Table S1. Previously reported sources of volatile organic compounds included in the analysis.

	Vap *in vivo* studies	**Emitted From Pathogens**	**Markers Of Oxidative Stress**	**Markers Of Airway Inflammation**	**Other Compounds In Breath And Ventilator Air Samples**
Sevoflurane					X[1–3]
Acetone	X[1,4]	X[5,6]	X[7]	X[8–10]	X[2,3,11,12]
2-propanol, 1,1,1,3,3,3-hexafluoro-					X[3]
Isoprene		X[5,6]		X[8]	X[2,3,11]
3-methylpentane		X[6,13]	X[14]		
Acetic acid		X[6,15]		X[8]	
2,3-butanedione		X[6,15]			
2-butanone		X[5]			
Hexane		X[6]	X[14]		
Ethyl acetate		X[5,6]			X[12]
Methyl cyclopentane					X[11]
Methyl propionate					X[16]
Tetrahydrofuran	X[4]	X[6]			
3-methylbutanal		X[5,6,17]	X[18]		
1-butanol		X[5,6]			
Benzene					X[11]
2-methylbutanal		X[5]	X[18]		
Cyclohexane		X[6,19]			
2-pentanone		X[5,6]	X[18]		
Heptane	X[4,20]	X[13,21]	X[14]		
Pentanal			X[18]		

3-pentanone		X[13]	X[18]		
Allyl methyl sulfide				X[8]	
Methyl thiocyanate		X[5,17]			
Methyl thioacetate		X[15]			
Ethylfuran		X[17]			
1,4-dioxane					X[22]
Acetoin		X[5,6]			
2,4,4-trimethyl-1-pentene				X[8]	
2,4 dimethylfuran		X[6]			
Methylcyclohexane			X[21]	X[8]	
Isoamyl alcohol		X[17]			
Methyl isobutyl ketone	X[1]				
Dimethyldisulfide		X[5,6,17]			
1,4-Heptadiene, 4-methyl-					X[23]
Pyridine		X[6]			
Methyl methacrylate		X[15]			
Pentanol		X[5,13]			X[2,24]
Toluene		X[5,6]		X[8]	
3-methylheptane			X[14]		
Cyclopentanone		X[17]			
Heptane, 3-methylene-					X[11]
Octane		X[13]	X[14]		
3-Penten-2-one, 4-methyl-			X[25]		
3-octene					X[23]
Hexanal		X[6,13]	X[18]		
Ethyl butanoate		X[5,6]			

2-octene					X[23]
Butyl acetate		X[6]			
2,4-dimethylheptane		X[5,6]	X[14]	X[8]	
Isovaleric acid		X[5,6]			
Furfural		X[6]			
2-Cyclopenten-1-one		X[6]			
2,4-dimethyl-1-heptene		X[6]			
2-methyl-1-pyrrole		X[26]			X
2-methylbutanoic acid					X[27]
Chlorobenzene				X[28]	X[3,29]
3-methyl-1-pyrrole		X[30]			X
Maleic anhydride					X[31]
2,3-dimethylheptane			X[14]	X[8]	
4-methyloctane		X[6]	X[14]	X[8]	
Ethylbenzene	X[4]	X[6]			
1-hexanol		X[13,21,26]			X[2,24]
P-xylene					X[11,22,23]
4-heptanone		X[5,32]	X[25]		
3-ethylheptane			X[14]		
2,4,6-trimethylheptane			X[14]		
Phenylethyne					X[2]
2,2,4-trimethylheptane			X[14]		
Cyclohexanol				X[9]	
4-ethyl-2,2-dimethylhexane			X[14]		
3-heptanone			X[25]		X[2 (a)]
Styrene				X[10]	

1-nonene		X[6]			
Cyclohexanone				X[8]	X[12]
3-heptanol					X[33]
Nonane			X[14]	X[8]	
Heptanal		X[6,13]	X[18]		
γ -Butyrolactone		X[6]			
p-bromofluorobenzene[(b)]					
α-pinene				X[8]	X[12,22,23,33]
3-Ethyl-3-methylheptane			X[14]		
2-ethylhexanal		X[34]	X[18]		X[34]
Camphene				X[8]	
Octane, 2,4,6-trimethyl-			X[18]		
Benzaldehyde		X[5,6]			
1-heptanol					X[24]
Dimethyltrisulfide		X[5,17]			
Octane, 2,2,6-trimethyl-			X[14]		
β-pinene		X[34]			
Phenol		X[5,6]		X[8]	
Benzonitrile		X[6]			
6-methyl-5-hepten-2-one			X[25]		X[27]
Heptane, 2,2,4,6,6-pentamethyl-			X[14]	X[8]	
Myrcene					X[11]
2-pentyl furan					X[23]
Decane		X[6]	X[14]	X[8]	
Octanal		X[6]		X[8]	

ß-Phellandrene					X[23]
3-carene	X[20]				
1,4-dichlorobenzene				X[10]	
α-terpinene					X[16]
p-cymene				X[35]	
2-ethyl-1-hexanol					X[2,12]
Limonene		X[5,6]			
Eucalyptol				X[8]	
Benzyl alcohol				X[8]	
Nonane, 4,5-dimethyl-			X[14]		
Pentanoic acid, 2-propyl-, methyl ester					X[(a)]
O-Hydroxybenzaldehyde		X[15]			
Decane, 2,6,7-trimethyl-			X[14]		
4-methyl decane		X[6]	X[14]		
γ -terpinene					X[16]
2-methyldecane			X[14]	X[8]	
Acetophenone		X[5,6]			
1-octanol		X[26]			X[36]
Hexanoic acid, 2-propenyl ester					X[37]
1-methyl-4-(1-methylethylidene)cyclohexene				X[8]	
1-undecene		X[6,17]			
Undecane			X[14]		X[3]
Nonanal	X[20]	X[6]	X[18]	X[8]	
Camphor					X[33]
Tetralin					X[38]

1-nonanol					X[36]
Benzene, 1,2,3-trichloro-					X[39]
Dodecane	X[4]		X[14]	X[8]	
Decanal		X[6]	X[18]	X[8]	
3,7-dimethylundecane			X[14]	X[8]	
Carvone					X[29]
M-Di-tert-butylbenzene				X[9]	X[12]
1-methyl indole					X[12]
2,6,11-trimethyldodecane				X[8]	
Tridecane			X[14]		
Indole		X[5,6]			
Undecanal			X[18]		
Tetramethylacetophenone					X[(c)]
Phthalic anhydride				X[9]	X[39]
Decane, 2,3,5,8-tetramethyl-			X[14]		
Nonane, 2,2,4,4,6,8,8-heptamethyl-			X[14]		
Propofol					X[2,3]
2,6,10-trimethyldodecane			X[14]	X[8]	
α-ylangene					X[33]
Decanoic acid		X[19]			
Tetradecane	X[4]		X[14]	X[8]	
Dodecanal			X[18]	X[8,9]	
Caryophyllene					X[40]
Cis-thujopsene					X[40]
Geranyl-acetone					X[34]

2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)				X[8]	
Pentadecane			X[14]		
Dibenzofuran					X[(d)]
Diethyl phthalate		X[19]			X[39]

[(a)] *Potential metabolite of valproic acid (known to interact with meropenem[41])*

[(b)] *Internal standard*

[(c)] *Ambient air pollutant: odour component in diesel engine exhaust*

[(d)] *Markes application note:* Monitoring VOC emissions from respiratory medical devices in accordance with the new ISO 18562 international standard (available: https://theanalyticalscientist.com/fileadmin/tas/issues/App_Notes/Markes_Application_Note_132.pdf; accessed 28.2.2022)

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Table S2. Changes in volatile organic compounds between baseline sampling and follow-up (48-72 hrs later) for patients with (VAP) and without (No VAP) ventilator-associated pneumonia using Wilcoxon's test. The difference between changes in VAP and non-VAP breath samples was also tested (Interaction). FDR-corrected p-values shown.

Compound	**No VAP**	**VAP**	**Interaction**
Heptane	0.276	0.009	0.885
Ethylbenzene	0.309	0.077	0.990
Nonane	0.246	0.019	0.885
Dodecane	0.276	0.015	0.885
Tetradecane	0.309	0.038	0.885
Cyclohexane	0.555	0.648	0.885
3 pentanone	0.309	0.019	0.565
Isoamyl alcohol	0.439	0.188	0.990
Pentanol	0.555	0.007	0.565
Butyl acetate	0.568	0.057	0.646
2,4 dimethylheptane	0.434	0.086	0.885
2,4-dimethyl-1-heptene	0.561	0.007	0.565
Benzaldehyde	0.000	0.007	0.885
Benzonitrile	0.358	0.451	0.990
4 methyldecane	0.555	0.127	0.885
Octane	0.333	0.077	0.885
Hexanal	0.246	0.035	0.990
2,3 dimethylheptane	0.903	0.067	0.565
4 methyloctane	0.309	0.185	0.990
4-ethyl 2,2- dimethylhexane	0.309	0.238	0.885
2,2,4,6,6-pentamethyl-heptane	0.932	0.680	0.990
Tridecane	0.309	0.093	0.885
Undecanal	0.188	0.008	0.885
2,2,4,4,6,8,8-heptamethyl-nonane	0.973	0.077	0.646
Dodecanal	0.309	0.007	0.885
Pentadecane	0.309	0.038	0.885
Methylcyclohexane	0.362	0.163	0.990
Styrene	0.276	0.050	0.990
Cyclohexanone	0.188	0.605	0.565
Benzene	0.469	0.537	0.990
Ethylfuran	0.555	0.084	0.885
(z)-3-octene	0.400	0.216	0.990
3-methyl-1-pyrrole	0.428	0.185	0.885
Phenylethyne	0.188	0.229	0.885
3-heptanol	0.188	0.774	0.565
2-ethyl-1-hexanol	0.246	0.007	0.678