

Bacterial identification by lipid profiling using liquid atmospheric pressure matrix-assisted laser desorption/ionization mass spectrometry

Article

Supplemental Material

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Supplemental Material for

“Bacterial identification by lipid profiling using liquid atmospheric pressure matrix-assisted laser desorption/ionization mass spectrometry”

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Table S1	Page S2
Figure S1	Page S3
Figure S2	Page S3
Table S2	Page S4
Table S3	Page S8

Table S1 – Bacterial species and NCTC strain number used for liquid AP-MALDI MS analysis.

Species	NCTC Strain Number
<i>Campylobacter jejuni</i>	11322
<i>Escherichia coli</i>	12241
<i>Enterococcus faecalis</i>	775
<i>Enterococcus hirae</i>	5855
<i>Klebsiella pneumoniae</i>	9633
<i>Lactobacillus brevis</i>	13386
<i>Pseudomonas aeruginosa</i>	12903
<i>Staphylococcus aureus</i>	6571
<i>Staphylococcus epidermidis</i>	13360
<i>Streptococcus pyogenes</i>	12696

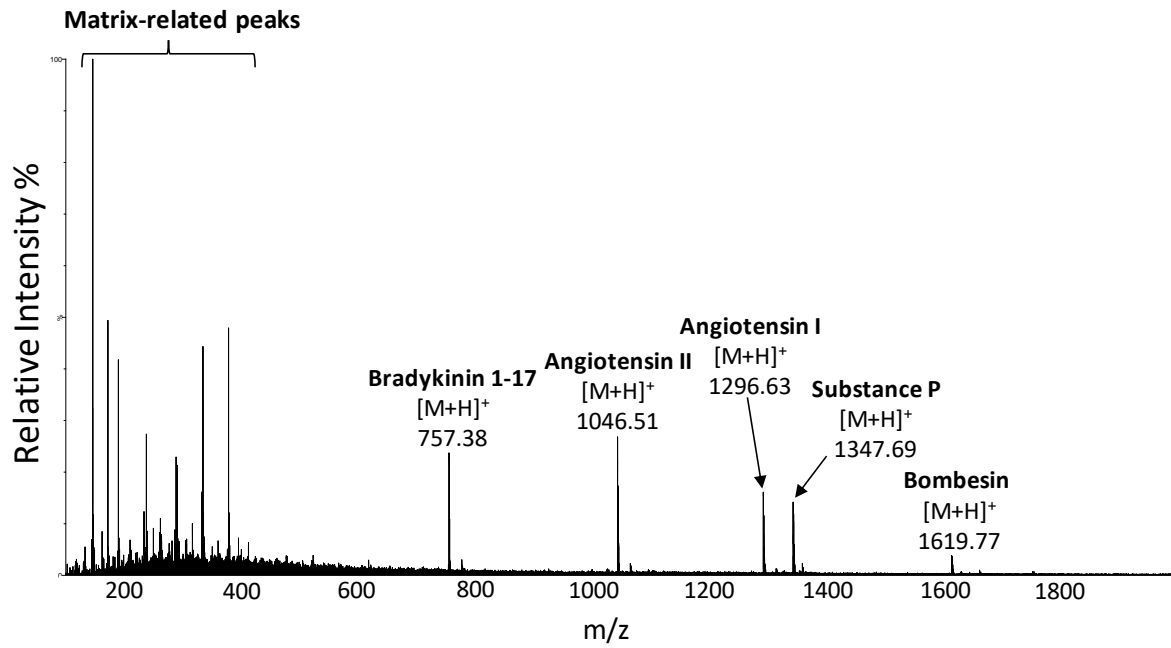


Figure S1 – Solid AP-MALDI mass spectrum of the peptide calibration standard mixture used in this study.

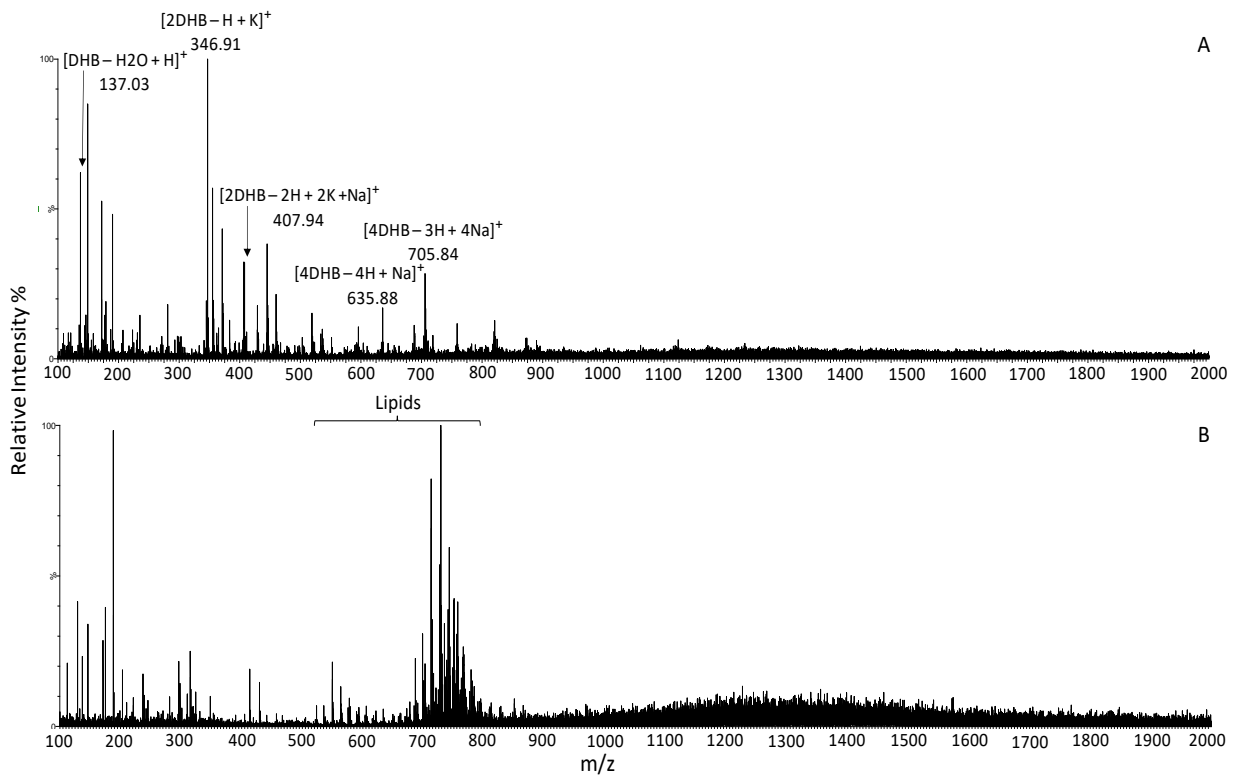


Figure S2 – AP-MALDI mass spectra of *E. coli* obtained from a solid (A) and liquid (B) MALDI sample, using DHB as the matrix chromophore compound.

Table S2 – Putative identification of lipid species observed in liquid AP-MALDI MS profiling of bacterial species (as seen in Figure 2), using accurate mass matching of entries in the LIPID MAPS Structure Database (LMSD; <https://www.lipidmaps.org/data/structure/LMSDSearch.php>).

m/z*	<i>C. jejuni</i>	<i>E. coli</i>	<i>E. faecalis</i>	<i>E. hirae</i>	<i>K. pneumoniae</i>	<i>L. brevis</i>	<i>P. aeruginosa</i>	<i>S. aureus</i>	<i>S. epidermidis</i>	<i>S. pyogenes</i>	Elemental Composition [#]	Putative Lipid Assignment [§]	LIPID MAPS Structure Database Accession Number
523.47	•	•			•						C ₃₂ H ₅₈ O ₅	Diacylglycerol	LMGL02010334
535.47		•									C ₃₃ H ₅₈ O ₅	Diacylglycerol or Isoprenoid	LMGL02010338, LMPRO1070021, LMPRO1070087, LMPRO1070088, LMPRO1070164
549.47	•	•			•						C ₃₈ H ₆₀ O ₂	Fatty Ester	LMFA07011032
563.50		•			•		•				C ₃₅ H ₆₂ O ₂	Diacylglycerol	LMGL02010343, LMGL02010386, LMGL02010409, LMGL02010454
577.51	•	•	•	•	•	•	•				C ₃₇ H ₆₈ O ₄	Fatty Alcohol	LMFA05000691
589.45		•	•	•	•						C ₃₇ H ₆₄ O ₅	Diacylglycerol	LMGL02010028, LMGL02010035, LMGL02010351, LMGL02010392, LMGL02010415, LMGL02010475, LMGL02010498
591.49	•				•			•	•	•	C ₃₇ H ₆₆ O ₅	Diacylglycerol	LMGL02010024, LMGL02010031, LMGL02010032, LMGL02010350, LMGL02010391, LMGL02010414, LMGL02010474
603.53	•	•			•						C ₃₉ H ₇₀ O ₄	Diacylglycerol	LMGL02070004, LMGL02070010, LMGL02070011, LMGL02070023, LMGL02070024
607.46								•	•	•	C ₃₇ H ₆₈ O ₄	Glycerophosphate	LMGP10020004, LMGP10020019
651.58							•				C ₄₁ H ₇₈ O ₅	Diacylglycerol or Sterols	LMGL02010081, LMGL02010082, LMGL02010105, LMGL02010106, LMGL02010113, LMGL02070009, LMGL02070018, LMGL02070020, LMGL02070031, LMGL02070032, LMST01020003, LMST01020054, LMST01020056, LMST01020094
664.48	•	•									C ₃₅ H ₇₀ NO ₈ P	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010700, LMGP01011244, LMGP01011262, LMGP01011317, LMGP01011339, LMGP01011363, LMGP01011409, LMGP01020176, LMGP02010106, LMGP02010297, LMGP02010302, LMGP02010316, LMGP02011207, LMGP02011215, LMGP02011255, LMGP02011261

676.49																$C_{36}H_{70}NO_8P$	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010392, LMGP01011319, LMGP01011341, LMGP01011364, LMGP01011381, LMGP01011432, LMGP01011473, LMGP02010005, LMGP02010353, LMGP02010355, LMGP02010371, LMGP02010390, LMGP02010410, LMGP02010429, LMGP02010480, LMGP02010507, LMGP02010518, LMGP02010563, LMGP02010636, LMGP02010793, LMGP02011235, LMGP02011267		
690.49																		$C_{37}H_{72}NO_8P$	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010735, LMGP01011321, LMGP01011343, LMGP01011365, LMGP01011382, LMGP01011411, LMGP01011433, LMGP01011474, LMGP01011521, LMGP02010372, LMGP02010395, LMGP02010432, LMGP02010456, LMGP02010482, LMGP02010520, LMGP02010541, LMGP02010565, LMGP02010622, LMGP02010794, LMGP02010841, LMGP02011199, LMGP02011228, LMGP02011247, LMGP02011268
704.50																		$C_{38}H_{74}NO_8P$	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010440, LMGP01010485, LMGP01011344, LMGP01011384, LMGP01011412, LMGP01011435, LMGP01011463, LMGP01011475, LMGP01011522, LMGP01011595, LMGP02010396, LMGP02010414, LMGP02010438, LMGP02010458, LMGP02010485, LMGP02010521, LMGP02010543, LMGP02010567, LMGP02010624, LMGP02010638, LMGP02010769, LMGP02010795, LMGP02010842, LMGP02011226, LMGP02011266
712.48																		$C_{39}H_{70}NO_8P$	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01011351, LMGP01011701, LMGP02010380, LMGP02010443, LMGP02010525, LMGP02010526, LMGP02010686, LMGP02010716, LMGP02010744, LMGP02010905, LMGP02010935, LMGP02011102, LMGP02011208, LMGP02011223, LMGP02011242
718.53																		$C_{39}H_{76}NO_8P$	Glycerophosphocholine, Glycerophosphoethanolamine or Glycerophosphoserine	LMGP01010002, LMGP01010008, LMGP01010535, LMGP01011328, LMGP01011347, LMGP01011367, LMGP01011386, LMGP01011437, LMGP01011464, LMGP01011477, LMGP01011523, LMGP01011596, LMGP01011756, LMGP02010009, LMGP02010010, LMGP02010099, LMGP02010311, LMGP02010378, LMGP02010415, LMGP02010440, LMGP02010462, LMGP02010491, LMGP02010524, LMGP02010544, LMGP02010569, LMGP02010770, LMGP02010797, LMGP02010824, LMGP02010843, LMGP02011040, LMGP02011204, LMGP03010098, LMGP03010117, LMGP03010168, LMGP03010206, LMGP03010251, LMGP03010280
726.49																		$C_{40}H_{72}NO_8P$	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010499, LMGP01010500, LMGP01010568, LMGP01010698, LMGP01011332, LMGP01011392, LMGP01011393, LMGP01011643, LMGP01011674, LMGP01011702, LMGP01011897, LMGP02010404, LMGP02010467, LMGP02010496, LMGP02010549, LMGP02010574, LMGP02010575, LMGP02010603, LMGP02010662, LMGP02010688, LMGP02010718, LMGP02010746, LMGP02010907, LMGP02010937, LMGP02011103
730.54																		$C_{40}H_{76}NO_8P$	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010494, LMGP01010496, LMGP01010682, LMGP01010684, LMGP01011330, LMGP01011390, LMGP01011414, LMGP01011440, LMGP01011526, LMGP01011555, LMGP01011597, LMGP01011616, LMGP01011835, LMGP02010403, LMGP02010465, LMGP02010494, LMGP02010528, LMGP02010546, LMGP02010572, LMGP02010601,

																						LMGP02010627, LMGP02010641, LMGP02010660, LMGP02010800, LMGP02010846, LMGP02010875, LMGP02011072					
735.55		•																					C ₄₀ H ₇₉ O ₉ P	Glycerophosphoglycerol	LMGP04020044, LMGP04020072, LMGP04020092, LMGP04030012, LMGP04030034, LMGP04030058		
740.52		•	•																					C ₄₁ H ₇₄ NO ₈ P	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01011356, LMGP01011418, LMGP01011445, LMGP01011446, LMGP01011645, LMGP01011676, LMGP01011704, LMGP01011898, LMGP02010096, LMGP02010111, LMGP02010112, LMGP02010421, LMGP02010532, LMGP02010643, LMGP02010691, LMGP02010749, LMGP02010909, LMGP02011104, LMGP02011174, LMGP02011190, LMGP02011197, LMGP02011203	
744.56		•																						C ₄₁ H ₇₈ NO ₈ P	Glycerophosphocholine or Glycerophosphoethanolamine	LMGP01010543, LMGP01011354, LMGP01011396, LMGP01011443, LMGP01011465, LMGP01011481, LMGP01011528, LMGP01011557, LMGP01011599, LMGP01011618, LMGP01011759, LMGP01011836, LMGP02010039, LMGP02010044, LMGP02010052, LMGP02010109, LMGP02010420, LMGP02010448, LMGP02010510, LMGP02010530, LMGP02010578, LMGP02010607, LMGP02010774, LMGP02010802, LMGP02010848, LMGP02010877, LMGP02011043, LMGP02011073, LMGP02011193, LMGP02011270	
753.54																									C ₄₃ H ₇₇ O ₈ P	Glycerophosphate	LMGP10010362, LMGP10010391, LMGP10010419, LMGP10010449, LMGP10010547, LMGP10010577, LMGP10010607, LMGP10010636, LMGP10010712, LMGP10010738, LMGP10010739, LMGP10010768, LMGP10010797, LMGP10010861, LMGP10010883,
795.53			•	•	•																				C ₄₁ H ₇₉ O ₁₂ P	Glycerophosphoinositol	LMGP06020008, LMGP06020022, LMGP06030008, LMGP06030031, LMGP06030057
915.58																									C ₄₉ H ₈₇ O ₁₃ P	Glycerophosphoinositol	LMGP06010332, LMGP06010361, LMGP06010389, LMGP06010419, LMGP06010517, LMGP06010547, LMGP06010577, LMGP06010606, LMGP06010682, LMGP06010708, LMGP06010709, LMGP06010738, LMGP06010767, LMGP06010831, LMGP06010853
931.56																									C ₅₁ H ₇₉ O ₁₃ P	Glycerophosphoinositol	LMGP06010616, LMGP06010808
941.60				•	•																				C ₅₁ H ₈₉ O ₁₃ P	Glycerophosphoinositol	LMGP06010524, LMGP06010585, LMGP06010613, LMGP06010642, LMGP06010689, LMGP06010717, LMGP06010747, LMGP06010776
945.57																									C ₄₅ H ₈₅ O ₁₈ P	Glycerophosphoinositolglycan	LMGP15010002
973.59																									C ₄₇ H ₈₉ O ₁₈ P	Glycerophosphoinositolglycan	LMGP15010003, LMGP15010014
1047.70				•	•																				C ₅₅ H ₁₀₂ N ₂ O ₁₆	Acidic glycosphingolipid	LMSP0601AA03

*measured monoisotopic m/z value of the protonated ion species, #obtained from LMSD with a mass tolerance of ±0.05 Da; §obtained from the main class category in LMSD. In general, flavonoids were excluded from the search results.

Table S3 – Most relevant lipid ion signals for the first 2 principle components of the PCA undertaken in this study (see Table S2 for accession number from LIPID MAPS structure database).

m/z	Putative lipid identification	Species detected in
607.50	Glycerophosphate	<i>S. aureus</i> , <i>S. epidermidis</i> , <i>S. pyogenes</i>
704.50	Glycerophosphocholine or Glycerophosphoethanolamine	<i>E. coli</i> , <i>K. pneumoniae</i>
730.50	Glycerophosphocholine or Glycerophosphoethanolamine	<i>C. jejuni</i> , <i>K. pneumoniae</i>
744.50	Glycerophosphocholine or Glycerophosphoethanolamine	<i>C. jejuni</i> , <i>K. pneumoniae</i>
915.50	Glycerophosphoinositol	<i>S. aureus</i> , <i>S. epidermidis</i> , <i>S. pyogenes</i>
931.50	Glycerophosphoinositol	<i>S. aureus</i> , <i>S. epidermidis</i> , <i>S. pyogenes</i>
941.50	Glycerophosphoinositol	<i>E. faecalis</i> , <i>E. hirae</i> , <i>L. brevis</i> , <i>S. pyogenes</i>
959.50	Glycerophosphoinositol	<i>E. faecalis</i> , <i>E. hirae</i> , <i>K. pneumoniae</i> , <i>S. epidermidis</i> , <i>S. pyogenes</i>