Supplementary Material (ESI) for Chemical Communications

Supporting Information

Rapid Ambient Mass Spectrometric Profiling of Fresh Intact Bacteria by using Desorption Electrospray Ionization

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Abstract: Additional information regarding bacteria preparation, mass spectrometric analysis and PCA is provided. Additional data are included for a typical DESI mass spectrum of *E. coli* JM109, low mass portions of the DESI mass spectra of *E. coli* DH10B, JM109 and *S. typhurium* TL212, and a loading plot of the first principal component (PC1).

All bacteria were obtained from the Department of Biochemistry, Purdue University. Bacteria were grown in 8 g/L nutrient broth for 12 hours and isolated by centrifuging the growth mixture at 13000g for 2 min. Isolated cells were washed twice with water and suspended in water at a concentration of approximately 1x108 cells/mL for immediate MS analysis. All mass spectra were recorded in the positive ion mode using a Thermo Finnigan LTQ mass spectrometer (San Jose, CA) equipped with a desorption electrospray ion source, (prototype Omni Spray Ion Source, Prosolia Inc., Indianapolis, IN) which is described elsewhere. [1, 2] Secondary ions generated from the bacterial samples were collected using a standard heated capillary interface with an orifice diameter of 500 μm. For tandem mass spectrometry, the precursor ions were isolated using a window of 1.5 mass/charge units (full-width) and dissociated by collisional activation with helium buffer gas for 30ms using a 30% collision energy setting (Thermo LTQ arbitrary unit).

Reproducibility of the data

Subtle but distinguishable differences are observable in Figure 1 by superimposing three spectra together with each spectrum in different color.

The data reported in this communication were all recorded using the standard CH_3OH/H_2O spray solvent. This solvent is the most widely used DESI spray and produces highly reproducible data. Although not reported in the communication, experiments were actually performed by doping acids, organic solvents and even surfactants into the spray. Spray solvent doping does have notable effects, which are being investigated further and will be reported in a more detailed study.

PCA Analysis

Principal component analysis (PCA) was performed using an in-house MatLab program (The MathWorks, Inc, version 7.1). Total intensity normalization was performed on each spectrum, using the full spectral range, then PCA was carried out after mean-centering preprocessing. In other words, covariance PCA was performed. In autoscaling preprocessing or correlation PCA, it is possible to overemphasize the effect of noise by scaling with the standard deviation.

The first two PCs captured 82% of the total X variance. Since first two PCs explain most of the variations, other PCs were not examined in this study.

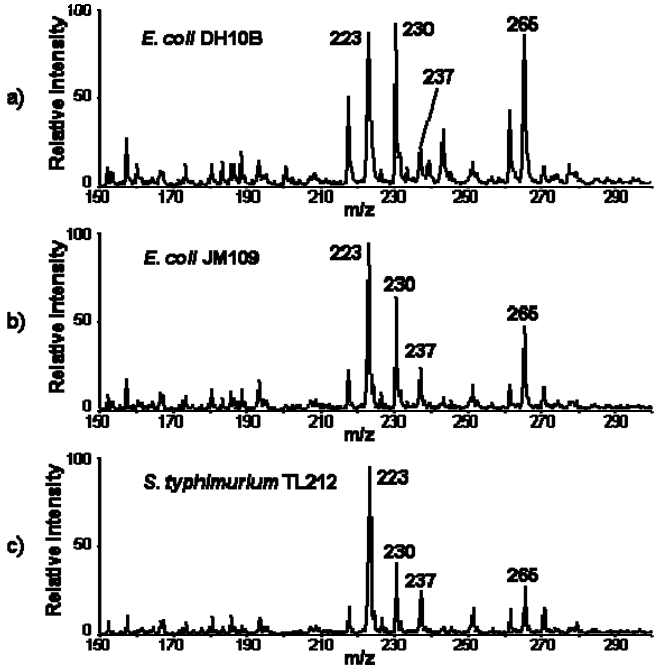

Figure S1. Typical low mass range DESI mass spectra of a) *E. coli* DH10B, b) *E. coli* JM109 and c) *S. typhimurium* TL212.

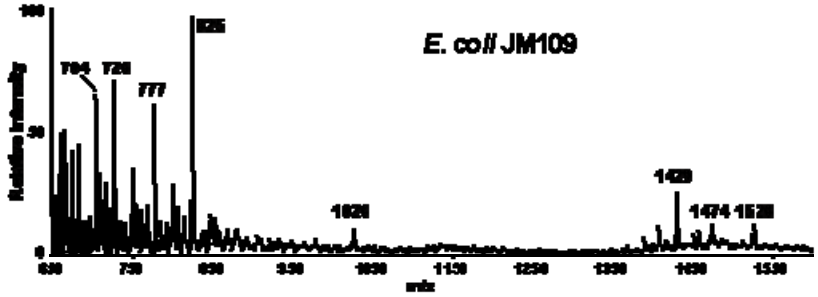

Figure S2. Typical DESI mass spectrum of *E. coli* JM109.

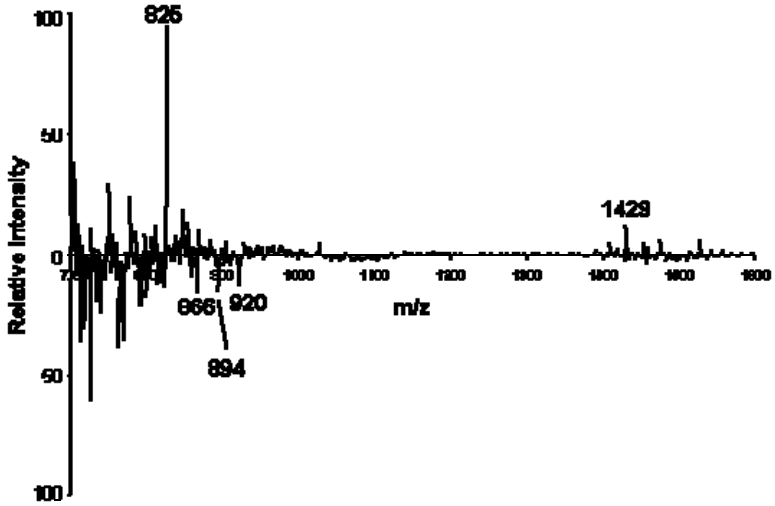

Figure S3. Loading plot of the first principal component (PC1).

Reference:

1 Z. Takats, J. Wiseman, B. Gologan and R. G. Cooks, *Science,* 2004, 306, 471.
2 Z. Takats, J. Wiseman and R. G. Cooks, *J. Mass Spectrom.,* 2005, 40, 1261.