Use of Matrix Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry (MALDI-TOF-MS) for detection of *Escherichia coli* in clinical urine samples

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SUPPLEMENTAL MATERIAL

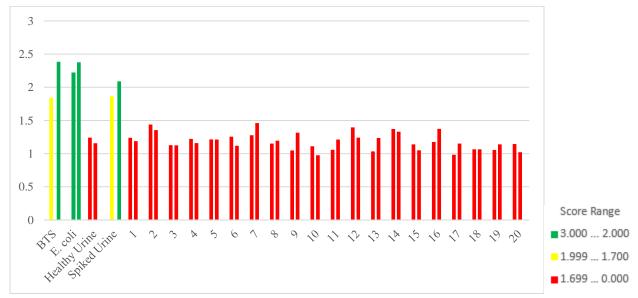


FIG. S1 Results of MALDI analysis of frozen clinical urine samples (Run 1).

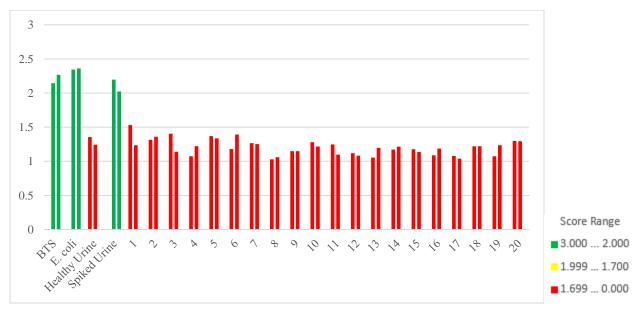


FIG. S2 Results of MALDI analysis of frozen clinical urine samples using 70% formic acid extraction (Run 2).

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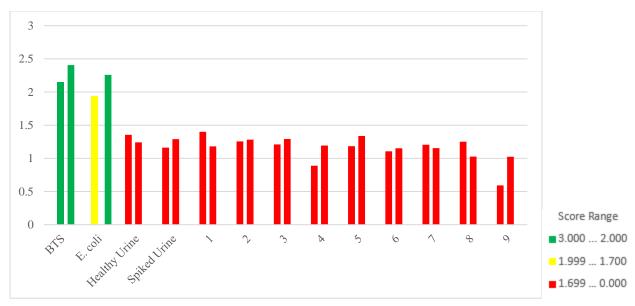


FIG. S3 Results of MALDI analysis of unfrozen clinical urine samples (Run 3).

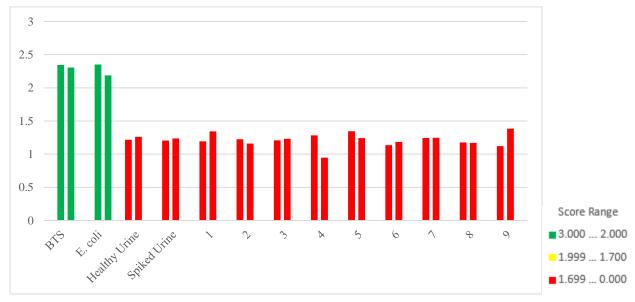


FIG. S4 Results of MALDI analysis of unfrozen clinical urine samples using 70% formic acid extraction (Run 4).

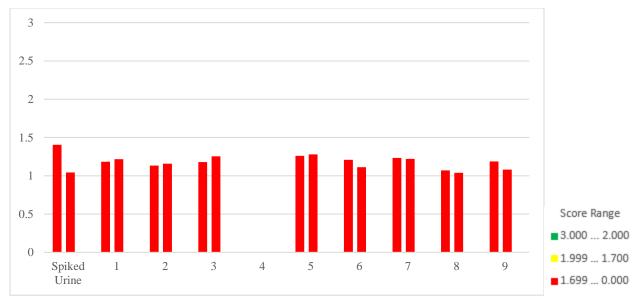


FIG. S5 Results of MALDI analysis of centrifuged unfrozen clinical urine samples (Run 5).

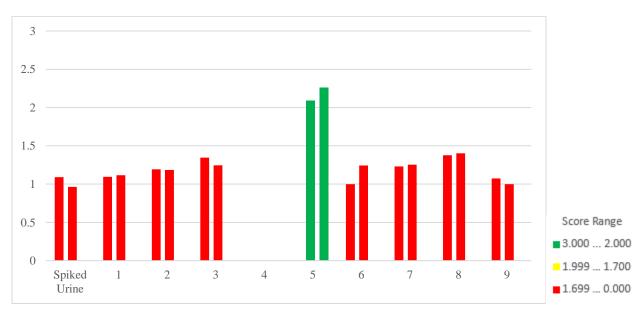
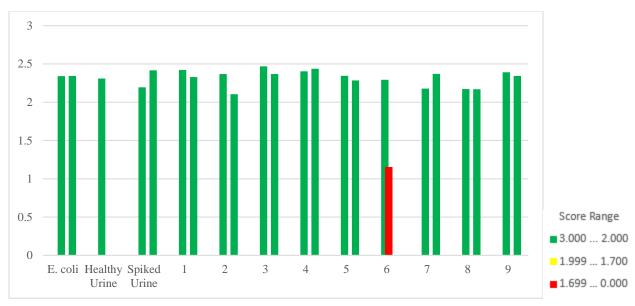


FIG. S6 Results of MALDI analysis of centrifuged unfrozen clinical urine samples using 70% formic acid extraction (Run 6).



 $FIG.\ S7\ Results\ of\ MALDI\ analysis\ of\ cultured\ unfrozen\ clinical\ urine\ samples\ (Run\ 7).$

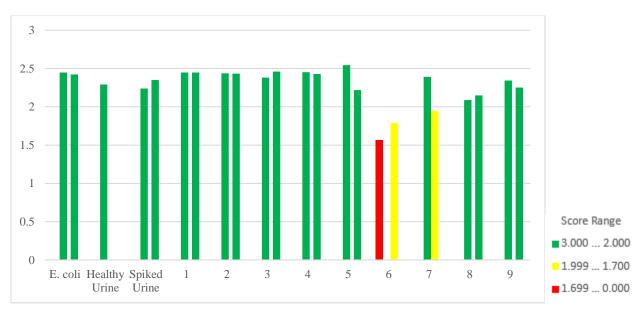


FIG. S8 Results of MALDI analysis of cultured unfrozen clinical urine samples using 70% formic acid extraction (Run 8).

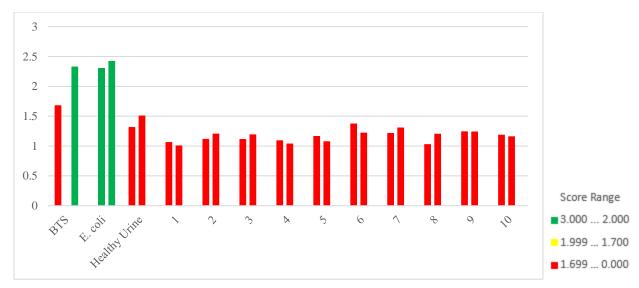


FIG. S9 Results of MALDI analysis of unfrozen clinical urine samples (Run 9).

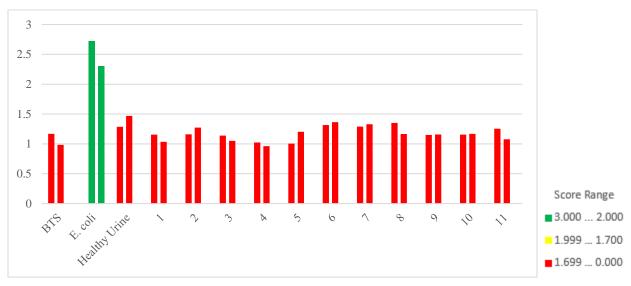
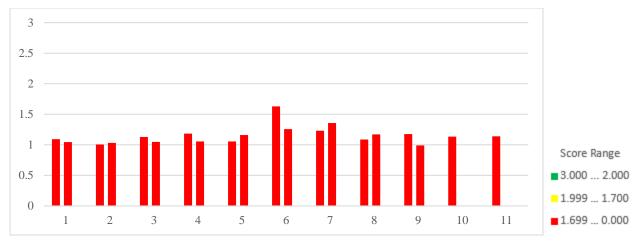


FIG. S10 Results of MALDI analysis of unfrozen clinical urine samples using 70% formic acid extraction (Run 10).



 $FIG.\ S11\ Results\ of\ MALDI\ analysis\ of\ centrifuged\ unfrozen\ clinical\ urine\ samples\ (Run\ 11).$

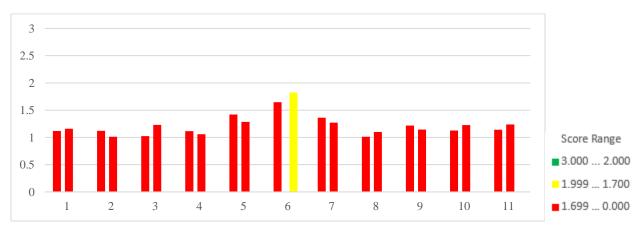


FIG. S12 Results of MALDI analysis of centrifuged unfrozen clinical urine samples using 70% formic acid extraction (Run 12).

TABLE SI Results of MALDI analysis of frozen clinical urine samples (Run 1) $\,$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>A1</u> (+)	BTS	Escherichia coli	1.842
<u>A2(+++)</u>	BTS	Escherichia coli	<u>2.385</u>
<u>A3(++)</u>	Solid E. coli	Escherichia coli	<u>2.221</u>
<u>A4</u> (+++)	Solid E. coli	Escherichia coli	2.376
<u>A5</u> (-)	1	not reliable identification	1.24
<u>A6</u> (-)	1	not reliable identification	1.188
<u>A7</u> (-)	2	not reliable identification	1.44
<u>A8</u> (-)	2	not reliable identification	1.355
<u>A9</u> (-)	3	not reliable identification	1.128
<u>A10</u> (-)	3	not reliable identification	1.125
<u>A11</u> (-)	4	not reliable identification	1.221
<u>A12</u> (-)	4	not reliable identification	1.16
<u>B1</u> (-)	5	not reliable identification	1.215
<u>B2</u> (-)	5	not reliable identification	1.213
<u>B3</u> (-)	6	not reliable identification	1,256
<u>B4(</u> -)	6	not reliable identification	1.119
<u>B5(</u> -)	7	not reliable identification	<u>1.277</u>
<u>B6(-)</u>	7	not reliable identification	1.461
<u>B7</u> (-)	8	not reliable identification	1.151
<u>B8</u> (-)	8	not reliable identification	1.196
<u>B9(</u> -)	9	not reliable identification	1.048
<u>B10</u> (-)	9	not reliable identification	1.315
<u>B11</u> (-)	10	not reliable identification	1.11
<u>B12(-)</u>	10	not reliable identification	0.977
<u>C1(-)</u>	11	not reliable identification	<u>1.059</u>
<u>C2(</u> -)	11	not reliable identification	1.212
<u>C3</u> (-)	12	not reliable identification	<u>1.395</u>

<u>C4(-)</u>	12	not reliable identification	<u>1.242</u>
<u>C5(-)</u>	13	not reliable identification	1.034
<u>C6(-)</u>	13	not reliable identification	1.236
<u>C7</u> (-)	14	not reliable identification	1.371
<u>C8(-)</u>	14	not reliable identification	1.33
<u>C9</u> (-)	15	not reliable identification	1.139
<u>C10</u> (-)	15	not reliable identification	1.051
<u>C11</u> (-)	16	not reliable identification	1.177
<u>C12</u> (-)	16	not reliable identification	1.374
<u>D1</u> (-)	17	not reliable identification	0.984
<u>D2(</u> -)	17	not reliable identification	1.153
<u>D3(</u> -)	18	not reliable identification	<u>1.065</u>
<u>D4(</u> -)	18	not reliable identification	1.064
<u>D5(</u> -)	19	not reliable identification	1.056
<u>D6(</u> -)	19	not reliable identification	1.139
<u>D7</u> (-)	20	not reliable identification	1.145
<u>D8</u> (-)	20	not reliable identification	1.022
<u>D9(</u> -)	Healthy Urine	not reliable identification	<u>1.241</u>
<u>D10</u> (-)	Healthy Urine	not reliable identification	1.157
<u>D11</u> (+)	Spiked Urine	Escherichia coli	1.864
<u>D12(++)</u>	Spiked Urine	Escherichia coli	2.089

 $TABLE\ S2\ Results\ of\ MALDI\ analysis\ of\ frozen\ clinical\ urine\ samples\ using\ 70\%\ formic\ acid\ extraction\ (Run\ 2)$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>E1</u> (++)	BTSF	Escherichia coli	2.146
<u>E2(++)</u>	BTSF	Escherichia coli	2.267
<u>E3(</u> +++)	Solid E. coli F	Escherichia coli	2.345
<u>E4(</u> +++)	Solid E. coli F	Escherichia coli	2.361
<u>E5(</u> -)	1F	not reliable identification	1.531
<u>E6</u> (-)	1F	not reliable identification	1.235
<u>E7</u> (-)	2F	not reliable identification	<u>1.315</u>
<u>E8</u> (-)	2F	not reliable identification	<u>1.36</u>
<u>E9(</u> -)	3F	not reliable identification	1.404
<u>E10</u> (-)	3F	not reliable identification	1.138
<u>E11</u> (-)	4F	not reliable identification	1.074
<u>E12</u> (-)	4F	not reliable identification	1.221
<u>F1</u> (-)	5F	not reliable identification	1.368
<u>F2</u> (-)	5F	not reliable identification	1.337
<u>F3(-)</u>	6F	not reliable identification	1.178
<u>F4(-)</u>	6F	not reliable identification	1.392
<u>F5(-)</u>	7F	not reliable identification	1.266
<u>F6(</u> -)	7F	not reliable identification	1.251
<u>F7(</u> -)	8F	not reliable identification	1.029
<u>F8</u> (-)	8F	not reliable identification	1.059
<u>F9(</u> -)	9F	not reliable identification	1.148
<u>F10(</u> -)	9F	not reliable identification	1.148
<u>F11(</u> -)	10F	not reliable identification	1.279
<u>F12</u> (-)	10F	not reliable identification	1.217
<u>G1</u> (-)	11F	not reliable identification	1.247
<u>G2</u> (-)	11F	not reliable identification	1.098
<u>G3</u> (-)	12F	not reliable identification	1.118

<u>G4(-)</u>	12F	not reliable identification	1.083
<u>G5(-)</u>	13F	not reliable identification	<u>1.054</u>
<u>G6</u> (-)	13F	not reliable identification	1.198
<u>G7</u> (-)	14F	not reliable identification	1.173
<u>G8</u> (-)	14F	not reliable identification	1.215
<u>G9</u> (-)	15F	not reliable identification	1.177
<u>G10</u> (-)	15F	not reliable identification	1.136
<u>G11</u> (-)	16F	not reliable identification	1.088
<u>G12(-)</u>	16F	not reliable identification	1.187
<u>H1</u> (-)	17F	not reliable identification	1.079
<u>H2(-)</u>	17F	not reliable identification	1.038
<u>H3(-)</u>	18F	not reliable identification	1.218
<u>H4(-)</u>	18F	not reliable identification	1.222
<u>H5(-)</u>	19F	not reliable identification	1.074
<u>H6(-)</u>	19F	not reliable identification	1.236
<u>H7</u> (-)	20F	not reliable identification	1.299
<u>H8</u> (-)	20F	not reliable identification	1.294
<u>H9</u> (-)	HUF	not reliable identification	1.335
<u>H10</u> (-)	HUF	not reliable identification	1.242
<u>H11(++)</u>	SUF	Escherichia coli	2.197
<u>H12(</u> ++)	SUF	Escherichia coli	2.024

TABLE S3 Results of MALDI analysis of unfrozen clinical urine samples (Run 3) $\,$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>A1</u> (++)	BTS	Escherichia coli	2.148
<u>A2(</u> +++)	BTS	Escherichia coli	2.407
<u>A3</u> (+)	Solid E. coli	Escherichia coli	1.94
<u>A4</u> (++)	Solid E. coli	Escherichia coli	<u>2.258</u>
<u>A5</u> (-)	Healthy Urine	not reliable identification	<u>1.076</u>
<u>A6</u> (-)	Healthy Urine	not reliable identification	1,097
<u>A7</u> (-)	Spiked Urine 10 μL	not reliable identification	<u>1.076</u>
<u>A8</u> (-)	Spiked Urine 10 μL	not reliable identification	1.144
<u>A9</u> (-)	Spiked Urine 100 μL	not reliable identification	1.179
<u>A10</u> (-)	Spiked Urine 100 μL	not reliable identification	1.065
<u>A11</u> (-)	Spiked Urine 1000 μL	not reliable identification	1.162
<u>A12</u> (-)	Spiked Urine 1000 μL	not reliable identification	1,29
<u>B1</u> (-)	1	not reliable identification	1.4
<u>B2</u> (-)	1	not reliable identification	1.18
<u>B3</u> (-)	2	not reliable identification	1,255
<u>B4</u> (-)	2	not reliable identification	1,283
<u>B5</u> (-)	3	not reliable identification	1.211
<u>B6</u> (-)	3	not reliable identification	1.292
<u>B7</u> (-)	4	not reliable identification	0.888
<u>B8</u> (-)	4	not reliable identification	1.192
<u>B9</u> (-)	5	not reliable identification	1.184
<u>B10</u> (-)	5	not reliable identification	1.338
<u>B11</u> (-)	6	not reliable identification	1.106
<u>B12</u> (-)	6	not reliable identification	<u>1.151</u>
<u>C1</u> (-)	7	not reliable identification	1.204
<u>C2</u> (-)	7	not reliable identification	1.155
<u>C3</u> (-)	8	not reliable identification	1.252

<u>C4(-)</u>	8	not reliable identification	1.027
<u>C5(</u> -)	9	not reliable identification	0.593
<u>C6(</u> -)	9	not reliable identification	1.023

 $TABLE\ S4\ Results\ of\ MALDI\ analysis\ of\ unfrozen\ clinical\ urine\ samples\ using\ 70\%\ formic\ acid\ extraction\ (Run\ 4)$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>D1</u> (+++)	BTSF	Escherichia coli	2.343
<u>D2(</u> +++)	BTSF	Escherichia coli	2.305
<u>D3(</u> +++)	Solid E. coli F	Escherichia coli	2.35
<u>D4(</u> ++)	Solid E. coli F	Escherichia coli	2.187
<u>D5(</u> -)	Healthy Urine F	not reliable identification	1.218
<u>D6(</u> -)	Healthy Urine F	not reliable identification	1.262
<u>D7</u> (-)	Spiked Urine 10 µL F	not reliable identification	1.203
<u>D8(</u> -)	Spiked Urine 10 µL F	not reliable identification	0.98
<u>D9(</u> -)	Spiked Urine 100 µL F	not reliable identification	1.068
<u>D10(</u> -)	Spiked Urine 100 µL F	not reliable identification	1.051
<u>D11(</u> -)	Spiked Urine 1000 µL F	not reliable identification	1.205
<u>D12</u> (-)	Spiked Urine 1000 µL F	not reliable identification	1.238
<u>E1</u> (-)	1F	not reliable identification	1.194
<u>E2(-)</u>	1F	not reliable identification	1.344
<u>E3(-)</u>	2F	not reliable identification	<u>1.226</u>
<u>E4(-)</u>	2F	not reliable identification	1.159
<u>E5(</u> -)	3F	not reliable identification	1.208
<u>E6(-)</u>	3F	not reliable identification	1.232
<u>E7(</u> -)	4F	not reliable identification	1.283
<u>E8(</u> -)	4F	not reliable identification	0.947
<u>E9(-)</u>	5F	not reliable identification	1.345
<u>E10</u> (-)	5F	not reliable identification	1.241
<u>E11</u> (-)	6F	not reliable identification	1.135
<u>E12</u> (-)	6F	not reliable identification	1.184
<u>F1</u> (-)	7F	not reliable identification	1.243
<u>F2</u> (-)	7F	not reliable identification	1.247
<u>F3</u> (-)	8F	not reliable identification	1.177

<u>F4(-)</u>	8F	not reliable identification	1.169
<u>F5</u> (-)	9F	not reliable identification	1.122
<u>F6(</u> -)	9F	not reliable identification	1.385

 $TABLE\ S5\ Results\ of\ MALDI\ analysis\ of\ centrifuged\ unfrozen\ clinical\ urine\ samples\ (Run\ 5)$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>C7</u> (-)	Spiked Urine	not reliable identification	1.045
<u>C8(</u> -)	Spiked Urine	not reliable identification	1.044
<u>C9(-)</u>	1	not reliable identification	1.184
<u>C10</u> (-)	1	not reliable identification	1.217
<u>C11</u> (-)	2	not reliable identification	1.133
<u>C12</u> (-)	2	not reliable identification	1.159
<u>F7</u> (-)	3	not reliable identification	1.178
<u>F8</u> (-)	3	not reliable identification	1.255
<u>F9</u> (-)	5	not reliable identification	<u>1.261</u>
<u>F10</u> (-)	5	not reliable identification	1.279
<u>F11</u> (-)	6	not reliable identification	1.208
<u>F12</u> (-)	6	not reliable identification	1.113
<u>G1</u> (-)	7	not reliable identification	1.233
<u>G2</u> (-)	7	not reliable identification	1.22
<u>G3</u> (-)	8	not reliable identification	1.071
<u>G4</u> (-)	8	not reliable identification	1.038
<u>G5</u> (-)	9	not reliable identification	1.187
<u>G6(-)</u>	9	not reliable identification	1.081

 $TABLE\ S6\ Results\ of\ MALDI\ analysis\ of\ centrifuged\ unfrozen\ clinical\ urine\ samples\ using\ 70\%\ formic\ acid\ extraction\ (Run\ 6).$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>G7</u> (-)	SUF	not reliable identification	1.09
<u>G8</u> (-)	SUF	not reliable identification	0.964
<u>G9</u> (-)	1F	not reliable identification	1.094
<u>G10</u> (-)	1F	not reliable identification	1.116
<u>G11</u> (-)	2F	not reliable identification	1.194
<u>G12</u> (-)	2F	not reliable identification	1.184
<u>H1</u> (-)	3F	not reliable identification	1.345
<u>H2(-)</u>	3F	not reliable identification	1.245
<u>H3(</u> ++)	5F	Escherichia coli	2.094
<u>H4(</u> ++)	5F	Escherichia coli	2.264
<u>H5(-)</u>	6F	not reliable identification	0.998
<u>H6(-)</u>	6F	not reliable identification	1.243
<u>H7</u> (-)	7F	not reliable identification	1.231
<u>H8</u> (-)	7F	not reliable identification	1.254
<u>H9(-)</u>	8F	not reliable identification	<u>1.377</u>
<u>H10</u> (-)	8F	not reliable identification	1.403
<u>H11</u> (-)	9F	not reliable identification	1.074
<u>H12(-)</u>	9F	not reliable identification	0.999

 $TABLE\ S7\ Results\ of\ MALDI\ analysis\ of\ cultured\ unfrozen\ clinical\ urine\ samples\ (Run\ 7).$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>A1</u> (++)	BTS	Escherichia coli	2.134
<u>A3(+++)</u>	BTS	Escherichia coli	2.414
<u>A5(</u> +++)	E. coli	Escherichia coli	2.34
<u>A6(</u> +++)	E. coli	Escherichia coli	2.343
<u>A9(</u> +++)	Healthy Urine (100 µL plate)	Escherichia coli	<u>2.31</u>
<u>B3(+++)</u>	Spiked Urine (10 µL plate)	Escherichia coli	2.346
<u>B4(++)</u>	Spiked Urine (10 μL plate)	Escherichia coli	2.277
<u>B5(++)</u>	Spiked Urine (100 µL plate)	Escherichia coli	2.194
<u>B6(</u> +++)	Spiked Urine (100 µL plate)	Escherichia coli	2.417
<u>B7(</u> +++)	1 (10 μL plate)	Escherichia coli	2.42
<u>B8(</u> +++)	1 (100 μL plate)	Escherichia coli	2.328
<u>B9(</u> +++)	2 (10 µL plate)	Escherichia coli	2.369
<u>B10(</u> ++)	2 (100 μL plate)	Escherichia coli	<u>2.105</u>
<u>B11</u> (+++)	3 (10 μL plate)	Escherichia coli	2.468
<u>B12(</u> +++)	3 (100 µL plate)	Escherichia coli	2.369
<u>C1</u> (+++)	4 (10 μL plate)	Escherichia coli	2.404
<u>C2(</u> +++)	4 (100 μL plate)	Escherichia coli	2.437
<u>C3(+++)</u>	5 (10 μL plate)	Escherichia coli	2.345
<u>C4(++)</u>	5 (100 μL plate)	Escherichia coli	2.284
<u>C5(++)</u>	6 (10 μL plate)	Escherichia coli	2.292
<u>A4</u> (++)	6 (10 μL plate)	Escherichia coli	2.284
<u>C6(</u> -)	6 (100 μL plate)	not reliable identification	1.15
<u>C7</u> (++)	7 (10 µL plate)	Escherichia coli	2.178
<u>C8(+++)</u>	7 (100 μL plate)	Escherichia coli	2.37
<u>C9(</u> ++)	8 (10 μL plate)	Escherichia coli	2.171
<u>C10(</u> ++)	8 (100 μL plate)	Escherichia coli	<u>2.17</u>
<u>C11</u> (+++)	9 (10 μL plate)	Escherichia coli	2.392

<u>C12</u> (+++)	9 (100 μL plate)	Escherichia coli	2.343

TABLE S8 Results of MALDI analysis of cultured unfrozen clinical urine samples using 70% formic acid extraction (Run 8)

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>A7</u> (+++)	E. coli F	Escherichia coli	2.447
<u>A8</u> (+++)	E. coli F	Escherichia coli	2.422
<u>A10(</u> ++)	Healthy Urine (100 μL plate) F	Escherichia coli	2.292
<u>D3</u> (+++)	Spiked Urine (10 µL plate) F	Escherichia coli	2.398
<u>D4</u> (+++)	Spiked Urine (10 µL plate) F	Escherichia coli	2.344
<u>D5(</u> ++)	Spiked Urine (100 µL plate) F	Escherichia coli	2.239
<u>D6</u> (+++)	Spiked Urine (100 µL plate) F	Escherichia coli	2.35
<u>D7</u> (+++)	1 (10 μL plate) F	Escherichia coli	<u>2.447</u>
<u>D8</u> (+++)	1 (100 µL plate) F	Escherichia coli	2.449
<u>D9(</u> +++)	2 (10 µL plate) F	Escherichia coli	2.437
<u>D10(</u> +++)	2 (100 µL plate) F	Escherichia coli	2.433
<u>D11(+++)</u>	3 (10 µL plate) F	Escherichia coli	2.381
<u>D12(</u> +++)	3 (100 µL plate) F	Escherichia coli	<u>2.46</u>
<u>E1</u> (+++)	4 (10 μL plate) F	Escherichia coli	2.452
<u>E2(</u> +++)	4 (100 µL plate) F	Escherichia coli	<u>2.429</u>
<u>E3(</u> +++)	5 (10 μL plate) F	Escherichia coli	2.544
<u>E4(++)</u>	5 (100 µL plate) F	Escherichia coli	2.218
<u>E5(</u> -)	6 (10 μL plate) F	not reliable identification	1.567
<u>E6(</u> +)	6 (100 μL plate) F	Escherichia coli	1.787
<u>E7(</u> +++)	7 (10 μL plate) F	Escherichia coli	2.392
<u>E8(</u> +)	7 (100 µL plate) F	Escherichia coli	1.946
<u>E9(</u> ++)	8 (10 μL plate) F	Escherichia coli	2.089
<u>E10</u> (++)	8 (100 µL plate) F	Escherichia coli	2.149
<u>E11</u> (+++)	9 (10 μL plate) F	Escherichia coli	2.344
<u>E12(</u> ++)	9 (100 μL plate) F	Escherichia coli	2.252

TABLE S9 Results of MALDI analysis of unfrozen clinical urine samples (Run 9).

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>BTS(</u> -)	BTS	not reliable identification	1.684
<u>BTS(</u> +++)	BTS	Escherichia coli	2.332
<u>EC(</u> +++)	EC	Escherichia coli	2.309
<u>EC(</u> +++)	EC	Escherichia coli	2.425
<u>HU</u> (-)	HU	not reliable identification	1.318
<u>HU</u> (-)	HU	not reliable identification	1.512
1(-)	1	not reliable identification	1.066
1(-)	1	not reliable identification	1.01
2(-)	2	not reliable identification	1.121
2(-)	2	not reliable identification	1.209
<u>3(-)</u>	3	not reliable identification	1.116
<u>3(-)</u>	3	not reliable identification	1.195
<u>4(-)</u>	4	not reliable identification	1.095
4(-)	4	not reliable identification	1.041
<u>5(</u> -)	5	not reliable identification	1.168
<u>5(</u> -)	5	not reliable identification	1.08
<u>6</u> (-)	6	not reliable identification	1.377
<u>6</u> (-)	6	not reliable identification	1.224
7(-)	7	not reliable identification	1.218
7(-)	7	not reliable identification	1.309
<u>8</u> (-)	8	not reliable identification	1.032
<u>8</u> (-)	8	not reliable identification	1.206
2(-)	9	not reliable identification	1.245
9(-)	9	not reliable identification	1.242
10(-)	10	not reliable identification	1.19
10(-)	10	not reliable identification	1.162

 $TABLE\ SI0\ Results\ of\ MALDI\ analysis\ of\ unfrozen\ clinical\ urine\ samples\ using\ 70\%\ formic\ acid\ extraction\ (Run\ 10)$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>BTSF</u> (-)	BTSF	not reliable identification	1.169
<u>BTSF</u> (-)	BTSF	not reliable identification	0.983
<u>ECF(</u> ++)	ECF	Escherichia coli	2.272
<u>ECF(</u> +++)	ECF	Escherichia coli	2.301
<u>HUF(-)</u>	HUF	not reliable identification	1.287
<u>HUF(-)</u>	HUF	not reliable identification	1.469
<u>1F(-)</u>	1F	not reliable identification	1.156
<u>1F(-)</u>	1F	not reliable identification	1.034
<u>2F(-)</u>	2F	not reliable identification	1.161
<u>2F(-)</u>	2F	not reliable identification	1.272
<u>3F(-)</u>	3F	not reliable identification	1.139
<u>3F(-)</u>	3F	not reliable identification	1.05
<u>4F(-)</u>	4F	not reliable identification	1.024
<u>4F</u> (-)	4F	not reliable identification	0.963
<u>5F(</u> -)	5F	not reliable identification	1.005
<u>5F(</u> -)	5F	not reliable identification	1.202
<u>6F</u> (-)	6F	not reliable identification	<u>1.316</u>
<u>6F</u> (-)	6F	not reliable identification	1.365
<u>7F(-)</u>	7F	not reliable identification	1.288
<u>7F(-)</u>	7F	not reliable identification	1.328
<u>8F(-)</u>	8F	not reliable identification	1.352
<u>8F(-)</u>	8F	not reliable identification	1.166
<u>9F(</u> -)	9F	not reliable identification	1.15
<u>9F(</u> -)	9F	not reliable identification	1.158
<u>10F(</u> -)	10F	not reliable identification	1.156
<u>10F(</u> -)	10F	not reliable identification	1.168
11F(-)	11F	not reliable identification	1,253

<u>11F</u> (-)	not reliable identification	<u>1.076</u>
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 $TABLE\ SI1\ Results\ of\ MALDI\ analysis\ of\ centrifuged\ unfrozen\ clinical\ urine\ samples\ (Run\ 11)$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>1C(-)</u>	1C	not reliable identification	1.092
<u>1C(</u> -)	1C	not reliable identification	1.045
<u>2C(-)</u>	2C	not reliable identification	1.005
<u>2C(-)</u>	2C	not reliable identification	1.031
<u>3C(</u> -)	3C	not reliable identification	1.129
<u>3C</u> (-)	3C	not reliable identification	1.049
<u>4C(-)</u>	4C	not reliable identification	1.184
<u>4C(-)</u>	4C	not reliable identification	1.055
<u>5C(</u> -)	5C	not reliable identification	1.056
<u>5C(</u> -)	5C	not reliable identification	1.16
<u>6C(</u> -)	6C	not reliable identification	1.629
<u>6C(-)</u>	6C	not reliable identification	1.258
<u>7C(-)</u>	7C	not reliable identification	1.231
<u>7C(-)</u>	7C	not reliable identification	1.358
<u>8C(-)</u>	8C	not reliable identification	1.088
<u>8C(-)</u>	8C	not reliable identification	1.17
<u>9C(</u> -)	9C	not reliable identification	1.176
<u>9C(-)</u>	9C	not reliable identification	0.99
<u>10C</u> (-)	10C	not reliable identification	1.134
11C(-)	11C	not reliable identification	1.139

 $TABLE\ SI2\ Results\ of\ MALDI\ analysis\ of\ centrifuged\ unfrozen\ clinical\ urine\ samples\ using\ 70\%\ formic\ acid\ extraction\ (Run\ 12)$

AnalyteName	AnalyteID	Organism(best match)	ScoreValue
<u>1CF(-)</u>	1CF	not reliable identification	1.117
<u>1CF(-)</u>	1CF	not reliable identification	1.16
<u>2CF(-)</u>	2CF	not reliable identification	1.122
<u>2CF(-)</u>	2CF	not reliable identification	1.013
<u>3CF(-)</u>	3CF	not reliable identification	1.025
<u>3CF(-)</u>	3CF	not reliable identification	1.23
4CF(-)	4CF	not reliable identification	1.115
4CF(-)	4CF	not reliable identification	1.058
<u>5CF(-)</u>	5CF	not reliable identification	1.421
<u>5CF</u> (-)	5CF	not reliable identification	1.284
<u>6CF(-)</u>	6CF	not reliable identification	1.648
<u>6CF(</u> +)	6CF	Escherichia coli	1.819
<u>7CF(-)</u>	7CF	not reliable identification	1.362
<u>7CF(-)</u>	7CF	not reliable identification	1.271
<u>8CF(-)</u>	8CF	not reliable identification	1.011
<u>8CF(-)</u>	8CF	not reliable identification	1.099
<u>9CF(-)</u>	9CF	not reliable identification	1.218
<u>9CF(-)</u>	9CF	not reliable identification	1.143
<u>10CF(-)</u>	10CF	not reliable identification	1.128
<u>10CF</u> (-)	10CF	not reliable identification	1.228
11CF(-)	11CF	not reliable identification	<u>1.141</u>
11CF(-)	11CF	not reliable identification	1.239

TABLE SI3 April 27^{th} urine sample appearances

Sample #	Description
1	Pale yellow, slightly cloudy, small amount of suspended material
2	Pale pink, moderately cloudy, small amount of suspended material
3	Vivid yellow, slightly cloudy
4	Vivid yellow, clear
5	Clear, colourless
6	Medium yellow, slightly cloudy
7	Vivid pink, clear, some suspended material
8	Medium yellow, slightly cloudy
9	Medium orange, opaque

TABLE SI4 June 7^{th} urine sample appearances

Sample #	Urine Sample Description	Pellet Description
1	Cloudy, pale orangish yellow Large, pinkish	
2	Slightly cloudy, pale yellow	Medium size, orangish
3	Cloudy, pale yellow	Medium size, orangish
4	Slightly cloudy, medium yellow	Large, yellowish
5	Slightly cloudy, pale yellow	Small, pale coloured
6	Clear, nearly colourless with a slight pinkish hue. Some suspended material	Very small, pale coloured
7	Clear, colourless	Very small, pale coloured
8	Slightly cloudy, pale yellow	Medium sized, orangish
9	Almost clear, pale yellow	Small, pale yellow
10	Almost clear, medium yellow	Medium sized, yellowish
11	Clear, medium yellow	Small, pale yellow