Supplementary Material

Sampling Dynamics for Volatile Organic Compounds Using Headspace Solid-Phase Microextraction Arrow for Microbiological Samples

Kevin E. Eckert [1], David O. Carter [2] and Katelynn A. Perrault [1,*]

[1] Laboratory of Forensic and Bioanalytical Chemistry, Forensic Sciences Unit, Division of Natural Sciences and Mathematics, Chaminade University of Honolulu, 3140 Waialae Ave., Honolulu, HI 96816, USA
[2] Laboratory of Forensic Taphonomy, Forensic Sciences Unit, Division of Natural Sciences and Mathematics, Chaminade University of Honolulu, 3140 Waialae Avenue, Honolulu, HI 96816, USA
* Correspondence: Katelynn.perrault@chaminade.edu

Table S1. Tabulated average peak area, standard deviation (s), and % Relative Standard Deviation (% RSD) for intraday and interday repeatability for reference volatile organic compounds using the optimized SPME Arrow method.

	Day 1 Area (counts*min)			**Day 2 Area (counts*min)**			**Day 3 Area (counts*min)**			**Inter-Day (counts*min)**		
Compound	Avg.	s	%RSD	Avg.	s	%RSD	Avg.	s	%RSD	Avg.	s	%RSD
benzene	1.68E+06	8.88E+04	5.3	1.42E+06	1.74E+04	1.2	1.40E+06	3.02E+04	2.2	1.50E+06	1.41E+05	9.4
heptane	2.80E+06	4.32E+04	1.5	2.38E+06	1.23E+05	5.2	1.98E+06	6.86E+04	3.5	2.39E+06	3.63E+05	15.2
toluene	5.03E+06	6.17E+04	1.2	4.53E+06	2.56E+05	5.6	4.18E+06	8.63E+04	2.1	4.58E+06	3.95E+05	8.6
octane	5.06E+06	1.04E+05	2.1	4.55E+06	6.71E+04	1.5	3.99E+06	6.74E+04	1.7	4.53E+06	4.67E+05	10.3
hexanal	3.35E+05	1.30E+04	3.9	3.28E+05	1.80E+04	5.5	2.57E+05	3.17E+04	12.4	3.07E+05	4.21E+04	13.7
ethylbenzene	6.76E+06	8.43E+04	1.2	6.34E+06	4.68E+05	7.4	5.74E+06	2.26E+05	3.9	6.28E+06	5.15E+05	8.2
m-xylene + p-xylene	1.69E+07	2.01E+05	1.2	1.60E+07	1.18E+06	7.4	1.45E+07	7.96E+05	5.5	1.58E+07	1.28E+06	8.1
nonane	8.99E+06	5.32E+04	0.6	8.30E+06	1.28E+05	1.5	7.04E+06	1.90E+05	2.7	8.11E+06	8.66E+05	10.7
o-xylene + styrene	1.39E+07	3.31E+05	2.4	1.27E+07	9.51E+05	7.5	1.18E+07	9.36E+05	7.9	1.28E+07	1.15E+06	8.9
n-decane	1.03E+07	2.06E+05	2.0	9.84E+06	8.85E+04	0.9	8.10E+06	5.73E+05	7.1	9.42E+06	1.05E+06	11.2
dimethyltrisulfide	1.92E+06	6.62E+04	3.5	1.96E+06	1.61E+05	8.2	1.86E+06	1.24E+05	6.7	1.91E+06	1.16E+05	6.0
1,2,3-trimethylbenzene	4.98E+06	2.77E+05	5.6	5.33E+06	6.53E+05	12.3	5.47E+06	4.87E+05	8.9	5.26E+06	4.83E+05	9.2
undecane	9.09E+06	3.00E+05	3.3	8.50E+06	2.15E+05	2.5	6.83E+06	6.86E+05	10.0	8.14E+06	1.09E+06	13.4
dodecane	4.91E+06	2.64E+05	5.4	4.80E+06	9.17E+04	1.9	3.74E+06	4.72E+05	12.6	4.48E+06	6.21E+05	13.9
naphthalene	4.57E+05	3.21E+04	7.0	4.72E+05	1.16E+05	24.5	3.59E+05	2.88E+04	8.0	4.29E+05	8.15E+04	19.0
tridecane	2.37E+06	1.73E+05	7.3	2.31E+06	1.02E+05	4.4	1.73E+06	1.82E+05	10.5	2.14E+06	3.36E+05	15.8
tetradecane	9.89E+05	8.16E+04	8.3	8.86E+05	9.70E+04	11.0	6.40E+05	2.38E+04	3.7	8.38E+05	1.68E+05	20.1
pentadecane	3.74E+05	8.75E+03	2.3	2.88E+05	4.93E+04	17.1	2.18E+05	9.73E+03	4.5	2.93E+05	7.24E+04	24.7
hexadecane	1.36E+05	2.64E+04	19.4	8.71E+04	1.80E+04	20.7	6.33E+04	1.16E+04	18.3	9.55E+04	3.64E+04	38.1

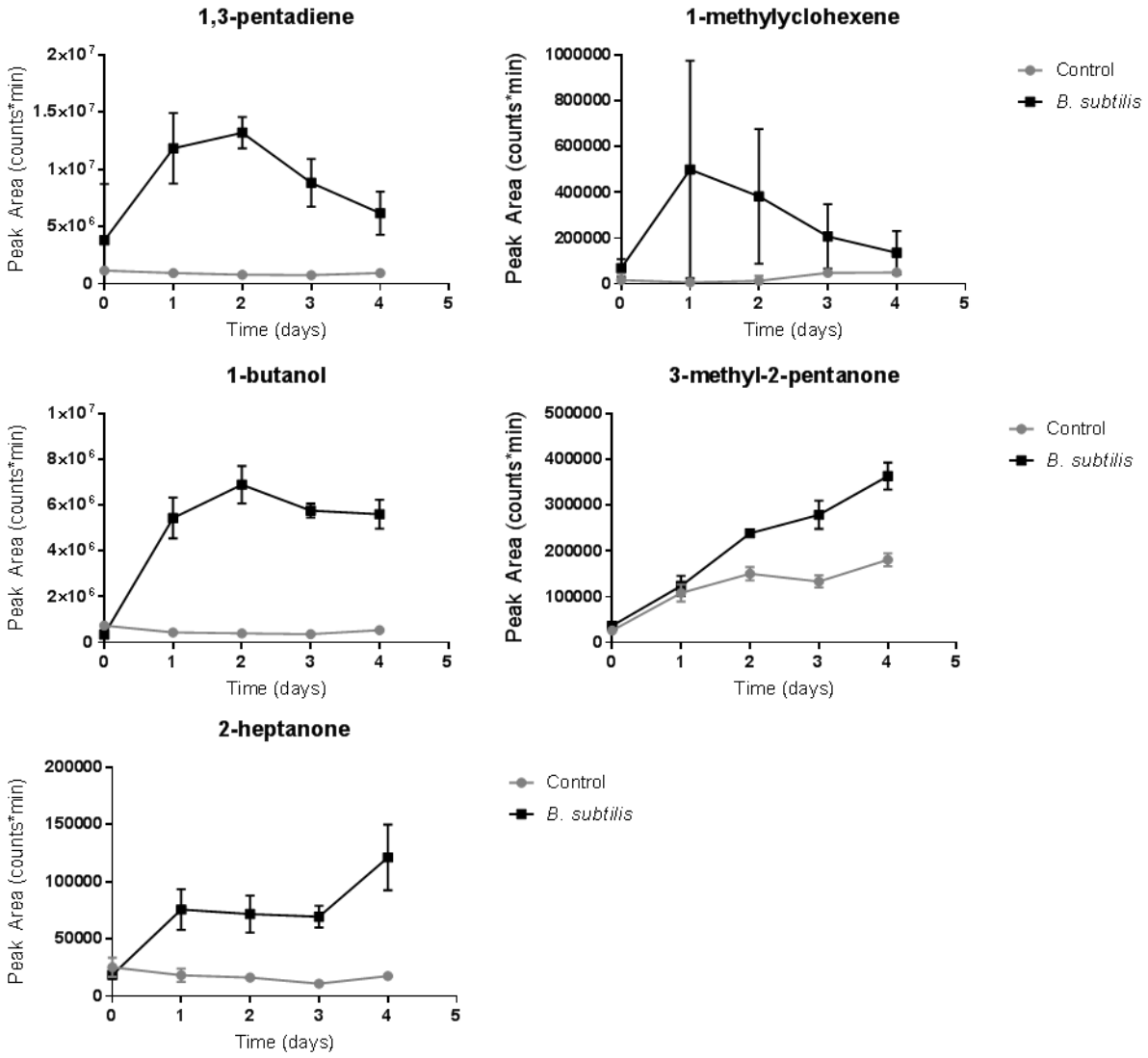
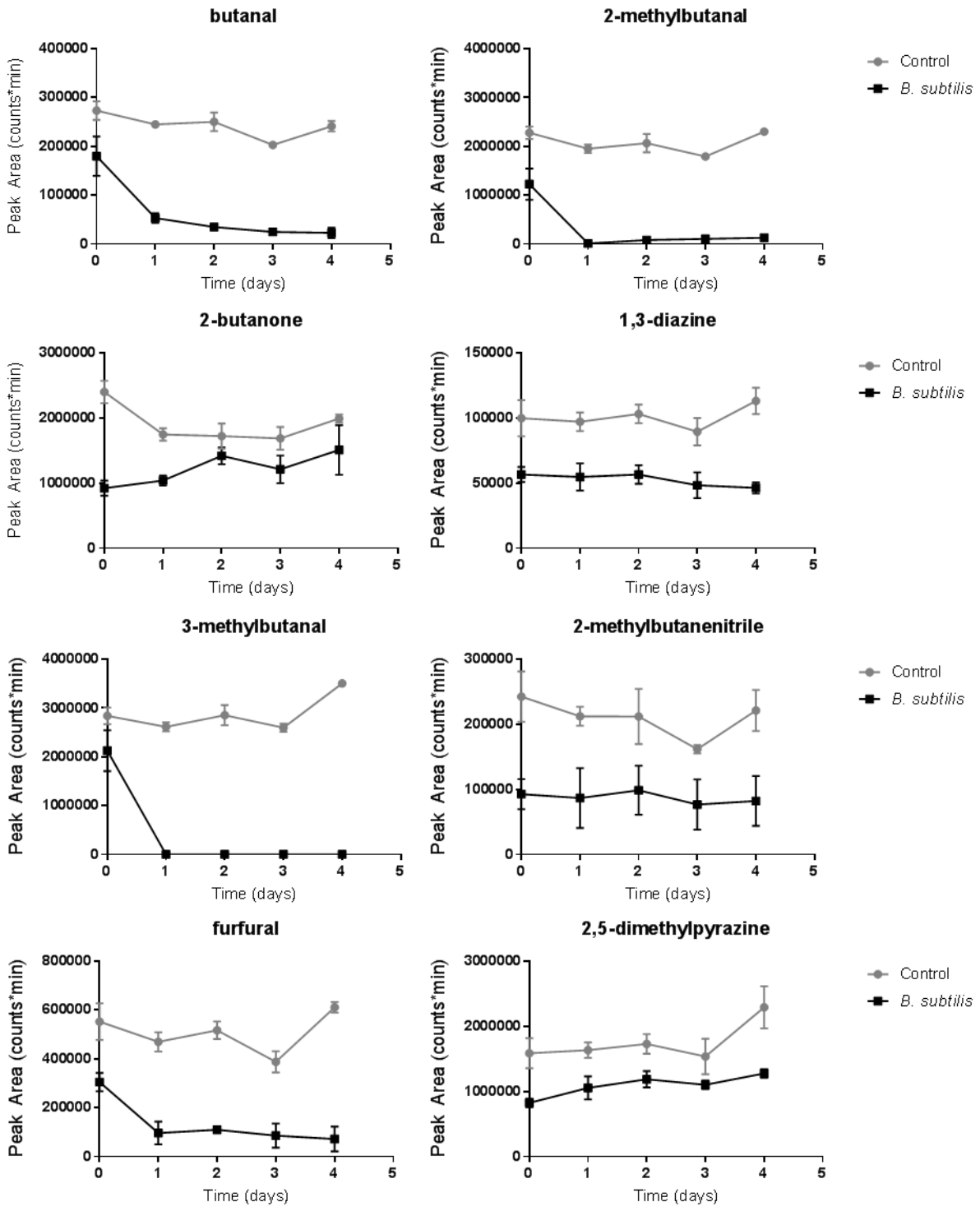


Figure S1. Category 1 compounds ("produced VOCs") detected from the headspace of *B. subtilis* samples incubated at 24 °C and monitored over a five day period using the optimized SPME Arrow method.


butanal
2-methylbutanal
2-butanone
1,3-diazine
3-methylbutanal
2-methylbutanenitrile
furfural
2,5-dimethylpyrazine
Peak Area (counts*min)
Time (days)
Control
B. subtilis

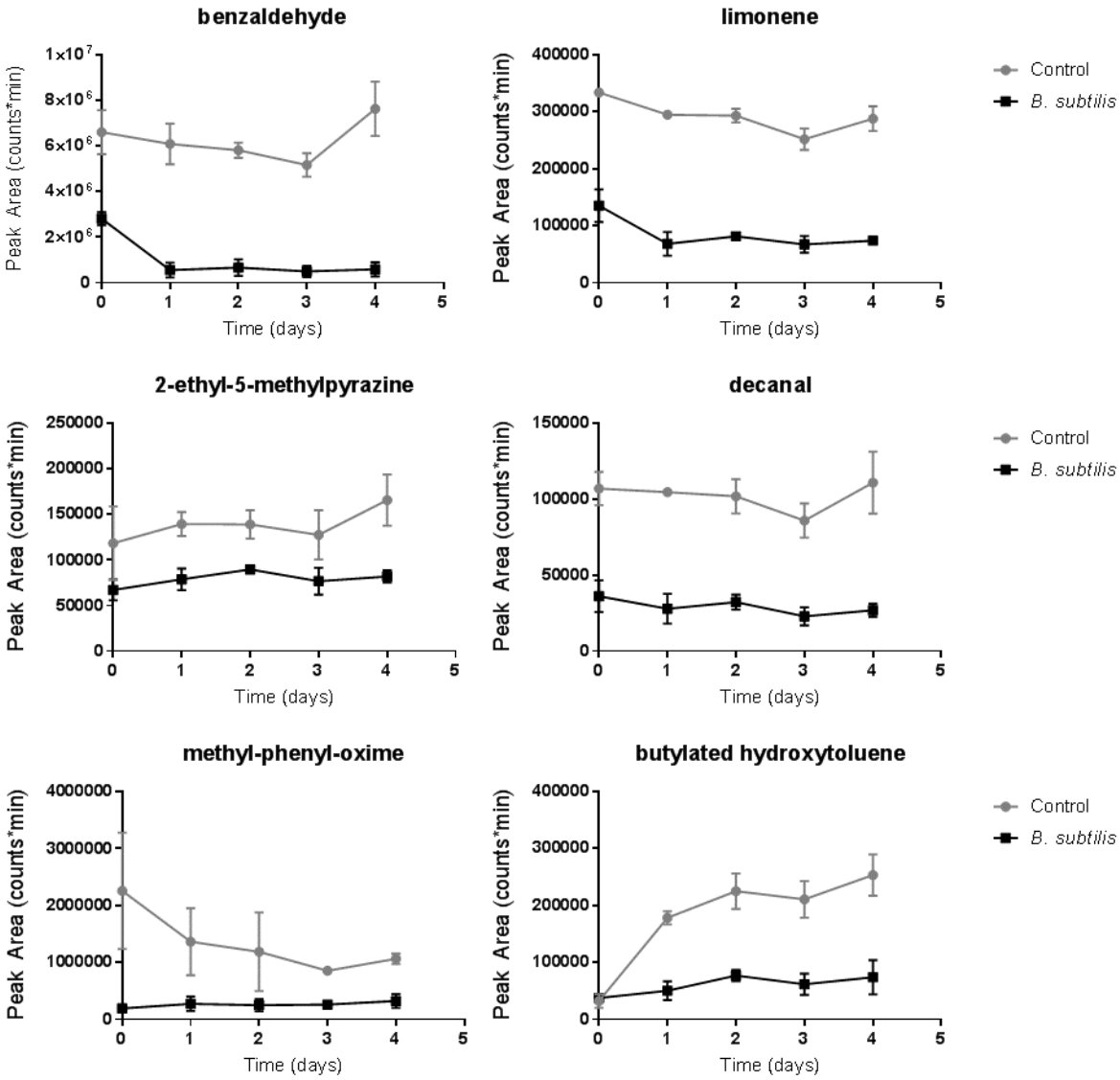


Figure S2. Category 2 compounds ("consumed VOCs") detected from the headspace of *B. subtilis* samples incubated at 24 °C and monitored over a five day period using the optimized SPME Arrow method.

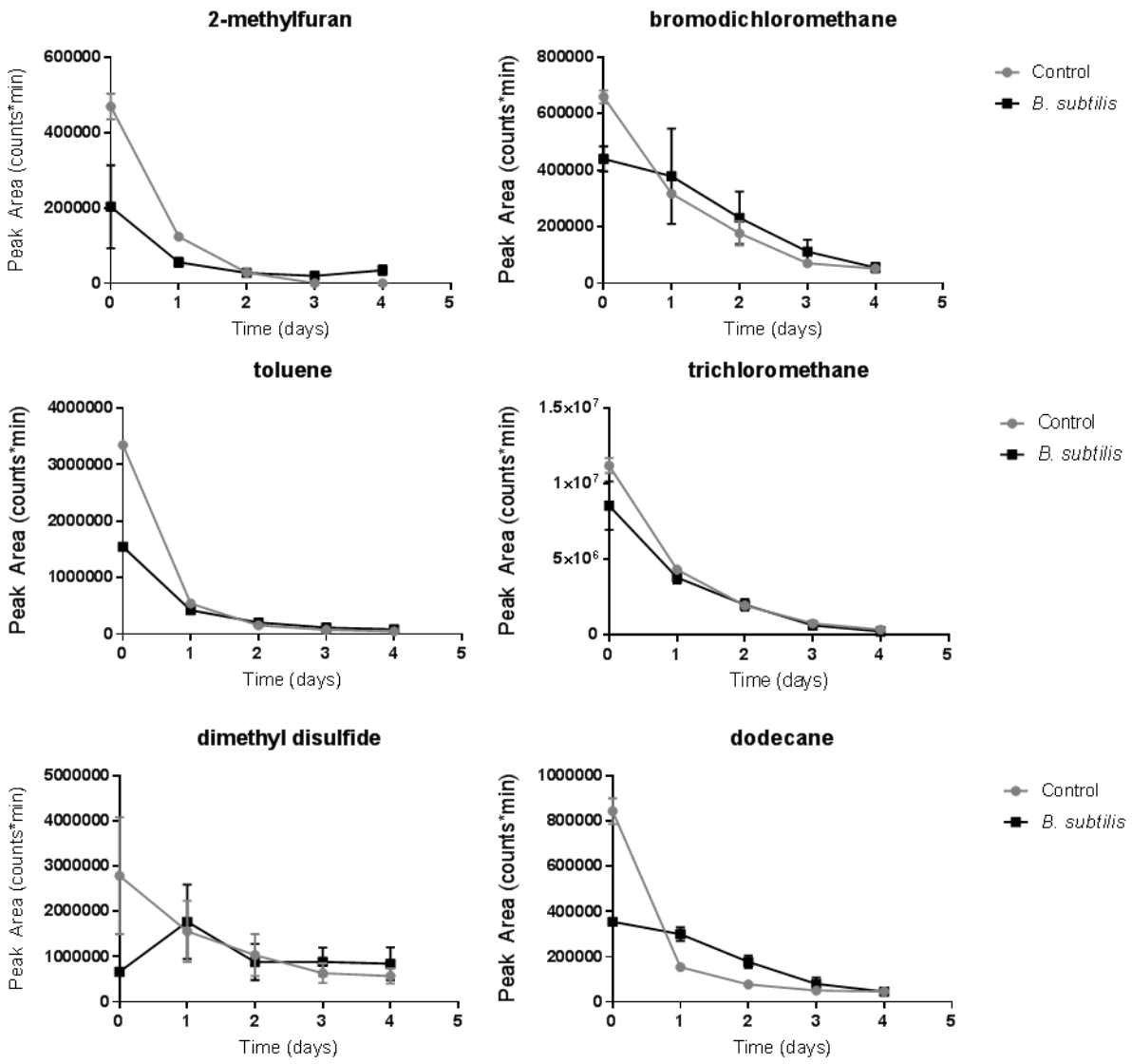


Figure S3. Category 3 compounds ("equilibrated VOCs") detected from the headspace of *B. subtilis* samples incubated at 24 °C and monitored over a five day period using the optimized SPME Arrow method.