Supplementary Material

Database-Assisted, Globally Optimized Targeted Secondary Electrospray Ionization High Resolution Mass Spectrometry (dGOT-SESI-HRMS) and Spectral Stitching Enhanced Volatilomics Analysis of Bacterial Metabolites

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Supplemental Figures

Figure S1: PLS-DA summarizing the differences in headspace chemical profiles among our bacteria cultures, media blanks and VOCQC samples.

Figure S2: Summary of dGOT method performance when incorporating three unique target list windows

Figure S3: Representative head to tail spectra of annotated MSMS features from dGOT-SESI-HRMS analysis of bacterial headspace volatiles.

Figure S4: Principal component analyses summarizing each of A) DDA, B) GOT and C) dGOT method's respective ability at distinguishing the volatile differences between each representative strain supplemented with either fructose or sucrose.

Figure S5: Heatmap summarizing the relative abundance of the annotated features detected with the dGOT method across all of our culture groups.

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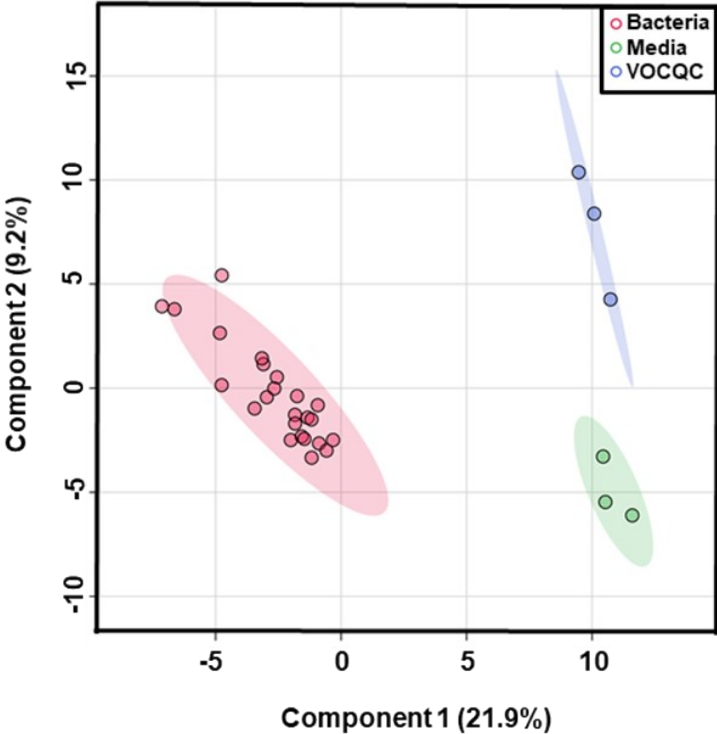
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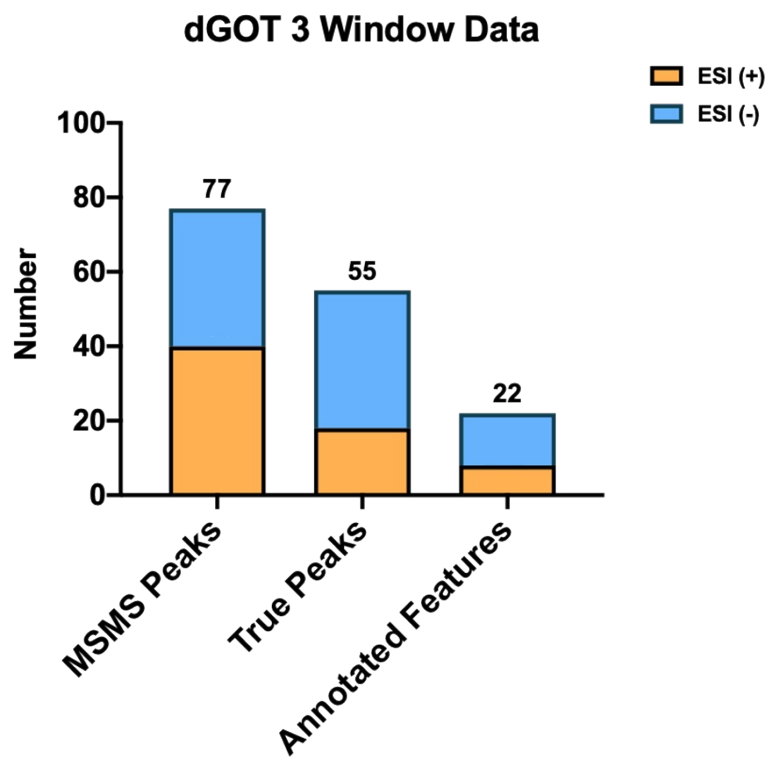
Figure S3: Representative head to tail spectra of annotated MSMS features from dGOT-SESI-HRMS analysis of bacterial headspace volatiles. A) 1-phenylpropan-2-one, B) 2-methylfuran, C) (methyltetrasulfanyl)methane and D) 2-ethylfuran
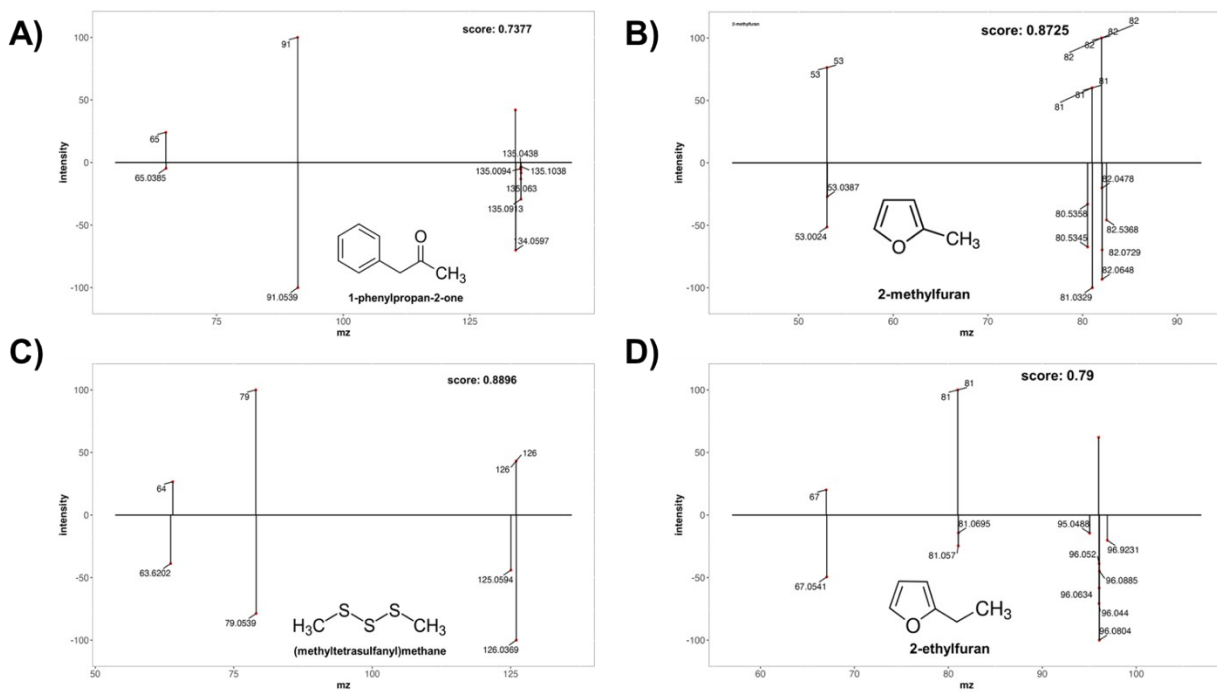
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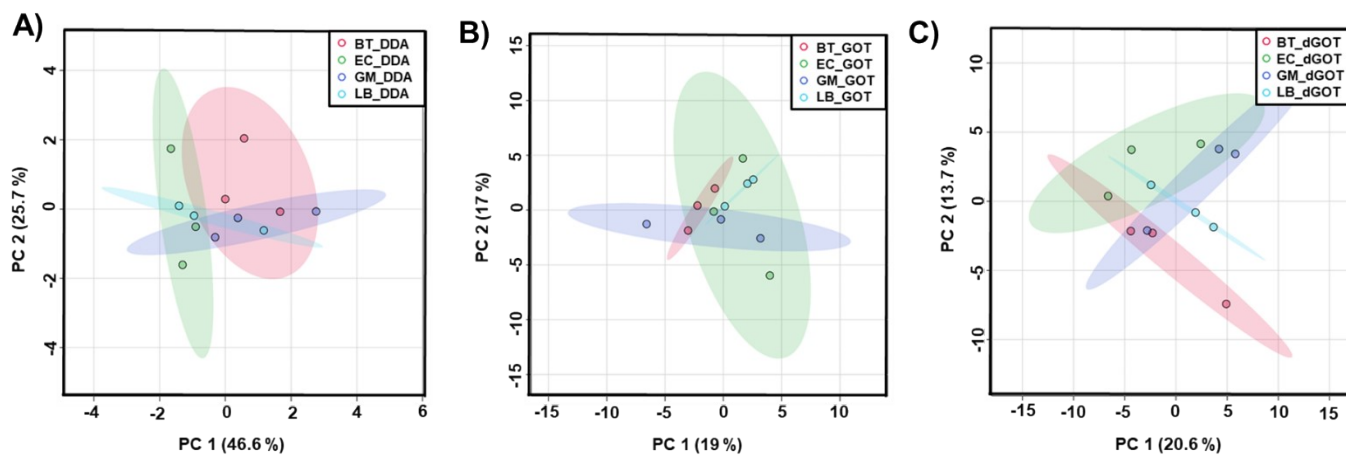
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