Supporting information

Title of main article: Strain-Level Differentiation of Bacteria by Paper Spray Ionization Mass Spectrometry

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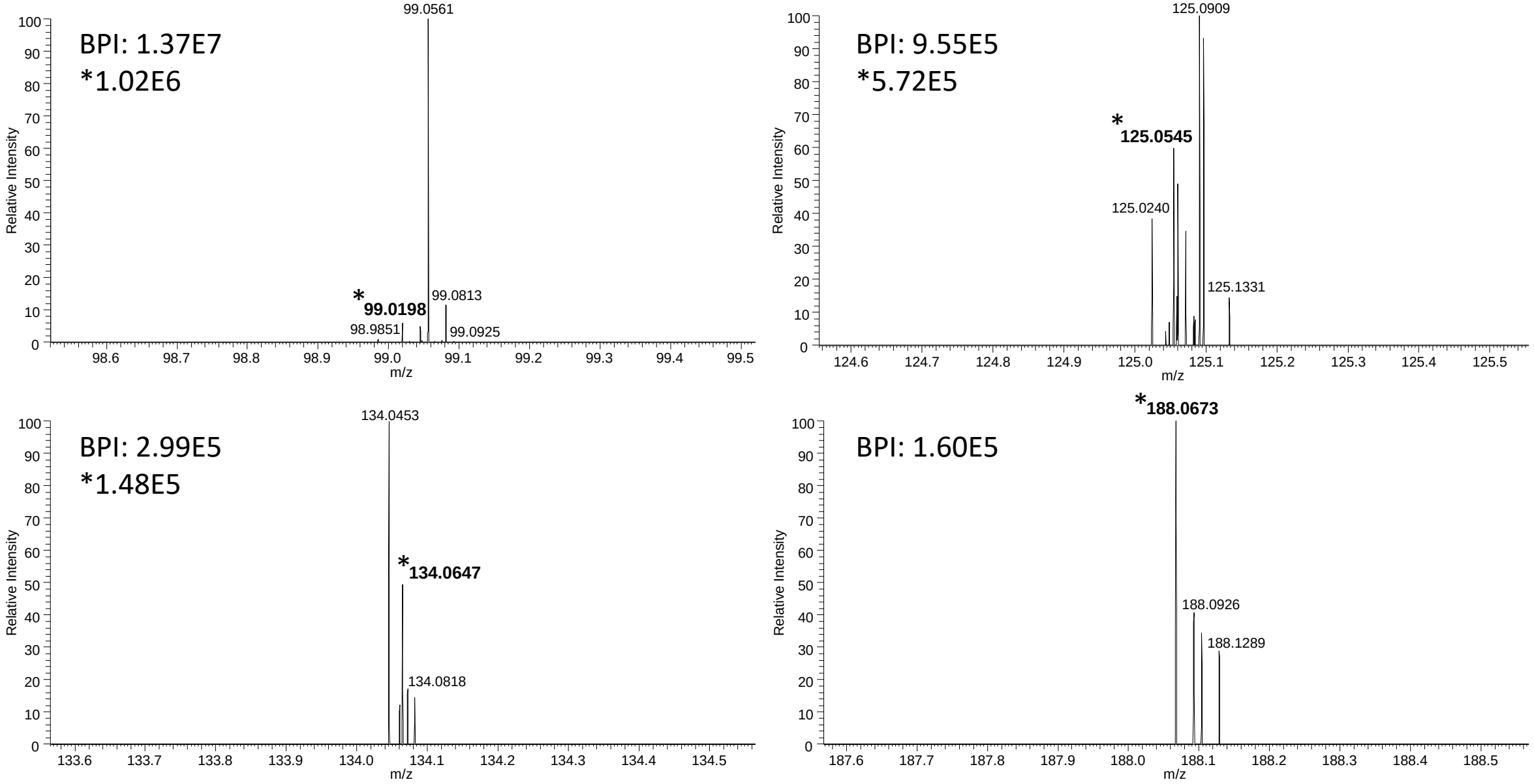

Figure S1. PSI-MS spectra obtained from OxWR lysates representing 4 of the strain-specific features: *m/z* 99.0198, 125.0545, 134.0647, 188.0673. 1 *m/z* windows centered on the targeted ion show competing ions at similar or much larger intensities, making MS/MS isolation even on HRMS difficult for identification purposes. BPI indicates Base Peak Intensity. Asterisk (*) indicates ion of interest and associated intensity level.

Table S1. Parameters for PSI-MS instrumentation and methodology

Mass Spectrometer	Thermo Q Exactive
Spray Voltage	4.5 kV
Capillary Temp	270° C
S-Lens RF	30%
Paper Spray System	Prosolia Velox 360
Solvent	4:1 H2O:ACN + 0.1% FA
Dispensing Steps	8
Dispense Volume	80 µL
Sample Dispense	5
Scan	Full MS
Mass Range	70 - 1,000 *m/z*
Resolution	140,000
Polarity	Positive

Table S2. Predicted chemical formula, adduct, and identification information for strain-exclusive features from CEU Mass Mediator screening the Human Metabolome Database, KEGG, Metlin, and Lipid Maps for exact mass matches (5ppm) to common ESI(+) adducts of known metabolites and lipids.

Experimental Mass (*m/z*)	Strain	Analysis	Formula	Adduct	Error (PPM)	Name
75.0325	OxWR	Lysates, Whole Cells				*No identifications found*
93.0384	OxWR	Whole Cells				*No identifications found*
99.0198	OxWR	Whole Cells				*No identifications found*
100.0276	OxWR	Lysates, Whole Cells				*No identifications found*
101.0988	OxWR	Lysates				*No identifications found*
105.0303	OxWR	Whole Cells				*No identifications found*
115.0145	OxWR	Lysates	C3H4N2O4	$[M+H-H2O]^+$	4	Oxalureate; Oxaluric acid; Monooxalylurea; Oxalurate; N-Carbamoyl-2-oxoglycine
121.0251	OxWR	Whole Cells				*No identifications found*
125.0545	OxWR	Lysates, Whole Cells				*No identifications found*
133.0250	OxWR	Lysates, Whole Cells	C3H4N2O4	$[M+H]^+$	5	Oxalureate; Oxaluric acid; Monooxalylurea; Oxalurate; N-Carbamoyl-2-oxoglycine
134.0647	OxWR	Whole Cells				*No identifications found*
135.0406	OxWR	Lysates, Whole Cells	C3H6N2O4	$[M+H]^+$	4	(R)-Ureidoglycolate; (+)-Ureidoglycolate; (+)-Ureidoglycolic acid
						(S)-Ureidoglycolic acid
			C4H12N2S2	$[M+H-H2O]^+$	3	Cystamine
135.0770	OxWR	Whole Cells	C4H10N2O3	$[M+H]^+$	4	L-Canaline
						N-Nitrosodiethanolamine
143.0649	OxWR	Lysates				*No identifications found*
157.0807	OxWR	Lysates				*No identifications found*
159.0406	OxWR	Lysates	C5H6N2O4	$[M+H]^+$	4	L-5-Carboxymethylhydantoin
						Ibotenic acid
						L-Dihydroorotic acid
						4,5-Dihydroorotic acid
			C5H8N2O5	$[M+H-H2O]^+$	3	3-(Carboxycarbonylamino)-L-alanine; N3-Oxalyl-L-2,3-diaminopropanoate; L-alpha-Amino-beta-oxalylaminopropionic acid; beta-ODAP
						N-Carbamoyl-DL-aspartic acid
						Ureidosuccinic acid
						L-3-Amino-2-(oxalylamino)propanoic acid
						L-2-Amino-3-(oxalylamino)propanoic acid
164.1018	OxWR	Lysates				*No identifications found*
174.0516	OxWR	Lysates, Whole Cells	C5H7N3O4	$[M+H]^+$	4	Azaserine
188.0673	OxWR	Lysates, Whole Cells	C6H9N3O4	$[M+H]^+$	4	1-(2-Hydroxyethyl)-2-hydroxymethyl-5-nitroimidazole
325.3667	HC1	Whole Cells				*No identifications found*
334.3476	HC1	Whole Cells				*No identifications found*
339.3823	HC1	Whole Cells				*No identifications found*
353.3978	HC1	Whole Cells				*No identifications found*