

TD/GC-MS analysis of volatile markers emitted from mono- and co-cultures of *Enterobacter cloacae* and *Pseudomonas aeruginosa* in artificial sputum

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Supplementary information

Chromatograms

Representative chromatograms for *E. cloacae* and *P. aeruginosa* mono- and co-culture bacterial samples are shown below (Fig S1).

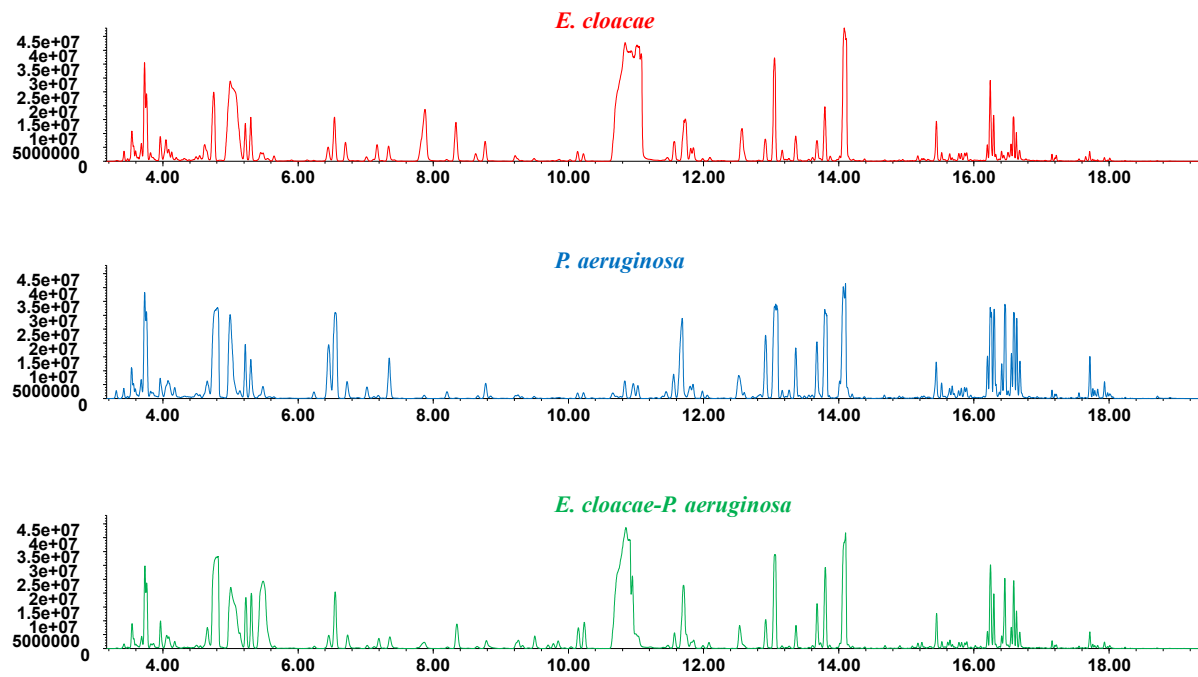


Fig S1. Representative chromatograms of *E. cloacae* and *P. aeruginosa* axenic cultures and co-culture.

Principal component (PC) tuning

Principal component analysis (PCA) was performed on X block data (VOC profile) to evaluate the number of PCs to input for DFA. Eight PCs were selected which accounts for approximately 64.5% of variance in the dataset (Fig S2).

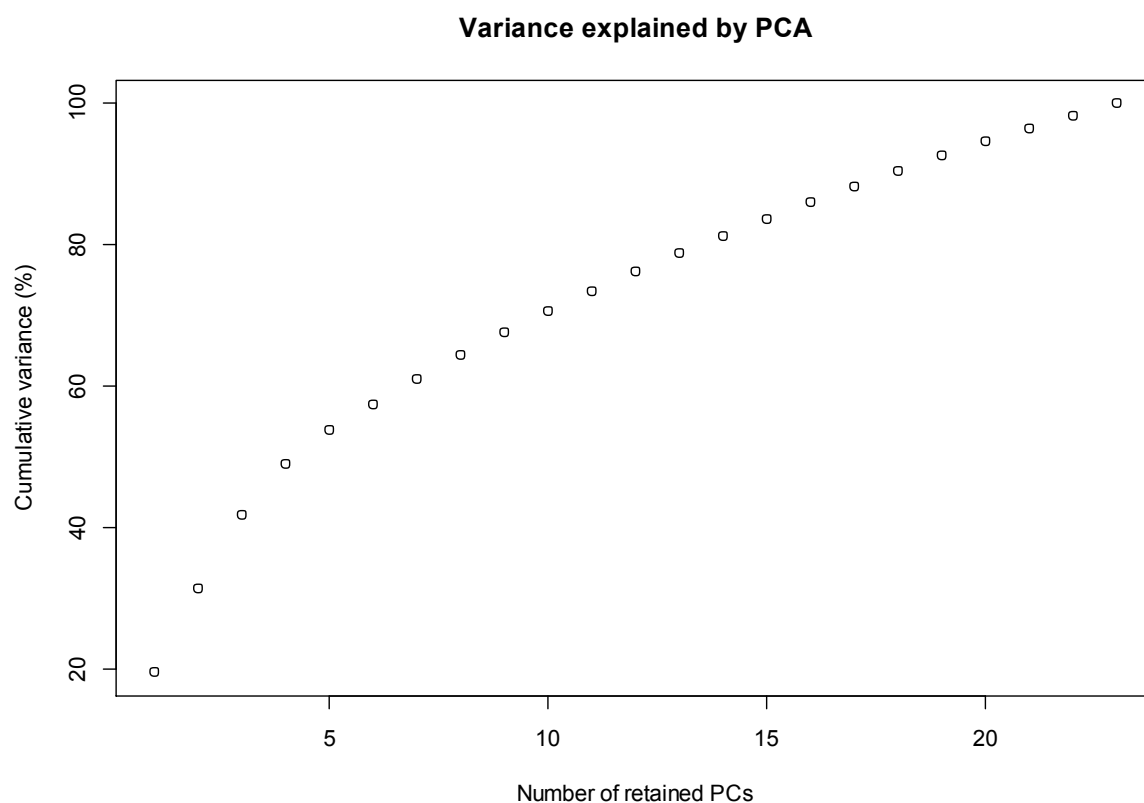


Fig S2. Scree plot of PCA indicating the number of retained principal components (PCs) extracted and the corresponding cumulative explained variance.

PC-DFA loadings plot

The loadings plots from PC-DFA analysis are shown in Fig S3. The fragments at the extremity of the loading plots were investigated as they are major contributors to the observed separation in the scores plot (Fig 5). Fragments 90, 465, & 2046 belong to 2-methyl-1-propanol and fragments 577, 859 to 1-undecene (Fig S3a). The identity of the other

fragments is still unknown. In the loadings plot of DF2, fragment 1083 originates from 3-methyl-1-butanol, 2012 from 2-methylbutyl acetate, and 1877 from isomayl butyrate.