

Bacteria-infected artificial urine characterization based on a combined approach using an electronic tongue complemented with ^1H -NMR and flow cytometry

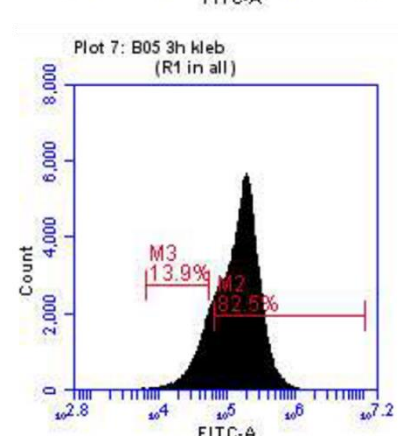
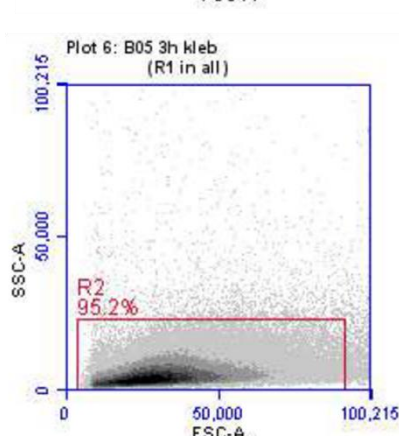
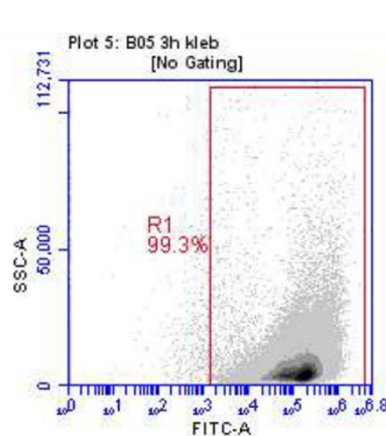
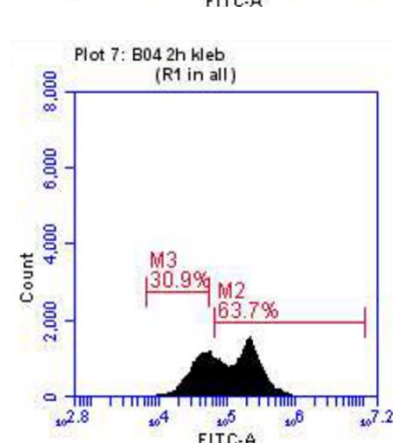
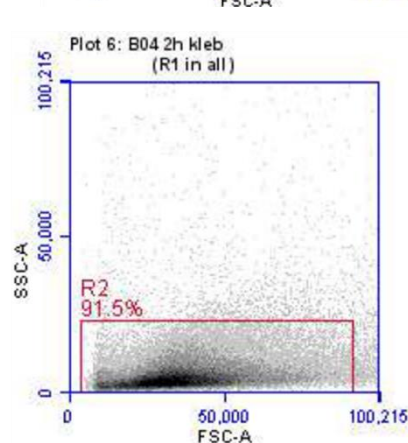
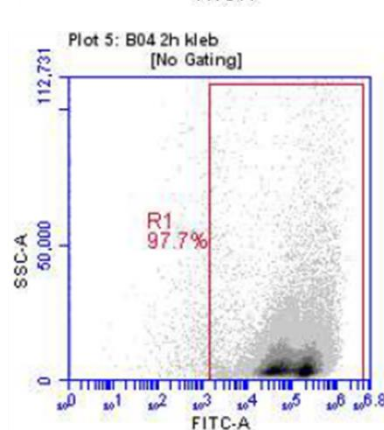
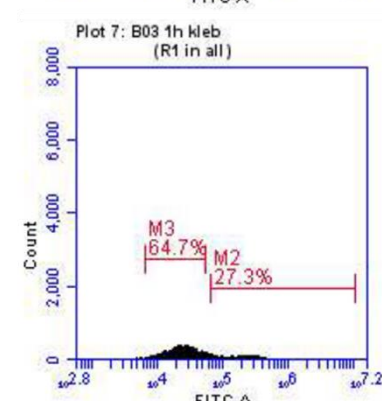
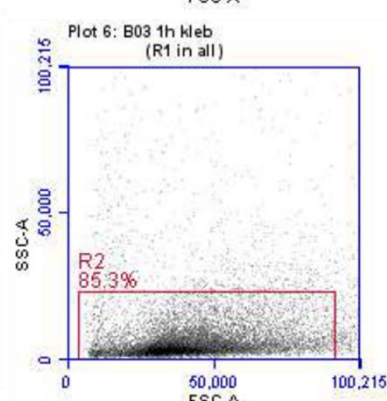
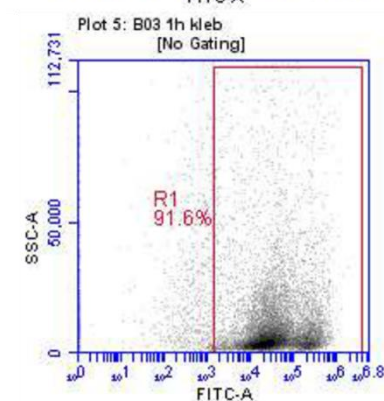
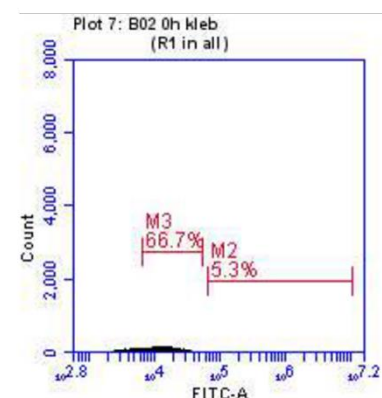
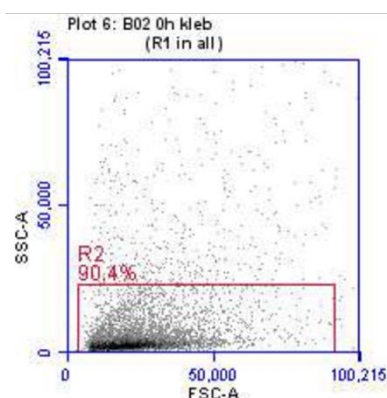
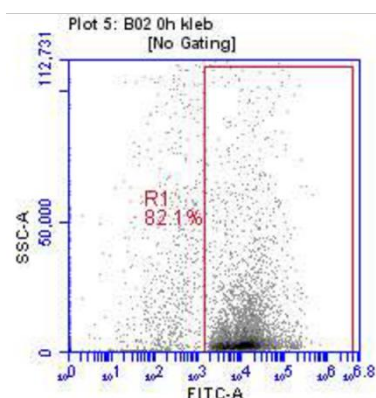
Carolin Psotta, Emelie J. Nilsson, Thomas Sjöberg and Magnus Falk*

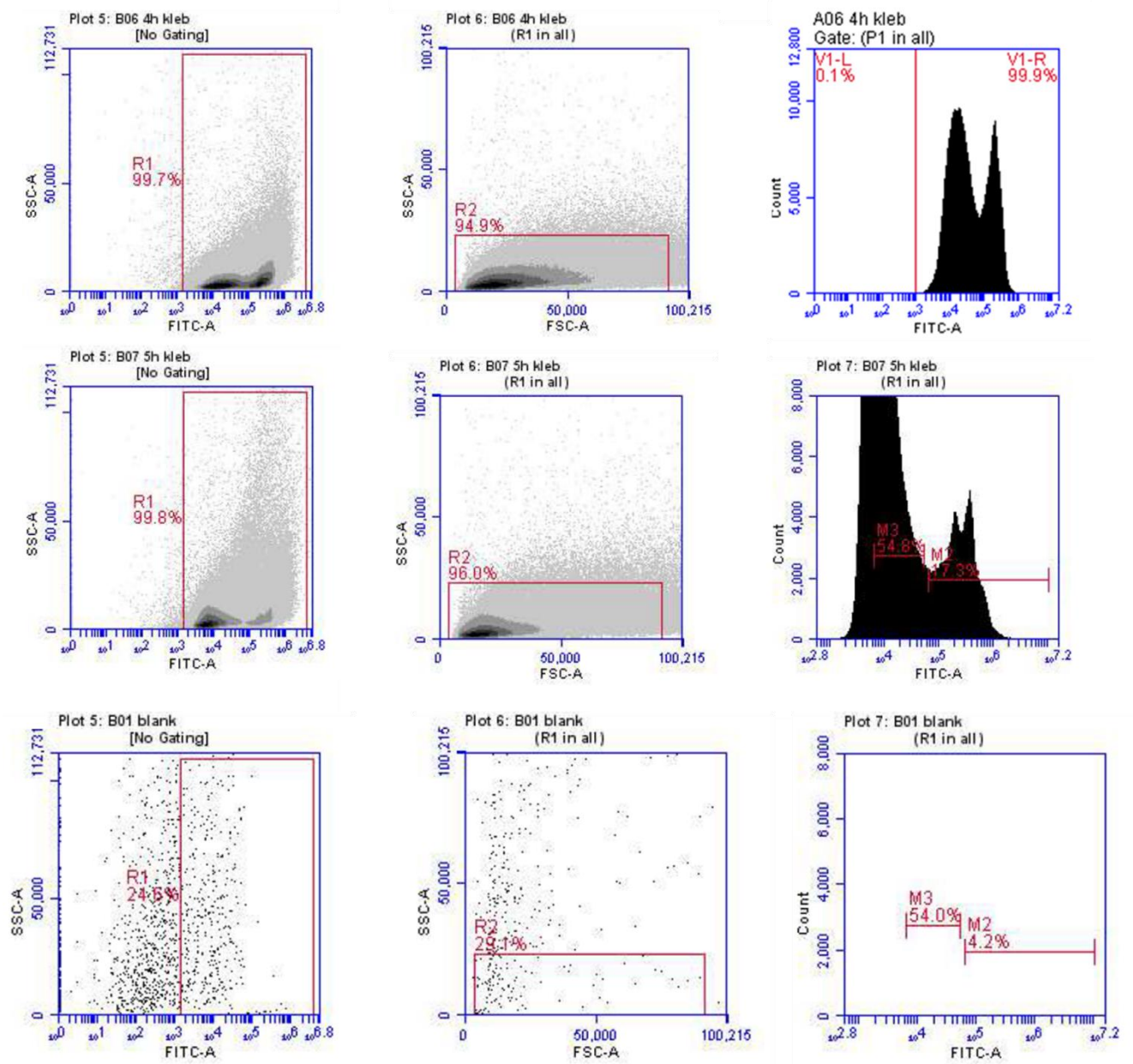
Department of Biomedical Science. Faculty of Health and Society. Malmö University.
Malmö 20506. Sweden

Biofilms-Research Center for Biointerfaces. Malmö University. Malmö 20506. Sweden

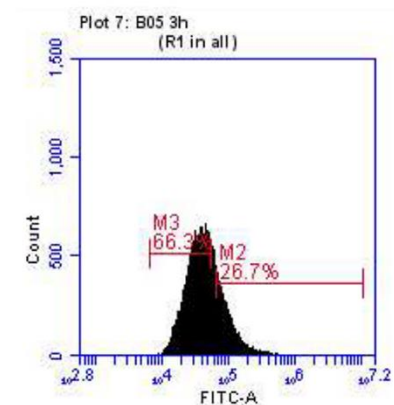
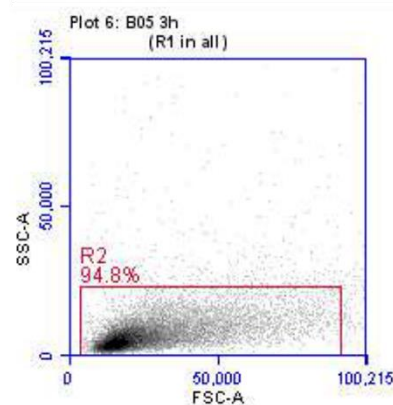
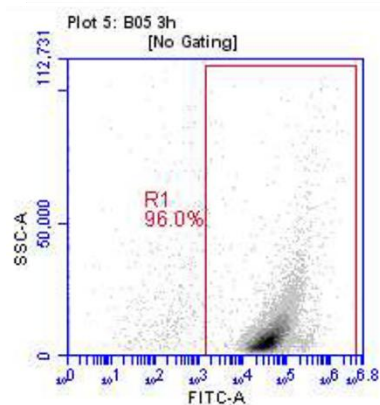
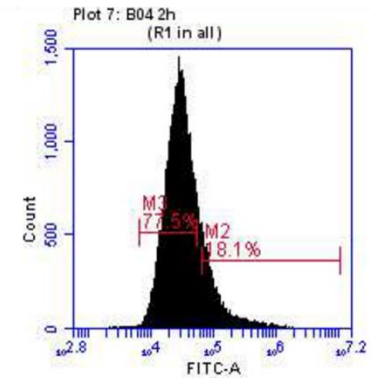
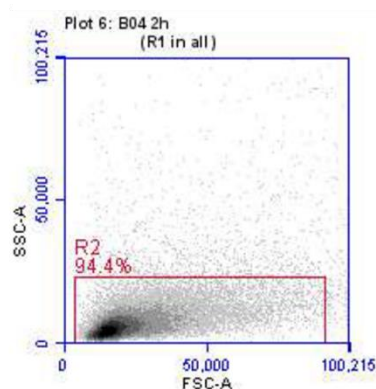
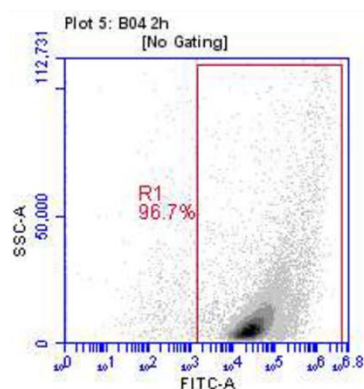
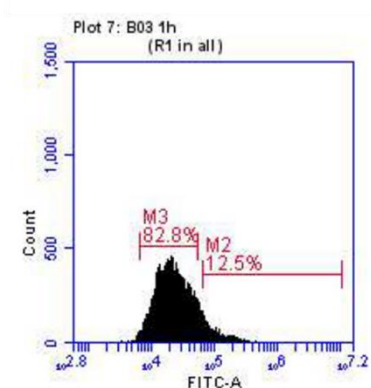
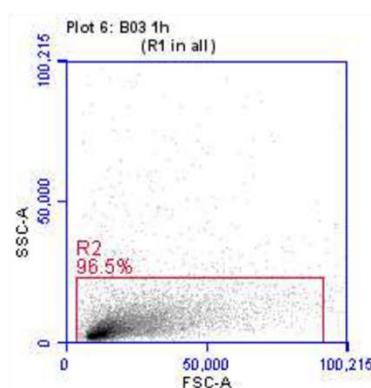
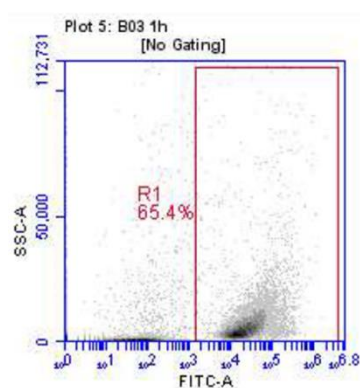
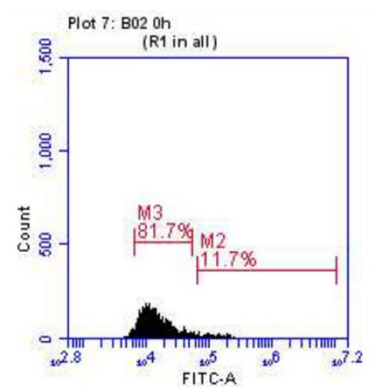
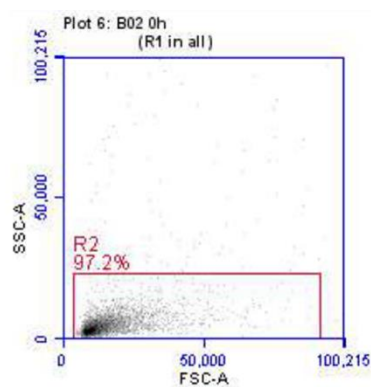
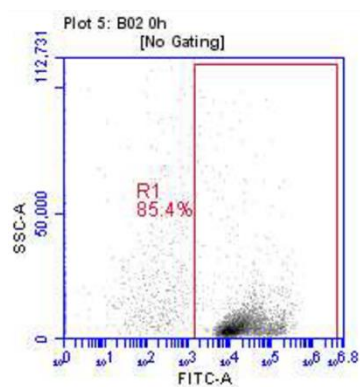
*corresponding author

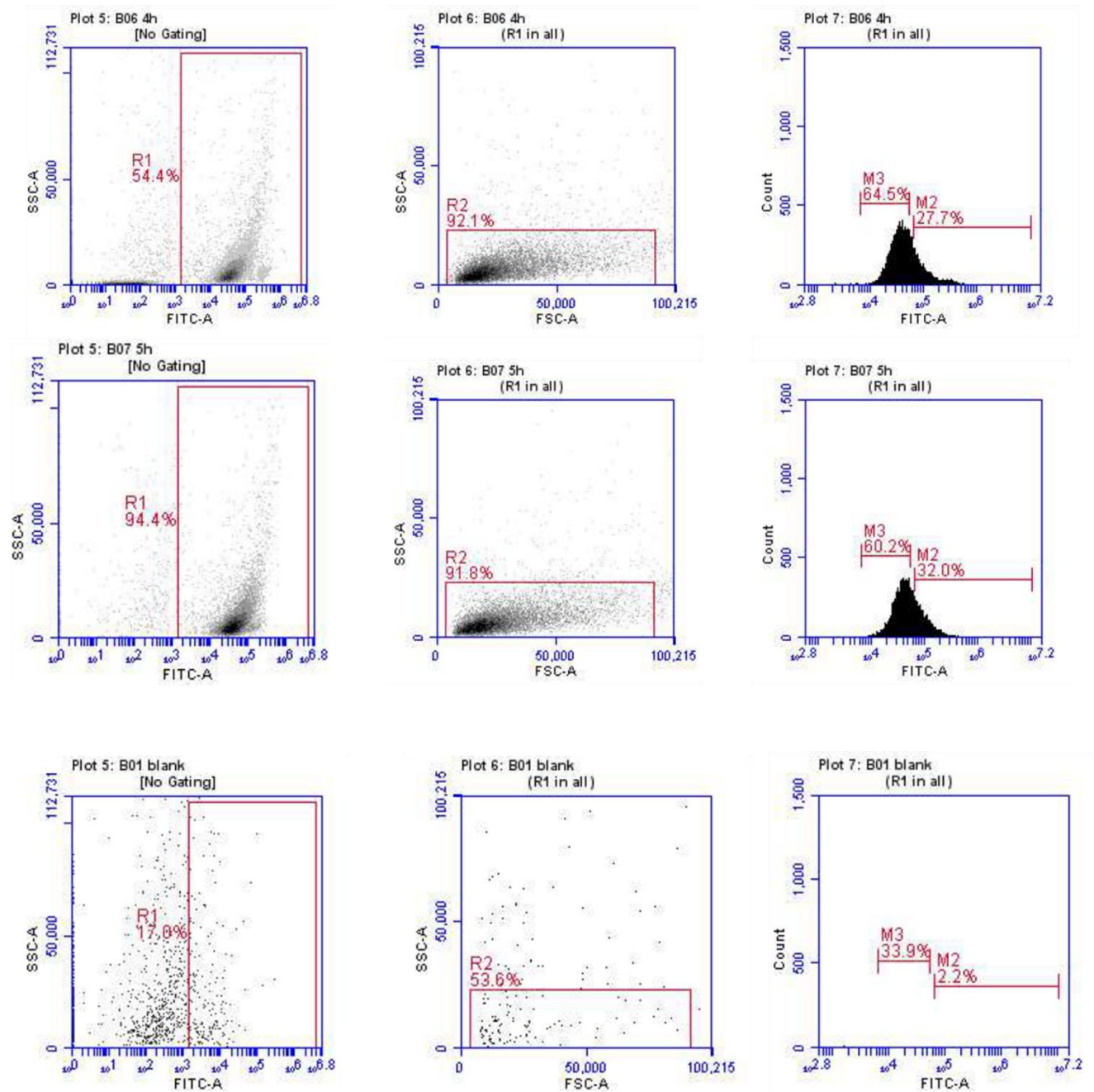
Supporting material



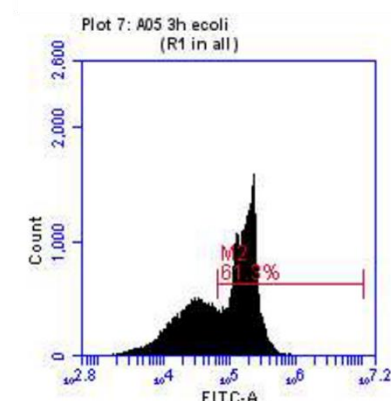
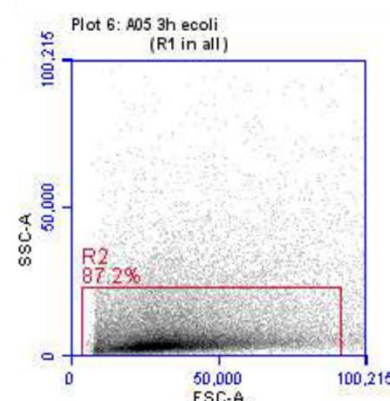
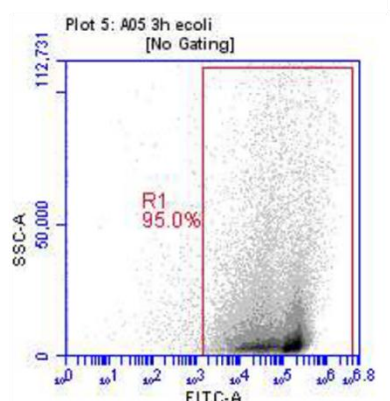
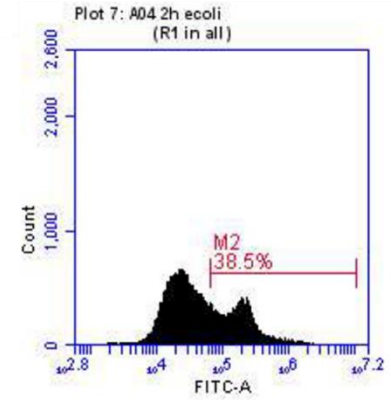
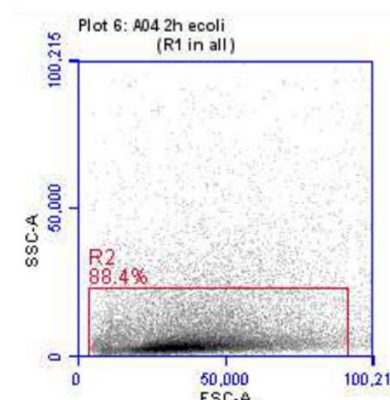
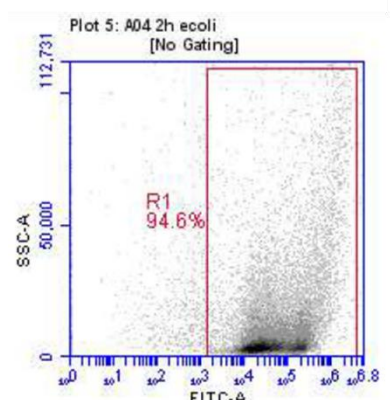
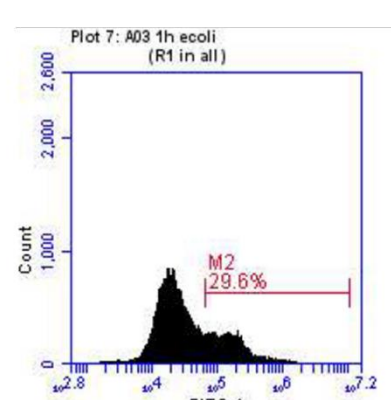
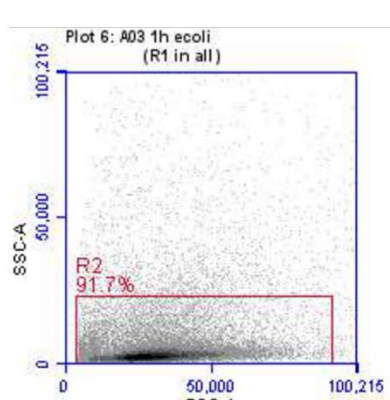
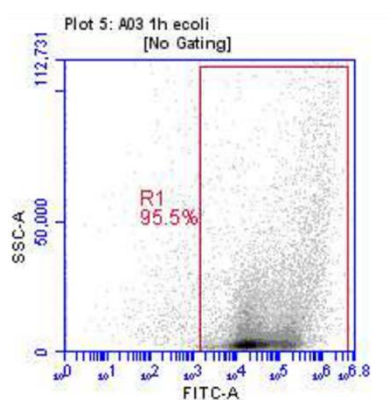
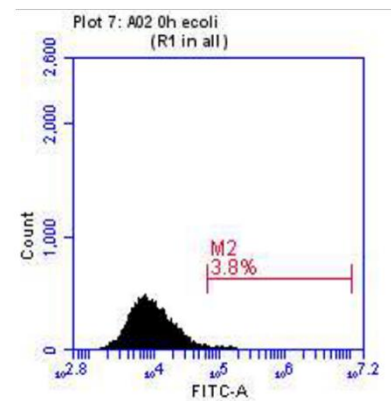
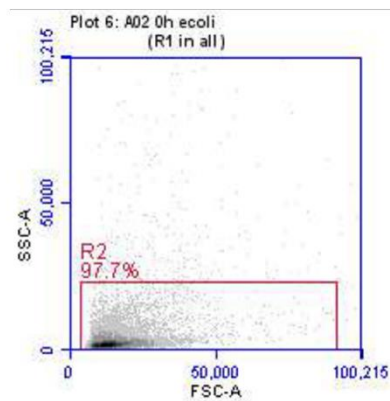
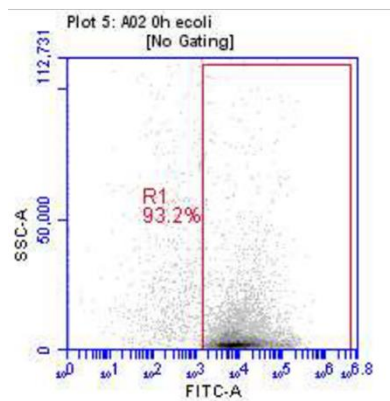


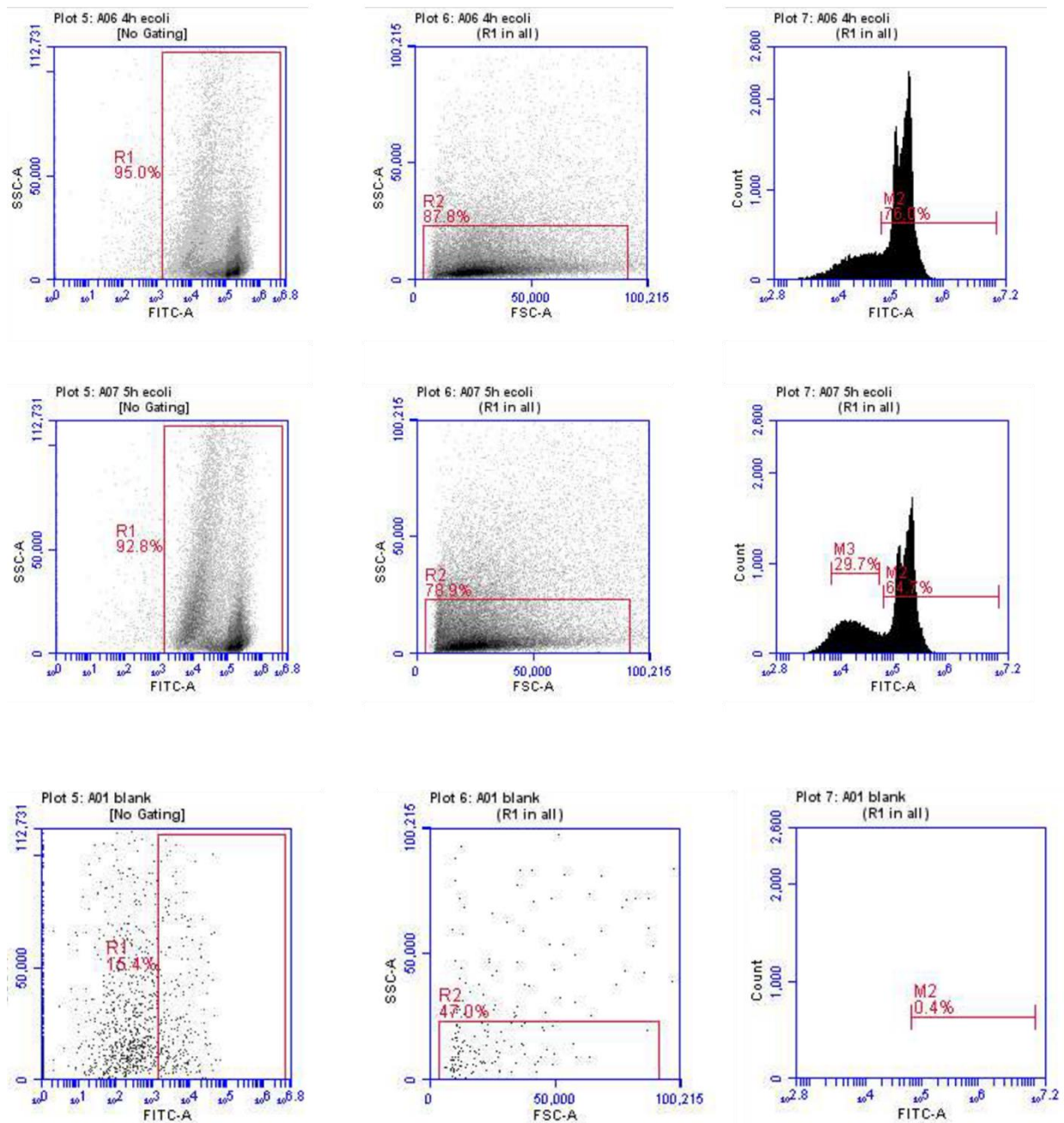
Supporting Figure S1: Flow cytometry results for *K.pneumoniae*, displaying FITC-A (Fluorescein isothiocyanate) vs. cell count.



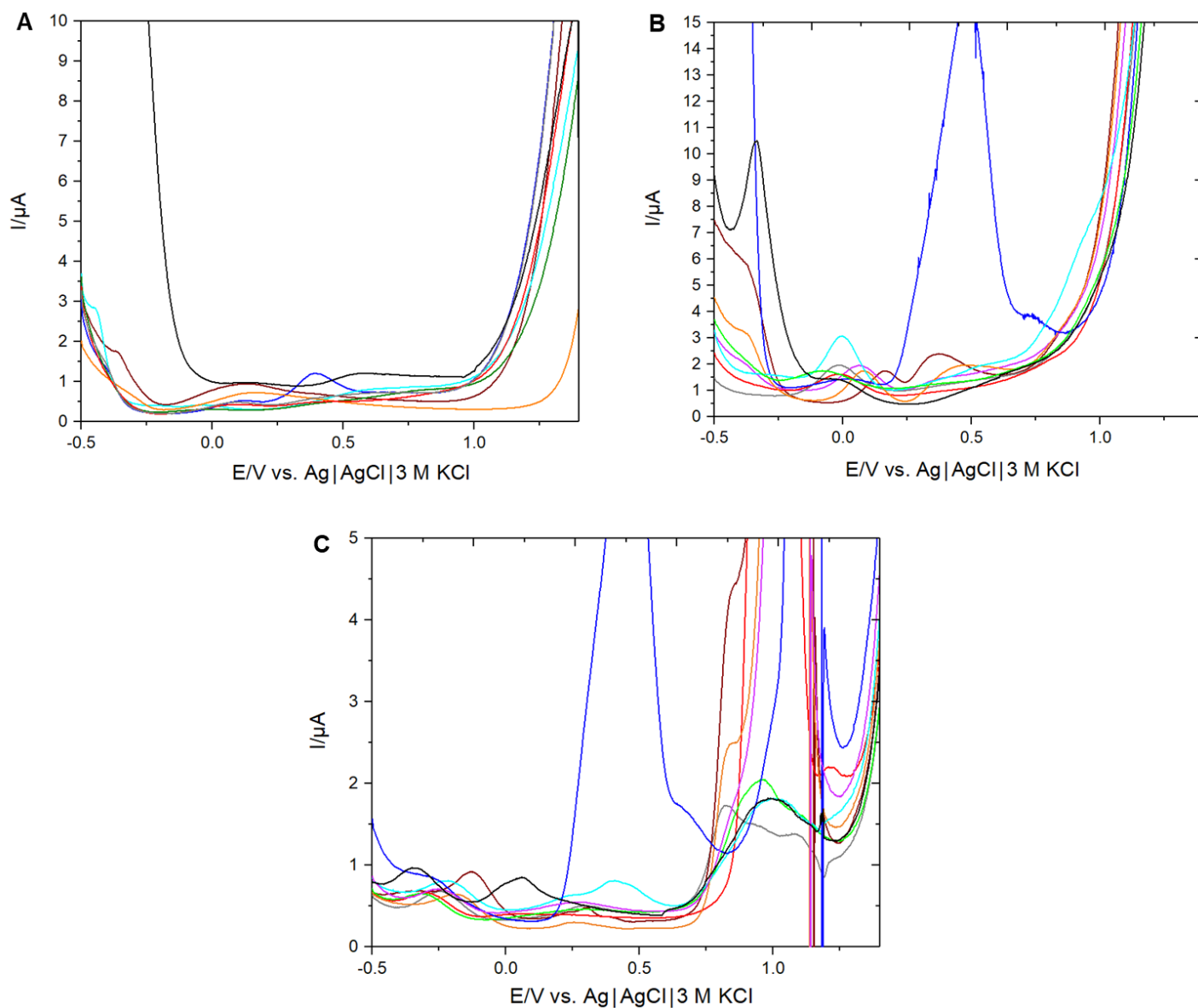


Supporting Figure S2: Flow cytometry results for *E. faecalis*, displaying FITC-A (Fluorescein isothiocyanate) vs. cell count.

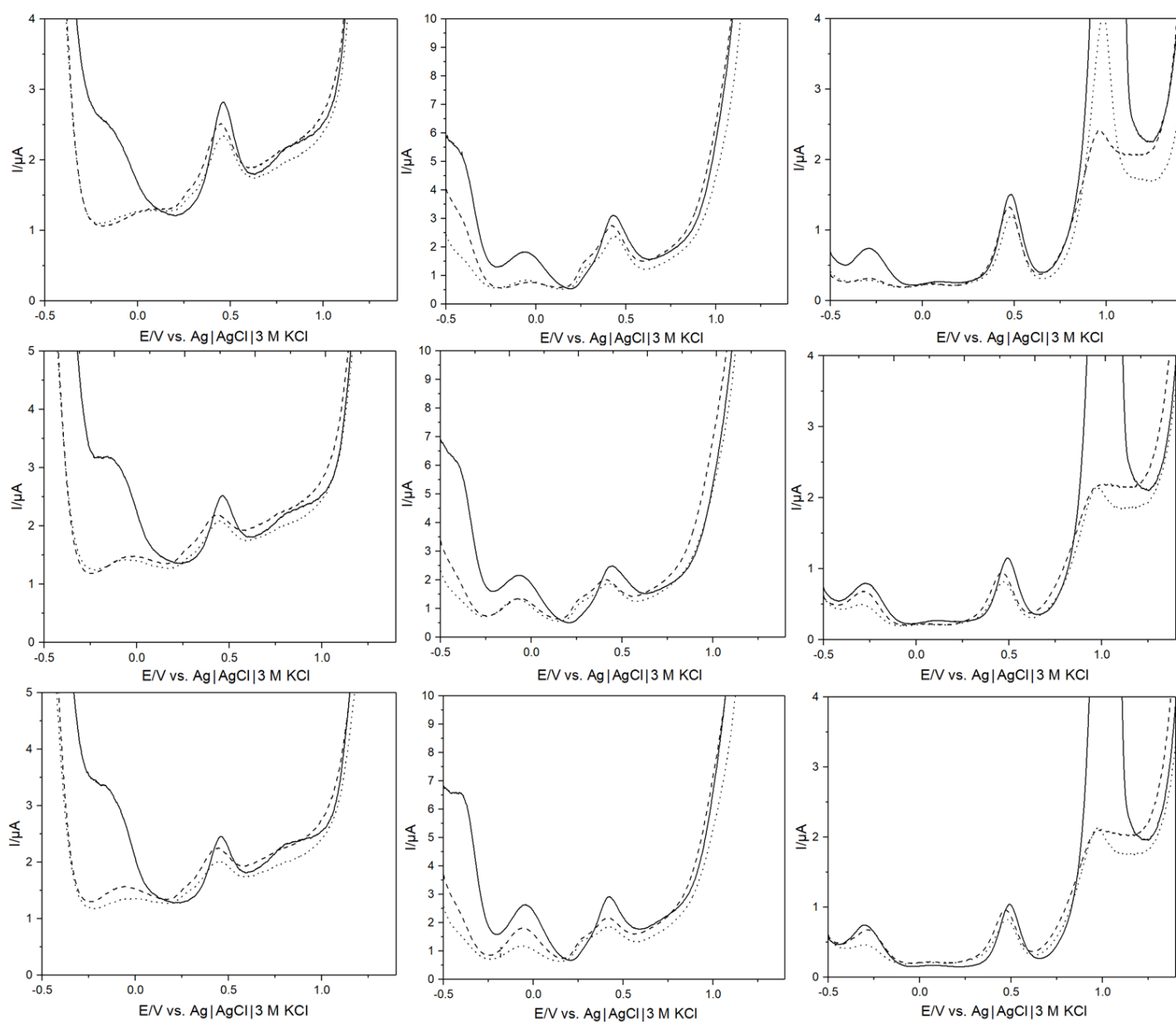




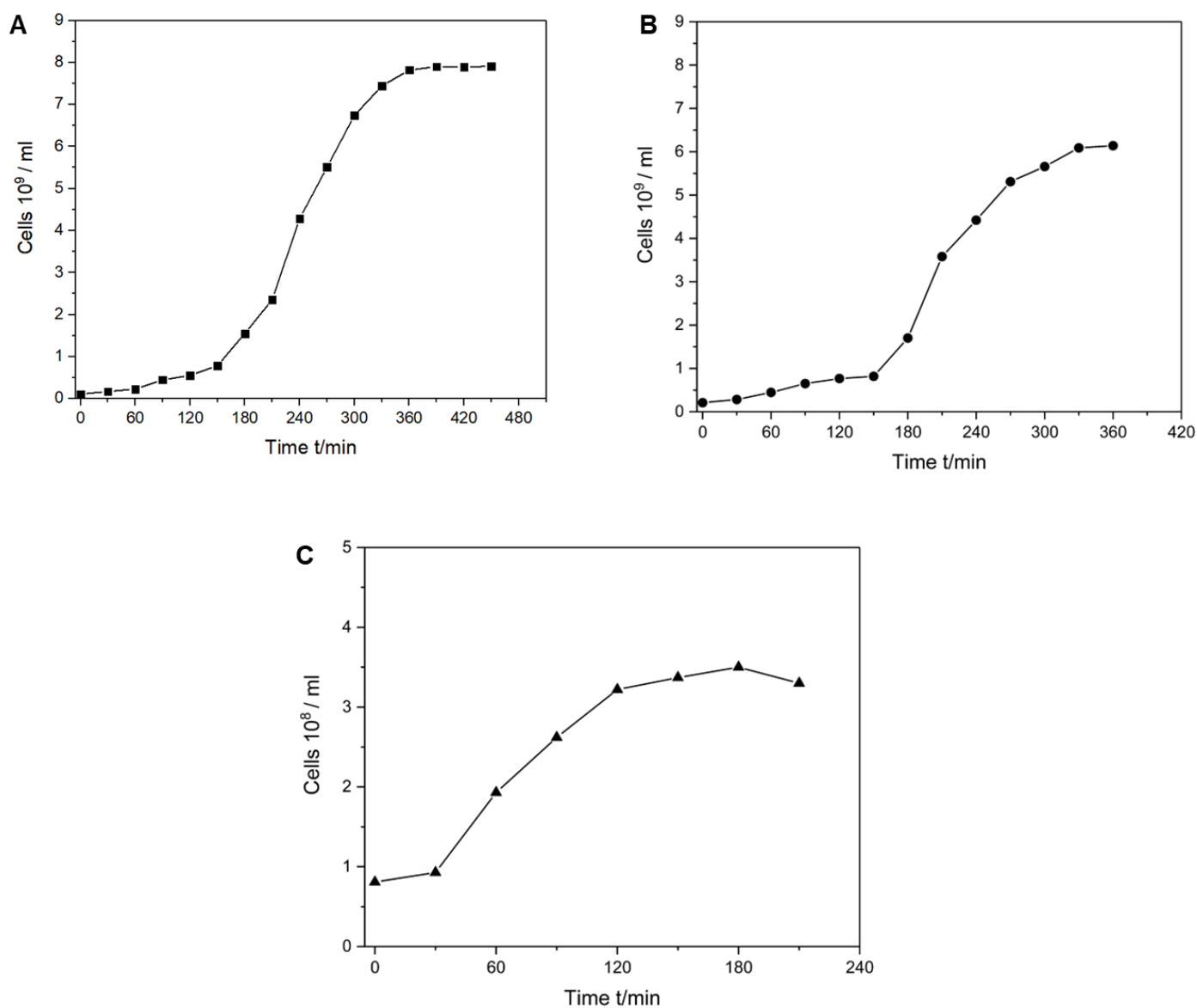
Supporting Figure S3: Flow cytometry results for *E. coli*, displaying FITC-A (Fluorescein isothiocyanate) vs. cell count.



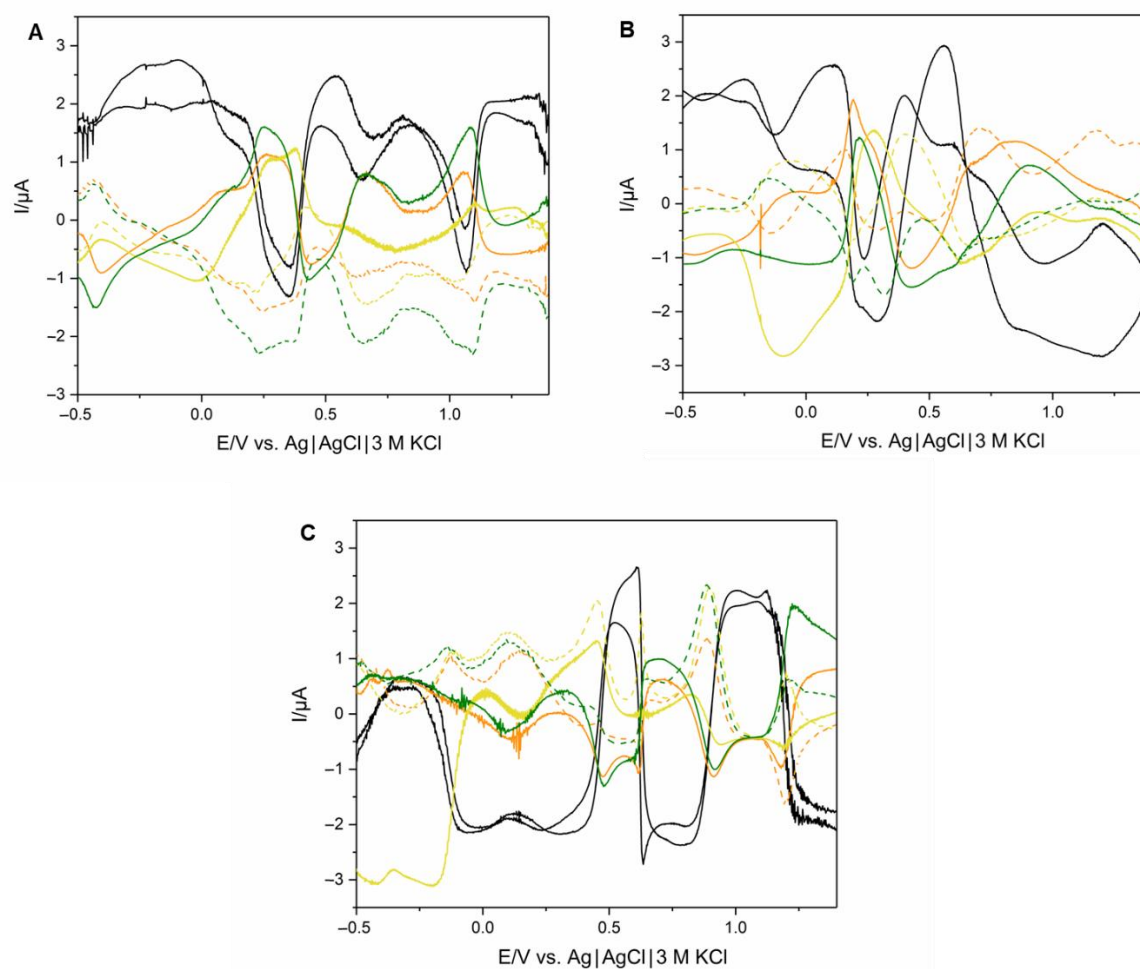
Supporting Figure S4: Investigation of Pt (A), Pd (B) and Au (C) electrodes using DPV in PBS and PBS with each of the metabolically relevant compounds in AUM, using the same concentrations as used in AUM (see Table 1, MS): PBS (black), acetic acid (grey), uric acid (dark blue), peptone (green), citric acid (dark red), lactic acid (orange), urea (cyan), creatinine (light red).



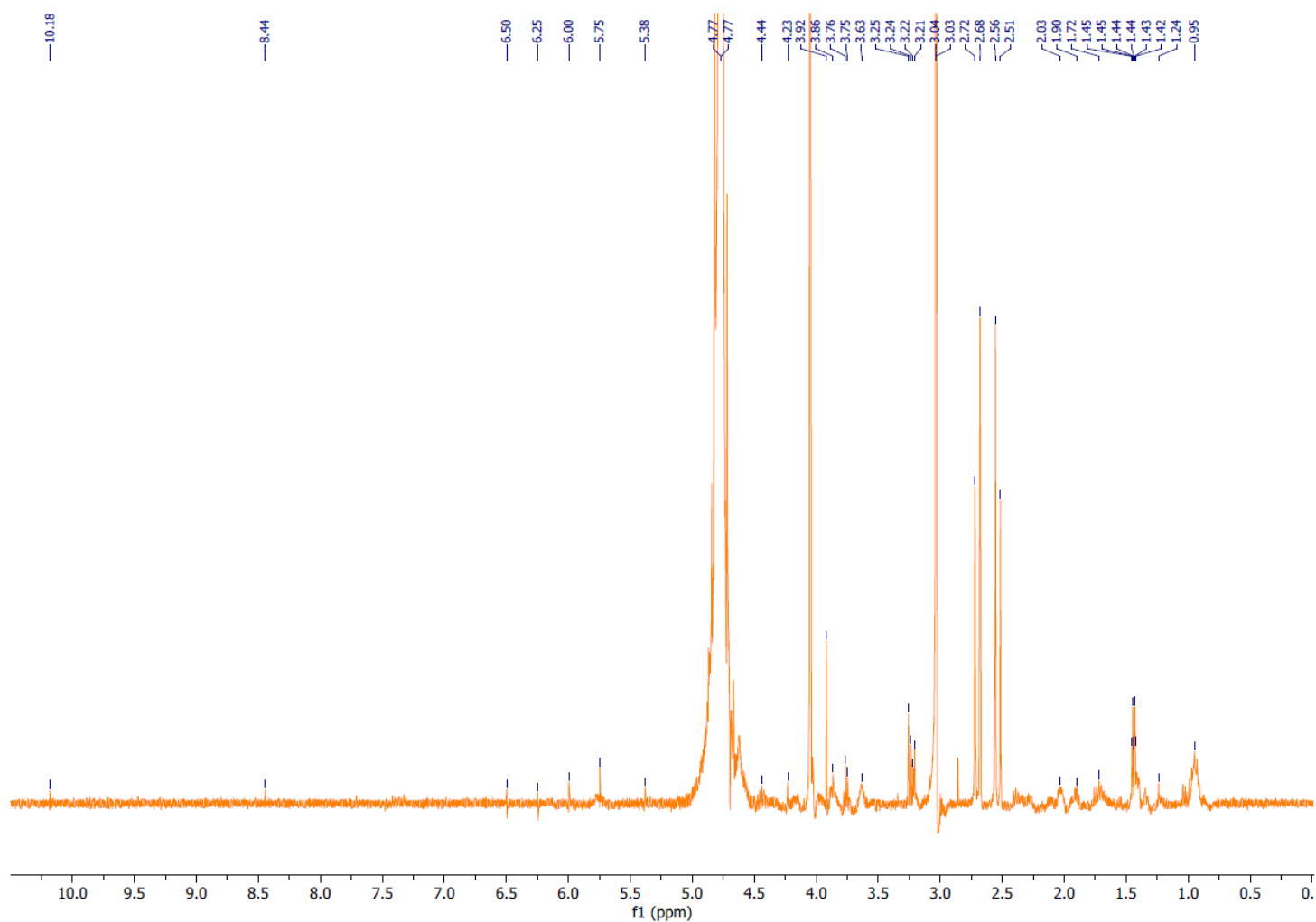
Supporting Figure S5: DPV comparing bacteria-infected AUM with the supernatant of the infected solution (solid = AUM; dashed = bacteria; dotted = supernatant): *K.pneumoniae* (top; $n = 3$), *E.faecalis* (middle; $n = 3$), *E.coli* (bottom; $n = 3$) and each electrode material (columns Pt (left) Pd (middle), Au (right)).



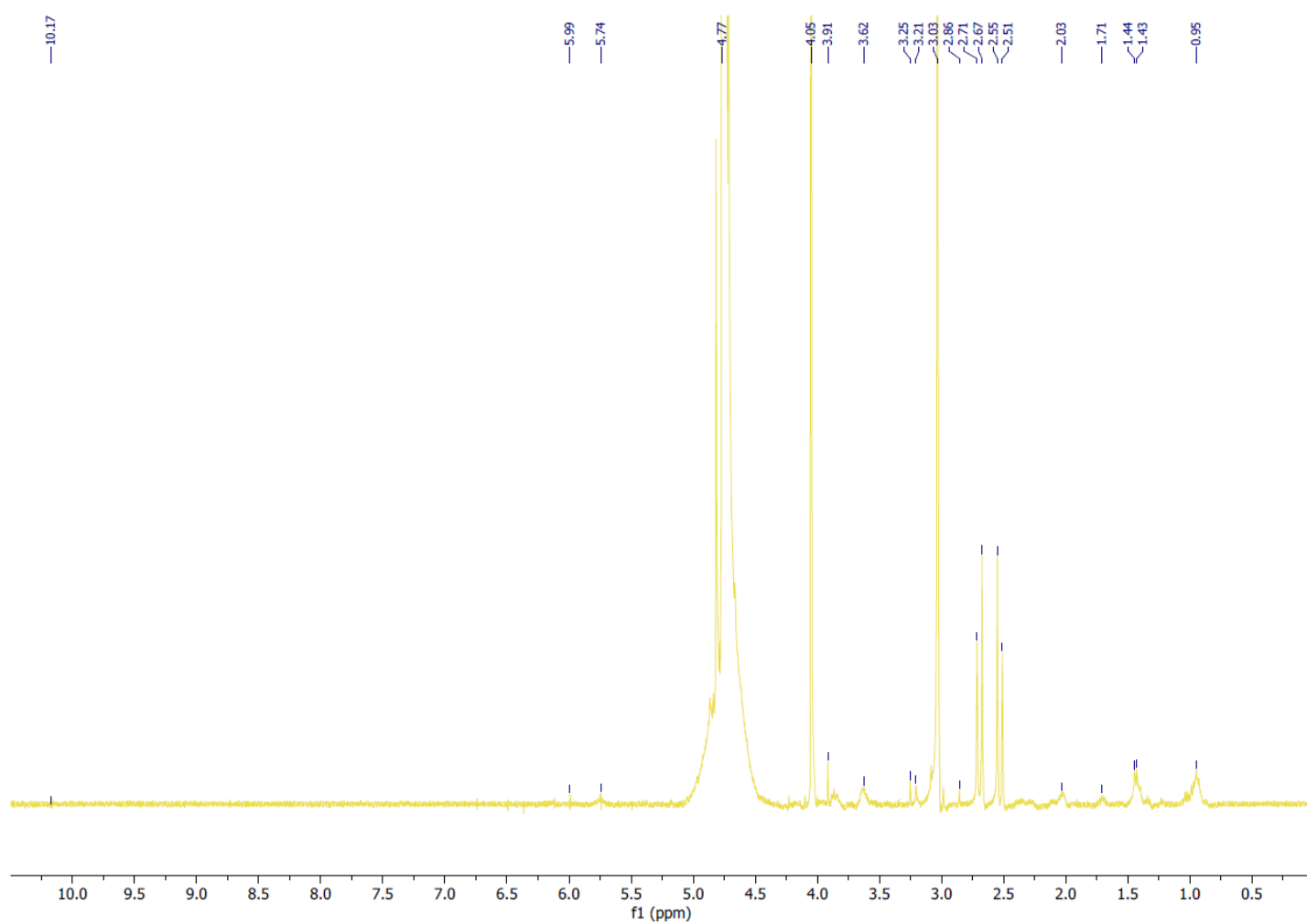
Supporting Figure S6: Bacterial growth curves in AUM obtained by measuring the optical density for *K.pneumoniae* (A), *E.coli*. (B) and *E.faecalis* (C)



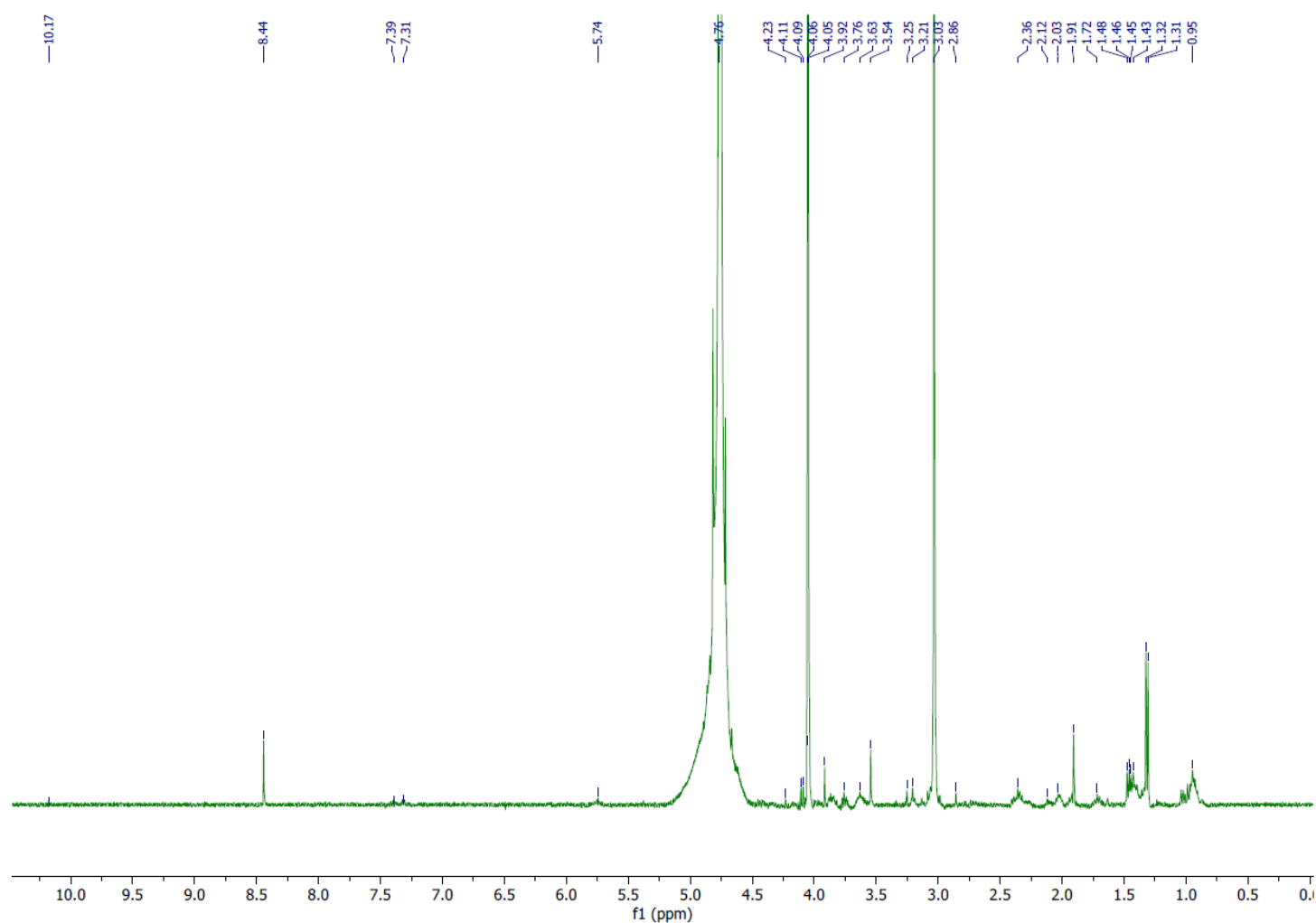
Supporting Figure S7: Normalized current response (subtracting the mean and dividing with the standard deviation) at each potential using the whole data set used for Fig. 4, (black = AUM; yellow = *K.pneumoniae*, green = *E.faecalis*, orange = *E.coli*, 1 h = dashed, 5 h = solid)) for the investigated electrode materials Pt (A), Pd (B), and Au (C)



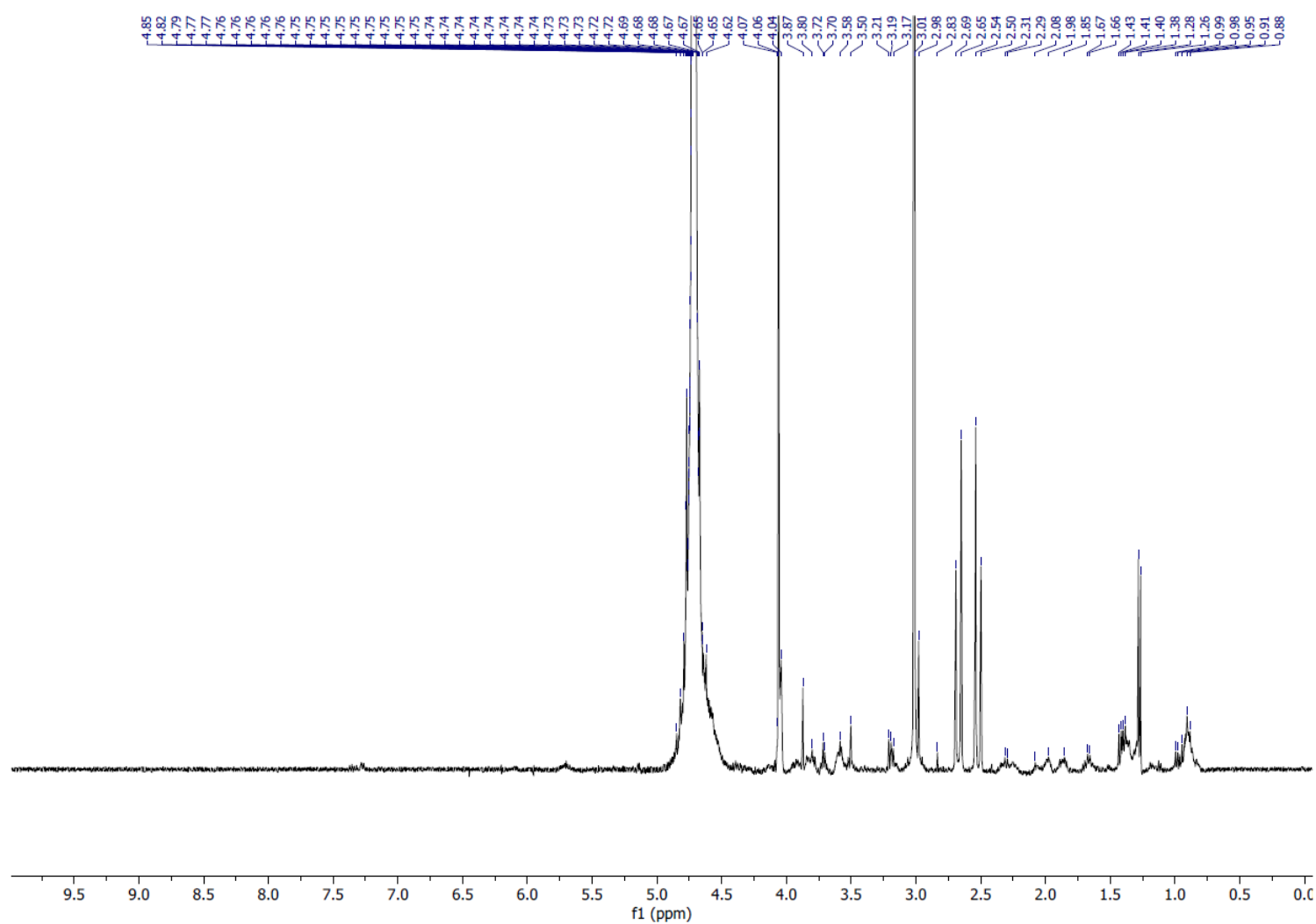
Supporting Figure S8: ^1H NMR spectrum of *E. coli* in AUM after 5h of bacterial growth (reference peak. positioned at 4.05 ppm relative to TMS (0 ppm)).



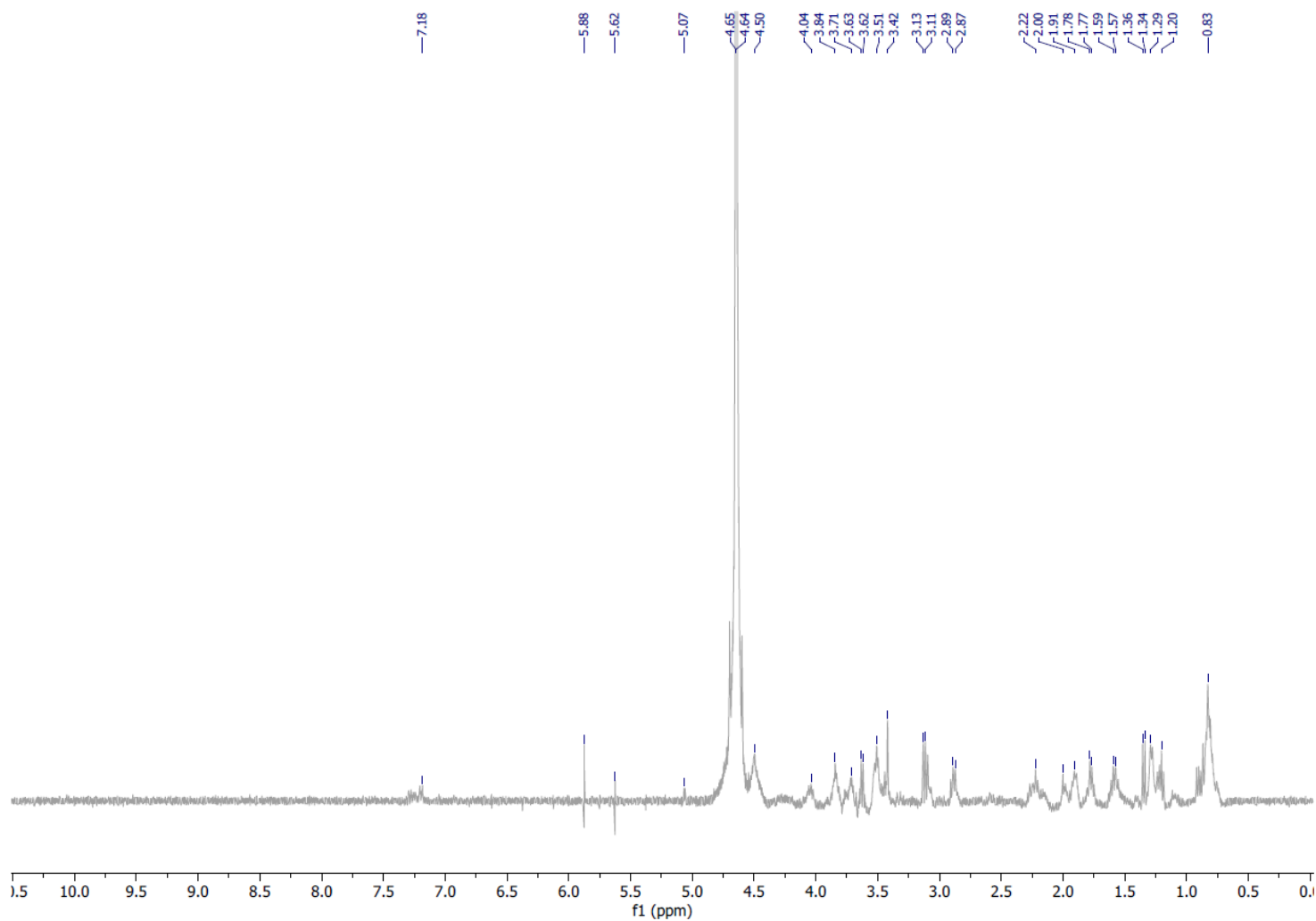
Supporting Figure S9: ^1H NMR spectrum of *K.pneumoniae* in AUM after 5h of bacterial growth (reference peak. positioned at 4.05 ppm relative to TMS (0 ppm)).



Supporting Figure S10: ^1H NMR spectrum of *E. faecalis* in AUM after 5h of bacterial growth (reference peak. positioned at 4.05 ppm relative to TMS (0 ppm)).



Supporting Figure S11: ^1H NMR spectrum of AUM (reference peak, positioned at 4.05 ppm relative to TMS (0 ppm)).



Supporting Figure S12: ¹H NMR spectrum of peptone in D₂O (reference peak, positioned at 4.05 ppm relative to TMS (0 ppm)).

Supporting Table S1: Score values related to the PCA of AUM and AUM incubated with three types of bacteria.

Sample name	Component 1	Component 2	Component 3	Component 4
ECfeac 1	0.174	0.554	-0.586	0.034
ECfeac 2	0.384	0.089	0.831	-0.121
ECfaec 3	0.006	-0.171	-0.267	-0.939
Ecoli 1	0.332	0.860	-0.113	0.225
Ecoli 2	0.311	0.875	-0.096	0.212
Ecoli 3	0.367	0.291	0.800	-0.039
Kleb 1	0.664	-0.347	-0.243	0.439
Kleb2	0.724	-0.500	0.025	0.345
Kleb 3	0.773	-0.463	-0.071	0.300
Aum1	-0.910	0.009	0.240	0.276
Aum2	-0.885	0.038	0.187	0.328
Aum 3	-0.844	-0.235	-0.167	0.370

Supporting Table S2: Score values related to the PCA of *K.pneumoniae* at different incubation times.

Sample name	Component 1	Component 2
Aum1	-.906	.336
Aum2	-.945	.106
Aum3	-.806	-.098
1h	.712	-.684
2h	.948	-.241
3h	.925	.205
4h	.884	.439
5h	.733	.633

Supporting Table S3: Score values related to the PCA of *E.faecalis* at different incubation times

Sample name	Component 1	Component 2
Aum1	-.902	.314
Aum2	-.945	.093
Aum3	-.842	.018
1h	.705	-.697
2h	.924	-.134
3h	.970	.146
4h	.792	.512
5h	.740	.613

Supporting Table S4: Score values related to the PCA of *E.coli* at different incubation times.

Sample name	Component 1	Component 2
Aum1	-.893	.240
Aum2	-.932	.150
Aum3	-.902	-.105
1h	.795	-.534
2h	.903	-.350
3h	.748	.344
4h	.880	.357
5h	.767	.559

Supporting Table S5: Score values related to the PCA of AUM and AUM incubated with three types of bacteria at different incubation times.

Sample name	Component 1	Component 2	Component 3	Component 4
Aum 1	-.946	-.238	.097	-.120
Aum2	-.914	-.324	-.060	-.110
Aum3	-.834	-.419	-.160	.089
Ecoli 1h	.595	-.104	-.628	.408
Ecoli 2h	.716	-.221	-.411	.458
Ecoli 3h	.525	-.428	.178	.383
Ecoli 4h	.718	-.387	.304	.375
Ecoli 5h	.591	-.353	.611	.193
Kleb 1h	.235	.576	-.691	-.202
Kleb2h	.162	.883	-.285	.010
Kleb 3h	.018	.918	.238	.221
Kleb 4h	.013	.868	.419	.211
Kleb 5h	-.092	.768	.433	.154
ECfeac 1h	.491	.041	-.788	-.301
ECfeac 2h	.765	-.096	-.362	-.421
ECfaec 3h	.889	-.066	.091	-.380
ECfaec 4h	.588	-.072	.605	-.408
ECfaec 5h	.494	-.038	.740	-.390