

Supplementary Information

Array-based specific classification of bacterial species via the ligands with dimethylamino/amino groups

Xizhe Li,^{a‡} Fan Yang,^{d‡} Haojie Li,^{a‡} Zhi Hu,^c Weiting Yu,^c Yuchen Zhang,^{b*} and Jie Gao^{a*}

a. *Interdisciplinary Research Center of Biology & Catalysis, School of Life Sciences, Northwestern Polytechnical University, Xi'an 710072, China. E. mail: jgao@nwpu.edu.cn*

b. *Department of Pharmacy, Xi'an No. 3 Hospital, The Affiliated Hospital of Northwest University, Xi'an 710021, China. E. mail: chenyuzhuonian1026@outlook.com*

c. *College of Environment, Zhejiang University of Technology, Hangzhou 310032, China.*

d. *Xingzichuan Drilling Company, Yanchang Oil Mine Management Bureau, Yanan 717400, China*

‡These authors contributed to this work equally.

1. Chemical structure of ligands

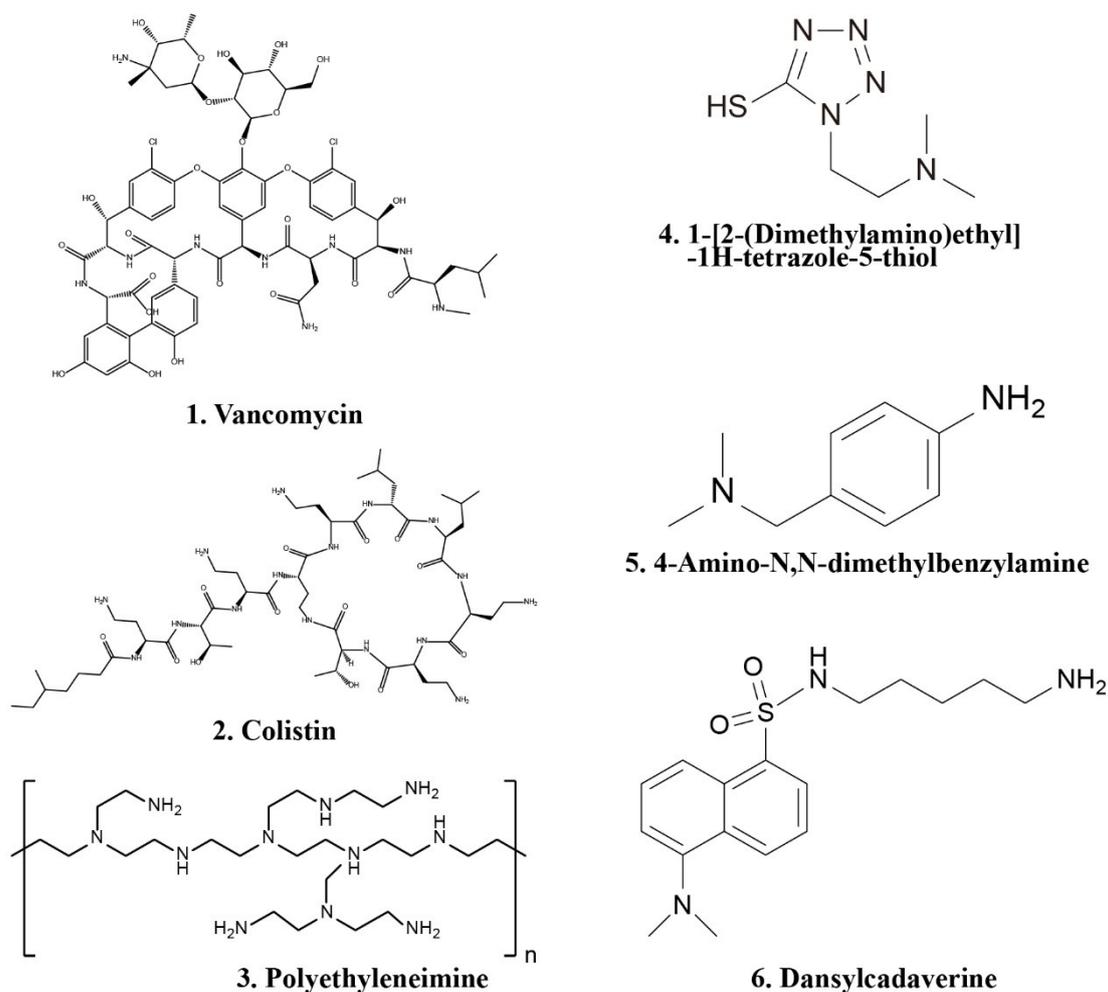


Figure S1. Chemical structure of the 6 ligands.

2. Detailed information of the ligands

Table S1. Detailed chemical information of the 12 ligands.

No	Compound	CAS number	Molecular mass	Molecular formula	LogP*	Abbr	Concentrations used in this study
1	Vancomycin	1404-93-9	1485.71	C ₆₆ H ₇₆ Cl ₃ N ₉ O ₂₄	-1.44	Vanco	0.6%
2	Colistin (Polymyxin E)	1264-72-8	1155.43	C ₅₂ H ₉₈ N ₁₆ O ₁₃	-3.68	Colistin	0.005%
3	PEI (Polyethyleneimine)	9002-98-6	~1800	(CH ₂ CH ₂ NH) _n	-5.41	PEI	5 mM
4	1-[2-(Dimethylamino)ethyl]-1H-tetrazole-5-thiol	61607-68-9	173.24	C ₃ H ₁₁ N ₅ S	0.28	MTZ	1.5 mM
5	4-Amino-N,N-dimethylbenzylamine	6406-74-2	150.2	C ₉ H ₁₄ N ₂	0.7	DMBA	15 mM
6	Dansylcadaverine (N-(Dimethyl-amino-naphtha-lene-sulfonyl)-1,5-pentane-diamine)	10121-91-2	335.46	C ₁₇ H ₂₃ N ₃ O ₂ S	2.83	Dansyl	3.5 mM

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

3. Detailed information of the bacteria

Table S2. Detailed information of the 16 kinds of bacteria.

No	Name of bacteria	Abbreviation	Gram species	Strains
1	<i>Staphylococcus aureus</i> 1	<i>S. aureus</i> 1	positive	
2	<i>Staphylococcus aureus</i> 2	<i>S. aureus</i> 2	positive	
3	<i>Staphylococcus aureus</i> 3	<i>S. aureus</i> 3	positive	
4	Methicillin-resistant <i>Staphylococcus aureus</i>	MRSA	positive	
5	<i>Listeria monocytogenes</i>	<i>L. monocytogenes</i>	positive	
6	<i>Enterococcus faecalis</i>	<i>E. faecalis</i>	positive	
7	<i>Bacillus subtilis</i>	<i>B. subtilis</i>	positive	
8	<i>Streptococcus mutans</i>	<i>S. mutans</i>	positive	
9	<i>Escherichia coli</i>	<i>E. coli</i>	negative	CMCC(B)44102
10	<i>Escherichia coli</i> BL21	<i>E.coli</i> BL21	negative	BL21
11	<i>Pseudomonas aeruginosa</i>	<i>P. aeruginosa</i>	negative	
12	<i>Pseudomonas fluorescens</i>	<i>P. fluorescens</i>	negative	
13	<i>Salmonella paratyphi</i> B	<i>S. paratyphi</i> B	negative	
14	<i>Shigella flexneri</i>	<i>Sh.flexneri</i>	negative	
15	<i>Enterobacter sakazakii</i>	<i>E. sakazakii</i>	negative	
16	<i>Enterobacter cloacae</i>	<i>E. cloacae</i>	negative	

4. UV-Vis spectra for 16 bacteria and 12 bacterial mixtures discrimination

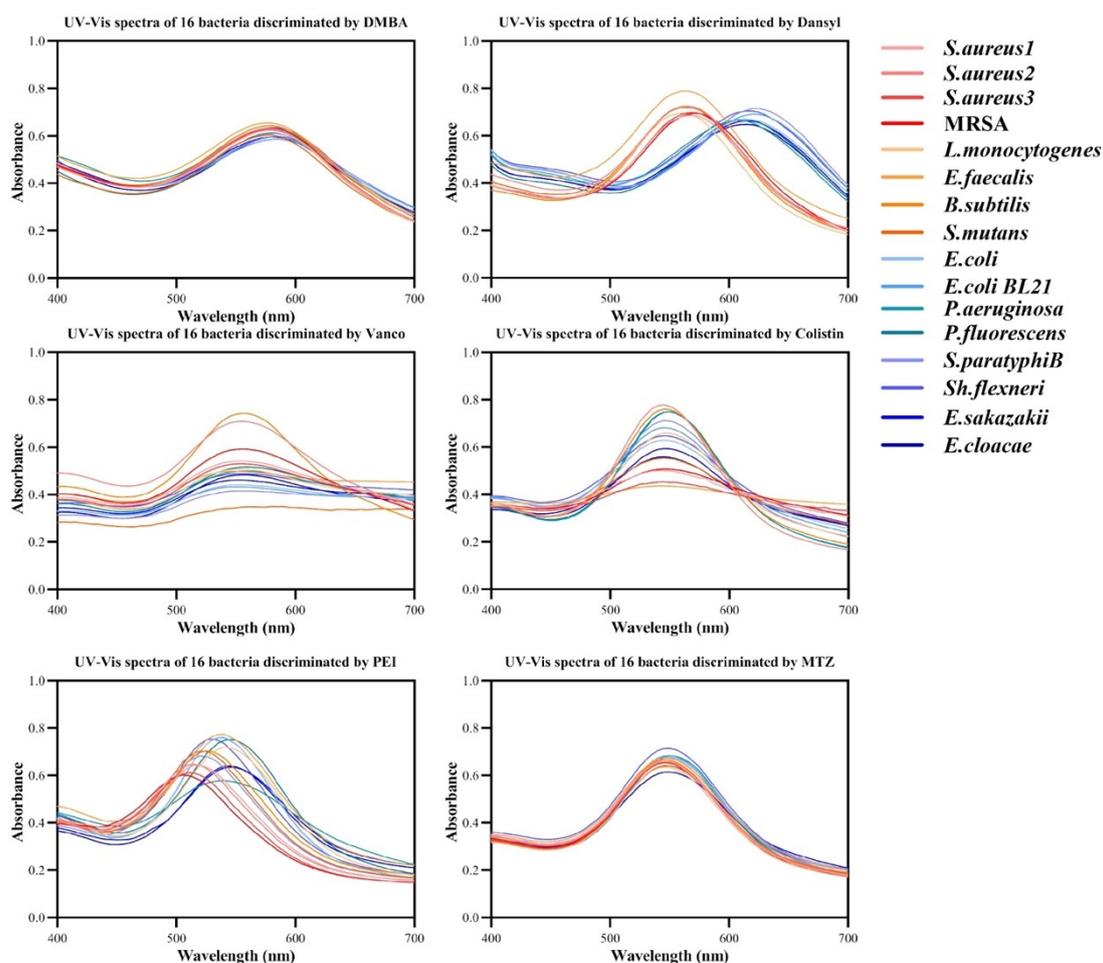


Figure S2. UV-Vis spectra of sensor arrays with 16 bacteria ($OD_{600}=0.05$).

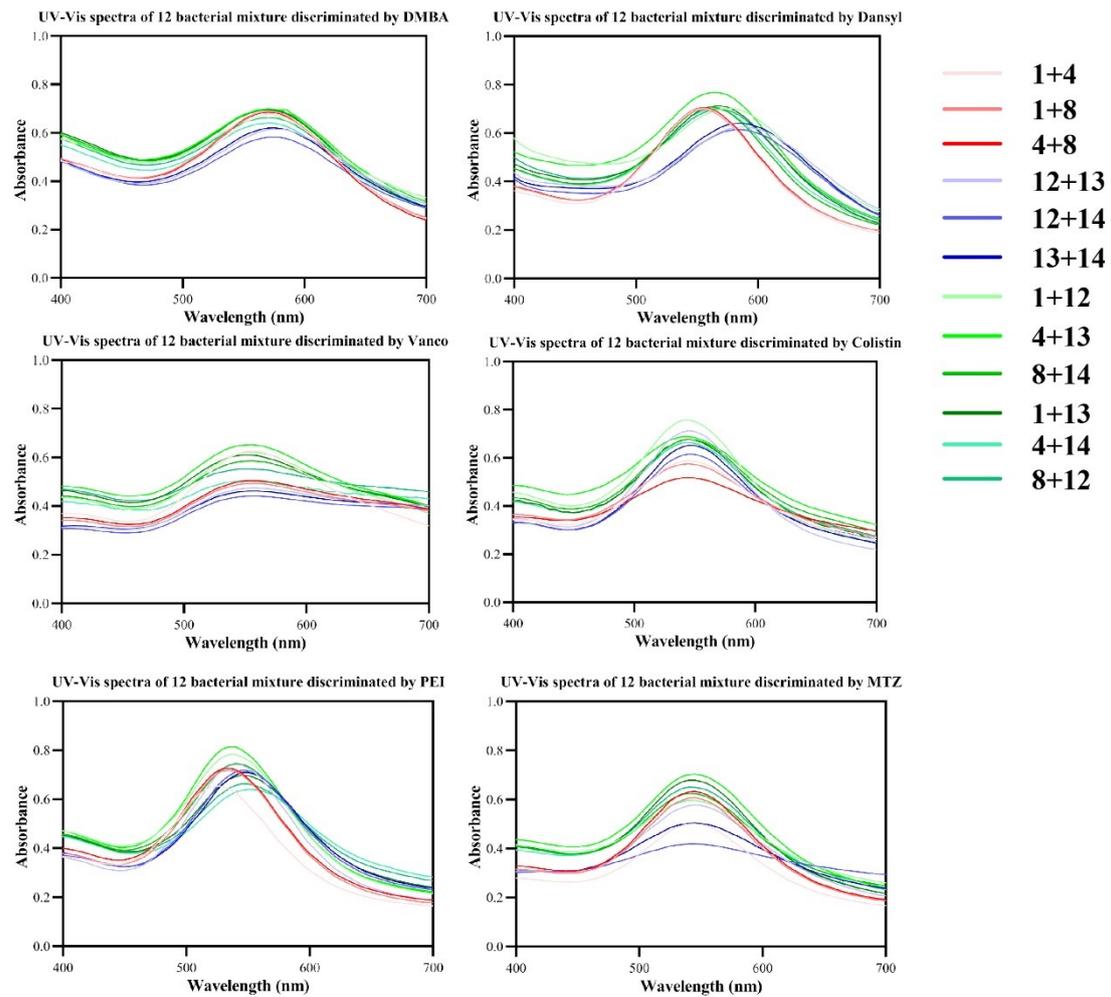


Figure S3. UV-Vis spectra of sensor arrays with 12 bacterial mixtures ($OD_{600}=0.05$).

5. Using the “houghcircles” function in open CV to identify various wells in microplate

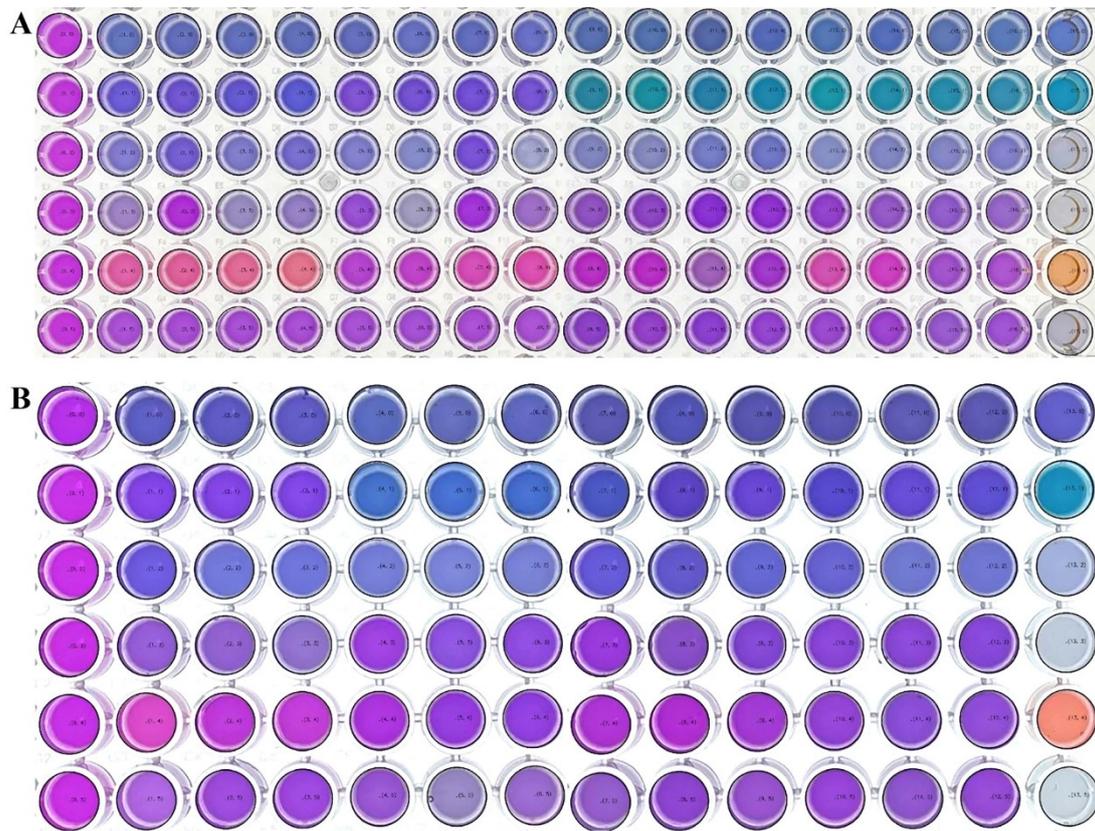


Figure S4. Discrimination of microplate wells by “houghcircles” function.

6. 4 LDA plots obtained by the 4 grayscale methods

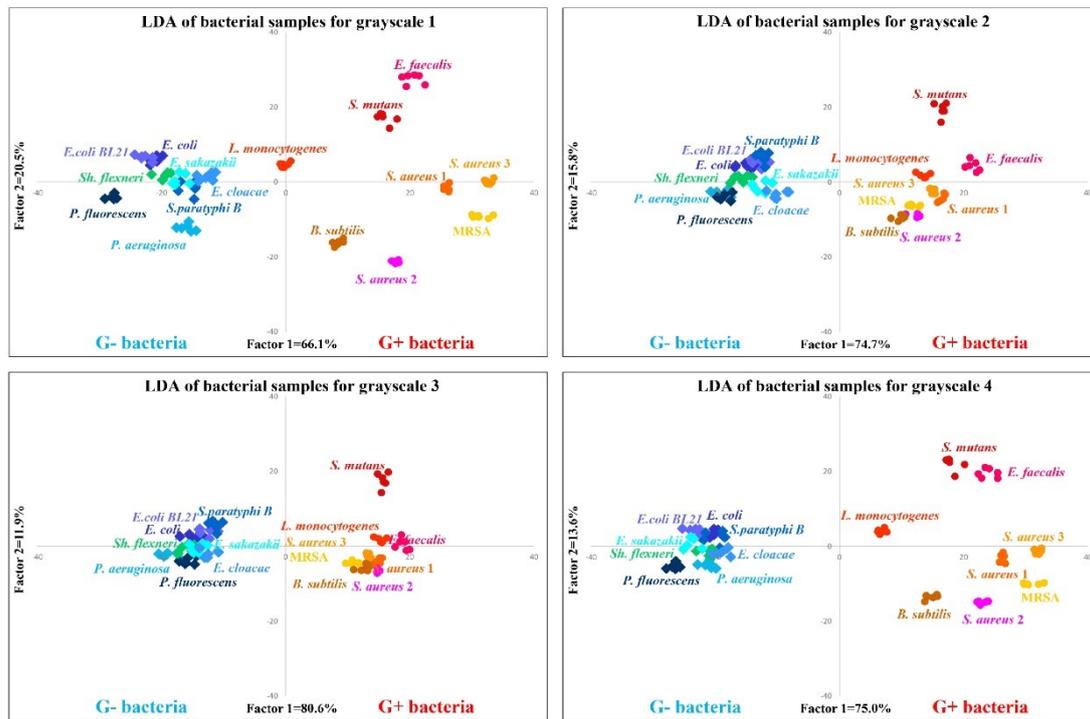


Figure S5. LDA plots of bacterial discrimination for the 4 grayscale methods

7. Colorimetric response patterns obtained by the grayscale value

Table S3. Colorimetric response patterns of 16 bacteria

	DMBA	Dansyl	Vanco	Colistin	PEI	MTZ
<i>S. aureus</i> 1	112.216	100.322	130.427	137.035	157.925	125.690
<i>S. aureus</i> 1	108.270	100.261	130.270	139.144	157.811	127.864
<i>S. aureus</i> 1	110.216	100.560	131.568	139.557	158.925	124.391
<i>S. aureus</i> 1	109.515	98.859	126.378	137.557	158.224	126.864
<i>S. aureus</i> 1	108.270	100.261	126.193	138.557	157.224	126.163
<i>S. aureus</i> 1	110.629	99.446	126.307	138.454	158.088	125.978
<i>S. aureus</i> 2	107.010	101.674	111.359	108.699	162.835	129.098
<i>S. aureus</i> 2	107.423	99.789	111.604	108.699	162.362	128.500
<i>S. aureus</i> 2	106.352	102.386	110.832	108.699	162.248	127.201
<i>S. aureus</i> 2	105.548	98.561	111.718	107.770	163.194	127.087
<i>S. aureus</i> 2	108.124	101.500	108.473	108.699	163.362	124.223
<i>S. aureus</i> 2	106.548	102.087	111.245	108.699	162.835	126.500
<i>S. aureus</i> 3	110.330	95.963	129.829	145.134	164.069	124.505
<i>S. aureus</i> 3	109.515	95.077	132.128	145.433	165.183	124.978
<i>S. aureus</i> 3	109.874	95.963	132.302	145.134	164.411	123.690
<i>S. aureus</i> 3	109.330	95.077	131.715	145.134	163.482	123.391
<i>S. aureus</i> 3	109.515	95.490	131.715	147.852	164.770	123.391
<i>S. aureus</i> 3	109.330	94.490	129.655	145.134	164.069	125.380
MRSA	111.439	97.371	119.512	135.775	168.440	123.804
MRSA	109.254	95.485	118.925	134.209	167.142	123.847
MRSA	110.439	95.485	119.512	134.373	166.266	124.032
MRSA	105.380	96.371	118.925	136.661	168.853	122.690
MRSA	111.439	91.882	119.626	136.486	169.081	125.092
MRSA	111.140	91.882	119.925	134.188	169.668	123.391
<i>nonocytogenes</i>	107.885	104.913	138.731	113.777	126.148	126.956
<i>nonocytogenes</i>	110.771	102.326	139.731	113.364	125.034	128.956
<i>nonocytogenes</i>	109.885	102.913	140.318	111.478	125.148	128.543
<i>nonocytogenes</i>	108.885	102.326	139.731	112.777	124.447	125.070
<i>nonocytogenes</i>	110.472	103.326	140.731	115.364	125.707	127.358
<i>nonocytogenes</i>	110.771	103.913	138.503	113.777	124.550	126.657
<i>E. faecalis</i>	113.628	97.142	145.396	165.065	130.716	123.701
<i>E. faecalis</i>	113.824	96.626	144.510	164.065	124.542	120.054
<i>E. faecalis</i>	113.813	98.625	147.695	160.521	128.770	123.956
<i>E. faecalis</i>	114.123	97.142	148.396	165.652	126.944	123.587
<i>E. faecalis</i>	113.650	96.843	150.695	163.065	126.656	123.587
<i>E. faecalis</i>	113.628	96.843	146.396	166.951	126.656	125.956
<i>B. subtilis</i>	110.330	98.587	105.788	104.520	142.738	126.554
<i>B. subtilis</i>	110.629	95.103	103.892	107.520	142.325	124.608
<i>B. subtilis</i>	110.330	96.587	105.788	105.808	143.738	127.739
<i>B. subtilis</i>	110.330	97.701	105.603	104.510	143.972	126.070
<i>B. subtilis</i>	104.700	95.701	104.603	106.509	141.869	128.326
<i>B. subtilis</i>	110.102	98.174	102.017	104.510	142.919	126.739
<i>S. mutans</i>	110.145	103.076	171.288	133.769	147.060	124.657
<i>S. mutans</i>	109.145	101.191	177.173	135.655	147.174	125.657
<i>S. mutans</i>	112.031	102.375	175.760	135.068	142.473	125.070
<i>S. mutans</i>	110.145	102.191	179.418	132.182	144.473	123.369
<i>S. mutans</i>	109.504	104.261	178.059	135.655	144.473	124.657
<i>S. mutans</i>	112.031	104.375	180.532	133.068	146.060	125.358
<i>E. coli</i>	103.687	111.039	130.675	103.405	106.405	98.105
<i>E. coli</i>	102.274	111.338	129.675	100.992	106.405	99.105
<i>E. coli</i>	102.274	109.224	130.675	101.992	104.879	97.105
<i>E. coli</i>	101.687	108.637	128.202	97.993	105.291	96.991
<i>E. coli</i>	98.687	109.925	128.789	100.992	104.476	96.105
<i>E. coli</i>	100.687	110.811	129.789	101.992	106.291	97.991
<i>E. coli</i> BL21	108.155	117.055	134.403	100.530	107.405	100.959
<i>E. coli</i> BL21	106.269	116.354	130.219	100.530	107.818	98.372
<i>E. coli</i> BL21	108.269	115.653	133.219	99.644	105.476	98.372
<i>E. coli</i> BL21	107.568	114.653	132.518	98.231	105.291	96.187
<i>E. coli</i> BL21	107.269	115.653	131.518	99.231	102.993	96.247
<i>E. coli</i> BL21	107.568	114.240	131.219	99.231	103.651	98.546
<i>. aeruginosa</i>	94.894	105.913	115.897	88.973	123.105	98.088
<i>. aeruginosa</i>	96.068	106.913	113.310	88.087	126.403	98.088
<i>. aeruginosa</i>	94.068	105.212	114.310	85.675	122.746	98.088
<i>. aeruginosa</i>	94.894	104.212	112.897	86.262	125.218	95.675
<i>. aeruginosa</i>	94.068	106.913	114.310	85.675	122.447	97.088
<i>. aeruginosa</i>	93.481	103.397	113.125	87.675	123.180	94.263
<i>. fluorescens</i>	93.985	109.342	112.108	89.446	99.910	100.333
<i>. fluorescens</i>	93.344	109.342	110.695	88.148	101.393	98.333
<i>. fluorescens</i>	94.572	109.342	107.923	88.560	99.980	100.333
<i>. fluorescens</i>	93.572	107.054	108.282	88.674	100.806	96.447
<i>. fluorescens</i>	90.854	109.342	108.108	87.920	98.568	99.447
<i>. fluorescens</i>	94.572	107.054	106.810	88.919	99.383	94.529
<i>paratyphi B</i>	105.970	116.930	139.534	94.589	125.766	102.485
<i>paratyphi B</i>	107.948	117.930	139.833	96.312	124.353	102.485
<i>paratyphi B</i>	110.731	115.044	136.648	94.703	123.353	103.257
<i>paratyphi B</i>	107.856	118.631	137.648	95.703	121.653	99.372
<i>paratyphi B</i>	108.856	118.930	133.649	92.899	127.353	101.485
<i>paratyphi B</i>	109.443	118.930	135.061	92.529	123.213	98.475
<i>Sh. flexneri</i>	96.670	114.120	124.370	103.884	111.817	97.768
<i>Sh. flexneri</i>	97.431	114.821	124.370	103.465	110.817	99.365
<i>Sh. flexneri</i>	97.431	114.120	121.485	100.547	110.817	98.953
<i>Sh. flexneri</i>	96.431	114.821	123.485	100.412	107.991	99.365
<i>Sh. flexneri</i>	97.143	111.419	121.958	101.878	110.518	94.540
<i>Sh. flexneri</i>	97.431	108.951	118.485	99.992	109.051	94.882
<i>E. sakazakii</i>	104.817	112.125	123.713	103.063	110.237	105.078
<i>E. sakazakii</i>	106.404	113.125	122.713	104.063	111.824	104.850
<i>E. sakazakii</i>	103.117	112.011	120.713	102.134	113.236	109.209
<i>E. sakazakii</i>	104.817	112.125	119.414	99.177	111.525	104.437
<i>E. sakazakii</i>	103.818	113.011	118.713	100.177	110.422	105.437
<i>E. sakazakii</i>	105.404	110.712	120.941	99.063	110.720	104.437
<i>E. cloacae</i>	105.970	114.505	118.092	112.917	116.051	104.812
<i>E. cloacae</i>	106.084	114.505	118.092	111.917	115.361	104.812
<i>E. cloacae</i>	105.970	111.918	114.320	109.733	115.845	103.926
<i>E. cloacae</i>	105.970	113.505	112.918	110.032	111.465	103.399
<i>E. cloacae</i>	105.084	112.918	117.978	105.733	115.144	103.513
<i>E. cloacae</i>	105.557	113.505	116.978	109.032	115.361	103.268

Table S4. Colorimetric response patterns of 12 bacterial mixtures

	DMBA	Dansyl	Vanco	Colistin	PEI	MTZ
1+4	87.309	93.783	93.393	106.992	122.176	135.698
1+4	87.608	93.783	93.795	106.878	123.193	135.111
1+4	87.309	92.897	92.094	107.405	123.062	133.111
1+4	86.309	92.370	91.796	105.291	123.492	135.698
1+4	88.309	92.783	92.795	107.106	124.079	135.285
1+4	86.309	91.783	92.322	106.878	122.421	135.698
1+8	85.309	90.534	112.515	111.954	115.343	113.415
1+8	85.423	90.936	112.102	111.367	114.343	115.529
1+8	84.537	90.534	113.401	111.894	113.756	112.529
1+8	85.309	89.708	113.401	110.367	114.642	115.415
1+8	84.423	89.936	112.287	110.666	115.169	114.116
1+8	83.722	89.050	113.689	111.068	114.229	113.828
4+8	85.010	92.392	114.102	121.564	114.702	115.034
4+8	83.950	90.979	123.502	121.852	114.816	114.149
4+8	84.239	91.979	115.102	120.678	115.115	113.035
4+8	85.238	92.278	114.515	121.564	114.115	115.034
4+8	84.413	90.979	115.102	120.151	115.115	114.736
4+8	83.239	89.865	115.102	121.379	113.816	114.035
12+13	103.463	106.953	117.292	97.946	106.230	111.062
12+13	104.523	107.654	119.178	98.349	107.072	111.351
12+13	104.284	107.768	118.292	97.946	106.773	109.764
12+13	104.463	106.953	118.292	97.946	107.001	111.062
12+13	103.115	106.366	117.292	97.648	105.062	111.351
12+13	102.876	106.067	118.292	97.762	105.475	110.764
12+14	107.116	105.185	125.152	103.616	97.604	138.952
12+14	108.116	104.186	127.151	104.730	98.191	138.952
12+14	106.116	103.887	126.151	102.915	97.490	138.952
12+14	106.529	101.186	125.152	103.915	96.490	138.952
12+14	105.117	104.598	125.152	103.029	95.964	137.952
12+14	107.116	103.186	126.151	102.328	96.490	138.952
13+14	100.023	101.186	123.152	99.703	102.248	121.852
13+14	101.023	102.599	123.266	99.404	103.949	121.151
13+14	101.414	100.186	119.793	98.589	102.949	122.852
13+14	100.550	101.186	122.739	97.404	103.835	121.151
13+14	100.436	102.186	124.152	98.703	102.949	121.852
13+14	102.012	101.186	124.152	97.290	101.949	119.966
1+12	102.713	91.805	95.943	97.768	108.964	118.106
1+12	103.300	91.919	95.117	96.469	109.665	117.992
1+12	102.713	90.392	95.117	97.469	108.964	117.107
1+12	103.414	92.218	95.117	98.469	109.964	118.106
1+12	102.012	91.919	95.943	97.480	108.964	117.694
1+12	101.599	90.919	95.117	98.708	108.964	117.107
4+13	91.859	82.177	97.227	104.095	107.128	106.410
4+13	91.642	80.291	96.227	103.095	108.302	106.182
4+13	91.457	82.938	97.227	102.981	107.416	105.595
4+13	91.642	83.237	95.928	104.095	107.829	106.708
4+13	92.044	82.291	96.227	101.868	107.074	106.182
4+13	93.310	83.237	97.227	101.982	106.829	106.708
8+14	93.392	88.921	102.157	100.307	107.339	112.937
8+14	93.278	86.921	102.157	100.307	107.883	112.937
8+14	94.392	88.921	101.869	98.720	106.410	113.051
8+14	93.392	87.921	102.157	99.606	106.823	111.938
8+14	93.392	87.035	101.570	99.606	106.524	113.937
8+14	93.278	88.921	102.456	100.307	106.410	112.937
1+13	91.392	80.237	102.091	99.763	102.502	111.149
1+13	90.392	82.237	102.091	98.763	103.089	109.263
1+13	90.919	81.009	98.977	99.763	102.388	110.263
1+13	90.278	80.237	101.977	98.763	101.790	110.149
1+13	90.164	79.824	101.749	99.763	102.502	108.562
1+13	92.392	82.650	101.091	99.763	104.089	107.562
4+14	99.914	86.188	116.957	100.122	101.422	117.704
4+14	99.501	85.661	116.843	98.823	102.721	114.292
4+14	99.273	86.258	115.669	100.122	102.422	116.704
4+14	100.561	84.373	114.555	100.122	99.422	113.531
4+14	97.974	84.960	115.669	100.122	100.835	115.705
4+14	99.675	85.960	116.256	99.122	103.422	114.292
8+12	96.675	84.488	112.011	99.986	100.868	111.269
8+12	98.974	83.901	111.310	97.976	101.868	108.682
8+12	97.974	81.026	112.011	97.976	100.868	110.269
8+12	98.974	83.200	110.652	99.687	101.868	108.383
8+12	95.974	82.026	111.897	97.976	100.868	109.682
8+12	97.974	81.428	111.310	98.976	101.868	107.796