Stain-free Gram staining classification of pathogens via Single-cell Raman spectroscopy combined with machine learning

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Table S1: Comparison of the four machine learning models in discriminating clinical samples. The best classification performance for each sample was annotated with bold black.

		#1	#2	#3	#4	#5	#6	#7	#8	#9	Overall
k-NN	GN	69	127	51	94	67	0	9	75	5	
	GP	2	18	1	3	38	71	57	16	74	0.806
	Acc.	0.972	0.876	0.981	0.969	0.638	1	0.864	0.176	0.937	
LDA	GN	60	119	52	95	88	0	0	1	1	
	GP	11	26	0	2	17	71	66	90	78	0.925
	Acc.	0.845	0.821	1	**0.979**	**0.838**	**1**	**1**	**0.989**	0.987	
GBM	GN	70	133	52	77	79	0	1	1	2	
	GP	1	12	0	20	26	71	65	90	77	0.919
	Acc.	0.986	0.917	**1**	0.794	0.752	1	0.985	**0.989**	0.975	
SVM	GN	71	135	51	94	88	0	0	1	0	
	GP	0	10	1	3	17	71	66	90	79	0.959
	Acc.	**1**	**0.931**	0.981	0.969	**0.838**	**1**	**1**	**0.989**	**1**	

The taxonomy: Sample 1−4, *E. coli*; Sample 5, *K. pneumoniae*; Sample 6−9, *E. faecalis*.