Table S1. Experimental parameters, spectral processing, Raman fingerprints, chemometric models, validation methods, and basis for molecular assignments of all studies reviewed.

Study Reference and Description of Samples Analyzed	**Scanning Details** *Wavelength; SERS; Surface; Liquid/Dried*	**Spectral Processing** *Raman shifts used; Baselining; Normalization*	**Dataset Size; Chemometric Methods; Software**	**Validation Methods** *For Predictive Models, if Present*	**Basis for Molecular Assignments**
Žukovskaja et al. [48]; Urine from mice with kidney disorders, Aspergillosis, asthma, and controls	785 nm; CaF_2 slide; Dried liquid	503-1,631 cm^{-1}; SNIP with 2nd order clipping filter, Wavelength calibration with 4-acetaminophenol; Area normalization	Mice with kidney disorders (n=18), Aspergillosis (n=14), Asthma (n=22); PCA, LDA; R	LOOCV (Leave one mouse out); Confusion matrix, accuracy, sensitivity, specificity	Spectra
Xu et al. [40]; THP-1 cells, monocyte-derived dendritic cells, macrophages infected with nontyphoidal *Salmonella enterica* serovar Typhimurium LT2 (ATCC 700220), clinical isolate STM-D32580, typhoidal *S. enterica* serovar Typhi Ty2 (ATCC 700931), *E. coli* DH5α	532 nm; Raman slide (surface details N/A); Fixed and dried cells	500-3,500 cm^{-1}; Polyline (LabSpec 6); Vector normalization	3 eukaryotic cultures, 3 bacterial strains, 6 time points; PCA, kNN, t-SNE; R	LOOCV; Sensitivity, accuracy	Spectra; PC1 loadings
Wichmann et al. [32]; Six bacterial species stored under five conditions	532 nm; Nickel slide; Dried cells	600-1,800 cm^{-1}, 2,700-3,200 cm^{-1}; AsLS; Vector normalization	6 species, 5 conditions; PLS; R	LOO (Leave one batch out); Accuracy, sensitivity, specificity	Spectra
Wang et al. [34]; *L. bulgaricus* exposed to penicillin G, ampicillin, vancomycin	780 nm; citrate-capped AuNPs SERS and gold surface; Dried cells	500-2,2000 cm^{-1}; Secondary derivative transformation; Citrate-reduced AgNP peak	1 strain, 3 antibiotics, 3 time points, 3 concentrations; PCA, PLSR	LOO	Spectra
Villa et al. [15]; *Gordonia*,	785 nm; AuNP	350-1,850 cm^{-1}; 1st derivative of	6 species, 190 spectra total; PLS-	⅔ dataset for training, ⅓ for	Spectra

Micobacterium, Brevibacterium species	SERS, coated porous filter paper; Dried cells	Savitzky-Golay smoothing; Mean centering	DA; PLS Toolbox in MATLAB v8.3	testing; FPR, FNR, STR, SPR, EFR; 100%	
Verma et al. [4]; *Mycobacterium indicus pranii, M. intracellulare*	514 and 785 nm; MgF_2; Dried cells	600-1,700 cm^{-1}; 3rd order polynomial Savitzky-Golay filtering, in-house algorithm; Vector normalization	3 isolates, 4 growth phases, 14 and 28 days; Quantification of intensities and ratios, ANOVA, PCA, HCA; GraphPad Prism 6, Unscrambler X	N/A	Spectra; standards
Senger et al. [47], Senger and Robertson [24]; Urine from end-stage kidney disease patients and healthy volunteers, peritoneal dialysis fluid	785 nm; Glass vials; Bulk liquid	400-1,800 cm^{-1}; Goldindec algorithm; Vector normalization	168; PCA, DAPC, TSD, TPD, ANOVA, Pairwise comparisons; Rametrix™ LITE and PRO Toolboxes in MATLAB r2018a	LOOCV (Leave one sample out); Accuracy, sensitivity, specificity, PPV, NPV	PC 1-4 and DAPC canonicals 1-4 loadings (Raman shift contributions)
Tanniche et al. [21,22]; *Synechocystis* PCC6803 metabolic and light-induced phenotypes	785 nm; Aluminum surface; Dried cells	400-1,800 cm^{-1}; Goldindec algorithm; Vector normalization	19 culture treatments total (triplicates); PCA, DAPC, TSD, TPD, TCD, ANOVA, Pairwise comparisons; Rametrix™ LITE and PRO Toolboxes in MATLAB r2018a	LOOCV (Leave one sample out); Accuracy, sensitivity, specificity	PC 1-4 and DAPC canonicals 1-4 loadings (Raman shift contributions)
Suzuki et al. [20]; Jurkat, HT29, PBMCs, whole blood cells	N/A; Microfluidic device; Live cells	2,800-3,100 cm^{-1}; N/A; N/A	~11,000 cells; CNN, t-SNE; N/A	10,000 (training), 1,000 (testing); Accuracy, confusion matrix	N/A
Shiramizu et al. [10]; Normal and non-Hodgkin lymphoma B-cells	785 nm; Aluminum slides; Dried cells	600-1,800 cm^{-1}; AsLS; Area normalization	2 cell types; PCA, kNN; MATLAB	N/A, Accuracy, specificity	N/A
Sherman et al. [37]; SERS spectra of 63	633 nm; AgNP	500-2,000 cm^{-1}; Blank subtraction;	63; Hierarchical tiers; MATLAB	N/A, Success rate	Spectra

metabolites	SERS, glass bottom well-plate; Liquid	N/A			
Sanchez et al. [42]; Healthy, LsoA- and LsoB Liberibacter infected tomatoes	831 nm; Hand-held spectrometer; Plant tissues	350-2,000 cm^{-1}; N/A; Mean centering, Vector normalization	150 surface spectra for all 3 groups; PLS-DA; PLS_Toolbox	N/A, Confusion matrix, Matthew's correlation coefficient	Spectra
Rüger et al. [39]; Dithiothreitol treated and untreated diatoms	785 nm; CaF_2 slide; Liquid cultures	650-1,800 cm^{-1}; EMSC, Pearson correlation coefficient cutoff; Area normalization	18 culture conditions over 8 hours; PLS-LDA; R hyperSpec, cbmodels packages	N/A	Spectra, PLS-LDA model coefficients
Rafferty et al. [44]; Glucose, lactate, and ammonia levels in CHO cell cultures	785 nm; Stainless steel probe; Liquid	100-3,425 cm^{-1}; Savitzky-Golay filtering, first derivative quadratic; SNV	5 batches (training), 1 batch (testing); PLS, RF, Cubist, SVMr; R	Cross validation, R-squared, RMSECV	N/A
Mondol et al. [19]; Grass, herb, shrub, and tree pollen samples	785 nm; CaF_2 slides; Dry particles	758-1,800 cm^{-1}; EMSC, Wavelength calibration with 4-acetaminophenol; Area normalization	37 pollen types; PCA, HCA, t-SNE, SVM, ANN; N/A	10-fold cross validation	Spectra
Moawad et al. [9]; *Burkholderia mallei*, *B. pseudo mallei*, other *Burkholderia* spp.	532 nm; Nickel foil surface; Dried cells	15-3,275 cm^{-1}; 3rd order polynomial, SNIP algorithm; Vector normalization	36 strains training, 12 strains testing, 3 batches each; PCA, SVM; Gnu R	LOBOCV; Sensitivity, confusion matrix	Spectra
Medeiros Neto et al. [27]; Normal thyroid tissue, goiter, cancer	785 nm; CaF_2 slides; Thyroid slices	400-1,800 cm^{-1}; 8th order polynomial; Vector normalization	30 (10 of each tissue); PCA, LDA, BLR; LabSpec5, OPUS, OriginPro 8, Minitab	LOO, Mean-Whitney test; Sensitivity, specificity	Spectra
M et al. [7]; *E. coli, Klebsiella pneumoniae, Staphylococcus aureus, Proteus vulgaris, Proteus mirabilis*	785 nm; Quartz coverslips; Bacterial colonies	450-1,800 cm^{-1}; 2nd order polynomial Savitzky-Golay filtering, 11-point moving average filtering, AsLS; Mean-centering, vector normalization	246 spectra total, 15 spectra per sample in testing set; PCA, PLS-DA, SVM with range 600-1,750 cm^{-1}; MATLAB 7.0	LOO, confusion matrix, 10 segments cross validation	Spectra and PC 1-3 loadings

Liu et al. [18]; Ten species of marine actinomycetes	532 nm; N/A; Single cell	425-1,942 cm^{-1}; Subtracting spectrum of blank solution, Savitzky-Golay filtering, polynomial fitting; Area normalization	10 species; PCA, LDA, KNN, SVM, HCA, 2DCNN, 1DCNN; MATLAB r2017a	10-fold cross-validation; 95%	Spectra
Lin et al. [8]; Colistin resistant *E. coli* ATCC 25922, *A. baumannii* ATCC 19606, *P. aeruginosa* ATCC 27853; Clinical isolates	532 nm; Glass slide; Dried cells	400-2,000 cm^{-1}; 2nd order polynomial smoothing; 10th order polynomial subtraction; Shifted to zero and area normalization; LabSpec 6 software	12 *E. coli*, 11 *A. baumannii*, 10 *P. aeruginosa*, 30 clinical isolates of each strain; PCA, HCA, Spectral distances; MATLAB r2016b	N/A	PC 1 loadings
Liang et al. [28]; Euploidy, Chromosome aneuploidy	785 nm; Gold coated quartz glass slide; N/A	65-3,200 cm^{-1}; Dark signal subtraction; Vector normalization over 600-1,800 cm^{-1}, Mean-centering	115 euploidy, 94 chromosome aneuploidy (5 replicates each); PCA over 900-1,500 cm^{-1}, Integration of bands for concentrations, kNN, RF, XGB; R	Training set to testing set ratio of 8:2; Precision, sensitivity, F1 score, Accuracy; 95%	PC 3 loadings
Li et al. [26]; *Acinetobacter baylyi* ADP1, *P. fluorescence*, *E. coli* JM109; Succinate, acetate, salicylate, glucose	785 nm; Aluminum surface on glass slide; Dried cells	500-2,000 cm^{-1}; N/A; Vector normalization	3 strains, 4 substrates; PCA, LDA, Dispersion indicator scores; IRootLab Toolbox for MATLAB R2013b	N/A	Spectra
Lemione et al. [43]; Brain cancer patients with glioma (grade II to IV), meningioma, lymphoma, and metastases	785 nm; Hand-held Raman device; Live tissues during surgery	728-1,730 cm^{-1}; Rolling ball algorithm (51 points); SNV	547 acquisitions from 65 surgeries; Bayesian model, MCMC, NUTS, PCA, LDA; Python, R	K-fold (10-fold), Log predictive density, nRMSE	Spectra, *a priori* literature search
Kumamoto et al. [17]; Human breast cancer cell line MCF-7 and a non-tumorigenic	532 nm; CaF_2 substrate; Live cells cultured on	1,397-1,501 cm^{-1} (multiple ranges); Iterative alternative-least-squares polynomial fitting;	2 cell lines, multiple cells and cell regions; PCA, Image analysis, SBR, Euclidean	LOO (spectral region); Accuracy; 90%	PC loadings (various numbers of PCs used)

epithelial cell line MCF-10A	substrate	N/A	distances; MATLAB 9.4		
Krige et al. [45]; *Geobacter sulfurreducens* strain PCA and modified versions ΔOmcS, ΔOmcZ, ΔPilA, KN400	532 nm; 3D printed cuvettes; Liquid cultures	30-1,550 cm^{-1}; Chromatogram baseline estimation and denoising filter using sparsity, Savitsky-Golay filtering; Curve integration	5 strains, multiple time points; N/A; MATLAB R2018	N/A	Spectra
Kopec et al. [31]; Medulloblastoma, breast cancer, and healthy tissues	532 nm; N/A; Fixed tissues	200-1,800 and 2,100-3,500 cm^{-1}; Savitsky-Golay filtering; Vector normalization	Medulloblastoma (n=5), breast cancer (n=7), healthy tissue; BAM, KMCA (imaging methods); WITec Project 4.1	N/A	Spectra
Kögler et al. [41]; *E. coli* cultures expressing HSPA1, Hsp27, and *h*CNTF	532 nm; TG-SERS and CW-Raman, AgNPs, Aluminum microwells; Liquid cultures	500-1,700 cm^{-1}; N/A; Peaks adjusted to [0,1] range	4 recombinant cultures (multiple time points); N/A; OriginPro Software, Timegate Instruments Oy	N/A (No chemometric analysis)	Spectra
Klein et al. [6]; *Brochothrix thermosphacta* DSM 20171, *E. coli* HB101, *E. coli* TOP10, *Micrococcus luteus*, *P. fuorescens* DSM 4358, *P. fuorescens* DSM 50090, *B. thuringiensis israelensis* DSM 5724	785 nm; Stainless steel surface; Blotted cells from agar plate	600-1,200 cm^{-1}; Concave rubber band method; Savitsky-Golay filtering; Minimum - Maximum normalization	7 species, 3,500 spectra; PCA, CDA; Origin Pro 2017G	K-fold; Confusion matrix, Accuracy; 96%	N/A
Kim et al. [49]; Human tears from breast cancer patients and healthy	785 nm; Au/HCP-PS SERS; Dried	417-1,782 cm^{-1}; Concave rubber band method, Savitsky-Golay filtering; Vector	5 control, 5 breast cancer patients; PC-LDA; R	LOOCV; Confusion matrix	Spectra

individuals	liquid	normalization			
Kim et al. [25]; *E. coli* ATCC25922 and six quinolone-resistant blood isolate strains	785 nm; Gold nanoparticle substrate, SERS; Dried cells	417-1,782 cm^{-1}; Concave rubber band method (10 iterations, 64 points); Z-score normalization	7 (1 control, 6 isolates); PCA, Multi SVMs; MATLAB	LOO	Spectra from different zones
Jaafreh et al. [5]; *Micrococcus luteus* DSM 20030, *Brochothrix thermosphacta* DSM 20171, *B. coagulans* DSM 1, *B. subtilis* DSM 10, *P. uorescens* DSM 4358, *P. uorescens* DSM 50090, *E. coli* K12, and *E. coli* HB101; Compared Raman microscope to portable fiber-optic system	785 nm; Stainless steel slide; Dried cells from agar plate	410-1,790 cm^{-1}; Concave rubber band correction method, Savitsky-Golay filtering; Vector normalization	8 (~115 scans/sample with microscope; ~25 scans/sample with fiber-optic); PCA, SVM	K-fold (75%/25%), Confusion matrix; Accuracy, sensitivity, specificity; 97%	Spectra with double standard deviations, PC 1-4 loadings
Huttanus et al. [46]; Urine from BCA, GU, ESKD patients, and healthy volunteers	785 nm; Glass vials; Bulk liquid	400-1,800 cm^{-1}; Goldindec algorithm; Vector normalization	168; PCA, DAPC, TSD, TPD, ANOVA, Pairwise comparisons; Rametrix™ LITE and PRO Toolboxes in MATLAB r2018a	LOOCV (Leave one sample out); Accuracy, sensitivity, specificity, PPV, NPV	PC 1-4 and DAPC canonicals 1-4 loadings (Raman shift contributions)
Huayhongthong et al. [11]; *E. coli* ATCC 25922, *B. cereus* ATCC 11778, *S. aureus* ATCC 13565 and *Salmonella typhimurium* ATCC 13311	785 nm; Aluminum slide, agar plate; Dried, live colonies	500-1,800 cm^{-1}; Specified joint (49 baseline points, 48 regions), Savitsky-Golay filtering; Calibration with Si crystalline wafer reference	73 total; PCA; PLS Toolbox in MATLAB r2018a	N/A (uninformed analysis)	Spectra
Ho et al. [12]; 30	633 nm; Gold-coated silica	381.98-1792.4 cm^{-1}; 5th-order polynomial	30 reference isolates plus MSSA	LOO, K-fold (5/30 samples),	N/A

bacterial and yeast isolates, including MRSA and MSSA; patient isolates	substrate; Dried monolayer cells	fit; Peaks adjusted to [0,1] range	at 3 reference times, 55 patient isolates; CNN, SVM, LR, PCA; Python	Confusion matrix, Welch's t-test; >80%	
García-Timermans et al. [38]; Three growth stages of *E. coli*	785 nm; CaF_2 slide; Dried cells	600-1,800 cm^{-1}; SNIP algorithm baselining; Area under curve normalization with MALDIquant package	9 (3x3; 60 replicates each); PCA, t-SNE, HCA, PhenoGraph, ARI, BA; R, RStudio, Python	N/A (uninformed analysis)	Boruta algorithm
Fisher et al. [23]; Enzyme kinetics, Culture growth, Chronic kidney disease	785 nm; Aluminum surface or glass vials; Dried cells or bulk liquid samples	200-2,000 cm^{-1}; Goldindec algorithm; Vector normalization	Varies for each study; PCA, DAPC, TCD; MATLAB r2018a with Rametrix™ LITE Toolbox	N/A	PC 1 loadings (Raman shift contributions)
Fallahzadeh et al. [29]; Normal, benign, and cancerous breast tissue samples	785 nm; N/A; Fixed tissue	500-3,200 cm^{-1}; Range independent algorithm, Savitsky-Golay filtering; Band height normalization	11 samples (49 spectra); ACO, QDA; MATLAB 7	LOO, Confusion matrix; 87%	Spectra
De Marchi et al. [35]; Metabolites secreted by *E. coli* and *Pseudomonas aeruginosa* in mixed populations	785 nm; AuNP films on glass slide covered by agar; Living colonies in agar	400-1,700 cm^{-1}; Performed with WiRE software v4.3	N/A	N/A	Spectra of cultures and experimental standards
Cordero et al. [30]; Bladder biopsies showing non-tumor, tumor, high grade, low grade cancer	785 nm; CaF_2 slide; Biopsied cells	400-3,200 cm^{-1}; AsLS, Dark spectrum subtraction, Savitsky-Golay filtering, Wavenumber calibration: peak position of N-acetyl p-aminophenol; Intensity calibration: White light source	67 samples from 28 patients; PLS, LDA; R	LOO, 2-layer cross validation (K-folds)	Mean spectra

Clèment et al. [50]; Detergent surfactants	785 nm; Quartz cuvette; Liquid	150-3,480 cm^{-1}; MSC	1 detergent, 3 components; PLSR, ICA-ML, ICA-JADE, FastICA; MATLAB r2016b with PLS Toolbox 8.2	Cross and external validation; RMSEC, RMSECV, RMSEP	Experimental standards
Chisanga et al. [33]; *Campylobacter jejuni* wild-type and mutants	785 nm; AgNPs; Spotted onto CaF_2 discs; Dried cells	400-1,800 cm^{-1}; AsLS; EMSC	Wild-type, 5 mutants, 10 replicates; PCA, DFA, HCA; MATLAB r2017a	Compared against MALDI-TOF-MS experimental data	Spectra, PC 1 and 2 loadings (Raman shift contributions)
Chen et al. [14]; *Staphylococcus aureus* ATCC 29213 *S. aureus* ATCC 25923, *Bacillus cereus, E. coli, Pseudomonas aeruginosa, Candida albicans;* MRSA, MSSA; multi-drug resistant isolates	532 nm; $AgNPs^{+}$; Dried cells	200-2,000 cm^{-1}; Automated function of LabSpec 6 software	1 sample per culture, 52 MSSA, 215 MRSA; PLS-DA, OPLS-DA; SIMCA 14.0	Correlation coefficient and predictive coefficient; K-fold (10-fold)	OPLS-DA Raman shift contributions
Cao et al. [36]; HEK293T cells with and without Cytochrome P450 2C9 expression	785 nm; AgNWs, AuNPs APTES functionalized silicon wafers; Dried cells	600-1,800 cm^{-1}; 5-point smoothing, normalization; Vertical movement with Micro Origin 8.0 software	1 sample per culture; PCA; MATLAB v.8.1	N/A	Spectra
Akanny et al. [13]; Discrimination of *Bacillus subtilis, Lactobacillus rhammosus GG, Escherichia coli*	785 nm; Uncoated spherical AuNPs, AgNPs; 1-cm quartz cell; Liquid	600-1,750 cm^{-1}; automatic weighted least squares; N/A	18 samples total; PCA, PLS-DA; MATLAB with PLS Toolbox	LOO; K-fold (20% of dataset); Sensitivity / Specificity; 100% each	VIP
Alunni Cardinali et al. [16]; *Candida albicans* CMC 1968, *C. tropicalis* CMC 2052, *C. parapsilosis* CMC 1841, and *C. glabrata* CMC 2032	532 nm, 20x microscope objective and 30 mm lens; Stainless steel substrate; Dried layers	800-3,100 cm^{-1}; Spline function; CH_2-CH_3 band (2,800-3,050 cm^{-1})	1 sample per culture; PCA excluding 1,780-2,640 cm^{-1}; R	N/A	First two PCs

Table S2. Definition of validation metrics.

Metric	Formula or Definition
TP	True positives
TN	True negatives
FP	False positives
FN	False negatives
Accuracy	(TP + TN) / (TP + TN + FP + FN)
Sensitivity [21,22,46,47]	TP / (FN + TP)
Specificity [21,22,46,47]	TN (TN + FP)
Positive predictive value (PPV) [21,22,46,47]	TP / (TP + FP)
Negative predictive value (NPV) [21,22,46,47]	TN / (TN + FN)
False positive rate (FPR) [15]	FP / (FP + TN) x 100
False negative rate (FNR) [15]	FN / (FN + TP) x 100
Sensitivity rate (STR) [15]	TP / (TP + FN) x 100
Specificity rate (SPR) [15]	TN / (TN + FP) x 100
Efficiency rate (EFR) [15]	EFR = 100 - (FPR + FNR)

ABBREVIATIONS

1DCNN: One-dimensional convolutional neural network
2DCNN: Two-dimensional convolutional neural network
ACO: Ant colony optimization
AgNPs: Silver nanoparticles
$AgNPs^{+}$: Positively-charged silver nanoparticles
AgNWs: Silver nanowires
ANN: Artificial neural network
ARI: Adjusted Rand Index
AsLS: Asymmetric least-squares fitting
Au/HCP-PS: Gold-decorated close-packed polystyrene nanosphere monolayer
AuNPs: Gold nanoparticles
BA: Boruta algorithm
BCA: Bladder cancer
BLR: Binary logistic regression
CDA: Canonical discriminant analysis
CNN: Convolutional neural network
CW: Continuous wave
DA: Discriminant analysis
DAPC: Discriminant analysis of principal components
DFA: Discriminant function analysis
EFR: Efficiency rate
EMSC: Extended multiplicative signal correction
ESKD: End-stage kidney disease
FN: False negative
FNR: False negative rate
FP: False positive
FPR: False positive rate
GU: Genitourinary cancer
HCA: Hierarchical cluster analysis
ICA-JADE: Independent component analysis - joint approximation diagonalization of eigenmatrices
ICA-ML: Independent component analysis - maximum likehood
kNN (KNN): k-Nearest neighbors
LDA: Linear discriminant analysis
LOBOCV: Leave-one-batch-out cross-validation
LOO: Leave-one-out
LOOCV: Leave-one-out cross-validation
LR: logistic regression
MCMC: Markov chain Monte Carlo sampling
MRSA: Methicillin-resistant *S. aureus*
MSC: Multiplicative signal correction
MSSA: Methicillin-sensitive *S. aureus*

N/A: Not available or not found in our analysis
NPV: Negative predictive value
nRMSE: Normalized root-mean squared error
NUTS: No-U-turn sampling
OPLS: Orthogonal projections to latent structures
PC-LDA: Linear discriminant analysis of principal components
PCA: Principal component analysis
PCs: Principal components
PLS: Partial least-squares
PLS-DA: Discriminant analysis of partial least-squares
PLS-LDA: Linear discriminant analysis of partial least-squares
PLSR: Partial least-squares regression
PPV: Positive predictive value
QDA: Quadratic discriminant analysis
RF: Random forests
RMSE: Root mean square error
RMSEC: Root mean square of calibration
RMSECV: Root mean square of cross validation
RMSEP: Root mean square of prediction
SBR: Signal-to-background ratio
SNIP: Sensitive nonlinear iterative peak
SNV: Standard variate normalization
SPR: Specificity rate
STR: Sensitivity rate
SVM: Support vector machines
SVMr: Support vector machines radial
TCD: Total canonical distance
TG-SERS: Time-gated surface enhanced Raman spectroscopy
TN: True negative
TP: True positive
TPD: Total principal component distance
TSD: Total spectral distance
t-SNE: t-distributed stochastic nearest neighbor embedding
VIP: Variable importance projection
XGB: Extreme gradient boosting