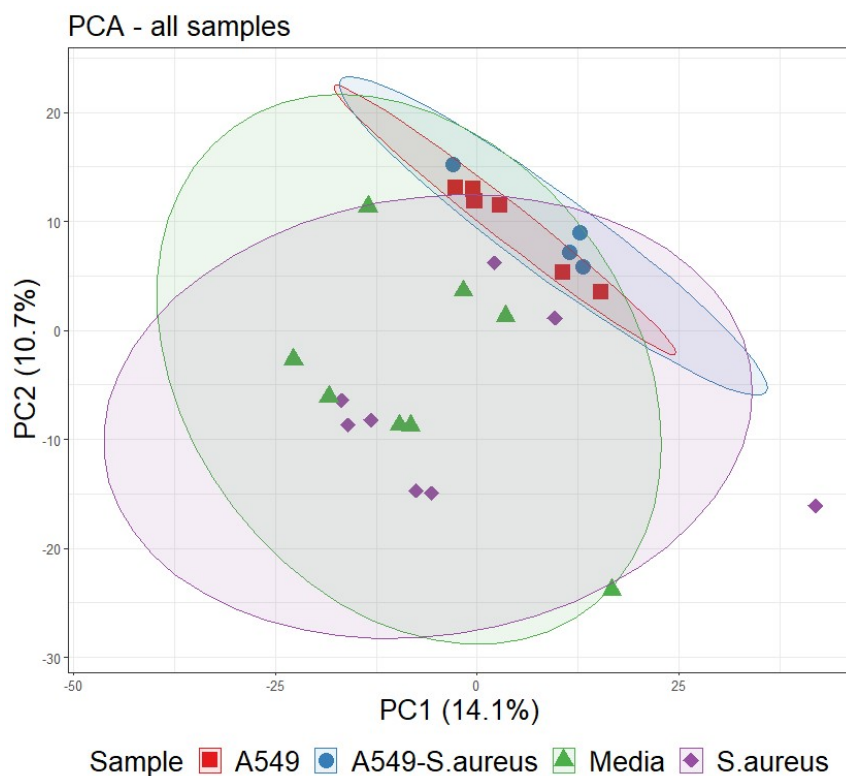


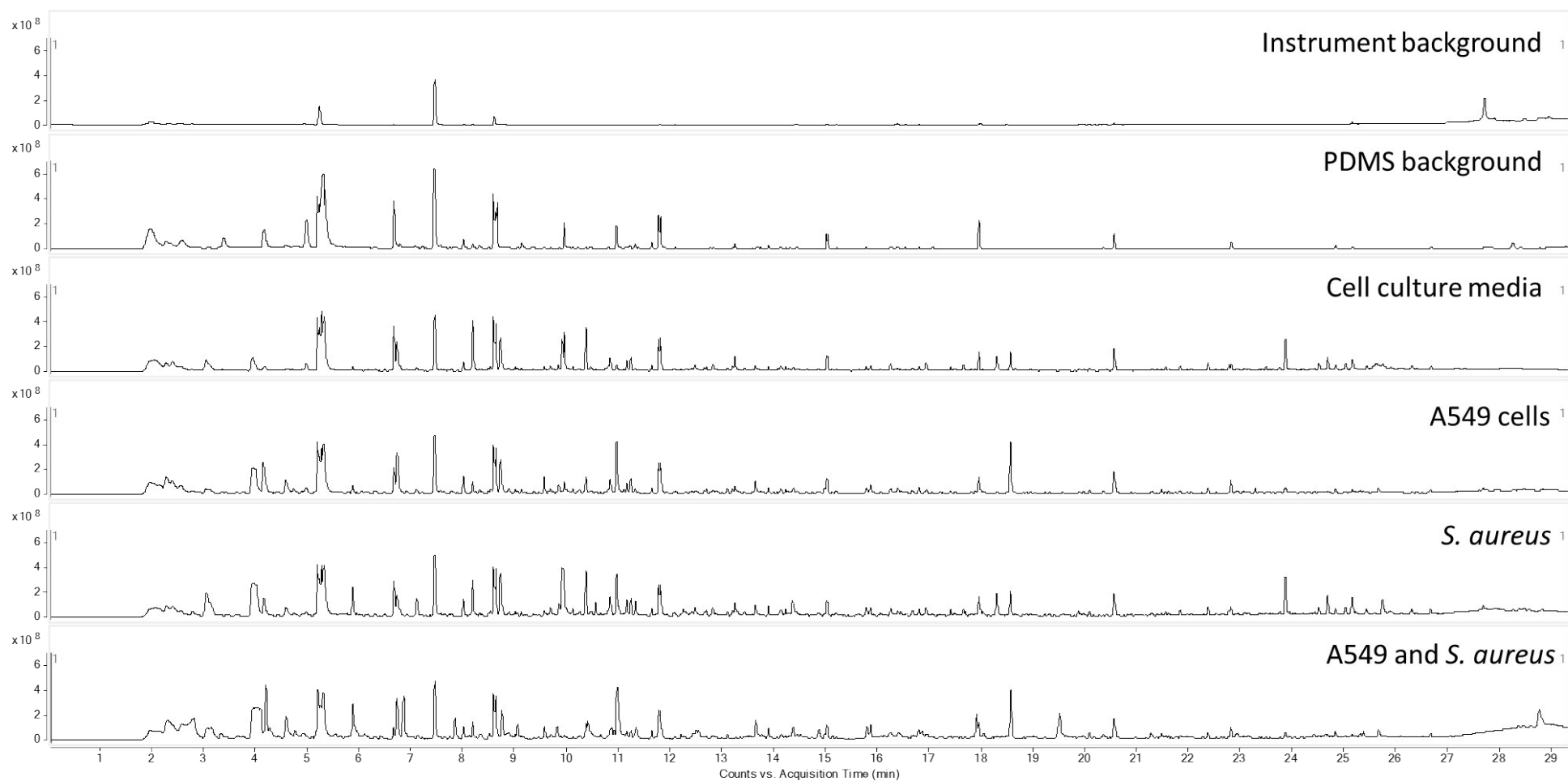
Supplementary information

Volatile metabolites differentiate air-liquid interface cultures after infection with *Staphylococcus aureus*

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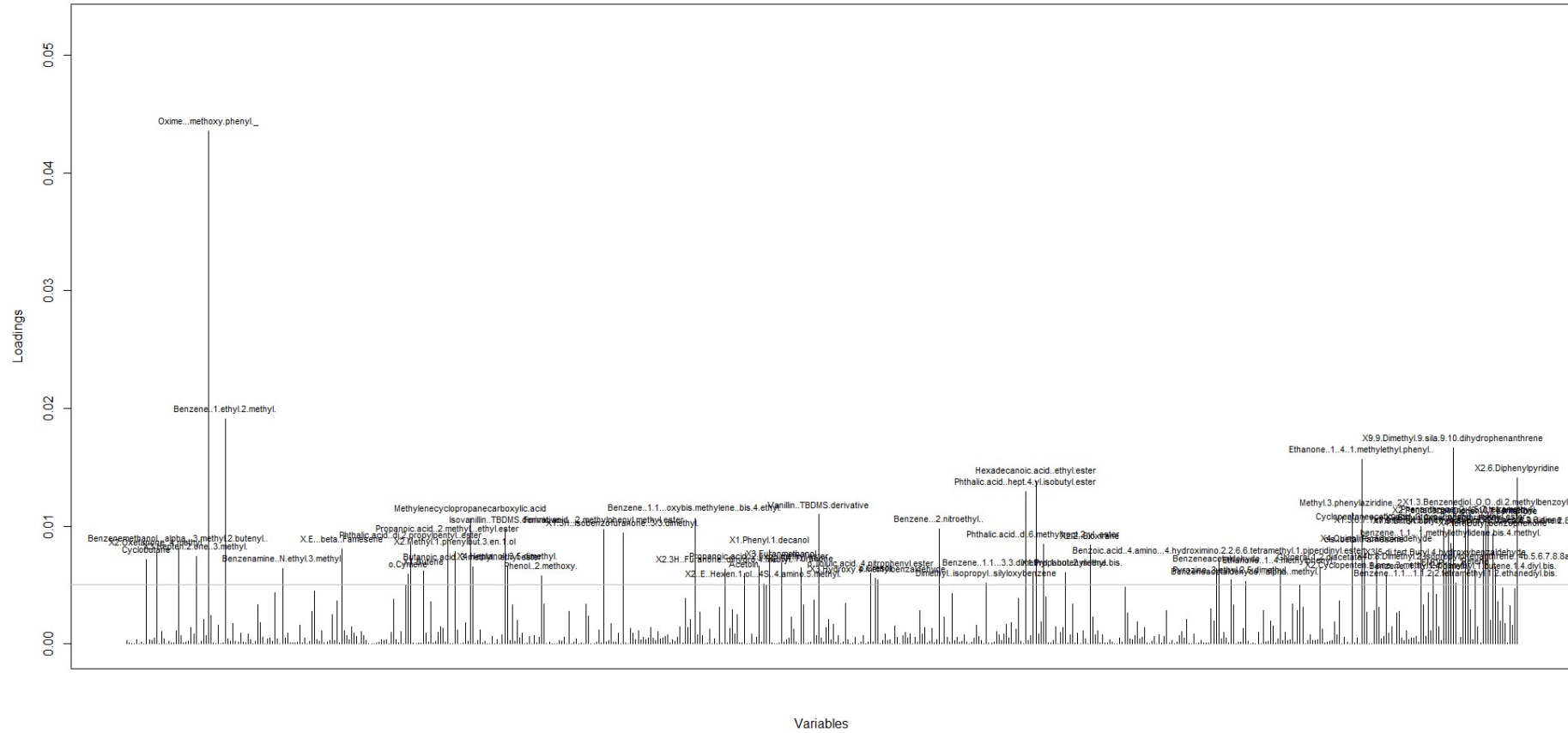


S1. PCA scores plot showing samples from infected cells, uninfected cells, media and *S. aureus*.



S2. Examples of total ion current chromatograms of samples, in order from top to bottom: instrument background (trap and column artefacts), PDMS sorbent material background, cell culture media (DMEM), A549 cells under normal growth conditions, *S. aureus* cultured in DMEM, and A549 cells infected with *S. aureus*.

DF 1



S3. PC-DFA loadings from the first discriminant function.

Table S1. List of VOCs extracted from PC-DFA (DF2) with NIST library references (where applicable)

VOC name (NIST ID)	RT (min)	NIST Library RI	Estimated RI	NIST Library RI reference
Triethylamine	3.441	711	693	Estevez, Ventanas, et al., 2005
2-Propenoic acid	3.813	NA	721	NA
Propanoic acid	3.824	NA	722	NA
2,2'-Bioxirane	3.939	NA	729	NA
Disulfide, dimethyl	4.102	722	740	Takeoka, Perrino, et al., 1996
Ethanamine, 2-chloro-N,N-dimethyl-	4.29	750	753	Jagadeshwar Reddy, Prabhakar, et al., 2006
2-Propenoic acid, 2-methyl-	4.633	711	776	Meynier, Novelli, et al., 1999
Acetyl valeryl	5.562	816	830	Wu, Liou, et al., 1987
Formic acid hydrazide	5.943	NA	849	NA
Butanoic acid, 2-methyl-	6.312	894	868	Alissandrakis E., Tarantilis P.A., et al., 2007
1-Butanol, 3-methyl-, acetate	6.417	867	874	Takeoka, Buttery, et al., 1992
Cyclopent-4-ene-1,3-dione	6.465	880	876	Kim and Chung, 2009
4-Heptanol, 3,5-dimethyl-	8.15	NA	958	NA
Furaneol	10.113	1097	1052	Jarunrattanasri, Theerakulkait, et al., 2007
Phenylethyl Alcohol	11.359	1086	1112	Hoskovec, Grygarová, et al., 2005
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	11.969	1134	1143	da Silva, Borba, et al., 1999
Dehydromevalonic lactone	12.223	1169	1155	Andriamaharavo, 2014
2-Isobutyl-4-methylpyridine	12.272	1154	1158	Machiels, van Ruth, et al., 2003
3-(2-Hydroxyethyl)-2-oxazolidinone	12.295	NA	1159	NA
Decanal	13.218	1200	1205	Asuming, Beauchamp, et al., 2005
Benzenepropanenitrile	13.821	1243	1237	Andriamaharavo, 2014
Benzoic acid, 2-hydroxy-, ethyl ester	14.45	1249	1270	Tudor and Moldovan, 1999
Indole	14.883	1292	1293	Dickens, 1999
Benzoic acid, 4-chloro-	15.691	NA	1337	NA
n-Decanoic acid	16.115	1387	1361	Alissandrakis E., Tarantilis P.A., et al., 2007
Benzeneacetamide	16.798	1412	1399	Andriamaharavo, 2014

cis-.beta.-Farnesene	17.705	1446	1453	Lucero, Fredrickson, et al., 2006
2(3H)-Furanone, 5-hexyldihydro-	17.92	1463	1465	Asuming, Beauchamp, et al., 2005
Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-	19.492	1492	1562	Yu, Liao, et al., 2007
Dodecanoic acid	19.53	1562	1564	Maia, Andrade, et al., 2000
Pyridine, 3-methyl-2-phenyl-	20.085	1513	1598	Rostad and Pereira, 1986
Pyridine, 2-hexyl-	24.792	NA	1915	NA
Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	24.88	1908	1921	Xu, Han, et al., 2012
Octadecanoic acid	27.688	2170	2111	Maia, Andrade, et al., 2000