-15.357	-11.023	-1.137
<i>L. monocytogenes</i>	-0.165	-20.285	-8.310	-9.916	-4.837	1.954	-1.450	8.265	-4.438	-11.346	-5.858	4.017
<i>L. monocytogenes</i>	1.814	-21.750	-5.831	-9.804	-7.357	0.271	0.853	6.526	3.706	5.630	-3.726	3.210
<i>L. monocytogenes</i>	-0.950	-17.416	-9.309	-9.933	-7.784	1.108	-2.121	2.522	-2.073	-12.651	-6.374	5.630
<i>E. faecalis</i>	1.168	-29.248	-4.616	-32.002	-8.837	0.247	9.838	12.789	-0.987	9.152	2.043	-6.859
<i>E. faecalis</i>	-2.897	-28.047	-7.792	-37.677	-3.353	1.330	8.713	-1.844	-14.295	-2.200	-11.812	-0.319
<i>E. faecalis</i>	0.389	-28.490	-4.010	-34.574	-2.264	-0.779	10.789	-1.426	0.293	9.662	-6.073	-7.038
<i>E. faecalis</i>	-1.902	-24.347	-6.623	-31.732	-3.337	-0.155	7.293	10.530	3.265	6.247	1.327	1.269
<i>E. faecalis</i>	-2.475	-28.263	-6.385	-37.779	-1.825	0.769	4.062	5.797	-6.540	5.158	-6.213	1.460
<i>E. faecalis</i>	0.094	-30.236	-2.589	-31.412	-3.013	-0.694	5.710	4.733	-1.046	9.718	1.532	0.814
<i>B. subtilis</i>	-10.456	-14.486	-15.839	-17.595	-4.705	1.020	-18.234	-4.565	-12.698	-33.111	-3.884	-8.744
<i>B. subtilis</i>	-7.862	-16.813	-16.250	-15.636	-3.502	1.068	-23.694	1.878	-10.895	-24.144	-2.765	-7.929
<i>B. subtilis</i>	-10.403	-20.121	-15.693	-20.119	-3.468	2.863	-17.676	2.074	-17.375	-37.277	-6.218	-11.084
<i>B. subtilis</i>	-9.515	-15.381	-16.400	-16.411	-4.064	0.945	-8.706	2.412	-5.766	-23.307	1.905	0.925
<i>B. subtilis</i>	-10.943	-12.944	-15.889	-16.633	-4.185	1.184	-6.076	7.481	-4.252	-18.670	3.404	-0.978
<i>B. subtilis</i>	-10.526	-18.482	-15.507	-16.263	-3.051	1.960	-9.422	4.480	-8.507	-26.530	3.210	-1.852
<i>S. mutans</i>	-18.978	-11.298	-6.933	-48.914	-15.423	-3.392	-15.033	-14.633	-6.057	-24.021	-2.504	-30.311
<i>S. mutans</i>	-20.227	-10.487	-9.245	-38.156	-16.470	-1.958	-3.698	-10.037	-3.576	-20.029	-2.645	-10.465
<i>S. mutans</i>	-20.592	-9.696	-9.395	-38.602	-14.917	-4.121	-18.789	-7.643	-11.365	-28.459	-5.491	-31.053
<i>S. mutans</i>	-15.362	-12.007	-6.087	-34.647	-15.509	-2.938	-2.071	-4.036	-3.577	-17.183	0.266	-12.423
<i>S. mutans</i>	-20.703	-12.514	-9.309	-39.800	-14.375	-3.209	-4.988	-12.789	-5.097	-27.059	-4.180	-16.371
<i>S. mutans</i>	-21.138	-8.294	-8.989	-39.669	-14.875	-3.429	-1.507	-10.076	-0.702	-16.624	-0.549	-14.805
<i>E. coli</i>	-50.363	-35.119	-41.424	-37.835	-21.518	-8.396	1.031	20.702	1.338	14.792	7.135	2.774
<i>E. coli</i>	-50.447	-46.966	-45.817	-48.829	-20.334	-5.983	1.286	13.050	-6.634	6.112	4.467	1.409
<i>E. coli</i>	-47.801	-39.677	-40.908	-35.695	-19.701	-8.108	4.018	21.510	2.237	14.176	5.227	2.041
<i>E. coli</i>	-43.363	-35.259	-34.264	-34.241	-18.938	-7.786	5.562	22.625	2.359	13.437	6.308	3.895
<i>E. coli</i>	-46.431	-45.087	-43.981	-44.261	-17.792	-7.982	1.670	16.350	-8.767	6.477	7.195	5.114
<i>E. coli</i>	-49.548	-34.532	-40.144	-34.538	-17.823	-8.415	2.411	20.461	0.624	13.440	7.714	2.619
<i>E. coli</i> 1	-84.446	-49.822	-26.488	-29.268	-16.191	-7.355	0.655	1.062	-3.058	-5.583	-30.284	0.333
<i>E. coli</i> 1	-80.221	-40.104	-25.413	-26.972	-16.306	-7.822	1.516	6.409	-2.450	1.522	-24.337	5.473
<i>E. coli</i> 1	-85.118	-50.536	-29.168	-28.385	-16.753	-4.805	0.546	0.198	-2.526	-5.084	-28.989	-1.578
<i>E. coli</i> 1	-84.002	-47.667	-27.419	-28.316	-14.040	-5.514	0.380	0.251	-0.390	-0.203	-25.082	2.240
<i>E. coli</i> 1	-75.801	-40.998	-22.253	-26.426	-14.941	-7.095	3.154	4.569	1.783	2.827	-21.793	3.098
<i>E. coli</i> 1	-83.223	-45.492	-29.123	-30.151	-15.567	-7.267	1.220	10.153	-1.389	1.818	-27.852	2.169
<i>E. coli</i> BL21	-11.629	-34.707	-33.466	-18.805	-20.757	-7.555	-0.073	-1.640	-0.899	-1.303	2.091	-5.162
<i>E. coli</i> BL21	-18.313	-42.187	-37.273	-28.041	-20.634	-39.361	-5.466	1.912	-4.755	-11.772	-1.321	3.704
<i>E. coli</i> BL21	-14.084	-35.036	-31.057	-21.272	-19.825	-45.679	-4.406	9.604	-3.944	-1.728	1.057	-7.399
<i>E. coli</i> BL21	-16.851	-31.097	-31.512	-14.056	-14.712	-44.133	-1.129	7.986	-1.813	0.188	2.563	1.885
<i>E. coli</i> BL21	-16.592	-38.961	-34.511	-28.038	-14.097	-38.243	-4.061	5.002	-3.113	-12.316	-0.849	0.861
<i>E. coli</i> BL21	-11.527	-32.462	-32.238	-21.564	-15.424	-44.970	1.096	4.242	-0.128	-1.471	0.668	-4.310
<i>P. aeruginosa</i>	-17.497	-37.843	-26.254	-35.765	-22.134	-19.363	-10.829	-23.496	-2.740	-12.271	0.342	-6.723
<i>P. aeruginosa</i>	-30.400	-37.739	-23.146	-37.222	-23.254	-20.716	-4.291	-11.832	2.066	-10.730	-0.518	-13.622
<i>P. aeruginosa</i>	-20.840	-36.121	-26.560	-31.379	-22.301	-17.085	-10.892	-13.051	-3.947	-20.426	-0.500	3.019
<i>P. aeruginosa</i>	-15.973	-39.789	-23.021	-35.897	-19.547	-16.504	-6.864	-15.945	-0.110	-10.577	1.560	1.290
<i>P. aeruginosa</i>	-21.185	-33.905	-21.865	-37.007	-19.587	-20.084	-8.326	-5.574	0.827	-18.489	0.970	1.937
<i>P. aeruginosa</i>	-17.039	-33.994	-24.866	-32.043	-18.738	-20.379	-7.650	-22.279	-0.997	-16.662	1.240	-3.626
<i>P. fluorescens</i>	-49.242	-37.650	-16.952	-28.484	-33.337	-3.016	0.832	11.240	-3.454	-4.758	5.970	5.869
<i>P. fluorescens</i>	-52.548	-40.396	-20.108	-33.148	-31.690	-3.189	-1.322	0.960	-5.700	-13.621	4.711	4.298
<i>P. fluorescens</i>	-50.857	-34.410	-23.472	-30.421	-30.348	-3.629	3.127	7.953	-2.253	-6.565	5.858	3.413
<i>P. fluorescens</i>	-43.667	-34.681	-20.294	-24.456	-27.481	-2.221	3.447	6.534	0.687	-7.188	7.504	5.157
<i>P. fluorescens</i>	-48.439	-40.500	-20.745	-28.084	-27.595	-1.958	-0.376	4.077	-2.570	-21.813	5.792	6.615
<i>P. fluorescens</i>	-46.385	-35.830	-17.286	-27.358	-26.134	-3.027	0.614	8.523	-3.879	-8.744	6.531	5.546
<i>S. paratyphi</i> B	-20.095	-19.023	-9.639	-29.369	-16.424	-8.725	-0.238	0.444	-2.675	-27.469	5.539	-0.509
<i>S. paratyphi</i> B	-19.100	-17.857	-7.269	-27.666	-13.556	-12.083	1.042	6.317	-3.320	-14.078	5.790	-1.101
<i>S. paratyphi</i> B	-20.561	-19.133	-10.874	-31.395	-13.291	-8.242	-0.210	-7.266	-5.122	-30.432	5.556	0.729
<i>S. paratyphi</i> B	-19.356	-18.315	-13.386	-27.502	-8.202	-11.404	1.954	-4.731	-2.488	-36.786	5.810	3.424
<i>S. paratyphi</i> B	-21.514	-14.403	-7.448	-24.757	-8.307	-12.871	3.576	4.235	2.211	-13.686	8.168	3.143
<i>S. paratyphi</i> B	-19.636	-19.071	-9.145	-29.610	-9.274	-8.501	0.676	-1.250	-0.096	-32.817	5.447	3.661
<i>Sh. flexneri</i>	-20.011	-29.255	-17.428	-23.001	-13.236	-45.471	-5.3					

Table S5. Fluorescent response patterns of training set in the detection of bacterial samples in serum.

	Vanco@AuNCs	Bacit@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Tsico@AuNCs	DMC-P@AuNCs	DMAL-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
<i>S. aureus</i> 1	-37.301	1.519	-9.709	-12.746	-10.812	1.801	-0.791	-1.389	-53.070	-8.139	3.397	-3.160
<i>S. aureus</i> 1	-38.141	1.165	-9.186	-11.973	-10.250	2.451	0.706	-0.882	-48.662	-6.925	2.779	-0.923
<i>S. aureus</i> 1	-34.569	2.925	-2.832	-6.473	-10.377	2.162	-0.022	0.978	-34.594	-2.827	-1.631	-1.179
<i>S. aureus</i> 1	-37.719	2.483	-10.716	-14.773	-10.134	2.767	1.019	-1.193	-49.335	-7.163	-5.680	-0.489
<i>S. aureus</i> 1	-37.181	1.566	-10.819	-11.818	-9.924	3.493	-0.061	-0.227	-41.681	-6.594	-4.791	-1.329
<i>S. aureus</i> 1	-37.775	5.635	-4.623	-5.641	-10.376	3.525	2.000	1.464	-34.166	-2.824	-2.595	-0.807
<i>S. aureus</i> 2	-44.603	4.387	-4.651	-6.619	-3.217	6.124	-2.515	-2.288	-45.014	1.211	-5.498	-4.055
<i>S. aureus</i> 2	-43.797	4.539	-3.895	-5.651	-2.594	6.785	-0.106	-0.045	-38.306	2.147	-4.407	-0.382
<i>S. aureus</i> 2	-46.606	2.703	-7.899	-5.738	-2.662	6.597	-1.027	-2.091	-42.871	-5.612	-5.667	-0.609
<i>S. aureus</i> 2	-43.174	3.586	-4.620	-5.543	-2.558	6.650	-0.220	0.062	-39.798	1.849	-4.329	-0.568
<i>S. aureus</i> 2	-40.989	5.015	-5.836	-3.985	-2.600	7.789	0.868	-1.041	-36.766	1.223	-4.588	0.575
<i>S. aureus</i> 2	-43.643	4.427	-7.373	-3.791	-2.752	7.707	0.084	-2.829	-39.284	-5.367	-5.158	0.453
<i>S. aureus</i> 3	-32.771	3.640	-9.357	-7.197	-4.292	4.980	-2.059	-4.381	-36.830	-6.838	-5.210	-1.880
<i>S. aureus</i> 3	-32.466	3.777	-8.851	-6.625	-4.284	5.168	-0.507	-2.588	-33.799	-5.515	-4.594	-0.543
<i>S. aureus</i> 3	-32.823	5.405	-0.983	-5.179	-4.500	4.808	-0.019	-0.881	-27.870	-0.115	-2.464	-0.796
<i>S. aureus</i> 3	-33.366	2.701	-9.639	-6.768	-3.969	4.808	-0.543	-1.637	-33.837	-4.983	-4.638	-0.862
<i>S. aureus</i> 3	-33.658	2.835	-6.944	-6.144	-4.106	6.371	-0.187	-1.611	-33.010	-4.486	-5.298	0.231
<i>S. aureus</i> 3	-32.255	4.876	-2.632	-3.704	-3.968	5.847	-0.083	0.361	-28.613	-0.201	-2.802	-0.584
MRSA	-34.304	5.941	0.479	-4.806	-7.458	4.929	-2.935	1.036	-43.487	-6.208	-3.899	-5.736
MRSA	-34.946	6.020	-0.463	-5.263	-7.239	5.527	-2.083	2.690	-37.777	-4.067	-2.702	-3.381
MRSA	-38.136	3.030	-8.428	-9.115	-7.425	5.119	-2.604	-1.129	-40.749	-6.764	-7.254	-2.810
MRSA	-39.036	6.289	0.535	-6.909	-7.364	5.382	-1.489	1.674	-36.448	-5.326	-3.244	-3.811
MRSA	-37.000	5.743	0.382	-6.003	-7.246	6.164	-0.656	2.505	-38.036	-3.506	-3.769	-2.988
MRSA	-38.802	1.960	-6.597	-7.929	-7.015	6.488	-1.956	0.027	-40.260	-6.324	-6.050	-3.469
<i>L. monocytogenes</i>	-47.312	0.396	-8.855	-10.938	-4.838	5.981	-1.513	-4.952	-47.914	-6.451	-10.734	-3.327
<i>L. monocytogenes</i>	-45.754	0.218	-8.164	-10.599	-4.475	6.740	1.467	-2.247	-42.997	-5.959	-8.365	-1.734
<i>L. monocytogenes</i>	-45.304	5.450	-4.931	-3.891	-4.566	6.048	2.549	-0.107	-36.778	-0.537	-7.096	-1.250
<i>L. monocytogenes</i>	-46.154	1.574	-9.626	-9.666	-4.846	6.096	1.299	-2.456	-43.823	-5.334	-9.271	-2.007
<i>L. monocytogenes</i>	-43.413	1.131	-8.177	-7.945	-4.434	7.421	1.460	-3.204	-41.568	-5.839	-7.800	-0.550
<i>L. monocytogenes</i>	-45.498	5.306	-3.178	-5.825	-4.543	7.389	3.174	-1.692	-32.527	-1.451	-7.128	-0.947
<i>E. faecalis</i>	-54.102	9.754	-5.748	-9.478	-5.780	8.460	-1.015	-7.117	-40.541	-4.396	-5.001	-5.524
<i>E. faecalis</i>	-51.646	9.575	-5.197	-8.442	-5.012	8.736	1.180	-3.233	-36.439	-3.595	-3.749	-1.598
<i>E. faecalis</i>	-51.413	5.108	-11.939	-8.457	-5.425	8.679	0.184	-4.005	-51.111	-5.366	-6.636	-2.275
<i>E. faecalis</i>	-50.704	9.365	-6.999	-8.425	-5.919	8.438	2.129	-3.974	-38.199	-3.604	-5.611	-2.226
<i>E. faecalis</i>	-47.672	8.863	-7.833	-5.905	-5.013	8.625	0.869	-3.326	-39.548	-2.765	-3.985	-0.939
<i>E. faecalis</i>	-48.701	4.385	-6.262	-5.055	-8.343	5.522	-5.063	-49.195	-4.458	-7.184	-0.386	-0.939
<i>B. subtilis</i>	-46.580	3.674	-11.081	-6.663	-7.210	6.317	-2.976	-5.440	-51.176	-6.817	-13.862	-2.420
<i>B. subtilis</i>	-45.194	3.635	-8.743	-5.720	-7.056	6.832	0.126	-2.794	-43.782	-5.178	-11.657	-0.056
<i>B. subtilis</i>	-43.960	6.520	-5.810	-5.021	-7.099	6.446	-0.338	-0.052	-39.104	0.502	-5.457	-0.848
<i>B. subtilis</i>	-44.670	2.042	-8.739	-7.279	-7.206	7.059	-0.360	-2.778	-41.822	-5.233	-11.977	-0.372
<i>B. subtilis</i>	-44.363	3.746	-6.660	-5.093	-6.882	7.757	0.323	-1.142	-41.380	-5.213	-9.643	-0.386
<i>B. subtilis</i>	-43.485	6.254	-6.161	-3.627	-6.792	7.272	-0.308	0.085	-39.781	0.229	-6.738	-0.317
<i>S. mutans</i>	-38.048	6.047	-7.592	-4.692	-4.430	5.664	4.030	2.171	-29.895	-7.912	-13.340	-9.314
<i>S. mutans</i>	-37.210	6.208	-6.798	-3.814	-4.344	6.579	4.656	2.698	-26.574	-2.005	-9.998	-3.137
<i>S. mutans</i>	-39.053	5.124	-9.041	-6.492	-4.254	6.241	3.897	2.112	-29.959	-9.105	-11.674	-3.801
<i>S. mutans</i>	-39.182	5.903	-6.554	-5.950	-4.171	6.495	4.202	2.758	-29.119	-2.386	-9.986	-3.668
<i>S. mutans</i>	-37.022	5.795	-5.421	-3.666	-4.181	7.541	4.655	2.440	-26.011	-3.585	-7.057	-2.015
<i>S. mutans</i>	-39.182	5.739	-7.574	-5.331	-4.282	7.500	3.885	2.297	-29.086	-9.263	-10.515	-1.373
<i>E. coli</i>	-38.721	5.856	-12.606	-6.443	-8.864	5.238	0.669	0.568	-35.124	-0.152	-5.357	-0.003
<i>E. coli</i>	-39.773	5.801	-10.921	-7.315	-8.405	5.480	0.807	1.297	-35.949	0.828	-5.183	0.371
<i>E. coli</i>	-44.188	5.721	-14.999	-9.015	-8.851	5.712	-0.505	-0.367	-42.824	-3.953	-4.796	-0.228
<i>E. coli</i>	-38.721	5.856	-12.606	-6.443	-8.819	5.238	0.696	1.304	-36.728	0.528	-5.105	0.304
<i>E. coli</i>	-35.869	7.008	-8.650	-3.503	-7.034	6.201	0.931	1.227	-38.319	-0.114	-4.835	0.713
<i>E. coli</i>	-43.256	6.479	-8.896	-3.578	-7.445	6.323	-0.678	-0.615	-41.569	-3.093	-5.738	0.928
<i>E. coli</i> 1	-65.582	-1.152	-10.963	-13.676	-5.351	2.537	21.977	0.055	-47.560	-9.497	-7.637	1.237
<i>E. coli</i> 1	-65.889	-1.918	-10.614	-14.738	-5.713	3.085	21.940	0.094	-45.316	-8.821	-6.654	1.639
<i>E. coli</i> 1	-63.462	-3.332	-3.689	-14.039	-6.053	1.916	21.799	4.962	-35.603	-7.894	-6.092	1.082
<i>E. coli</i> 1	-65.582	-1.152	-10.963	-13.676	-5.268	2.537	21.964	-0.212	-45.913	-9.022	-6.661	1.335
<i>E. coli</i> 1	-54.083	-0.774	-7.987	-8.392	-5.040	4.283	12.705	1.605	-44.784	-7.778	-5.887	1.177
<i>E. coli</i> 1	-53.559	-1.881	-4.245	-8.029	-4.842	4.510	12.782	3.875	-36.278	-6.152	-5.853	1.275
<i>E. coli</i> BL21	-67.422	-3.397	-9.990	-11.372	-7.191	4.824	8.143	6.138	-44.721	-1.205	-5.351	-2.229
<i>E. coli</i> BL21	-68.436	-1.969	-11.778	-10.369	-6.374	4.833	8.222	7.026	-43.231	-4.306	-4.306	-1.501
<i>E. coli</i> BL21	-67.169	-2.931	-12.581	-11.181	-6.924	4.590	7.728	4.726	-43.721	-5.253	-5.823	-2.356
<i>E. coli</i> BL21	-67.422	-3.397	-9.990	-11.372	-6.877	4.824	7.193	7.125	-42.419	-1.465	-5.045	-1.872
<i>E. coli</i> BL21	-56.611	0.394	-7.339	-6.638	-5.499	6.960	6.811	6.842	-40.601	-2.982	-3.991	-1.615
<i>E. coli</i> BL21	-55.880	0.018	-7.925	-6.224	-5.590	7.101	7.576	3.553	-42.152	-5.688	-5.256	-1.424
<i>P. aeruginosa</i>	-58.364	-0.251	-14.613	-9.767	-15.557	2.909	3.455	-6.001	-43.829	-7.946	-5.794	-6.948
<i>P. aeruginosa</i>	-57.067	-0.023	-14.824	-9.186	-15.334	1.954	3.866	-2.581	-40.637	-6.839	-5.140	-6.692
<i>P. aeruginosa</i>	-59.707	0.241	-14.892	-7.310	-15.375	1.832	4.034	-2.073	-37.221	-2.733	-5.224	-6.863
<i>P. aeruginosa</i>	-58.364	-0.251	-14.613	-9.767	-14.613	2.909	3.610	-3.307	-41.274	-6.247	-5.596	-6.066
<i>P. aeruginosa</i>	-47.551	0.758	-10.329	-5.084	-13.487	3.152	3.583	-2.978	-38.740	-5.312	-5.680	-6.008
<i>P. aeruginosa</i>	-48.255	0.674	-10.069	-4.909	-14.162	2.723	3.267	-0.249	-37.365	-2.880	-4.953	-6.044
<i>P. fluorescens</i>	-47.254	-1.345	-6.983	-12.062	-6.284	5.272	2.044	-2.373	-50.293	-4.614	-4.818	-1.841
<i>P. fluorescens</i>	-41.575	-2.648	-7.007	-12.384	-5.206	5.076	3.008	-2.902	-47.390	-3.403	-4.455	-0.621
<i>P. fluorescens</i>	-48.462	-4.590	-10.101	-11.870	-5.459	4.846	2.347	-2.441	-48.388	-14.829	-6.123	-0.553
<i>P. fluorescens</i>	-47.254	-1.345	-6.983	-12.062	-5.214	5.272	3.054	-3.255	-46.605	-3.419	-4.999	-0.823
<i>P. fluorescens</i>	-41.748	-0.981	-4.959	-8.217	-5.019	5.926	3.332	-2.523	-46.457	-4.392	-4.691	-0.061
<i>P. fluorescens</i>	-41.625	-4.614	-6.367	-8.329	-4.926	6.053	2.384	-1.781	-48.056	-14.281	-5.319	-0.264
<i>S. paratyphi</i> B	-57.801	-3.739	7.719	-11.041	-6.918	2.768	4.272	0.184	-48.398	-21.814	-9.124	-2.123
<i>S. paratyphi</i> B	-56.765	-5.036	8.100	-11.686	-6.384	2.843	4.170	0.507	-48.601	-18.305	-8.217	-0.254
<i>S. paratyphi</i> B	-51.109	-1.701	2.876	-11.510	-6.867	2.406	4.645	3.702	-36.879	-13.641	-6.143	-0.515
<i>S. paratyphi</i> B	-57.801	-3.739	7.719	-11.041	-6.068	2.768	4.398	0.197	-47.454	-17.379	-8.977	-0.281
<i>S. paratyphi</i> B	-50.302	-1.745	8.089	-7.245	-5.770	5.503	4.271	-0.521	-46.343	-18.092	-8.400	-0.135
<i>S. paratyphi</i> B	-50.547	1.886	3.403	-7.253	-6.341	5.149	3.880	3.285	-32.939	-13.107	-5.827	-0.355
<i>Sh. flexneri</i>	-56.899	3.815	-13.915	-11.756	-13.405	4.866	4.634	-3.763	-29.103	-6.699	-7.760	-2.660
<i>Sh. flexneri</i>	-61.865	4.358	-12.363	-11.802	-12.843	5.175	5.371	-3.173	-30.380	-3.053	-7.130	-0.50

Table S6. Fluorescent response patterns of training set in the detection of bacterial samples in urine.

	Vanco@AuNCs	Bacit@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Tcico@AuNCs	DMC-P@AuNCs	DMAL-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
<i>S. aureus</i> 1	-1.876	-0.822	-20.841	-7.605	1.545	-2.299	-1.143	-14.094	-10.485	-2.229	-4.256	-9.566
<i>S. aureus</i> 1	1.075	-0.200	-18.381	-5.764	2.507	2.497	1.299	-10.530	-5.913	2.117	-1.910	-4.408
<i>S. aureus</i> 1	3.148	1.046	-14.805	-3.928	1.658	0.902	1.530	-8.167	-6.009	3.092	-1.774	-4.611
<i>S. aureus</i> 1	0.292	-1.492	-19.644	-5.696	1.524	1.098	0.557	-11.720	-6.803	1.544	-2.244	-3.582
<i>S. aureus</i> 1	2.790	0.057	-14.940	-3.817	2.081	2.426	1.671	-8.899	-4.923	1.689	-1.011	-4.680
<i>S. aureus</i> 1	3.998	2.921	-12.582	-2.937	1.253	2.626	2.646	-9.063	-3.489	4.403	-1.887	-3.094
<i>S. aureus</i> 2	1.758	-0.471	-12.445	-3.867	-1.508	-11.926	0.956	-12.612	2.691	6.354	-1.970	-2.211
<i>S. aureus</i> 2	2.433	1.165	-7.735	-1.699	-1.086	-7.140	1.732	-7.320	6.630	6.463	-0.954	2.643
<i>S. aureus</i> 2	1.005	-2.820	-11.213	-4.075	-1.834	-6.362	-0.580	-10.714	3.866	2.938	-1.215	-0.156
<i>S. aureus</i> 2	4.876	-0.574	-9.387	-2.111	-2.430	-7.529	0.300	-9.672	6.514	6.057	-0.485	2.173
<i>S. aureus</i> 2	3.952	2.197	-9.096	-0.461	-2.415	-5.023	0.647	-7.500	6.437	5.248	0.951	3.504
<i>S. aureus</i> 2	2.843	0.037	-9.159	-2.974	-1.820	-5.027	-0.489	-11.417	5.800	2.440	-0.437	1.777
<i>S. aureus</i> 3	-2.010	-2.585	-2.499	-0.924	0.441	-0.307	0.584	-13.102	2.059	0.064	-2.099	-4.537
<i>S. aureus</i> 3	-0.397	-0.734	-1.388	1.477	0.700	0.627	1.585	-9.926	6.073	3.800	-0.024	-0.339
<i>S. aureus</i> 3	-0.748	0.477	2.050	1.492	-0.398	0.494	1.034	-7.392	7.922	3.391	0.232	-0.684
<i>S. aureus</i> 3	-0.436	-1.251	-0.629	0.515	0.450	0.271	0.873	-10.576	5.626	3.242	0.244	-0.457
<i>S. aureus</i> 3	1.921	2.069	0.715	1.362	0.704	2.543	1.689	-7.852	5.419	3.393	0.188	0.287
<i>S. aureus</i> 3	1.513	1.967	1.729	2.419	0.820	1.640	1.186	-4.534	6.281	4.312	0.763	-0.097
MRSA	-1.559	0.374	-1.588	-5.969	0.225	-3.279	-0.666	0.350	-10.853	1.130	-4.131	-3.895
MRSA	0.397	2.363	-1.136	-2.821	1.535	-1.534	3.419	1.408	-10.526	4.056	-1.894	-0.509
MRSA	-0.617	0.129	-3.563	-4.653	1.182	-1.770	2.076	-1.807	-20.640	2.830	-3.278	-1.538
MRSA	-0.056	1.124	-1.682	-5.160	0.730	-2.122	1.693	0.482	-9.948	3.538	-2.175	-0.707
MRSA	2.226	1.332	0.181	-3.465	0.536	-0.016	4.264	0.647	-7.069	4.657	-1.665	-0.132
MRSA	0.644	1.664	-2.733	-5.297	-0.013	-0.639	2.158	-0.648	-20.046	4.032	-2.713	-0.738
<i>L. monocytogenes</i>	-2.155	-0.439	-3.670	0.604	1.809	-0.733	-3.390	-2.618	0.422	2.407	-2.184	-2.461
<i>L. monocytogenes</i>	-0.684	2.069	-2.132	2.067	2.739	1.092	0.191	-1.320	2.980	3.935	-0.921	-1.875
<i>L. monocytogenes</i>	-0.278	1.964	-1.673	3.096	2.408	0.461	0.343	-1.185	3.805	4.197	-1.224	-1.520
<i>L. monocytogenes</i>	-1.260	0.852	-2.397	1.979	2.217	0.096	-0.103	-2.176	1.637	3.841	-2.643	-0.522
<i>L. monocytogenes</i>	0.423	1.619	0.025	2.775	2.250	2.359	1.035	-1.209	3.464	3.455	-0.403	-1.182
<i>L. monocytogenes</i>	1.270	1.946	1.198	2.832	2.657	0.923	0.352	-1.258	4.725	4.616	-0.486	-0.976
<i>E. faecalis</i>	-2.305	-0.336	-3.722	-0.526	-3.477	-0.064	-0.857	-0.404	3.650	5.334	-0.896	-3.534
<i>E. faecalis</i>	0.644	0.340	0.588	1.334	-3.320	1.975	1.297	-0.044	5.004	6.645	0.435	-0.580
<i>E. faecalis</i>	-2.365	0.178	-4.133	-0.635	-3.295	1.476	0.189	-0.306	2.089	4.400	-0.288	-1.550
<i>E. faecalis</i>	-0.503	0.467	-2.576	1.360	-3.205	1.477	0.701	0.938	4.427	6.487	-0.155	-0.918
<i>E. faecalis</i>	-0.740	1.978	-0.366	1.409	-3.831	2.826	1.157	2.724	4.248	6.741	0.754	-0.053
<i>E. faecalis</i>	-1.080	-0.976	-1.994	-0.726	-3.262	2.204	0.398	-0.845	3.666	5.401	-1.061	-0.547
<i>B. subtilis</i>	0.418	0.805	-6.131	-5.461	2.319	-0.722	2.421	-1.504	1.977	5.259	-2.925	3.598
<i>B. subtilis</i>	1.938	0.571	-3.520	-5.476	2.731	1.112	3.760	0.139	2.584	6.038	-1.094	5.112
<i>B. subtilis</i>	4.714	0.501	-0.956	-3.561	1.403	-0.021	2.517	1.844	3.399	7.048	-0.893	4.214
<i>B. subtilis</i>	1.373	0.447	-4.695	-5.514	2.071	1.057	2.957	-0.460	2.684	5.905	-1.833	4.762
<i>B. subtilis</i>	2.370	2.131	-5.014	-3.379	2.185	0.760	3.847	1.695	2.981	6.346	-0.330	4.062
<i>B. subtilis</i>	3.069	2.689	-2.435	-1.446	1.061	0.691	4.399	1.844	4.274	7.133	-1.455	4.695
<i>S. mutans</i>	2.380	-0.427	-5.131	-4.532	-1.622	1.826	2.244	-3.441	3.310	4.172	0.812	-2.025
<i>S. mutans</i>	1.886	2.378	-3.185	-6.631	-1.192	2.163	1.355	-1.189	4.439	6.061	2.699	0.721
<i>S. mutans</i>	1.233	-0.657	-9.605	-5.749	-1.605	0.465	0.736	-3.775	1.350	4.680	1.876	-0.777
<i>S. mutans</i>	1.395	1.783	-2.859	-4.676	-0.985	1.772	2.462	-1.174	4.087	5.964	2.162	0.268
<i>S. mutans</i>	3.572	2.130	-6.024	-1.653	-1.939	2.705	2.993	0.471	5.376	5.932	3.416	0.749
<i>S. mutans</i>	1.514	1.103	-9.084	-4.680	-1.666	1.432	1.243	-3.610	2.878	3.759	2.517	-0.510
<i>E. coli</i>	-0.113	0.691	-5.782	-1.771	-1.467	-5.434	4.811	7.054	2.595	5.936	-0.024	2.338
<i>E. coli</i>	-1.400	2.528	-5.866	0.113	-1.192	-4.817	6.265	5.559	4.233	6.787	-0.113	2.798
<i>E. coli</i>	-4.383	0.429	-7.053	-1.640	-0.157	-4.395	4.191	-0.457	0.418	4.023	-0.093	1.971
<i>E. coli</i>	-2.207	2.603	-5.395	-0.158	-1.552	-3.351	5.795	6.398	4.050	6.499	-0.299	2.361
<i>E. coli</i>	2.435	2.591	-3.980	1.694	-1.038	-2.653	5.812	3.272	4.041	6.515	-0.073	2.715
<i>E. coli</i>	-3.757	0.842	-4.797	0.249	-0.523	-2.957	3.573	-1.816	0.800	3.960	0.654	2.771
<i>E. coli</i> 1	-0.140	-0.708	-12.998	-8.221	2.175	-7.681	1.425	-3.632	-3.413	3.214	0.165	-1.514
<i>E. coli</i> 1	2.182	-0.330	-6.313	-3.653	2.309	-2.684	3.004	-5.232	-0.053	3.451	0.623	-0.401
<i>E. coli</i> 1	3.148	0.534	-4.822	-1.964	1.961	-4.713	3.027	3.932	2.379	5.219	0.455	-0.417
<i>E. coli</i> 1	0.874	-0.256	-7.111	-4.012	2.698	-4.406	2.213	-4.810	-0.020	3.050	0.177	0.159
<i>E. coli</i> 1	3.420	0.309	-4.613	-0.949	3.204	-1.495	2.732	-5.087	1.325	3.518	0.618	0.267
<i>E. coli</i> 1	3.614	1.072	-4.196	-0.052	4.057	-1.815	2.219	3.136	2.416	4.341	0.619	0.288
<i>E. coli</i> BL21	-4.902	-0.498	-3.760	-5.175	-2.549	-3.729	1.536	-2.217	0.120	4.433	-0.083	0.708
<i>E. coli</i> BL21	-2.411	-0.064	1.379	-1.238	-0.809	-0.241	1.744	1.760	1.313	5.099	0.786	1.386
<i>E. coli</i> BL21	-4.767	-1.756	-5.021	-3.785	-0.704	-0.471	0.605	-1.556	-2.043	3.761	0.184	1.505
<i>E. coli</i> BL21	-2.686	-0.003	-1.687	-1.695	-1.740	-0.716	2.940	3.418	0.444	4.243	-0.071	1.286
<i>E. coli</i> BL21	-0.865	0.726	0.406	-0.219	0.384	1.506	1.733	2.622	0.931	5.526	0.522	1.328
<i>E. coli</i> BL21	-2.844	0.223	-2.730	-1.741	-0.967	1.015	1.812	-1.250	-1.493	4.450	-0.555	0.661
<i>P. aeruginosa</i>	-4.497	-6.954	-3.623	-2.333	4.001	-6.852	-0.936	-4.696	2.946	6.168	1.126	-2.019
<i>P. aeruginosa</i>	0.485	-4.081	-0.607	2.211	2.989	-2.120	1.030	-1.965	4.127	6.710	2.911	-1.257
<i>P. aeruginosa</i>	0.099	-2.910	1.009	1.393	3.494	-2.752	2.008	-1.356	5.076	7.050	1.778	-1.386
<i>P. aeruginosa</i>	-0.420	-5.536	-0.408	1.710	3.635	-2.093	0.495	-2.560	3.773	6.071	1.973	-1.288
<i>P. aeruginosa</i>	2.227	-4.606	2.034	4.373	4.650	0.095	2.033	-1.192	4.790	7.419	2.947	-1.697
<i>P. aeruginosa</i>	3.894	-3.918	2.723	3.429	4.495	-0.442	2.562	-1.587	6.551	7.599	1.529	-1.732
<i>P. fluorescens</i>	-1.379	-0.581	-2.081	-4.849	-1.019	-3.622	0.570	-3.214	2.601	3.064	1.597	-2.253
<i>P. fluorescens</i>	-0.992	1.302	-2.167	0.316	-0.256	-1.234	1.375	-2.767	4.137	4.130	3.284	-1.415
<i>P. fluorescens</i>	-1.271	-0.806	-3.879	-1.948	-0.488	-1.923	-1.056	-5.594	1.032	2.235	3.208	-1.500
<i>P. fluorescens</i>	-1.057	0.083	-0.978	-1.601	-0.222	-1.626	0.054	-2.685	3.020	3.236	2.669	-1.687
<i>P. fluorescens</i>	0.367	1.046	-0.177	0.710	0.626	-0.215	1.341	-1.292	3.806	3.895	3.725	-0.892
<i>P. fluorescens</i>	0.353	-1.119	-1.638	-0.470	0.832	-0.723	0.042	-4.640	1.900	2.679	2.770	-0.755
<i>S. paratyphi</i> B	-13.842	-3.856	-5.165	-4.218	0.261	-1.100	-0.409	-2.640	2.806	2.573	-4.584	1.670
<i>S. paratyphi</i> B	-11.691	-0.157	-1.205	-1.077	1.002	1.972	2.159	-0.293	3.448	4.238	-3.309	2.777
<i>S. paratyphi</i> B	-10.780	1.659	-0.807	1.645	1.042	1.238	1.576	5.658	5.069	5.244	-1.945	1.847
<i>S. paratyphi</i> B	-12.186	-0.736	-1.648	-0.104	1.044	0.637	1.309	-0.214	3.358	4.005	-3.647	1.686
<i>S. paratyphi</i> B	-10.984	0.193	-0.338	1.517	1.698	1.988	3.023	0.876	4.167	5.131	-3.126	2.527
<i>S. paratyphi</i> B	-12.440	1.676	-0.096	2.115	1.446	2.447	2.869	5.472	5.239	5.618	-1.975	1.957
<i>Sh. flexneri</i>	-3.892	-0.511	-8.883	-2.657	-1.192	-10.043	-2.464	-3.319	1.550	4.070	-1.379	-0.110
<i>Sh. flexneri</i>	-0.042	-1.627	-2.421	-0.565	0.225	-6.050	1.806	1.258	2.492	7.923	-0.859	1.358
<i>Sh. flexneri</i>	-2.624	-2.805	-6.433	-3.324	1.019	-5.223	-0.792	-5.020	0.644	4.248	-2.116	1.048
<i>Sh. flexneri</i>	-1.275	-0.621	-3.826	-0.197	1.032	-6.666						

Table S7. Fluorescent response patterns of training set in the detection of mixed bacteria.

	Vanco@AuNCs	Baci@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Teico@AuNCs	DMC-P@AuNCs	DMAE-1@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
3+4	-1.935	-1.168	-0.087	6.774	-2.191	11.483	-6.971	-5.154	1.981	-28.093	-3.742	-9.471
3+4	-0.998	5.371	0.370	7.532	0.211	9.192	-13.388	-0.301	-5.521	-25.532	-2.121	-5.095
3+4	-0.964	-1.200	-1.023	6.870	3.894	12.318	-3.196	-1.856	0.538	-25.918	-4.347	1.535
3+4	0.087	5.928	0.264	7.500	4.410	10.293	-0.107	1.731	0.111	-18.076	-1.755	-4.575
3+4	-2.594	-2.190	-6.962	1.795	-0.303	10.423	-8.811	-12.911	-7.483	-38.567	-11.165	-3.570
3+4	-2.816	-5.433	-6.182	-1.411	0.873	9.855	-8.827	-10.972	-9.613	-35.244	-8.296	-11.803
4+7	7.505	-9.659	-4.431	-9.032	0.206	4.223	2.297	-4.929	-2.831	-34.916	-12.526	-26.496
4+7	7.730	-8.266	-7.163	-8.283	-1.146	2.801	2.359	-3.999	-4.357	-38.339	-11.331	-26.189
4+7	8.156	-6.521	-5.442	-6.709	3.621	4.469	3.773	-3.400	1.828	-29.664	-10.770	-20.731
4+7	6.638	-5.638	-7.854	-6.674	2.667	2.943	4.920	-0.684	-8.973	-30.602	-9.547	-22.569
4+7	10.851	0.028	1.447	-2.198	-1.451	1.964	3.078	5.325	11.077	-24.618	-0.952	-23.729
4+7	10.432	-2.377	-0.903	-2.702	-2.295	1.995	-3.580	7.953	4.335	-23.900	0.475	-23.654
7+8	-3.179	-0.261	-2.890	-2.633	0.263	-1.342	12.308	-17.967	12.617	-7.009	-13.739	-5.047
7+8	-1.448	-0.155	-1.586	-2.289	0.217	-5.184	9.936	-22.805	11.299	7.049	-13.774	-2.157
7+8	-0.964	0.374	-2.191	-0.625	0.489	-4.368	15.292	-9.567	18.770	10.392	-10.973	-0.317
7+8	1.300	2.005	0.356	0.515	0.978	-3.811	9.580	-10.918	4.754	8.582	-2.006	2.475
7+8	-6.318	-8.679	-9.846	-3.115	0.799	-3.041	7.295	-26.285	7.614	-3.722	-15.995	-2.476
7+8	-5.652	-12.741	-7.835	-2.569	0.786	-2.550	7.979	-21.977	-9.624	-9.855	-20.624	2.681
11+14	-10.402	4.896	3.340	-2.833	3.793	-7.500	4.318	1.675	1.232	-6.932	-14.181	-4.576
11+14	-6.889	3.533	3.215	-4.233	0.603	-8.502	10.078	-0.995	2.492	-0.065	-15.908	-3.502
11+14	-6.089	3.622	3.422	-4.390	3.783	-7.310	8.293	8.049	6.891	1.401	-12.723	0.087
11+14	-8.774	5.205	0.890	-0.926	2.657	-7.011	14.469	2.118	13.967	4.842	-13.933	2.034
11+14	-11.408	-7.909	-4.014	-6.996	3.227	-4.118	9.219	-5.083	-3.280	-13.825	-23.840	-5.124
11+14	-11.566	-3.726	-8.127	-6.579	0.286	-6.018	8.935	-2.820	-2.288	-9.697	-22.373	-5.636
15+16	-19.769	-6.301	-3.239	0.284	-0.868	-12.369	6.326	-8.629	-4.511	-35.378	-4.850	0.205
15+16	-18.730	-2.375	-4.502	1.154	0.057	-13.837	1.602	-9.703	-6.161	-33.080	-5.683	0.143
15+16	-14.005	-2.163	-2.353	2.426	0.282	-10.592	10.198	-4.325	1.499	-27.466	-2.459	6.434
15+16	-20.296	1.330	-4.600	2.457	1.120	-11.378	9.785	-0.442	-2.425	-26.256	-4.792	4.575
15+16	-24.319	-7.546	-8.204	-1.706	-0.370	-9.690	2.654	-18.235	-5.098	-45.742	-7.159	4.857
15+16	-25.058	-8.566	-9.340	-1.151	0.614	-10.395	3.256	-15.677	-10.599	-45.657	-11.842	-2.895
11+16	-0.468	-7.695	-11.002	1.064	-5.012	-3.518	-1.486	-26.598	-2.856	-50.072	-13.599	-4.146
11+16	-0.088	-2.713	-13.294	2.860	0.195	-1.413	-0.291	-26.317	-1.529	-51.102	-17.383	-4.512
11+16	-0.008	-4.396	-10.101	1.766	2.614	0.461	3.657	-22.717	3.645	-39.454	-11.163	6.425
11+16	-0.106	-3.619	-11.651	2.520	-1.679	-0.217	5.589	-20.491	-12.892	-44.053	-15.137	-0.864
11+16	1.102	-2.953	-6.649	3.241	-4.788	-5.746	3.307	-20.232	8.075	-34.920	-9.054	-6.185
11+16	-0.440	-2.576	-6.547	4.128	-1.082	-5.300	-1.968	-14.498	-3.011	-37.373	-8.207	-7.065
4+14	-18.819	-1.080	-5.606	2.893	-1.670	11.786	18.259	1.675	11.541	-1.938	5.569	11.603
4+14	-15.340	-5.740	-5.104	0.880	-4.101	9.712	17.260	1.842	5.129	-6.164	4.777	10.798
4+14	-14.548	-6.664	-3.334	3.072	0.176	12.776	18.436	2.311	6.948	-5.059	6.361	11.650
4+14	-15.730	-7.627	-2.680	0.406	-2.108	10.815	18.826	1.311	6.778	-5.859	4.266	10.175
4+14	-16.939	-7.921	-2.182	0.571	-3.303	9.444	18.843	0.996	6.782	-6.559	4.107	10.362
4+14	-17.494	-5.735	-5.025	0.152	0.165	9.344	17.802	-0.005	7.205	-5.705	4.802	9.900
7+15	-9.862	-5.711	-12.094	5.692	-6.973	10.034	17.232	-12.481	7.914	-13.040	5.563	9.805
7+15	-8.347	-6.185	-13.341	4.081	-5.575	8.485	17.221	-14.504	9.290	-10.861	4.672	10.357
7+15	-9.169	-5.845	-10.562	8.715	-2.673	10.717	17.065	-14.434	8.597	-11.127	5.568	10.969
7+15	-7.901	-7.078	-6.294	5.910	-2.316	10.914	17.333	-16.737	7.674	-12.146	5.143	10.414
7+15	-9.279	-7.903	-6.125	5.151	-3.299	8.803	17.272	-16.278	7.366	-13.596	4.489	10.081
7+15	-8.498	-7.816	-8.414	5.251	-10.266	9.865	16.974	-13.730	7.252	-12.844	5.022	10.021
8+16	-34.233	0.157	-2.970	-14.277	-9.012	-9.147	18.758	9.990	4.518	3.526	5.679	10.746
8+16	-32.526	1.502	-3.045	-11.359	-9.596	-9.138	18.373	13.443	3.106	3.083	6.040	11.111
8+16	-32.591	-2.608	-4.483	-14.525	-2.399	-3.910	18.833	14.196	6.848	3.547	6.043	11.507
8+16	-34.933	1.164	-9.738	-18.746	-3.387	-4.727	17.532	13.303	7.479	3.803	6.199	10.964
8+16	-36.971	-0.012	-10.571	-21.178	-9.714	-8.494	18.013	13.404	7.373	2.898	5.510	11.153
8+16	-35.636	0.075	-9.192	-18.031	-9.646	-8.444	19.976	11.433	5.439	3.212	5.201	10.491
3+4+7+11+14+15	4.841	-8.523	-22.857	1.758	-10.680	18.620	16.803	-9.142	8.760	6.020	2.496	3.439
3+4+7+11+14+15	4.648	-9.234	-22.279	1.774	-9.232	18.623	16.677	-6.325	7.071	6.316	3.494	6.391
3+4+7+11+14+15	7.559	-6.707	-23.922	3.276	-3.179	18.035	16.538	-8.142	7.858	6.738	2.985	3.364
3+4+7+11+14+15	6.110	-6.005	-23.635	6.120	-3.856	19.632	17.011	-12.383	9.042	8.457	4.580	5.495
3+4+7+11+14+15	5.276	-6.673	-24.580	3.560	-9.838	18.965	16.502	-13.994	7.395	5.666	3.718	5.292
3+4+7+11+14+15	5.591	-7.801	-24.998	4.459	-8.035	19.453	17.200	-10.322	7.785	6.409	3.408	4.634

Table S8. Fluorescent response patterns of training set in the detection of bacteria with gradient concentrations.

	Vanco@AuNCs	Bacit@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Teico@AuNCs	DMC-P@AuNCs	DMAE-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
S1	-15.932	0.197	6.694	4.802	-4.247	-4.051	-0.499	-2.027	1.628	-2.401	-2.840	-0.062
S1	-15.629	3.976	9.649	3.474	-4.615	-6.336	-2.715	-1.173	0.050	-3.765	-3.477	-1.475
S1	-8.297	3.917	9.871	10.120	-3.527	6.200	-0.244	-1.203	1.229	-2.191	-3.166	0.255
S1	-9.643	8.231	9.109	8.961	-4.002	2.948	-1.885	-2.079	0.898	-3.414	-3.688	-1.168
S1	-10.192	7.846	8.996	8.702	-4.567	2.851	-3.438	-1.051	-0.116	-2.769	-4.346	-0.789
S1	-9.316	8.566	9.340	8.509	-4.008	3.401	-2.001	-1.492	-0.052	-2.489	-4.646	-1.217
S2	4.495	-4.634	-2.785	-13.475	-2.386	6.028	-2.121	0.472	3.418	-2.032	1.200	-0.456
S2	4.307	-3.639	-1.711	-14.767	-3.503	5.083	-2.753	0.933	2.111	-1.892	0.350	-2.010
S2	3.499	-2.186	-3.077	-12.763	-4.078	3.591	-2.360	1.637	2.586	-2.548	1.130	-2.572
S2	3.480	-2.591	-3.655	-14.225	-2.937	3.503	-2.662	0.325	2.624	-2.700	0.823	-1.312
S2	8.057	1.237	0.613	-1.351	-2.218	11.610	-3.107	1.688	3.365	-2.527	0.512	-2.562
S2	8.275	1.833	1.114	-2.160	-1.437	12.184	-2.873	0.845	3.950	-2.791	0.707	-2.570
S3	-7.787	8.025	7.660	4.801	-3.177	4.808	-2.379	0.821	2.137	-1.025	1.079	0.488
S3	-7.158	8.727	7.709	3.832	-2.896	4.399	-3.089	-0.184	3.331	-1.454	1.424	0.630
S3	-6.362	8.011	7.243	4.871	-2.052	4.096	-4.220	0.973	2.624	-1.931	1.193	0.607
S3	-6.446	8.027	7.527	5.791	-3.264	4.055	-2.847	0.743	2.075	-1.356	0.686	0.535
S3	-3.644	6.943	11.255	4.275	-1.979	14.044	-3.836	0.859	2.092	-1.661	0.239	0.512
S3	-3.710	7.278	11.463	3.884	-1.286	12.974	-3.809	1.147	2.279	-1.875	-0.193	0.141
S4	-12.420	-9.567	-2.965	-15.661	-3.017	7.672	-1.598	-5.900	-0.351	-3.697	1.579	0.611
S4	-11.344	-8.322	-2.759	-16.509	-2.741	7.764	-1.576	-5.950	0.472	-3.092	0.884	0.701
S4	-11.893	-8.995	-3.748	-17.039	-2.931	7.601	-1.778	-4.987	-0.397	-2.981	0.975	0.021
S4	-12.350	-9.293	-6.574	-17.596	-3.037	5.819	-1.776	-4.995	-0.308	-3.501	1.062	0.419
S4	-8.868	-10.790	4.272	-3.451	-2.324	16.200	-1.911	-6.404	-0.215	-2.710	0.271	1.295
S4	-8.350	-10.827	4.441	-2.862	-1.994	15.741	-2.339	-5.372	-0.670	-2.634	0.335	0.257
S5	-5.239	-0.385	6.787	-0.884	-2.313	6.327	-3.025	0.345	2.370	-1.744	2.204	0.729
S5	-5.869	-1.047	6.542	-1.106	-2.664	6.816	-1.791	0.077	3.247	-2.102	1.598	1.320
S5	-6.333	-1.671	5.692	-1.967	-1.941	6.156	-1.955	-0.692	3.017	-2.051	1.683	1.085
S5	-6.346	-2.423	4.983	-1.764	-2.694	5.992	-2.730	1.211	2.297	-1.973	1.691	0.597
S5	-2.571	1.552	12.938	7.408	-2.346	12.332	-2.231	-0.710	2.955	-1.798	1.139	0.724
S5	-4.578	1.224	12.678	7.713	-2.156	12.178	-2.200	-0.614	3.262	-1.877	1.151	0.735
S6	-14.371	-4.262	-2.092	-2.031	-2.630	-4.538	-2.998	-0.766	1.170	-1.212	0.899	0.973
S6	-13.485	-5.693	-3.071	-2.380	-2.659	-4.306	-2.892	-0.020	1.193	-0.774	0.839	0.198
S6	-9.537	-1.041	5.629	5.755	-1.809	2.501	-3.616	-1.087	0.928	-1.009	0.731	0.806
S6	-9.238	-1.317	5.254	4.651	-1.426	1.013	-3.710	0.369	1.248	-1.840	0.905	1.267
S6	-9.923	-1.725	4.905	5.235	-2.580	2.262	-3.184	-0.033	2.155	-1.417	1.459	0.737
S6	-10.160	-1.735	5.199	5.175	-2.407	1.048	-4.010	-0.846	1.243	-0.969	2.043	1.407
S7	0.551	-5.914	9.572	7.010	-1.631	5.872	-1.454	1.069	2.605	-1.846	1.305	2.174
S7	0.341	-1.586	8.411	7.148	-1.544	6.094	-2.585	2.326	1.712	-1.774	1.155	2.355
S7	3.634	1.429	10.329	12.310	0.058	12.107	-0.844	1.314	2.726	-1.452	0.240	2.120
S7	1.781	3.011	10.368	11.621	0.606	12.016	-1.816	1.172	2.943	-1.942	1.750	2.243
S7	3.198	2.575	10.004	11.582	0.435	11.422	-2.689	2.200	2.082	-1.848	1.462	2.302
S7	1.671	2.545	9.965	11.601	0.535	11.184	-1.291	1.365	2.635	-1.376	0.334	2.287
S8	3.140	-5.357	-0.532	1.476	-1.620	3.081	-2.256	-4.782	1.567	-1.724	-0.861	0.861
S8	3.499	-5.009	-0.636	1.372	-1.111	2.687	-2.044	-3.774	0.044	-3.337	-1.625	-0.801
S8	2.543	-5.158	-0.898	0.831	-1.139	2.247	-2.237	-3.758	1.201	-4.177	-0.766	-0.796
S8	3.164	-4.297	-1.249	1.077	-2.217	2.752	-2.550	-4.335	1.729	-3.976	-1.490	0.282
S8	5.135	-0.724	2.412	5.572	-0.104	5.437	-2.020	-3.226	1.051	-2.667	-1.262	-0.406
S8	4.891	1.095	3.130	6.039	-0.462	5.770	-2.274	-3.883	1.444	-3.533	-1.202	0.585
S9	-5.491	-0.054	4.346	0.526	-6.769	4.633	-1.023	-7.176	2.266	-0.437	0.076	-0.297
S9	-2.368	-0.849	4.890	1.789	-6.664	4.629	-1.162	-7.768	1.449	-0.926	0.614	-0.178
S9	-3.484	-0.930	5.020	-0.238	-7.098	4.201	-2.343	-5.872	2.116	-0.523	0.356	-0.650
S9	-3.090	-1.622	5.258	0.499	-6.861	4.662	-0.515	-6.787	1.780	0.072	0.028	-0.630
S9	-1.533	-0.178	11.484	5.197	-5.027	7.307	-1.794	-6.140	2.617	0.211	0.573	0.243
S9	1.232	-1.085	11.184	4.880	-5.697	7.167	-1.147	-7.074	2.906	-0.221	0.104	0.322
E1	-5.040	10.596	5.114	2.395	-5.327	-9.398	-3.222	-0.617	0.328	1.030	-0.887	0.689
E1	-5.775	10.284	4.845	1.915	-5.178	-9.756	-2.527	-2.427	1.605	0.993	-1.515	0.487
E1	-5.694	10.266	4.870	2.156	-4.793	-9.074	-2.999	-3.729	1.810	0.569	-0.877	0.035
E1	-3.122	10.065	6.379	3.779	-5.415	-8.011	-3.565	-1.552	0.448	0.538	-1.356	0.517
E1	-3.799	10.034	6.460	3.085	-5.033	-8.310	-3.005	-3.199	1.584	-0.171	-1.923	0.551
E1	-4.824	10.251	6.231	2.849	-4.339	-8.105	-5.016	-0.733	0.933	0.211	-1.196	0.358
E2	-3.857	5.965	7.144	3.886	-3.349	-4.634	-3.972	1.204	-0.855	-0.899	0.187	1.222
E2	-4.676	5.777	6.992	3.298	-3.398	-5.087	-4.328	0.223	-0.554	-1.421	-0.213	0.973
E2	-4.509	5.868	6.932	3.085	-3.145	-4.878	-3.876	0.240	-1.146	-0.022	0.490	1.540
E2	-3.146	6.747	8.039	4.537	-3.326	-2.609	-3.991	0.400	0.004	0.048	0.320	1.193
E2	-3.756	6.278	7.992	4.437	-2.660	-3.007	-3.877	0.155	0.607	-0.497	-1.289	1.786
E2	-4.241	6.223	7.608	4.342	-3.486	-3.503	-4.303	0.868	-0.853	-0.657	-1.308	1.186
E3	2.943	6.916	13.207	9.227	3.357	4.204	-5.550	6.023	4.382	1.466	1.381	1.217
E3	3.607	7.309	13.279	9.346	3.628	4.175	-3.971	5.330	4.796	1.584	1.603	3.084
E3	3.324	7.916	14.638	10.824	3.504	5.664	-4.870	4.860	5.060	1.570	1.857	4.142
E3	4.872	7.304	14.628	10.742	3.533	5.525	-5.610	5.256	4.379	1.499	1.854	3.658
E3	4.464	6.512	13.494	9.829	3.269	5.230	-4.156	4.923	4.487	1.710	0.927	3.691
E3	4.160	7.022	14.031	9.973	3.323	5.020	-4.496	5.241	4.943	1.726	1.178	3.512
E4	1.702	7.057	6.326	1.988	0.819	-4.723	-6.444	0.998	1.682	0.692	-1.071	0.858
E4	1.729	7.169	6.649	2.471	0.516	-4.479	-6.531	0.671	2.330	-0.200	-1.525	1.093
E4	3.062	7.735	7.586	5.014	1.379	-3.618	-6.632	-0.149	2.415	0.166	-1.190	1.795
E4	3.201	7.842	7.235	5.156	1.019	-3.237	-6.232	0.927	1.687	-0.227	-1.976	0.568
E4	2.247	7.455	6.604	4.701	1.506	-3.559	-6.585	-0.082	2.032	-0.526	-1.070	1.190
E4	2.347	7.345	6.845	4.840	-0.091	-3.600	-6.392	-0.016	1.868	0.020	-1.796	1.918
E5	-2.042	12.681	13.169	7.178	1.379	-0.951	-5.445	2.616	3.048	1.638	2.890	1.871
E5	-1.850	12.849	13.456	6.999	0.555	-1.006	-4.791	2.461	3.441	1.625	2.954	1.441
E5	-2.030	12.257	12.757	6.038	0.697	-1.129	-5.493	1.831	3.331	1.520	2.486	1.834
E5	-0.912	11.075	14.031	4.878	0.383	-1.427	-6.379	2.908	3.083	1.750	2.924	1.833
E5	0.029	11.907	14.975	7.670	0.275	-0.331	-5.824	1.192	3.349	1.031	1.223	1.989
E5	-1.028	11.986	13.325	6.550	0.747	-0.405	-7.136	2.112	2.695	1.241	2.035	1.586
E6	-7.111	8.129	11.318	1.891	2.511	-2.475	-4.489	0.727	2.441	0.063	1.832	1.070
E6	-6.685	7.966	10.881	2.266	1.199	-3.144	-4.667	0.733	2.648	-0.471	2.011	1.673
E6	-7.469	8.047	10.921	1.579	2.068	-3.376	-4.801	0.093	2.038	0.133	0.786	2.212
E6	-8.058	7.957	10.559	3.310	1.343	-3.928	-4.187	0.631	2.598	0.192	0.365	1.472
E6	-5.229	7.561	11.547	4.516	1.728	-1.848	-6.028	0.260	2.215	-0.874	0.891	1.674
E6	-5.073	7.833	11.568	3.758	1.693	-2.245	-5.712	-0.293	1.990	-0.374	0.094	2.387
E7	5.836	9.357	7.743	10.966	1.675	-4.748	-6.257	0.405	3.122	0.690	0.507	2.710
E7	5.132	8.553	7.190	9.919	1.032	-5.090	-5.223	-0.528	3.840	1.068	-0.441	2.

Table S9. Fluorescent response patterns of testing set in the detection of bacterial samples in water.

No	Verification	Vanco@AuNCs	Bacit@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Teico@AuNCs	DMC-P@AuNCs	DMAE-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
1	<i>S. aureus</i> 1	2.665	-1.850	-1.037	-11.038	-0.892	3.946	17.340	-7.828	-9.794	-2.800	-17.467	0.618
2	<i>S. aureus</i> 1	2.552	-0.712	-1.906	-7.538	-2.255	2.691	16.754	7.564	-14.266	9.923	-8.720	-3.773
3	<i>S. aureus</i> 2	2.560	-1.169	-1.910	-5.443	-2.599	4.568	-7.672	2.161	3.144	-0.057	2.294	-5.778
4	<i>S. aureus</i> 2	2.250	-2.102	-4.826	-7.165	-4.079	3.664	-11.968	-7.778	-12.232	-9.811	-5.012	-11.998
5	<i>S. aureus</i> 3	-7.106	-3.478	-1.724	-15.310	-1.448	2.804	2.327	-1.270	-7.747	-37.291	2.584	-11.016
6	<i>S. aureus</i> 3	-5.775	-4.430	-4.026	-13.070	-2.484	2.542	3.729	3.922	9.954	-25.876	4.401	-8.520
7	<i>E. faecalis</i>	1.246	-28.963	-4.424	-31.951	-3.088	0.234	8.950	12.511	-1.169	8.164	1.919	-7.983
8	<i>E. coli</i>	-50.202	-34.814	-11.102	-37.780	-20.524	-8.411	-0.052	20.483	1.164	13.940	7.023	1.841
9	<i>E. coli</i>	-50.286	-46.618	-45.480	-48.768	-19.556	-5.998	0.208	12.775	-6.835	5.050	4.349	0.449
10	<i>E. coli</i> 1	-84.229	-49.464	-26.219	-29.218	-15.271	-7.370	-0.436	0.697	-5.247	-4.879	-30.493	-0.649
11	<i>E. coli</i> 1	-80.012	-39.780	-25.148	-26.924	-15.384	-7.837	0.444	6.084	-2.637	0.349	-24.530	4.593
12	<i>P. aeruginosa</i>	-17.388	-37.528	-25.986	-35.712	-21.131	-19.382	-12.175	-24.045	-2.928	-13.779	0.213	-7.844
13	<i>P. fluorescens</i>	-49.083	-37.336	-16.717	-28.436	-32.178	-3.030	-0.256	10.951	-3.644	-6.084	5.855	4.997
14	<i>P. fluorescens</i>	-52.383	-40.071	-19.862	-33.096	-30.555	-3.203	-2.457	0.594	-5.898	-17.209	4.593	3.395
15	<i>Sh. flexneri</i>	-19.898	-28.971	-17.191	-22.955	-12.357	-45.496	-6.620	7.407	-14.893	-16.028	8.141	-5.098
16	<i>Sh. flexneri</i>	-18.155	-29.089	-17.444	-30.263	-11.614	-41.802	-10.610	1.393	-34.526	-26.344	4.091	-2.196
17	<i>E. sakazakii</i>	-58.343	-23.069	-12.060	-54.883	-8.554	-40.694	-2.979	-8.450	-3.257	-20.681	4.097	2.265
18	<i>E. sakazakii</i>	-59.119	-19.654	-9.901	-52.430	-11.538	-42.255	-1.182	4.241	1.261	-15.195	7.520	1.839
19	<i>E. cloacae</i>	-6.933	-19.169	-9.315	-13.548	-7.338	-31.591	-0.534	4.241	1.261	-15.195	7.520	1.839
20	<i>E. cloacae</i>	-10.399	-21.231	-12.569	-16.911	-5.542	-31.966	-5.796	-10.916	-2.434	-9.514	3.489	-29.891

Table S10. Fluorescent response patterns of testing set in the detection of bacterial samples in serum.

No	Verification	Vanco@AuNCs	Bacit@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Teico@AuNCs	DMC-P@AuNCs	DMAE-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
1	<i>S. aureus</i> 1	-38.101	1.144	-12.359	-11.498	-10.498	2.296	-0.235	-1.033	-51.149	-8.688	3.761	-3.080
2	<i>S. aureus</i> 3	-30.552	6.011	-1.862	-3.092	-4.356	4.839	-1.187	-2.869	-29.390	-1.682	-2.797	-2.094
3	MRSA	-35.468	6.490	0.766	-5.659	-7.301	5.009	-2.723	1.123	-43.690	-4.577	-3.515	-5.587
4	MRSA	-36.922	1.999	-6.334	-10.052	-8.024	5.487	-8.836	-2.027	-46.478	-8.989	-8.101	-6.207
5	<i>E. faecalis</i>	-52.285	10.326	-7.562	-7.852	-5.316	8.697	-2.460	-5.390	-41.578	-4.422	-3.949	-5.162
6	<i>E. faecalis</i>	-53.529	6.733	-13.326	-9.784	-5.242	8.728	-3.021	-6.531	-54.143	-5.479	-8.718	-4.652
7	<i>B. subtilis</i>	-45.444	3.463	-10.435	-6.233	-7.045	6.499	-2.952	-5.714	-51.383	-6.384	-12.833	-3.469
8	<i>B. subtilis</i>	-46.169	7.029	-8.938	-3.713	-7.399	5.911	-2.287	-3.191	-47.321	-0.718	-8.268	-3.663
9	<i>S. mutans</i>	-38.479	5.861	-8.557	-8.533	-4.311	6.143	3.561	1.819	-29.897	-12.277	-13.254	-8.062
10	<i>E. coli</i> 1	-63.462	-3.332	-3.689	-14.039	-5.631	1.916	21.743	4.565	-40.213	-7.788	-6.823	0.957
11	<i>E.coli</i> BL21	-68.436	-1.969	-11.778	-10.369	-7.128	4.833	8.141	6.447	-44.287	-1.004	-5.134	-2.218
12	<i>E.coli</i> BL21	-67.169	-2.931	-12.581	-11.181	-6.912	4.590	8.012	4.633	-46.793	-6.313	-5.659	-2.819
13	<i>P. aeruginosa</i>	-57.067	-0.023	-14.824	-9.186	-15.246	1.954	3.756	-5.784	-43.304	-7.972	-5.046	-7.314
14	<i>P. aeruginosa</i>	-59.707	0.241	-14.892	-7.310	-15.644	1.832	3.971	-4.076	-36.004	-3.176	-5.188	-8.413
15	<i>P. fluorescens</i>	-41.575	-2.648	-7.007	-12.384	-5.806	5.076	2.311	-2.600	-50.384	-4.296	-4.727	-1.611
16	<i>S.paratyphi</i> B	-56.765	-5.036	8.100	-11.686	-6.716	2.843	4.471	0.424	-47.119	-21.808	-8.758	-1.904
17	<i>S.paratyphi</i> B	-51.109	-1.701	2.876	-11.510	-6.443	2.406	4.729	3.202	-36.788	-13.180	-7.552	-1.350
18	<i>Sh. flexneri</i>	-61.865	4.358	-12.363	-11.802	-13.234	5.175	4.513	-2.180	-28.772	-6.931	-7.605	-2.353
19	<i>E. cloacae</i>	-41.433	5.829	-8.822	-7.620	-8.559	12.960	4.255	0.759	-32.552	-0.722	-12.247	-4.601
20	<i>E. cloacae</i>	-45.349	5.113	-10.682	-8.901	-8.092	12.503	3.204	0.482	-38.118	-6.238	-13.859	-3.472

Table S11. Fluorescent response patterns of testing set in the detection of bacterial samples in urine.

No	Verification	Vanco@AuNCs	Bacit@AuNCs	Aeros@AuNCs	Colistin@AuNCs	PEI@AuNCs	Teico@AuNCs	DMC-P@AuNCs	DMAE-T@AuNCs	DMA-BA@AuNCs	DMA-HP@AuNCs	DMA-N@AuNCs	DMA-BT@AuNCs
1	<i>S. aureus</i> 3	-1.560	-3.111	-1.735	-0.026	-0.466	-0.746	0.886	-12.216	1.935	0.489	-1.758	-4.070
2	<i>S. aureus</i> 3	-0.938	-0.011	0.854	0.587	-0.257	-0.807	0.378	-10.022	7.634	5.780	-2.526	-5.761
3	MRSA	-1.540	1.600	-1.689	-5.585	0.570	-2.699	0.178	-0.570	-10.479	1.721	-3.461	-3.495
4	MRSA	-2.584	-1.125	-3.729	-6.938	0.398	-2.851	-0.332	-2.638	-21.144	0.118	-3.987	-3.709
5	<i>L. monocytogenes</i>	-1.530	0.752	-3.369	1.547	1.923	-0.320	-2.850	-2.331	1.524	2.360	-1.959	-3.680
6	<i>L. monocytogenes</i>	-2.951	1.619	-1.655	1.623	1.112	-0.479	-1.868	-1.773	2.009	3.422	-2.065	-3.927
7	<i>E. faecalis</i>	-0.628	-0.248	-0.989	-0.161	-3.302	0.196	0.247	0.505	4.151	5.135	-0.334	-2.959
8	<i>E. faecalis</i>	-3.055	-0.784	-5.353	-1.784	-3.795	-0.663	-2.204	-0.618	1.003	3.717	-1.064	-3.050
9	<i>S. mutans</i>	1.675	1.700	-4.029	-5.302	-1.788	1.832	2.692	2.784	2.460	4.274	1.483	-1.581
10	<i>E. coli</i>	-1.444	2.513	-9.945	-0.907	-1.373	-8.423	5.326	6.473	2.614	6.613	0.196	2.058
11	<i>E. coli</i>	-4.399	-0.502	-11.637	-5.687	-0.734	-8.186	3.688	-1.195	0.225	4.465	-0.309	1.784
12	<i>P. aeruginosa</i>	-3.528	-5.016	-4.114	-1.404	2.231	-5.857	-0.047	-3.861	2.644	6.745	1.507	-1.021
13	<i>P. aeruginosa</i>	-0.361	-3.999	-1.485	-1.999	3.106	-7.232	1.090	-0.714	4.611	6.563	1.632	-1.614
14	<i>P. fluorescens</i>	-4.433	-2.181	-8.748	-6.232	0.725	-4.112	-1.775	-4.584	0.293	0.821	1.609	-2.194
15	<i>S. paratyphi</i> B	-12.900	-2.007	-3.826	-5.466	-0.123	-0.700	0.281	-1.889	2.123	2.920	-3.913	2.063
16	<i>S.paratyphi</i> B	-13.034	1.134	-2.856	-2.299	0.386	-0.813	-0.122	1.238	4.885	3.880	-2.990	1.519
17	<i>E. sakazakii</i>	-2.131	-5.764	-8.614	-12.831	0.161	-5.317	-2.260	-6.357	-5.904	0.616	0.197	0.595
18	<i>E. sakazakii</i>	0.258	-5.312	-6.574	-7.775	0.800	-5.948	2.693	-0.290	-3.073	3.987	-0.262	1.827
19	<i>E. cloacae</i>	-11.432	0.301	-7.090	-6.626	-3.934	-3.861	-2.344	2.458	2.316	2.175	-2.773	2.211
20	<i>E. cloacae</i>	-13.993	-5.024	-16.139	-9.721	-2.922	-4.214	-4.290	-3.893	-4.074	-1.916	-6.577	0.812

7. HCA and OPLS-DA results

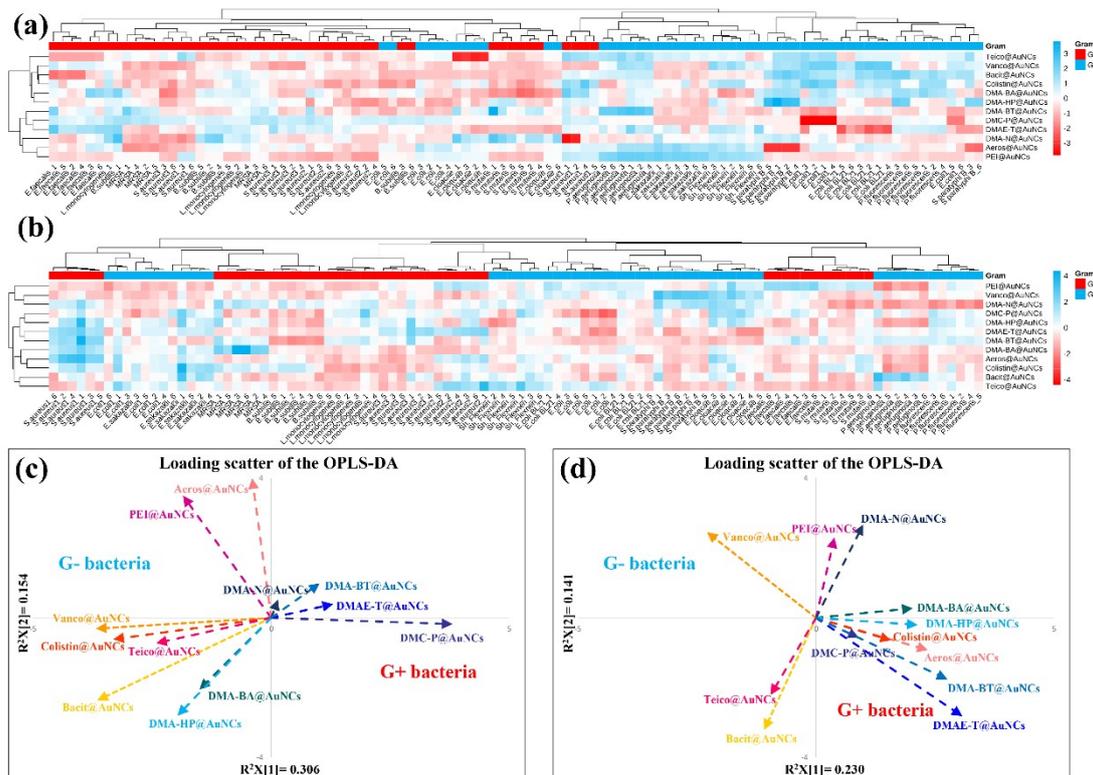


Figure S5. Heatmap and HCA results for the detection of bacterial samples in serum and urine, respectively (a, b); Loading scatter of the OPLS-DA for for the detection of bacterial samples in serum and urine, respectively (c, d).

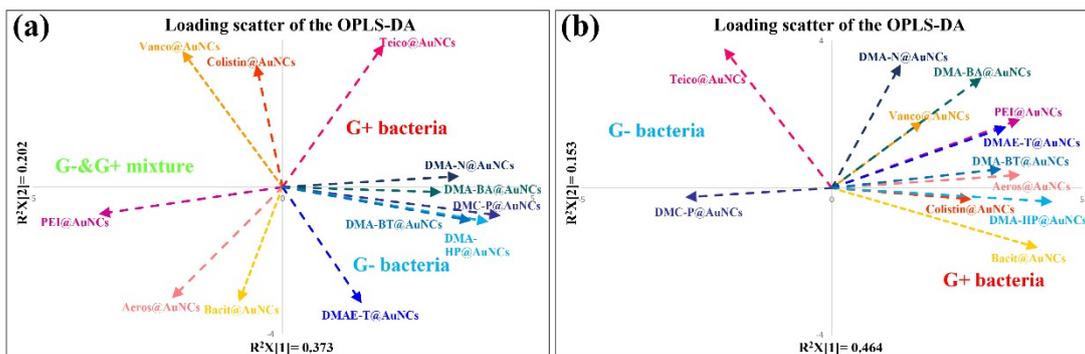


Figure S6. Loading scatter of the OPLS-DA for the detection of mixed bacteria and bacterial samples with gradient concentrations, respectively (a, b).

Table S16. Misclassification table for the training set in the detection of bacterial samples in serum.

Members	Correct	S. aureus 1	S. aureus 2	S. aureus 3	MRSA	L. monocytogenes	E. faecalis	B. subtilis	S. mutans	E. coli	E. coli 1	E. coli BL21	P. aeruginosa	P. fluorescens	S. paratyphi B	Sh. flexneri	E. sakazakii	E. cloacae
S. aureus 1	6	100%	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S. aureus 2	6	100%	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S. aureus 3	6	100%	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0
MRSA	6	100%	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0
L. monocytogenes	6	100%	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0
E. faecalis	6	100%	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0
B. subtilis	6	100%	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0
S. mutans	6	100%	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0
E. coli	6	100%	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0
E. coli 1	6	100%	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0
E. coli BL21	6	100%	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0
P. aeruginosa	6	100%	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0
P. fluorescens	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0
S. paratyphi B	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0
Sh. flexneri	6	83.33%	0	1	0	0	0	0	0	0	0	0	0	0	0	0	5	0
E. sakazakii	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6
E. cloacae	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6
Total	102	99.02%	6	7	6	6	6	6	6	6	6	6	6	6	6	5	6	6

Table S17. Misclassification table for the testing set in the detection of bacterial samples in serum.

Verification	Correc	S. aureus 1	S. aureus 2	S. aureus 3	MRSA	L. monocytogenes	E. faecalis	B. subtilis	S. mutans	E. coli	E. coli 1	E. coli BL21	P. aeruginosa	P. fluorescens	S. paratyphi B	Sh. flexneri	E. sakazakii	E. cloacae
1 S. aureus 3	100%	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2 S. aureus 3	100%	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3 MRSA	100%	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
4 MRSA	100%	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
5 L. monocytogenes	100%	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
6 L. monocytogenes	100%	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
7 E. faecalis	100%	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
8 E. faecalis	100%	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
9 S. mutans	100%	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
10 E. coli	100%	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
11 E. coli	0%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12 P. aeruginosa	100%	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
13 P. aeruginosa	100%	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
14 P. fluorescens	100%	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
15 S. paratyphi B	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
16 S. paratyphi B	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
17 E. sakazakii	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
18 E. sakazakii	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
19 E. cloacae	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
20 E. cloacae	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Table S18. Misclassification table for the training set in the detection of mixed bacteria.

Members	Correct	3+4	4+7	7+8	11+14	15+16	11+16	4+14	7+15	8+16	3+4+7+11+14+15	
3+4	6	100%	6	0	0	0	0	0	0	0	0	
4+7	6	100%	0	6	0	0	0	0	0	0	0	
7+8	6	100%	0	0	6	0	0	0	0	0	0	
11+14	6	100%	0	0	0	6	0	0	0	0	0	
15+16	6	100%	0	0	0	0	6	0	0	0	0	
11+16	6	100%	0	0	0	0	0	6	0	0	0	
4+14	6	100%	0	0	0	0	0	0	6	0	0	
7+15	6	100%	0	0	0	0	0	0	0	6	0	
8+16	6	100%	0	0	0	0	0	0	0	0	6	
3+4+7+11+14+15	6	100%	0	0	0	0	0	0	0	0	0	6
Total	60	100%	6	6	6	6	6	6	6	6	6	6

Table S19. Misclassification table for the training set in the detection of bacteria with gradient concentrations.

Members	Correct	S1	S2	S3	S4	S5	S6	S7	S8	S9	E1	E2	E3	E4	E5	E6	E7	E8	E9
S1	6	100%	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S2	6	100%	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S3	6	100%	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S4	6	100%	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0
S5	6	50%	0	0	0	0	3	1	0	0	2	0	0	0	0	0	0	0	0
S6	6	100%	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0
S7	6	100%	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0
S8	6	100%	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0
S9	6	100%	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0
E1	6	100%	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0
E2	6	100%	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0
E3	6	100%	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0
E4	6	83.33%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
E5	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0
E6	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0
E7	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0
E8	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0
E9	6	100%	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6
Total	108	96.3%	6	7	6	6	6	6	6	6	6	6	6	5	6	6	7	6	6

Table S20. Variable importance for projection (VIP) values of OPLS-DA for the detection of bacterial samples in the different situation.

	Water		Serum		Urine		Mixture		Gradient concentration	
	VIP value	SE of mean	VIP value	SE of mean						
Vanco@AuNCs	0.977	0.043	1.025	0.076	0.982	0.124	0.974	0.077	1.065	0.053
Bacit@AuNCs	0.981	0.052	0.980	0.103	1.065	0.096	1.105	0.215	1.021	0.058
Aeros@AuNCs	1.011	0.062	0.949	0.100	1.016	0.104	1.089	0.132	0.965	0.044
Colistin@AuNCs	1.010	0.059	1.040	0.254	0.974	0.084	1.042	0.144	1.026	0.104
PEI@AuNCs	1.000	0.078	0.992	0.100	1.037	0.056	0.995	0.288	0.995	0.042
Teico@AuNCs	0.977	0.071	0.993	0.160	1.081	0.041	0.990	0.091	0.999	0.129
DMC-P@AuNCs	1.039	0.055	0.994	0.081	1.068	0.115	0.926	0.094	1.054	0.074
DMAE-T@AuNCs	1.036	0.081	1.036	0.064	0.981	0.072	1.104	0.098	1.065	0.059
DMA-BA@AuNCs	1.115	0.105	1.072	0.084	0.945	0.193	0.912	0.177	1.021	0.139
DMA-HP@AuNCs	1.045	0.077	0.929	0.054	0.999	0.118	1.040	0.072	0.925	0.077
DMA-N@AuNCs	0.998	0.102	1.063	0.146	1.012	0.095	0.929	0.201	1.089	0.042
DMA-BT@AuNCs	1.054	0.066	1.084	0.084	1.031	0.179	0.982	0.077	1.033	0.019