Supplemental Material

Detection and Classification of Bacterial Cells After Centrifugation and Filtration of Liquid Specimens Using Laser-Induced Breakdown Spectroscopy

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Table S1. Identification of the 19 emission lines observed in LIBS spectra used to create ratios for bacteria and water differentiation.

Element symbol	Emission line wavelength (nm)	Ionization state	Variable designation for ratios
C	247.856	I	c
P	213.618	I	p1
P	214.914	I	p2
P	253.398	I	p3
P	253.56	I	p4
P	255.326	I	p5
P	255.491	I	p6
Mg	279.079	II	mgii1
Mg	279.553	II	mgii2
Mg	279.806	II	mgii3
Mg	280.271	II	mgii4
Mg	277.983	I	mgi1
Mg	285.213	I	mgi2
Ca	317.933	II	caii2
Ca	393.366	II	caii3
Ca	396.847	II	caii4
Ca	422.673	I	cai1
Na	588.995	I	na1
Na	589.593	I	na2

Table S2. List of 145 ratios constructed from the 19 measured LIBS emission line intensities to construct predictor variables for discrimination. The identities of the 19 lines is provided in Table SI.

p1/c	p2/na2	p4/na1	p6/cai1	mgii4/caii2	caii3/na2
p1/mgii1	p3/c	p4/na2	p6/na1	mgii4/caii3	caii4/c
p1/mgii2	p3/mgii1	p5/c	p6/na2	mgii4/caii4	caii4/na1
p1/mgii3	p3/mgii2	p5/mgii1	mgii1/c	mgii4/cai1	caii4/na2
p1/mgii4	p3/mgii3	p5/mgii2	mgii1/caii2	mgii4/na1	cai1/c
p1/mgi1	p3/mgii4	p5/mgii3	mgii1/caii3	mgii4/na2	cai1/na1
p1/mgi2	p3/mgi1	p5/mgii4	mgii1/caii4	mgi1/c	cai1/na2
p1/caii2	p3/mgi2	p5/mgi1	mgii1/cai1	mgi1/caii2	c/na1
p1/caii3	p3/caii2	p5/mgi2	mgii1/na1	mgi1/caii3	c/na2
p1/caii4	p3/caii3	p5/caii2	mgii1/na2	mgi1/caii4	mgi1/mgii1
p1/cai1	p3/caii4	p5/caii3	mgii2/c	mgi1/cai1	mgi1/mgii2
p1/na1	p3/cai1	p5/caii4	mgii2/caii2	mgi1/na1	mgi1/mgii3
p1/na2	p3/na1	p5/cai1	mgii2/caii3	mgi1/na2	mgi1/mgii4
p2/c	p3/na2	p5/na1	mgii2/caii4	mgi2/c	mgi2/mgii1
p1/mgii1	p4/c	p5/na2	mgii2/cai1	mgi2/caii2	mgi2/mgii2
p2/mgii2	p4/mgii1	p6/c	mgii2/na1	mgi2/caii3	mgi2/mgii3
p2/mgii3	p4/mgii2	p6/mgii1	mgii2/na2	mgi2/caii4	mgi2/mgii4
p1/mgii4	p4/mgii3	p6/mgii2	mgii3/c	mgi2/cai1	cai1/caii2
p2/mgi1	p4/mgii4	p6/mgii3	mgii3/caii2	mgi2/na1	cai1/caii3
p2/mgi2	p4/mgi1	p6/mgii4	mgii3/caii3	mgi2/na2	cai1/caii4
p2/caii2	p4/mgi2	p6/mgi1	mgii3/caii4	caii2/c	
p2/caii3	p4/caii2	p6/mgi2	mgii3/cai1	caii2/na1	
p2/caii4	p4/caii3	p6/caii2	mgii3/na1	caii2/na2	
p2/cai1	p4/caii4	p6/caii3	mgii3/na2	caii3/c	
p2/na1	p4/cai1	p6/caii4	mgii4/c	caii3/na1	

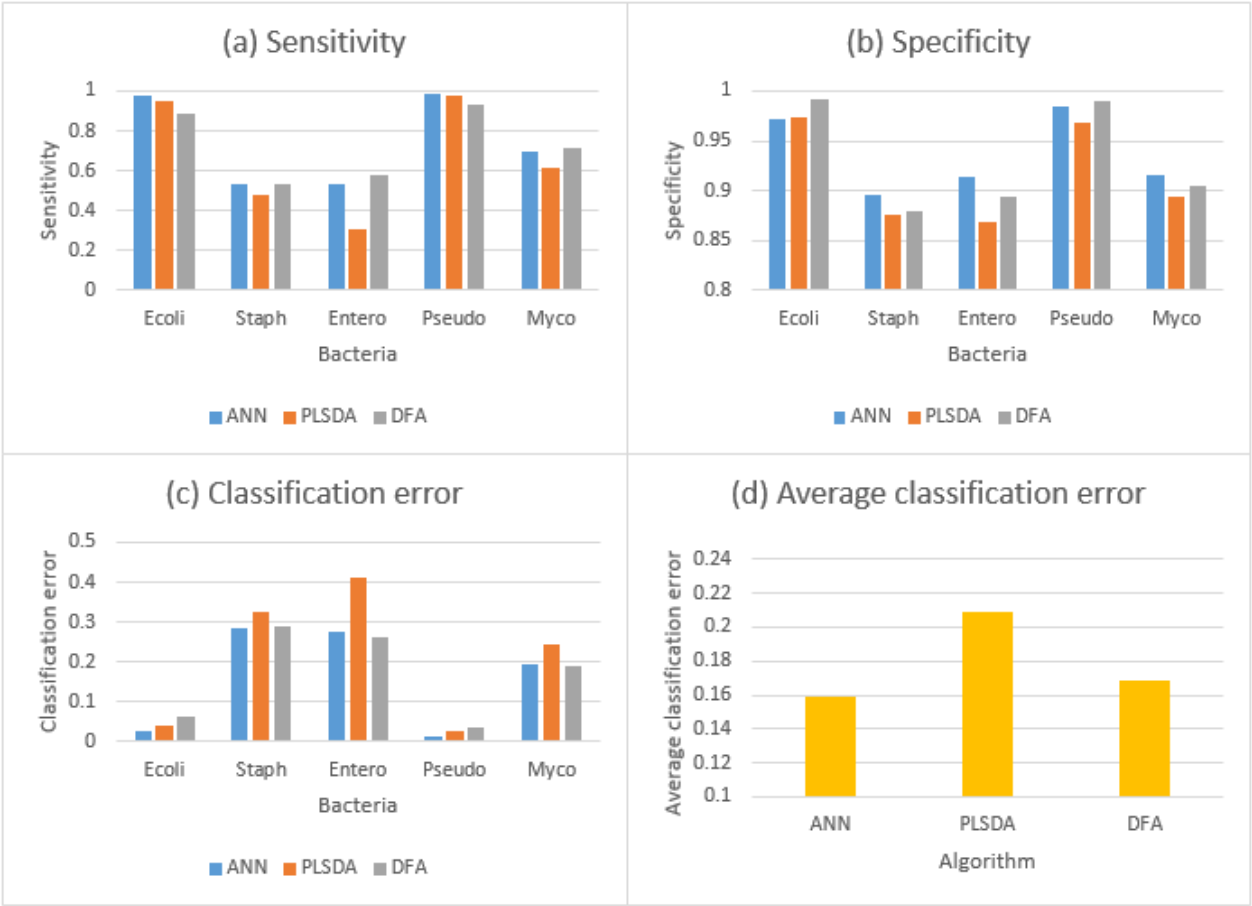

Figure S1. (a) Sensitivity, (b) specificity, and (c) classification error for classification tests performed on five species of bacterial pseudodata classified with three different chemometric algorithms. (d) The average of the classification errors for the five species. "Ecoli" = *E. coli*. "Staph" = *S. epidermidis*. "Entero" = *E. cloacae*. "Pseudo" = *P. aeruginosa*. "Myco" = *M. smegmatis*. ANN= artificial neural network. PLSDA = partial least squares discriminant analysis. DFA = discriminant function analysis.