***Supplementary Information***

# Rapid discrimination of *Enterococcus faecium* strains using multiple physicochemical analytical techniques

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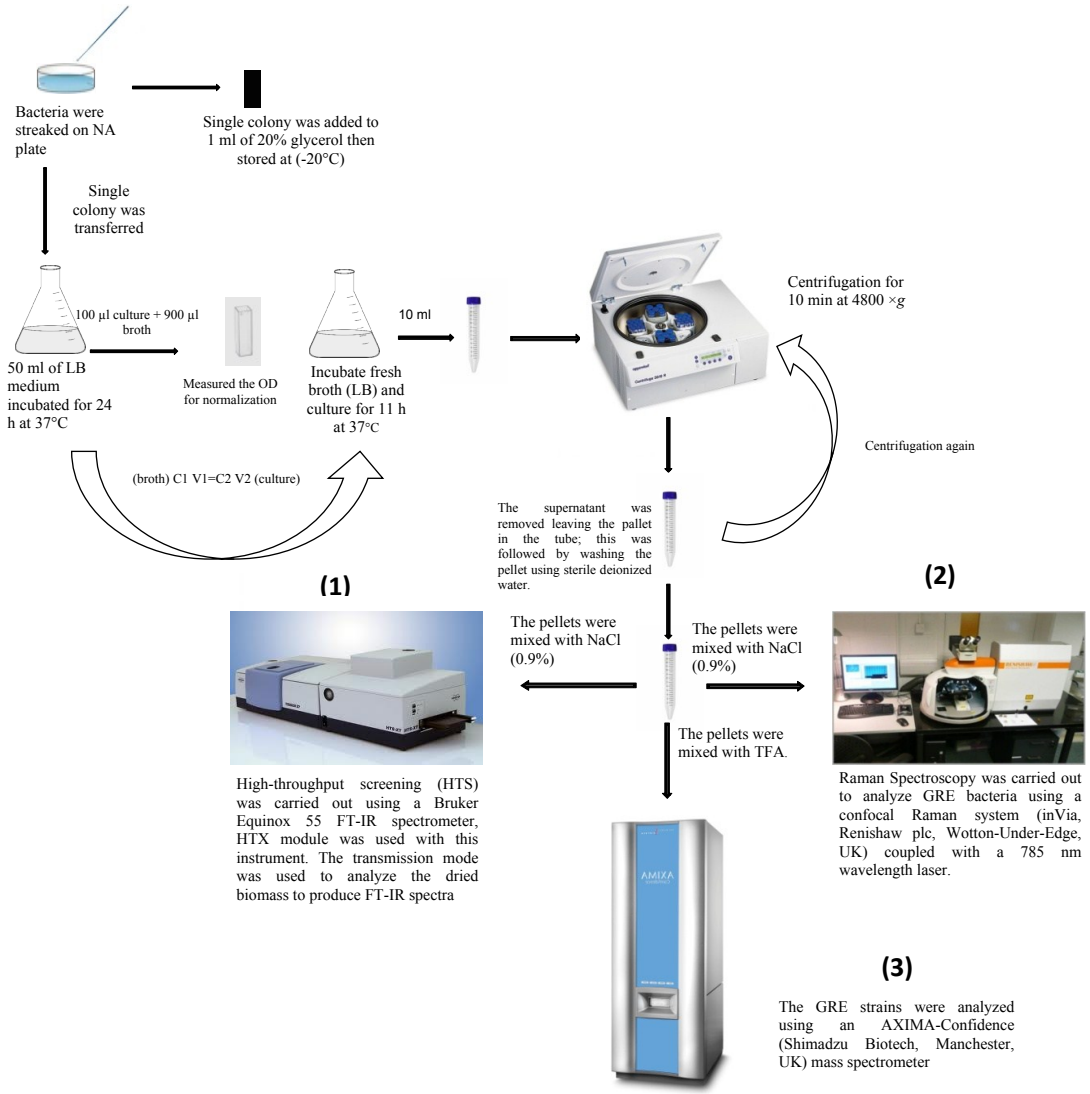



Figure S1: Schematic of sample preparation for: (1) FT-IR spectroscopy, (2) Raman spectroscopy and (3) MALDI-TOF-MS analysis of bacteria samples.

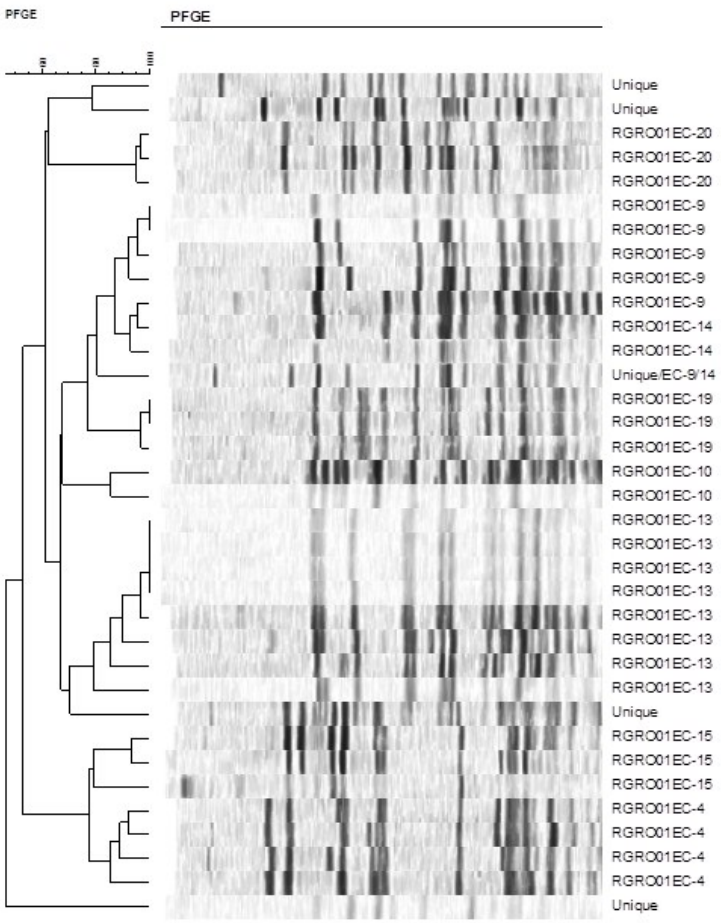



Figure S2: Dendrogram generated from pulsed field gel electrophoresis (PFGE) of the 35 enterococci isolates. The top strain A13960776 is strain 178; the others follow in the sequence: 214, 192, 198, 204, 160, 233, 211, 205, 133, 194, 203, 219, 174, 175, 173, 139, 151, 154, 155, 149, 152, 144, 185, 177, 167, 191, 190, 223, 224, 179, 193, 170, 109, and 156**.**

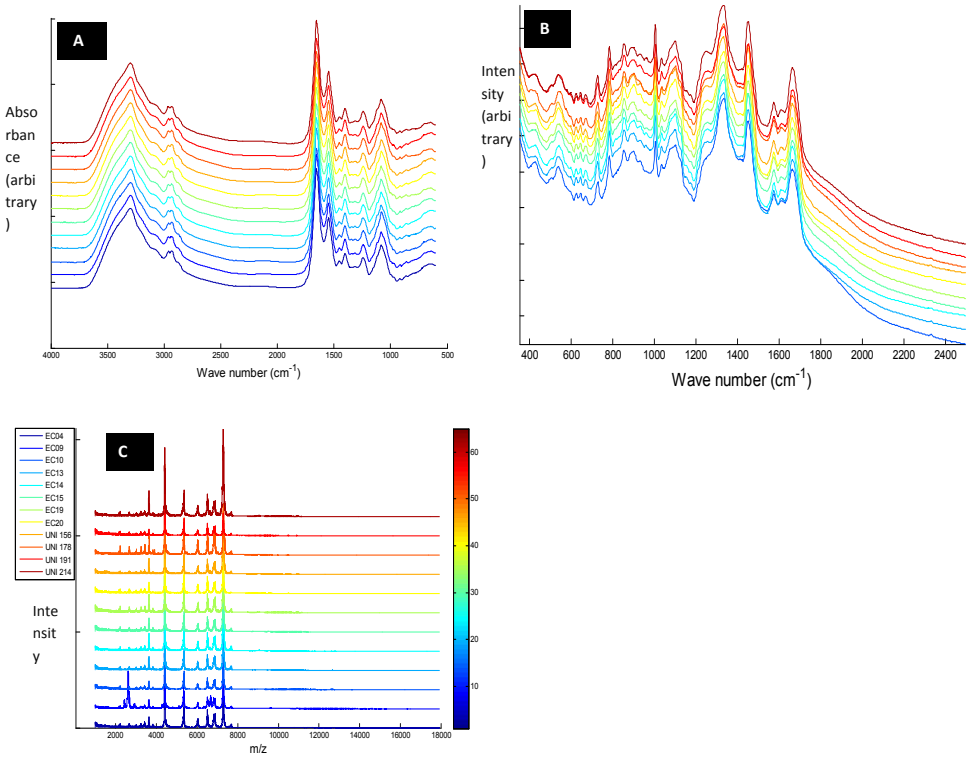



Figure S3: Typical spectra from: (A) FT-IR spectroscopy, (B) Raman spectroscopy and (C) MALDI-TOF-MS for the 12 enterococci strains (EC04, EC09, EC10, EC13, EC14, EC15, EC19, EC20, UNI 156, UNI 178, UNI 191 and UNI 214). The spectra from each analytical technique were plotted after pre-processing.

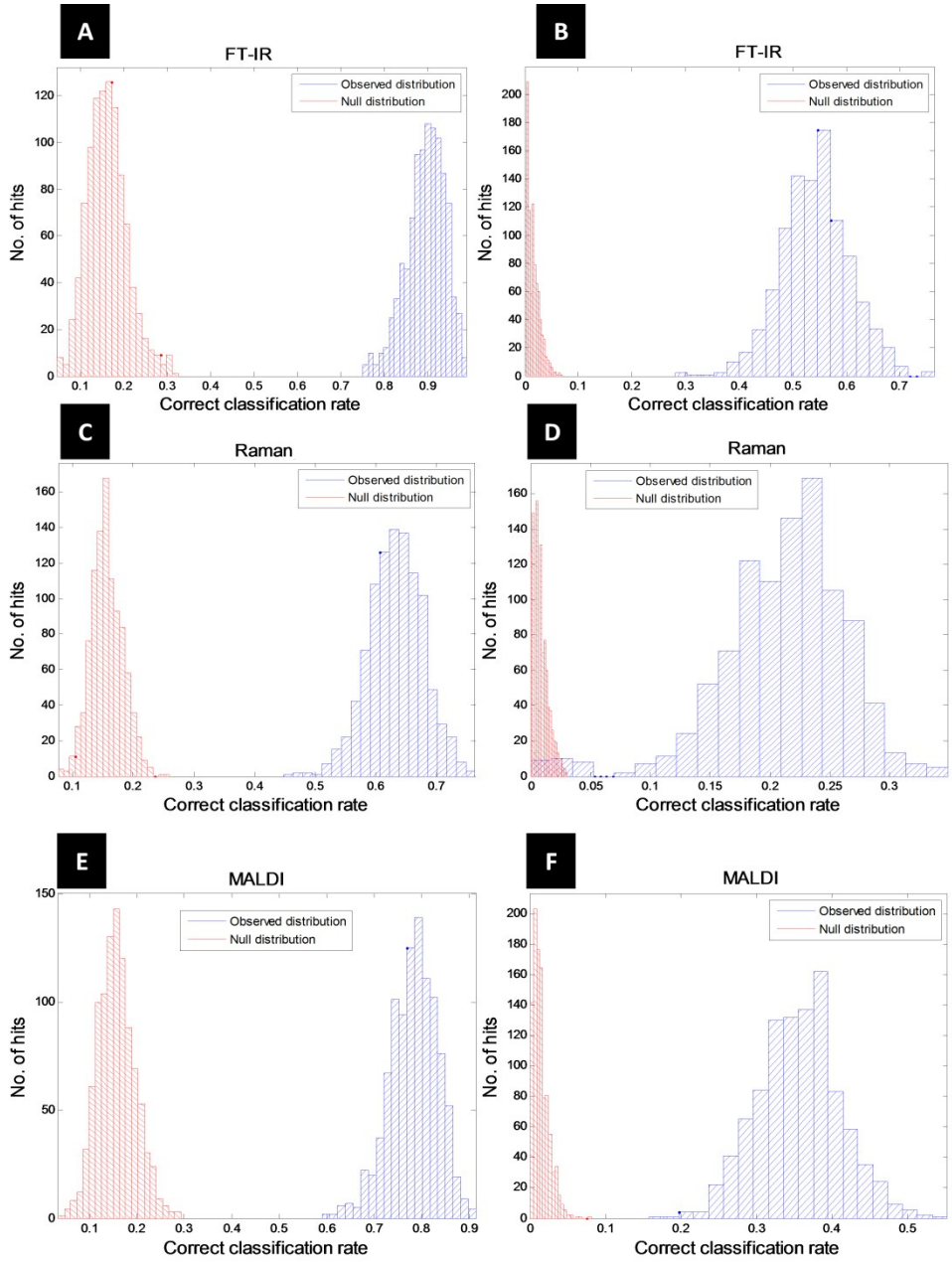



Figure S4: The predictive accuracies expressed as correct classification rates (CCRs) generated from FT-IR spectroscopy data (A-B), Raman spectroscopy data (C-D) and MALDI-TOF-MS data (E-F) based on 1,000 bootstrapping re-sampling (blue bars). The null distribution (red bars) was obtained by permuting the order of the labels and conducting the same PLS-DA classification procedure. Not a single case out of 1,000 bootstrap cases had a model using permuted labels that obtained a higher CCR than the one using the known labels (A, C and E) at the strain level (12 classes) based on FT-IR spectroscopy, Raman spectroscopy and MALDI-TOF-MS data; the mean CCRs = 89.4%, 69.3% and 78.2%, respectively. At the isolate level (35 classes), based on FT-IR spectroscopy, Raman spectroscopy and MALDI-TOF-MS data, the mean CCRs were 54.3%, 21.1%, and 35.7%, respectively.

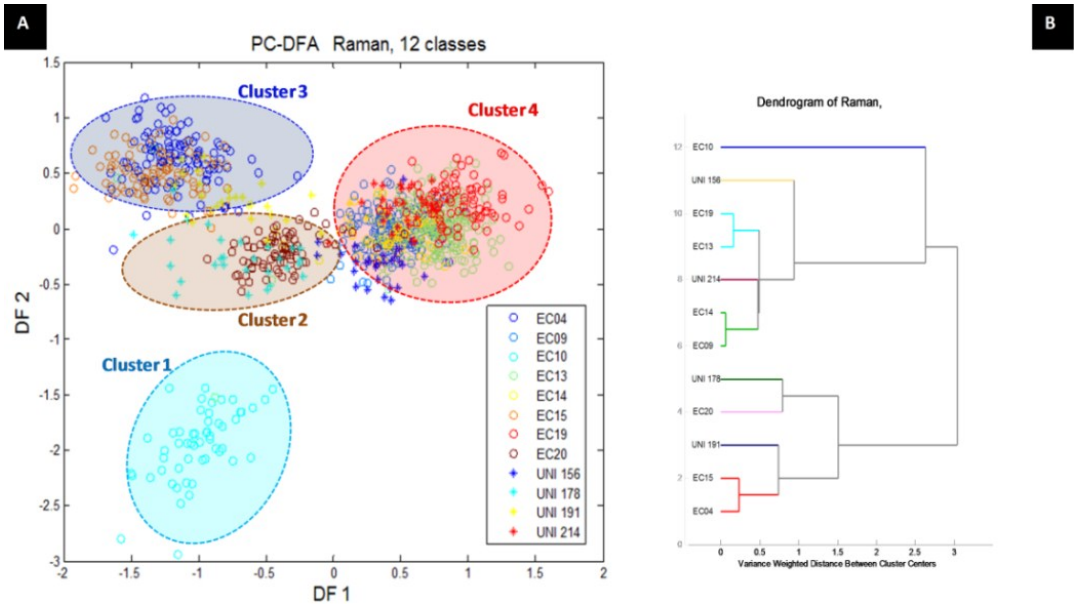



Figure S5**:** (A) PC-DFA plot from Raman data after pre-processing illustrating the relationship between the 12 enterococcal strains. (B) Cluster analysis on averaged DFA scores (12 classes/strains) using Ward's linkage.

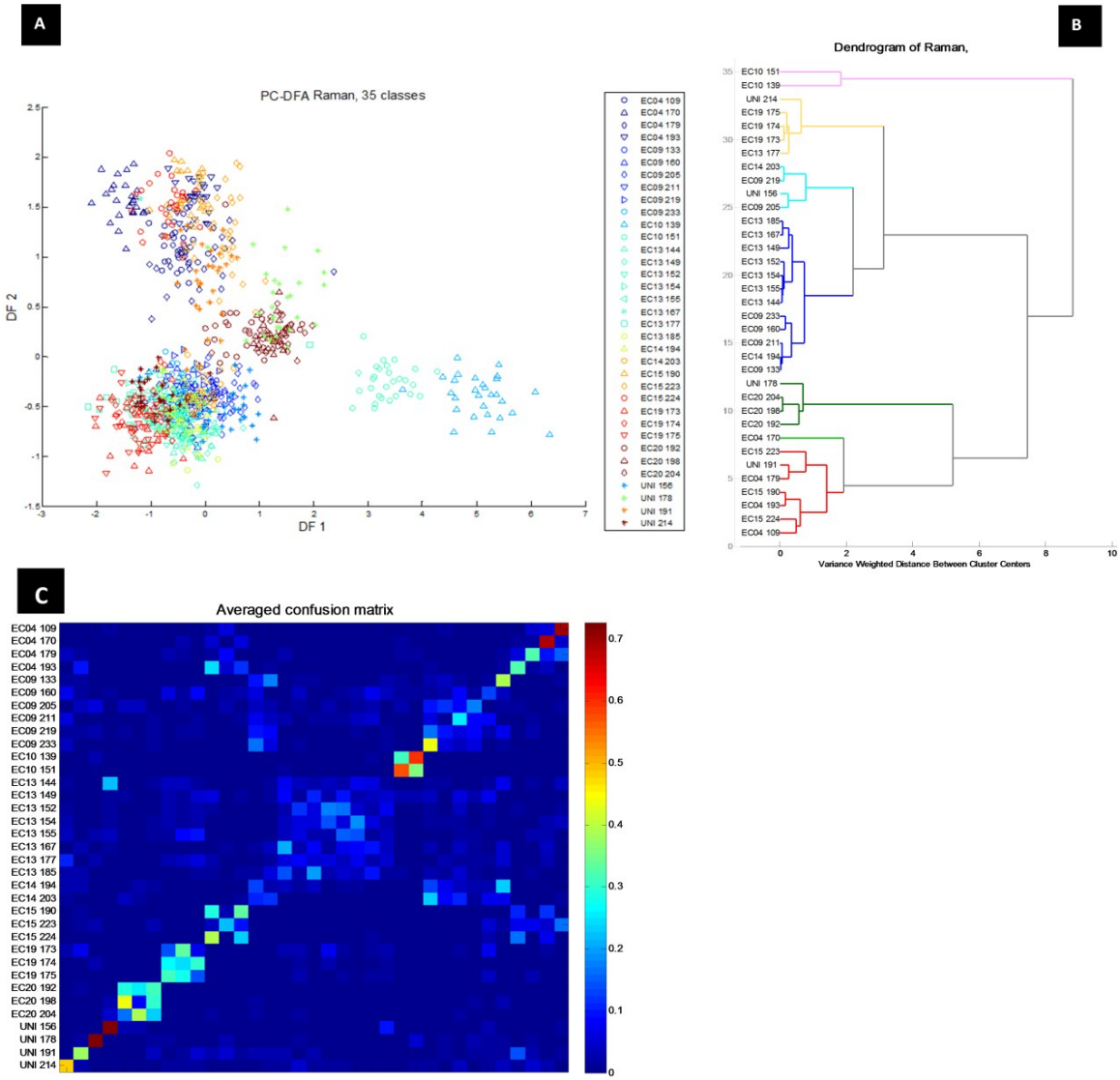



Figure S6: (A) PC-DFA plot of Raman spectroscopy data after pre-processing illustrating the relationship between the 35 isolates. (B) Hierarchical cluster analysis on averaged PC-DFA scores (35 classes), using the Ward's linkage algorithm. (C) PLS-DA trained on 35 classes (i.e. 35 isolates) generated from Raman spectroscopy data.

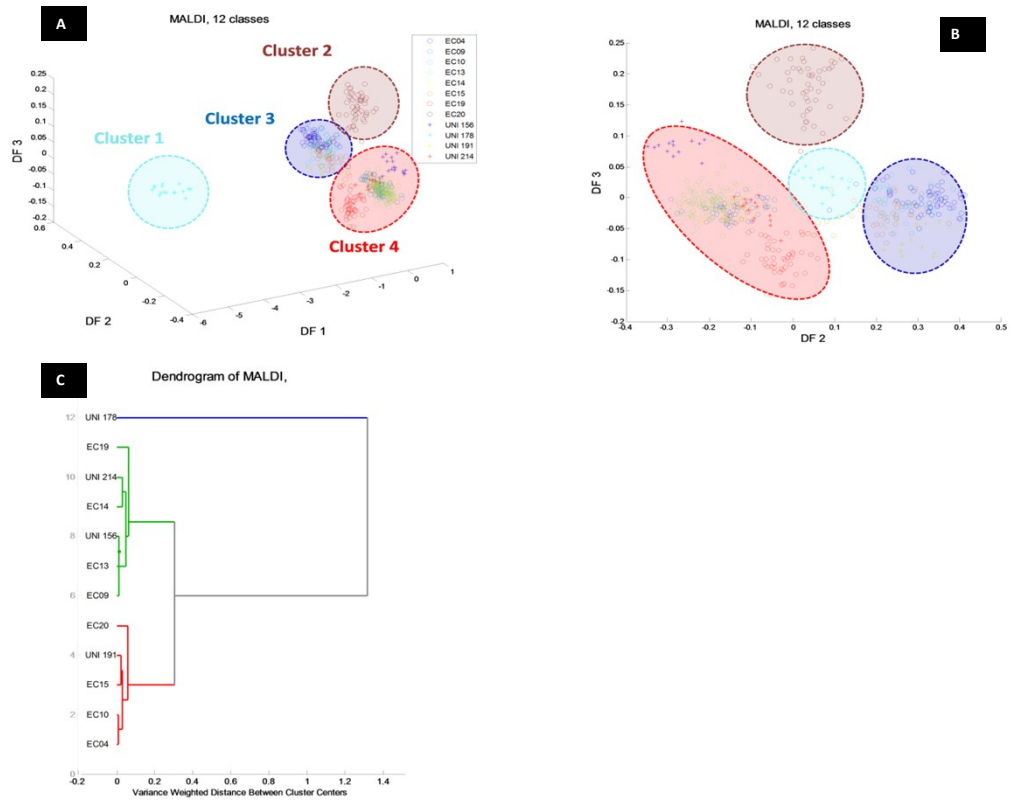
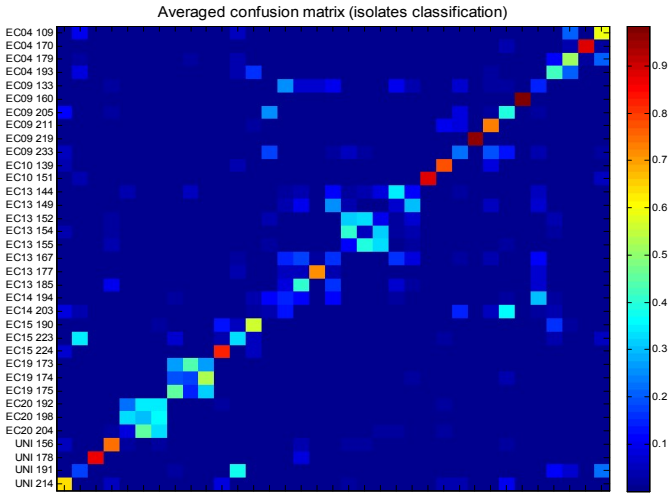
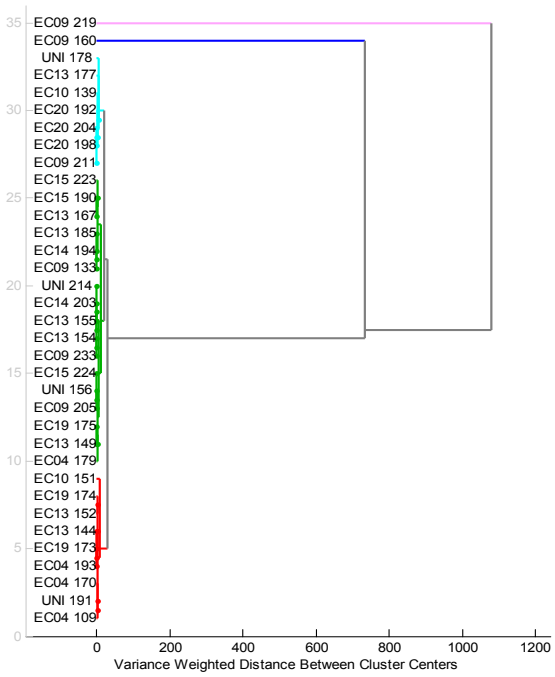



Figure S7: (A) 3-D PC-DFA plot from MALDI-TOF-MS data after pre-processing, illustrating the relationship between the 12 enterococci strains. (B) DFA plot for DF2 *v.* DF3. (C) Hierarchical cluster analysis on averaged DFA scores from MALDI-TOF-MS data of the 12 strains using Ward's linkage.

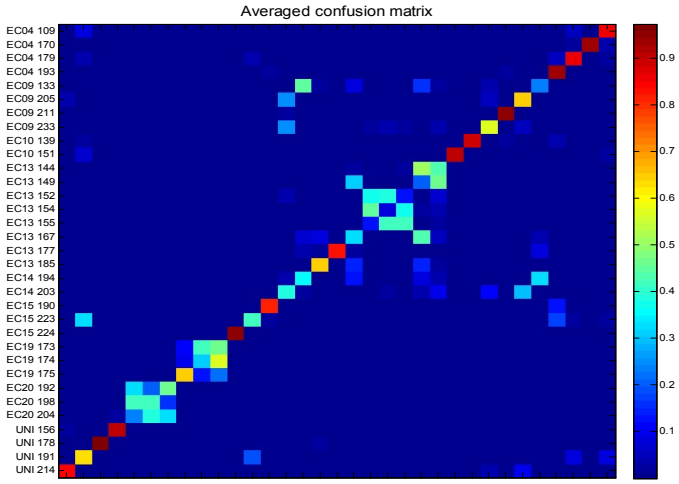
**A**


Averaged confusion matrix (isolates classification)
EC04 109
EC04 170
EC04 179
EC04 193
EC09 133
EC09 160
EC09 205
EC09 211
EC09 219
EC09 233
EC10 139
EC10 151
EC13 144
EC13 149
EC13 152
EC13 154
EC13 155
EC13 167
EC13 177
EC13 185
EC14 194
EC14 203
EC15 190
EC15 223
EC15 224
EC19 173
EC19 174
EC19 175
EC20 192
EC20 198
EC20 204
UNI 156
UNI 178
UNI 191
UNI 214
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

**B**


EC09 219
EC09 160
UNI 178
EC13 177
EC10 139
EC20 192
EC20 204
EC20 198
EC09 211
EC15 223
EC15 190
EC13 167
EC13 185
EC14 194
EC09 133
UNI 214
EC14 203
EC13 155
EC13 154
EC09 233
EC15 224
UNI 156
EC09 205
EC19 175
EC13 149
EC04 179
EC10 151
EC19 174
EC13 152
EC13 144
EC19 173
EC04 193
EC04 170
UNI 191
EC04 109
35
30
25
20
15
10
5
0
0
200
400
600
800
1000
1200
Variance Weighted Distance Between Cluster Centers

**C**


Averaged confusion matrix
EC04 109
EC04 170
EC04 179
EC04 193
EC09 133
EC09 205
EC09 211
EC09 233
EC10 139
EC10 151
EC13 144
EC13 149
EC13 152
EC13 154
EC13 155
EC13 167
EC13 177
EC13 185
EC14 194
EC14 203
EC15 190
EC15 223
EC15 224
EC19 173
EC19 174
EC19 175
EC20 192
EC20 198
EC20 204
UNI 156
UNI 178
UNI 191
UNI 214
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

**D**

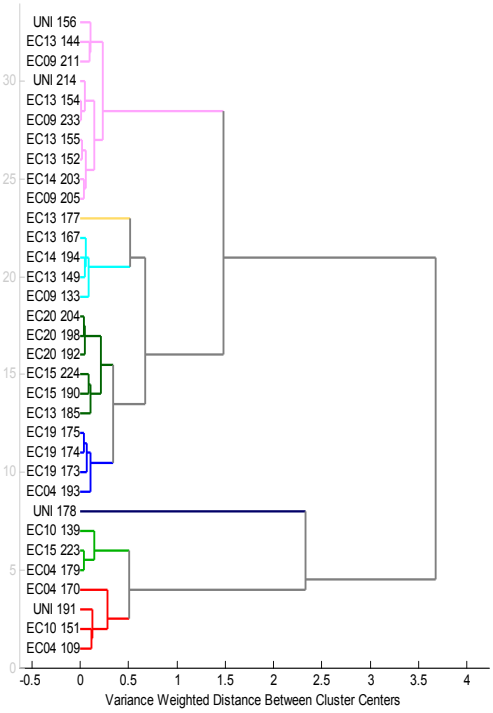

UNI 156
EC13 144
EC09 211
UNI 214
EC13 154
EC09 233
EC13 155
EC13 152
EC14 203
EC09 205
EC13 177
EC13 167
EC14 194
EC13 149
EC09 133
EC20 204
EC20 198
EC20 192
EC15 224
EC15 190
EC13 185
EC19 175
EC19 174
EC19 173
EC04 193
UNI 178
EC10 139
EC15 223
EC04 179
EC04 170
UNI 191
EC10 151
EC04 109
30
25
20
15
10
5
0
-0.5
0
0.5
1
1.5
2
2.5
3
3.5
4
Variance Weighted Distance Between Cluster Centers

Figure S8: (A) PLS-DA trained based on MALDI-TOF-MS data for the 35 isolates (i.e. 35 classes). (B) Hierarchical cluster analysis based on averaged DFA scores of 35 isolates (i.e. 35 classes) using Ward's linkage. (C) PLS-DA results trained on MALDI-TOF-MS data for 33 isolates (i.e. 33 classes) where species 160 and 219 were removed. (D) Hierarchical cluster analysis based on mean DFA scores of the 33 isolates (i.e. 33 classes) using Ward's linkage.

Table S1 The 35 enterococci isolates used in this study.

| No. | Isolate | Strain |
|---|---|---|
| 1 | 139 | EC10 |
| 2 | 151 | EC10 |
| 3 | 144 | EC13 |
| 4 | 149 | EC13 |
| 5 | 152 | EC13 |
| 6 | 154 | EC13 |
| 7 | 155 | EC13 |
| 8 | 167 | EC13 |
| 9 | 177 | EC13 |
| 10 | 185 | EC13 |
| 11 | 194 | EC14 |
| 12 | 203 | EC14 |
| 13 | 190 | EC15 |
| 14 | 223 | EC15 |
| 15 | 224 | EC15 |
| 16 | 173 | EC19 |
| 17 | 174 | EC19 |
| 18 | 175 | EC19 |
| 19 | 192 | EC20 |
| 20 | 198 | EC20 |
| 21 | 204 | EC20 |
| 22 | 109 | EC04 |
| 23 | 170 | EC04 |
| 24 | 179 | EC04 |
| 25 | 193 | EC04 |
| 26 | 133 | EC09 |
| 27 | 160 | EC09 |
| 28 | 211 | EC09 |
| 29 | 205 | EC09 |
| 30 | 219 | EC09 |
| 31 | 233 | EC09 |
| 32 | 156 | UNI |
| 33 | 178 | UNI |
| 34 | 191 | UNI |
| 35 | 214 | UNI |

*UNI = Unique*

Table S2 The prediction accuracies of the 12 enterococci strains using (A) Raman spectroscopy data and (B) MALDI-TOF-MS data.

| **A** **Class Known** /Predicted | **EC04** | **EC09** | **EC10** | **EC13** | **EC14** | **EC15** | **EC19** | **EC20** | **UNI 156** | **UNI 178** | **UNI 191** | **UNI 214** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| EC04 | 71.5% | 2.3% | 0.6% | 2.1% | 0.3% | 21.5% | 1.4% | 0.1% | 0.0% | 0.0% | 0.1% | 0.0% |
| EC09 | 0.6% | 69.3% | 0.0% | 17.4% | 7.4% | 0.9% | 2.8% | 0.9% | 0.0% | 0.0% | 0.1% | 0.5% |
| EC10 | 0.1% | 7.0% | 88.8% | 3.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.8% | 0.0% | 0.0% |
| EC13 | 1.0% | 6.9% | 0.4% | 82.3% | 0.5% | 0.7% | 4.4% | 1.2% | 2.1% | 0.4% | 0.0% | 0.1% |
| EC14 | 0.2% | 77.6% | 0.0% | 10.0% | 7.3% | 0.5% | 0.6% | 3.7% | 0.0% | 0.0% | 0.0% | 0.1% |
| EC15 | 33.3% | 2.3% | 0.0% | 4.4% | 0.2% | 58.5% | 0.8% | 0.3% | 0.0% | 0.1% | 0.1% | 0.0% |
| EC19 | 0.4% | 4.9% | 0.0% | 25.5% | 0.0% | 0.0% | 68.9% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% |
| EC20 | 0.5% | 3.3% | 0.2% | 2.4% | 0.7% | 2.2% | 0.2% | 90.2% | 0.1% | 0.1% | 0.0% | 0.0% |
| UNI 156 | 1.2% | 4.1% | 0.0% | 42.6% | 0.1% | 0.1% | 1.5% | 16.1% | 34.1% | 0.0% | 0.0% | 0.0% |
| UNI 178 | 4.0% | 14.4% | 1.3% | 14.5% | 0.2% | 4.7% | 10.4% | 4.9% | 0.0% | 45.4% | 0.2% | 0.0% |
| UNI 191 | 39.1% | 11.9% | 0.0% | 9.8% | 4.7% | 19.3% | 4.1% | 5.6% | 0.0% | 0.1% | 5.4% | 0.0% |
| UNI 214 | 6.0% | 41.7% | 0.0% | 31.5% | 2.1% | 0.3% | 12.4% | 0.0% | 0.0% | 0.0% | 0.1% | 5.8% |

| **B** **Class known**/Predicted | **EC04** | **EC09** | **EC10** | **EC13** | **EC14** | **EC15** | **EC19** | **EC20** | **UNI 156** | **UNI 178** | **UNI 191** | **UNI 214** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| EC04 | 93.8% | 1.0% | 0.1% | 0.4% | 0.3% | 3.8% | 0.1% | 0.1% | 0.0% | 0.0% | 0.3% | 0.0% |
| EC09 | 1.0% | 71.5% | 0.1% | 11.0% | 13.7% | 0.3% | 0.5% | 0.2% | 0.2% | 0.0% | 0.1% | 1.5% |
| EC10 | 0.4% | 3.7% | 83.1% | 4.4% | 0.1% | 2.6% | 1.6% | 2.8% | 0.0% | 0.0% | 1.0% | 0.3% |
| EC13 | 0.3% | 2.5% | 0.0% | 95.8% | 0.7% | 0.6% | 0.0% | 0.0% | 0.1% | 0.0% | 0.1% | 0.0% |
| EC14 | 0.0% | 58.7% | 0.0% | 15.0% | 25.8% | 0.3% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC15 | 7.8% | 2.7% | 0.9% | 0.8% | 1.3% | 77.0% | 0.8% | 0.4% | 0.2% | 0.0% | 8.0% | 0.1% |
| EC19 | 0.0% | 0.4% | 0.0% | 1.8% | 0.0% | 0.0% | 97.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC20 | 0.1% | 0.2% | 0.1% | 1.1% | 0.1% | 0.4% | 0.0% | 97.6% | 0.5% | 0.0% | 0.0% | 0.0% |
| UNI 156 | 0.0% | 10.8% | 0.0% | 18.7% | 0.5% | 0.1% | 0.0% | 12.1% | 56.1% | 0.0% | 0.0% | 1.7% |
| UNI 178 | 0.6% | 4.4% | 0.0% | 8.2% | 0.0% | 3.1% | 0.4% | 0.0% | 0.0% | 83.2% | 0.0% | 0.0% |
| UNI 191 | 51.6% | 0.4% | 0.7% | 0.0% | 0.2% | 29.1% | 4.7% | 0.0% | 0.0% | 0.0% | 13.2% | 0.0% |
| UNI 214 | 0.6% | 20.6% | 0.8% | 13.9% | 1.4% | 0.9% | 1.1% | 0.0% | 2.8% | 0.0% | 0.0% | 57.9% |

Table S3 The prediction accuracies of the 35 enterococci isolates using a PLS-DA model generated from FT-IR spectroscopy data

| | EC04 109 | EC04 170 | EC04 179 | EC04 193 | EC09 133 | EC09 160 | EC09 205 | EC09 211 | EC09 219 | EC09 233 | EC10 139 | EC10 151 | EC13 144 | EC13 149 | EC13 152 | EC13 154 | EC13 155 | EC13 167 | EC13 177 | EC13 185 | EC14 194 | EC14 203 | EC15 190 | EC15 223 | EC15 224 | EC19 173 | EC19 174 | EC19 175 | EC20 192 | EC20 198 | EC20 204 | UNI 156 | UNI 178 | UNI 191 | UNI 214 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| EC04 109 | 95.0% | 0.8% | 0.9% | 1.0% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 0.0% | 0.0% | 0.0% | 0.3% | 0.0% | 0.6% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% |
| EC04 170 | 0.2% | 96.4% | 0.1% | 0.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.1% | 0.0% | 0.6% | 0.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.6% |
| EC04 179 | 1.5% | 0.2% | 76.3% | 0.4% | 0.0% | 0.1% | 0.0% | 0.8% | 0.0% | 0.0% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.0% | 0.1% | 0.3% | 0.1% | 0.2% | 0.0% | 0.0% | 0.0% | 15.6% | 0.3% | 0.0% | 0.1% | 0.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 2.9% | 0.1% |
| EC04 193 | 0.0% | 0.3% | 0.0% | 76.8% | 0.0% | 0.0% | 0.2% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.8% | 1.8% | 0.6% | 0.1% | 15.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 3.3% | 0.0% |
| EC09 133 | 0.1% | 0.0% | 0.0% | 0.0% | 78.3% | 1.2% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 6.0% | 9.4% | 0.0% | 0.0% | 0.0% | 3.0% | 0.0% | 0.0% | 1.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC09 160 | 0.0% | 0.0% | 0.4% | 0.0% | 2.0% | 79.3% | 0.5% | 3.2% | 0.0% | 0.8% | 0.0% | 0.0% | 0.0% | 0.3% | 3.9% | 1.1% | 0.4% | 0.2% | 0.1% | 0.1% | 0.9% | 5.4% | 0.0% | 0.4% | 0.0% | 0.1% | 0.0% | 0.5% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.1% |
| EC09 205 | 0.0% | 0.0% | 0.0% | 0.9% | 0.0% | 0.0% | 64.9% | 0.9% | 28.3% | 0.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.8% | 0.0% | 0.4% | 0.9% | 0.1% | 0.0% | 0.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.5% | 0.6% | 0.0% | 0.0% | 0.2% | 0.0% |
| EC09 211 | 0.0% | 0.0% | 0.8% | 0.4% | 0.0% | 3.7% | 1.3% | 56.5% | 1.3% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.2% | 2.1% | 0.5% | 12.0% | 0.0% | 0.0% | 0.2% | 0.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 19.9% |
| EC09 219 | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 35.5% | 0.7% | 50.9% | 10.6% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.1% | 0.9% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.1% | 0.1% |
| EC09 233 | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.1% | 0.1% | 0.3% | 5.4% | 82.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.6% | 0.0% | 3.1% | 7.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.0% | 0.5% |
| EC10 139 | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 95.6% | 3.8% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.1% |
| EC10 151 | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 3.2% | 96.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC13 144 | 0.0% | 0.0% | 0.2% | 0.0% | 7.8% | 0.0% | 0.0% | 0.0% | 0.1% | 0.9% | 0.0% | 0.0% | 27.1% | 16.2% | 18.8% | 7.7% | 12.2% | 2.2% | 1.2% | 3.4% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 1.1% | 0.8% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC13 149 | 0.0% | 0.0% | 0.0% | 0.0% | 14.8% | 2.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 11.9% | 15.4% | 4.0% | 1.0% | 0.6% | 40.8% | 0.6% | 8.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC13 152 | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 2.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 6.5% | 0.4% | 21.9% | 54.3% | 13.3% | 0.2% | 0.8% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC13 154 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.9% | 0.0% | 0.1% | 0.2% | 0.0% | 0.0% | 0.0% | 5.8% | 0.4% | 43.1% | 25.3% | 23.0% | 0.5% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% |
| EC13 155 | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 1.2% | 0.0% | 0.4% | 0.3% | 0.0% | 0.0% | 0.0% | 7.2% | 3.3% | 18.2% | 30.6% | 32.9% | 0.9% | 0.4% | 0.5% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.1% | 0.4% | 1.6% | 0.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.9% |
| EC13 167 | 0.0% | 0.0% | 0.0% | 0.0% | 2.1% | 0.0% | 0.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 26.7% | 0.1% | 0.5% | 0.0% | 49.7% | 0.0% | 19.7% | 0.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC13 177 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.8% | 0.2% | 0.0% | 1.3% | 0.0% | 0.1% | 0.9% | 0.6% | 5.4% | 7.7% | 0.2% | 0.4% | 77.5% | 1.3% | 0.0% | 0.0% | 0.1% | 0.5% | 0.3% | 0.1% | 0.0% | 1.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% |
| EC13 185 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.8% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 5.4% | 0.0% | 0.0% | 0.1% | 24.6% | 0.6% | 55.8% | 8.7% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 0.0% | 0.0% | 0.0% | 2.1% | 0.0% |
| EC14 194 | 0.0% | 0.1% | 0.0% | 1.2% | 3.2% | 1.9% | 0.4% | 4.4% | 0.3% | 5.7% | 0.0% | 0.0% | 3.9% | 0.3% | 0.0% | 0.0% | 0.0% | 0.6% | 0.0% | 11.5% | 32.3% | 21.7% | 0.3% | 1.4% | 1.8% | 0.0% | 0.1% | 3.0% | 0.0% | 5.1% | 0.1% | 0.0% | 0.0% | 0.4% | 0.0% |
| EC14 203 | 0.0% | 0.0% | 0.0% | 0.2% | 0.1% | 1.2% | 1.6% | 9.5% | 1.7% | 18.7% | 0.0% | 0.0% | 4.1% | 0.0% | 0.1% | 0.1% | 0.2% | 1.1% | 0.0% | 0.7% | 25.7% | 33.1% | 0.4% | 0.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.6% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC15 190 | 0.0% | 0.2% | 0.0% | 1.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.1% | 0.2% | 94.4% | 0.1% | 3.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC15 223 | 0.5% | 0.0% | 3.6% | 2.1% | 0.0% | 0.4% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.6% | 0.0% | 0.0% | 0.0% | 0.3% | 91.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.8% | 0.0% |
| EC15 224 | 0.0% | 0.4% | 0.0% | 8.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 4.6% | 0.0% | 8.7% | 0.3% | 3.6% | 0.1% | 73.7% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC19 173 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 53.4% | 41.9% | 4.6% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC19 174 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 36.8% | 55.8% | 6.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC19 175 | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 4.7% | 0.2% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 0.3% | 0.1% | 0.1% | 0.1% | 1.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 15.3% | 14.6% | 62.2% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC20 192 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.6% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.0% | 0.0% | 0.8% | 0.1% | 1.6% | 0.0% | 0.0% | 0.5% | 38.8% | 23.4% | 32.3% | 0.0% | 0.0% | 0.0% | 0.1% |
| EC20 198 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.6% | 0.0% | 0.2% | 0.1% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 5.7% | 0.6% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 18.2% | 25.8% | 48.1% | 0.0% | 0.0% | 0.0% | 0.0% |
| EC20 204 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.1% | 0.0% | 0.1% | 0.2% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.4% | 0.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 28.0% | 50.8% | 18.1% | 0.0% | 0.0% | 0.0% | 0.0% |
| UNI 156 | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.3% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.8% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.3% | 0.0% | 0.1% | 97.9% | 0.0% | 0.0% | 0.0% |
| UNI 178 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 1.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 98.0% | 0.2% | 0.0% |
| UNI 191 | 0.0% | 0.0% | 0.6% | 3.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.2% | 0.0% | 0.0% | 0.0% | 1.5% | 0.0% | 3.1% | 0.1% | 0.0% | 0.0% | 1.1% | 0.2% | 0.1% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 0.0% | 0.0% | 88.5% | 0.2% |
| UNI 214 | 0.0% | 0.1% | 0.4% | 0.0% | 0.0% | 2.5% | 0.0% | 19.0% | 1.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.9% | 0.3% | 0.2% | 1.7% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.1% | 0.4% | 0.0% | 0.1% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 5.2% | 67.6% |

*The different colours represent the strain level identification.*

Table S4 The prediction accuracies of the 35 enterococci isolates using a PLS-DA model generated from MALDI-TOF-MS data

| | EC04 109 | EC04 170 | EC04 179 | EC04 193 | EC09 133 | EC09 160 | EC09 205 | EC09 211 | EC09 219 | EC09 233 | EC10 139 | EC10 151 | EC13 144 | EC13 149 | EC13 152 | EC13 154 | EC13 155 | EC13 167 | EC13 177 | EC13 185 | EC14 194 | EC14 203 | EC15 190 | EC15 223 | EC15 224 | EC19 173 | EC19 174 | EC19 175 | EC20 192 | EC20 198 | EC20 204 | UNI 156 | UNI 178 | UNI 191 | UNI 214 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| EC04 109 | 59.6% | 1.1% | 20.9% | 0.8% | 0.3% | 0.0% | 0.1% | 0.1% | 0.0% | 0.5% | 0.3% | 0.8% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 5.5% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 9.5% | 0.0% |
| EC04 170 | 1.9% | 87.0% | 4.0% | 0.0% | 0.0% | 0.0% | 3.7% | 0.1% | 0.0% | 0.0% | 0.0% | 1.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.2% | 0.4% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.0% |
| EC04 179 | 23.1% | 1.5% | 49.9% | 11.5% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.1% | 0.7% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.6% | 0.0% | 1.0% | 0.0% | 0.0% | 0.5% | 3.2% | 0.2% | 0.0% | 2.0% | 1.2% | 0.0% | 0.2% | 0.1% | 0.4% | 0.0% | 2.9% | 0.1% |
| EC04 193 | 1.5% | 0.0% | 19.0% | 42.0% | 0.0% | 0.0% | 0.0% | 2.7% | 0.0% | 0.3% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.3% | 0.8% | 16.5% | 4.2% | 1.2% | 0.0% | 0.0% | 0.0% | 0.3% | 1.0% | 0.4% | 0.0% | 0.0% | 9.5% | 0.2% |
| EC09 133 | 0.1% | 0.0% | 0.3% | 0.0% | 15.5% | 0.0% | 2.2% | 2.0% | 0.0% | 5.7% | 0.4% | 0.0% | 2.9% | 11.1% | 0.3% | 0.0% | 0.0% | 8.0% | 8.0% | 7.7% | 27.5% | 1.3% | 1.2% | 0.1% | 0.7% | 0.5% | 0.0% | 0.9% | 0.0% | 0.0% | 0.1% | 2.3% | 0.0% | 0.6% | 0.5% |
| EC09 160 | 0.1% | 0.3% | 0.0% | 0.1% | 0.0% | 97.2% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 0.5% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% |
| EC09 205 | 0.0% | 0.3% | 0.1% | 0.0% | 2.0% | 0.0% | 36.4% | 2.3% | 0.0% | 9.6% | 0.0% | 0.0% | 0.1% | 0.0% | 0.2% | 1.0% | 1.4% | 1.0% | 0.0% | 1.8% | 1.1% | 26.6% | 1.4% | 0.0% | 0.1% | 0.5% | 0.1% | 0.4% | 0.0% | 0.0% | 0.0% | 2.1% | 0.0% | 0.0% | 11.4% |
| EC09 211 | 0.0% | 0.0% | 0.1% | 0.4% | 0.3% | 0.0% | 2.3% | 69.8% | 0.0% | 10.1% | 11.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.1% | 0.2% | 0.0% | 0.1% | 0.0% | 1.9% | 1.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.2% | 0.0% | 0.0% | 0.3% |
| EC09 219 | 0.0% | 0.0% | 0.0% | 0.7% | 0.0% | 0.0% | 0.3% | 0.0% | 96.2% | 0.0% | 0.0% | 0.1% | 0.1% | 0.0% | 0.3% | 0.0% | 0.0% | 0.1% | 0.0% | 0.9% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.3% | 0.6% |
| EC09 233 | 2.1% | 0.0% | 0.0% | 0.1% | 4.9% | 0.0% | 14.6% | 21.0% | 0.0% | 18.9% | 0.3% | 0.1% | 1.0% | 0.0% | 1.2% | 2.9% | 5.4% | 2.0% | 0.0% | 0.2% | 0.7% | 17.7% | 0.2% | 0.0% | 1.3% | 0.0% | 0.1% | 0.1% | 0.2% | 0.0% | 0.0% | 0.5% | 0.0% | 0.2% | 4.4% |
| EC10 139 | 0.6% | 0.0% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 7.5% | 0.0% | 0.0% | 80.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 2.9% | 0.0% | 0.9% | 0.4% | 0.9% | 0.2% | 0.2% | 0.9% | 0.0% | 0.0% | 1.2% | 2.9% |
| EC10 151 | 4.8% | 0.1% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.6% | 89.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.3% | 0.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 3.3% | 0.0% |
| EC13 144 | 0.0% | 0.0% | 0.0% | 0.7% | 4.8% | 0.0% | 0.3% | 0.2% | 0.0% | 2.0% | 0.1% | 0.2% | 9.8% | 38.7% | 8.2% | 2.8% | 2.1% | 11.1% | 0.0% | 4.2% | 1.7% | 1.6% | 0.2% | 0.0% | 0.7% | 0.9% | 5.4% | 0.4% | 0.1% | 0.1% | 3.2% | 0.5% | 0.0% | 0.0% | 0.2% |
| EC13 149 | 0.0% | 0.0% | 0.8% | 0.0% | 8.9% | 0.0% | 0.0% | 4.8% | 0.0% | 0.7% | 0.1% | 0.0% | 28.4% | 6.3% | 1.0% | 2.1% | 3.4% | 24.6% | 0.1% | 13.0% | 2.8% | 0.0% | 0.2% | 0.1% | 0.0% | 0.0% | 0.5% | 0.3% | 0.0% | 0.0% | 1.1% | 0.1% | 0.0% | 0.1% | 0.5% |
| EC13 152 | 0.1% | 0.0% | 0.0% | 2.8% | 0.1% | 0.0% | 0.6% | 0.5% | 0.0% | 1.3% | 0.5% | 0.0% | 5.7% | 3.1% | 10.7% | 34.1% | 29.7% | 0.0% | 0.0% | 0.3% | 0.0% | 4.9% | 0.3% | 0.4% | 0.0% | 0.4% | 1.3% | 0.4% | 0.0% | 0.1% | 0.1% | 1.7% | 0.0% | 0.7% | 0.3% |
| EC13 154 | 0.1% | 0.0% | 0.0% | 3.4% | 0.0% | 0.0% | 0.3% | 1.1% | 0.0% | 1.0% | 0.0% | 0.0% | 3.5% | 2.1% | 29.1% | 5.9% | 40.7% | 0.8% | 0.1% | 0.6% | 0.0% | 1.0% | 1.2% | 0.0% | 0.1% | 1.0% | 1.2% | 0.5% | 0.0% | 0.2% | 0.1% | 2.7% | 0.0% | 0.0% | 3.3% |
| EC13 155 | 0.0% | 0.0% | 0.0% | 1.2% | 0.0% | 0.0% | 2.1% | 1.2% | 0.0% | 1.2% | 0.0% | 0.0% | 1.2% | 0.4% | 32.6% | 41.6% | 9.7% | 0.2% | 0.0% | 0.2% | 0.0% | 2.7% | 0.0% | 0.7% | 0.0% | 0.1% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 3.8% | 0.0% | 0.0% | 0.9% |
| EC13 167 | 0.0% | 0.0% | 0.3% | 0.0% | 10.6% | 0.0% | 0.9% | 3.7% | 0.0% | 2.4% | 0.0% | 0.0% | 9.0% | 19.1% | 0.3% | 0.1% | 0.2% | 13.0% | 2.5% | 21.3% | 11.9% | 0.3% | 0.0% | 1.6% | 0.1% | 0.1% | 0.0% | 0.8% | 0.6% | 0.0% | 0.2% | 0.9% | 0.0% | 0.0% | 0.1% |
| EC13 177 | 0.1% | 0.5% | 1.2% | 0.0% | 6.1% | 0.0% | 0.0% | 0.8% | 0.0% | 0.0% | 0.0% | 0.2% | 0.1% | 0.3% | 0.0% | 0.0% | 0.0% | 3.7% | 70.4% | 7.2% | 6.1% | 0.0% | 0.1% | 2.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.1% |
| EC13 185 | 0.1% | 0.0% | 0.9% | 0.0% | 5.5% | 0.0% | 0.6% | 0.5% | 0.0% | 1.3% | 0.0% | 0.5% | 1.7% | 8.8% | 0.3% | 0.1% | 0.1% | 13.8% | 0.2% | 42.3% | 9.3% | 0.5% | 1.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.3% | 0.6% | 0.2% | 10.5% | 0.0% | 0.3% | 0.0% |
| EC14 194 | 0.1% | 0.0% | 0.2% | 1.8% | 27.0% | 0.0% | 3.7% | 0.9% | 0.0% | 0.4% | 0.0% | 0.0% | 0.7% | 3.7% | 0.0% | 0.3% | 0.0% | 10.2% | 1.3% | 13.4% | 15.6% | 12.5% | 3.1% | 0.1% | 0.0% | 1.0% | 1.4% | 1.6% | 0.0% | 0.3% | 0.0% | 0.2% | 0.0% | 0.4% | 0.0% |
| EC14 203 | 0.0% | 0.0% | 0.0% | 2.9% | 2.1% | 0.0% | 36.5% | 6.5% | 0.0% | 13.8% | 0.0% | 0.0% | 0.7% | 0.3% | 0.5% | 1.1% | 0.3% | 0.0% | 0.0% | 0.2% | 12.9% | 4.3% | 2.8% | 0.3% | 0.0% | 0.2% | 0.2% | 0.0% | 0.0% | 0.0% | 0.5% | 0.3% | 0.0% | 3.3% | 10.2% |
| EC15 190 | 0.0% | 0.0% | 2.1% | 16.3% | 0.4% | 0.0% | 0.2% | 1.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.1% | 0.3% | 0.4% | 0.1% | 0.0% | 0.0% | 0.1% | 1.4% | 0.2% | 57.0% | 5.1% | 12.9% | 0.2% | 0.0% | 0.0% | 1.4% | 0.0% | 0.0% | 0.1% | 0.0% | 0.3% | 0.0% |
| EC15 223 | 4.9% | 0.4% | 0.6% | 3.6% | 0.9% | 0.0% | 0.3% | 0.1% | 0.0% | 0.7% | 3.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.6% | 0.0% | 0.0% | 0.0% | 0.0% | 4.9% | 32.4% | 3.3% | 0.3% | 0.0% | 7.2% | 0.5% | 0.9% | 0.2% | 0.2% | 0.0% | 34.7% | 0.0% |
| EC15 224 | 0.0% | 0.2% | 0.0% | 0.3% | 1.4% | 0.0% | 0.4% | 0.0% | 0.0% | 0.5% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 5.7% | 0.3% | 81.9% | 0.1% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 1.1% | 0.0% | 0.0% | 7.3% |
| EC19 173 | 0.0% | 0.2% | 0.0% | 0.1% | 0.2% | 0.0% | 0.4% | 0.1% | 0.0% | 0.0% | 0.6% | 0.0% | 0.1% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.1% | 0.0% | 24.6% | 47.2% | 24.7% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.7% |
| EC19 174 | 0.4% | 0.2% | 0.1% | 0.4% | 0.0% | 0.0% | 3.3% | 0.0% | 0.0% | 0.3% | 0.2% | 0.2% | 1.5% | 0.0% | 0.3% | 1.0% | 0.1% | 0.0% | 0.0% | 0.1% | 0.0% | 0.1% | 0.1% | 0.1% | 0.0% | 53.2% | 20.1% | 17.8% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.5% | 0.0% |
| EC19 175 | 0.3% | 0.2% | 0.0% | 0.0% | 0.8% | 0.0% | 0.1% | 0.0% | 0.0% | 0.4% | 0.5% | 0.0% | 1.2% | 0.1% | 0.0% | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.5% | 0.0% | 0.0% | 0.3% | 0.0% | 30.6% | 15.0% | 47.3% | 0.6% | 0.5% | 0.0% | 0.5% | 0.0% | 0.9% | 0.0% |
| EC20 192 | 0.0% | 0.0% | 0.2% | 0.2% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 1.5% | 0.0% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.9% | 0.1% | 0.0% | 1.4% | 0.1% | 2.0% | 0.0% | 0.0% | 0.7% | 32.3% | 34.9% | 24.2% | 0.2% | 0.0% | 0.1% | 0.0% |
| EC20 198 | 0.0% | 0.1% | 0.7% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 0.0% | 0.0% | 32.4% | 30.8% | 34.5% | 0.1% | 0.0% | 0.1% | 0.0% |
| EC20 204 | 0.0% | 0.0% | 0.2% | 0.4% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 2.8% | 0.0% | 0.4% | 2.1% | 1.3% | 0.0% | 0.0% | 0.4% | 0.0% | 0.4% | 0.0% | 0.3% | 0.0% | 0.8% | 0.0% | 0.0% | 0.0% | 0.0% | 31.5% | 43.6% | 12.0% | 3.0% | 0.0% | 0.4% | 0.2% |
| UNI 156 | 0.3% | 0.0% | 0.0% | 0.0% | 0.9% | 0.0% | 2.6% | 0.4% | 0.0% | 0.6% | 0.0% | 0.0% | 0.0% | 0.0% | 1.7% | 1.8% | 1.6% | 0.9% | 0.0% | 4.7% | 0.3% | 0.0% | 0.0% | 0.2% | 0.1% | 0.0% | 0.0% | 1.1% | 1.6% | 0.5% | 1.7% | 73.6% | 0.0% | 0.0% | 5.4% |
| UNI 178 | 0.0% | 0.0% | 0.1% | 0.1% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.3% | 0.0% | 8.3% | 0.0% | 0.0% | 1.0% | 0.0% | 0.1% | 0.0% | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 89.2% | 0.0% | 0.0% |
| UNI 191 | 19.7% | 0.1% | 6.4% | 11.9% | 0.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.2% | 0.1% | 0.1% | 0.3% | 36.4% | 0.0% | 0.2% | 0.1% | 2.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 21.2% | 0.0% |
| UNI 214 | 0.0% | 0.0% | 0.1% | 0.2% | 0.5% | 0.0% | 11.4% | 0.1% | 0.0% | 5.0% | 4.5% | 0.0% | 0.1% | 0.0% | 0.1% | 0.2% | 1.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.4% | 0.0% | 0.0% | 8.9% | 0.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 4.9% | 0.0% | 0.0% | 61.9% |

*The different colours represent the strain level identification*

Table S5 The 4 main clusters (including SMCs) observed from the three different analytical techniques based on PC-DFA plots of 12 classes (12 strains)

| | **Cluster 1** | **Cluster 2** | | **Cluster 3** | | **Cluster 4** | |
|---|---|---|---|---|---|---|---|
| **FT-IR** | EC10 | EC20 | UN 156 | EC04/EC15/UN 191 | | EC13/EC19/EC14/EC09/UN 214 | UN 178 |
| **Raman** | EC10 | EC20 | UN 178 | EC04/EC15/UN 191 | | EC13/EC19/EC14/EC09/UN 214/ UN156 | |
| **MALDI** | UN 178 | EC20 | | EC04/EC15/UN 191 | EC10 | EC13/EC19/EC14/EC09/UN 214/ UN156 | |