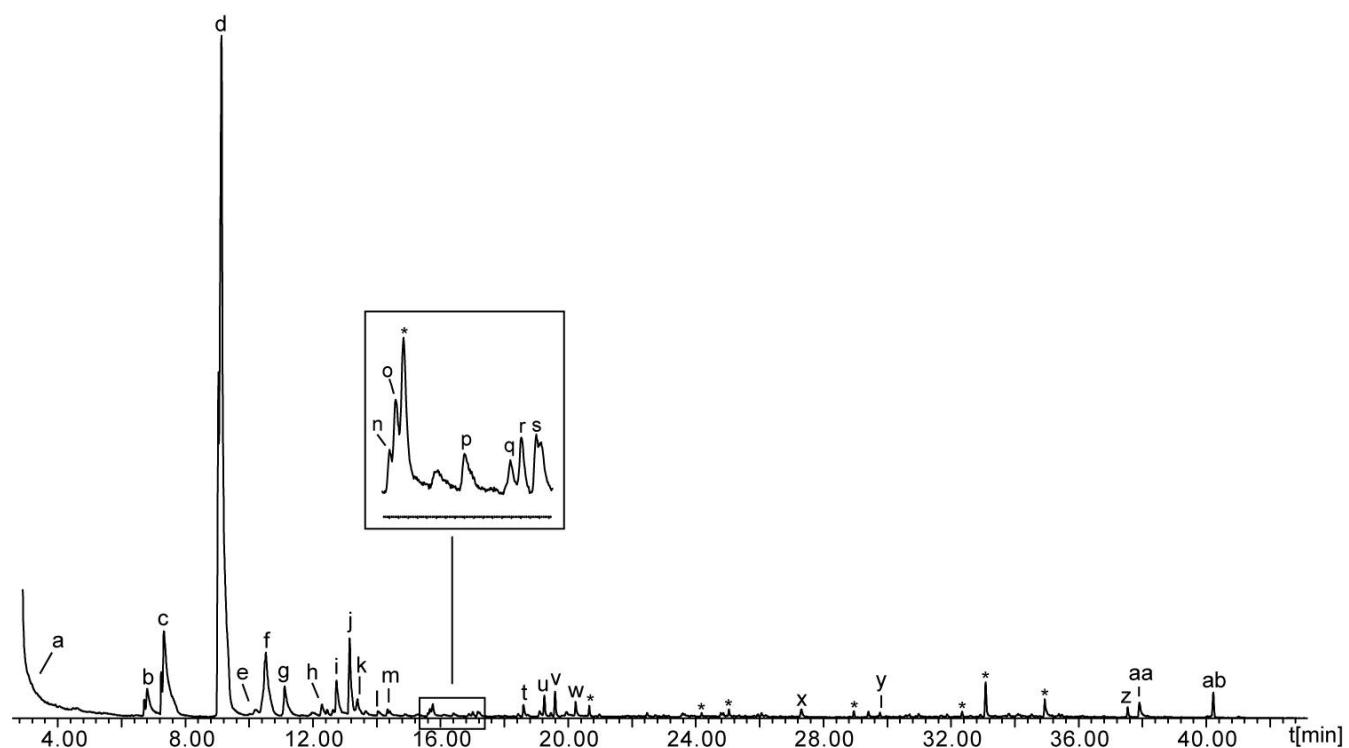


Figure S2 GC-MS chromatograms of medium and bacterial headspace

Figure S2A Total ion chromatogram of medium headspace and compounds identified. Largest peaks are indicated with a letter which corresponds with the list of compounds below.



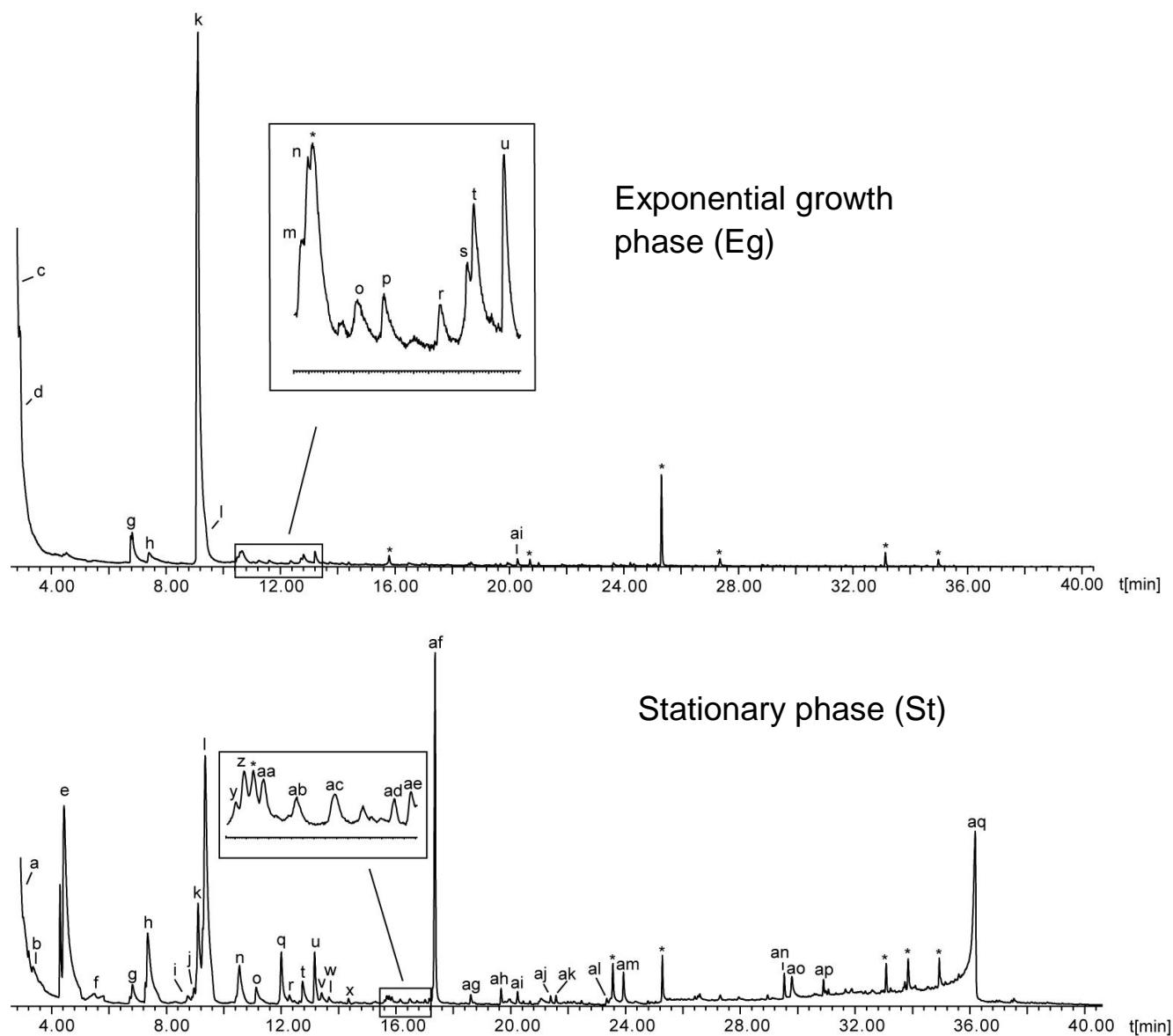
| GC ^{a)} | Compound | Retention index ^{b)} | Intensity |
|------------------|-------------------------------|-------------------------------|-----------|
| a | 1-Butanol | n.d. ^{c)} | ++++ |
| b | Cyclohexanone | 901 | ++ |
| c | 2,5-Dimethylpyrazine | 915 | +++ |
| d | Benzaldehyde | 963 | ++++ |
| e | Butylbutyrate | 997 | ++ |
| f | Trimethylpyrazine | 999 | +++ |
| g | 2-Acetylthiazol | 1016 | ++ |
| | 2-Hydroxybenzaldehyde | 1040 | + |
| h | Pyrazin M: 136 | 1050 | ++ |
| | m/z: 57, 85, 41, 129 | 1055 | + |
| | m/z: 57, 85, 41, 129 | 1060 | + |
| i | Acetophenone | 1063 | ++ |
| j | 2-Ethyl-3,6-dimethylpyrazine | 1075 | ++ |
| k | Pyrazin M: 136 | 1082 | ++ |
| l | Nonanal | 1104 | ++ |
| m | m/z: 43, 123, 101, 138 | 1111 | + |
| | m/z: 43, 69, 131, 114, 85 | 1113 | + |
| n | Pyrazin M: 164 | 1151 | ++ |
| o | 2,6-Di-(1-Methylethyl)pyrazin | 1153 | ++ |
| * | Silanozan | 1156 | ++ |

| | | | |
|----|--|------|----|
| p | Naphthalene | 1176 | ++ |
| q | Pyrazin, M=164 | 1193 | ++ |
| r | Dimethyl-(2-methylpropyl)-pyrazine M=164 | 1196 | + |
| s | Decanal | 1201 | + |
| | m/z: 107, 135, 91, 150, 80 | 1203 | + |
| t | 2-Butyl-3,6-dimethylpyrazine | 1253 | ++ |
| | α -Ethylidenebenzeneacetaldehyde | 1272 | ++ |
| u | m/z: 145, 76, 120, 46, 192 | 1277 | ++ |
| | Isobornylacetate | 1285 | ++ |
| v | m/z: 145, 118, 192, 46 | 1289 | ++ |
| | Pyrazine | 1302 | ++ |
| w | 2,5-Dimethyl-3-(3-methylbutyl)-pyrazine | 1313 | ++ |
| * | Siloxane* | 1329 | ++ |
| * | Unknown | 1465 | ++ |
| | Hexasulfur | 1487 | ++ |
| | Pentadecane | 1498 | + |
| * | Cyclosiloxane* | 1499 | + |
| | sesquiterpene | 1513 | + |
| | m/z: 71, 57, 85, 43, 99 | 1537 | + |
| | m/z: 205, 190, 174, 73 | 1542 | + |
| x | Hexadecane | 1596 | ++ |
| * | Cyclosiloxane | 1669 | + |
| y | Hydrocarbon | 1706 | + |
| * | Unknown | 1829 | + |
| | m/z: 157, 143, 185, 270 | 1857 | + |
| * | Bis(2-methylpropyl)phthalat | 1866 | ++ |
| | m/z: 205, 217, 220, 175 | 1917 | + |
| | m/z: 160, 145, 270, 95, 105 | 1943 | + |
| * | Dibutylphthalat | 1961 | ++ |
| | m/z: 239, 183, 253, 268 | 1988 | + |
| z | 2-Ethylhexyl dodecanoate,* | 2099 | ++ |
| aa | m/z: 121, 179, 137, 292 | 2120 | ++ |
| ab | m/z: 149, 91, 121, 79 | 2253 | ++ |
| | m/z: 112, 70, 57 | 2300 | + |

^{a)}Peak in chromatogram, ^{b)}Abundance relative to the largest peak in the total ion chromatogram: + 0 – 0.5%; ++ 0.5 – 10%; +++ 10 – 30%; +++++ 30 – 100%, ^{c)}not determined, *) artifact

Figure S2B Total ion chromatogram and compounds identified of *C. minutissimum* headspace.

Largest peaks are indicated with a letter which corresponds with the list of compounds below.



| GC ^{a)} | Compound | Retention index ^{b)} | | Intensity |
|------------------|----------------------------------|-------------------------------|----|-----------|
| | | Eg | St | |
| a | Ethylacetate* | n.d. ^{c)} | | ++++ |
| b | Toluol | n.d. | | ++ |
| c | 1-Butanol | n.d. | ++ | |
| d | 3-Methyl-1-butanol | n.d. | ++ | |
| e | Butylacetate | 826 | | ++++ |
| f | 3-Methylbutanoic acid | 863 | | ++ |
| g | Cyclohexanone | 901 | ++ | ++ |
| h | 2,5-Dimethylpyrazine | 915 | ++ | ++++ |
| i | 3-Hydroxy-2-heptanon or isomeric | 952 | | ++ |
| j | Butylisobutyrate | 958 | | ++ |

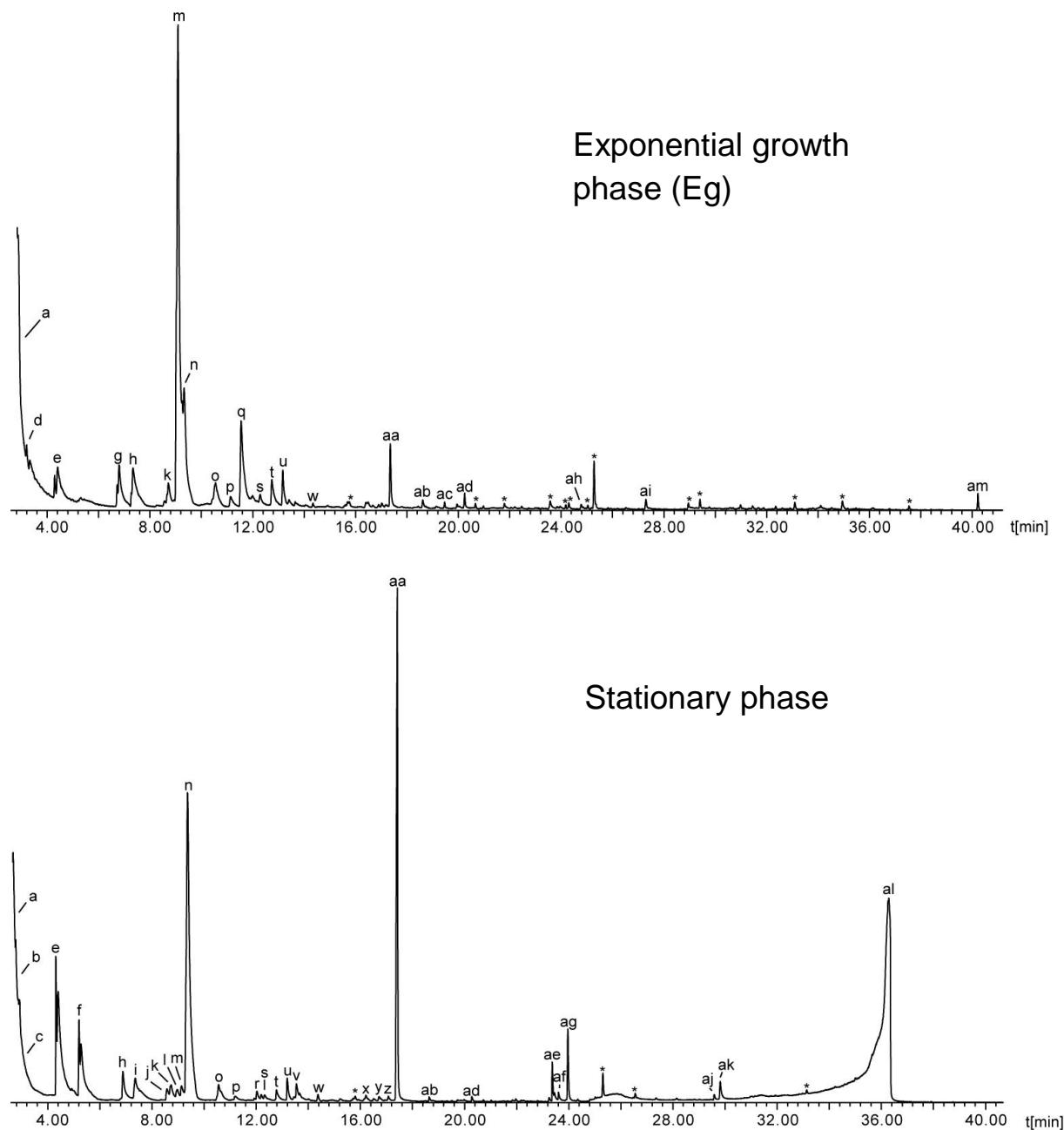
| | | | | |
|----|---|------|------|------|
| k | Benzaldehyde | 963 | ++++ | ++++ |
| l | Dimethyltrisulfide | 968 | ++ | ++++ |
| m | Butylbutyrate | 997 | + | |
| n | Trimethylpyrazine | 999 | ++ | +++ |
| o | 2-Acetylthiazol | 1016 | + | ++ |
| p | 2-Ethyl-1-hexanol* | 1029 | + | |
| q | Butyl-2-methylbutanoate | 1042 | | +++ |
| r | Pyrazine, M: 136 | 1050 | + | ++ |
| s | S-Methylmethanthiosulphonate | 1062 | + | |
| t | Acetophenone | 1063 | ++ | ++ |
| u | 2-Ethyl-3,6-dimethylpyrazine | 1075 | ++ | +++ |
| v | Pyrazine, M: 136 | 1082 | | ++ |
| w | m/z: 123, 58, 43, 138 | 1090 | | ++ |
| x | m/z: 43, 123, 101, 138 | 1111 | + | ++ |
| y | 2,6-Di(1-Methylethyl)pyrazine | 1153 | | ++ |
| z | Pyrazine M: 150 | 1155 | + | ++ |
| * | Silanolane | 1156 | ++ | |
| aa | 7-Methyl-2-nanone | 1160 | | ++ |
| ab | Methyl(2-methyl-3-furyl)disulfide | 1168 | | + |
| ac | m/z: 160, 91, 45 Pyrazine, M=164 | 1179 | | + |
| | | 1193 | + | |
| ad | Dimethyl-(2-methylpropyl)-pyrazine, M=164 | 1196 | + | |
| ae | Decanal | 1201 | | ++ |
| af | Dimethyltetrasulfide | 1208 | | ++++ |
| ag | 2-Butyl-3,6-dimethylpyrazine | 1253 | + | ++ |
| | Isobornylacetate | 1285 | + | |
| ah | 2-Undecanone | 1292 | | ++ |
| | m/z: 57, 143, 87, 69, 159 | 1301 | + | |
| | Pyrazine | 1302 | + | + |
| ai | 2,5-Dimethyl-3-(3-methylbutyl)-pyrazine | 1313 | + | ++ |
| | m/z: 69, 43, 85, 111, 154 | 1321 | | + |
| | m/z: 138, 95, 83, 193, 57 | 1340 | + | |
| aj | 10-Methyl-2-undecanone | 1359 | | + |
| ak | 9-Methyl-2-undecanone | 1363 | | ++ |
| | Artifact | 1371 | + | |
| | Tetradecane | 1397 | + | + |
| al | Isobutyl-2-phenylacetate | 1432 | | ++ |
| | Pentathiane | 1437 | | ++ |
| am | Dimethylpentasulfide | 1455 | | ++ |
| | Artifact | 1465 | + | |
| | Artifact | 1470 | + | |
| | Hexasulfur | 1487 | + | |
| | 5-Methyl-2-phenyl-2-hexenal | 1488 | + | + |
| | 12-Methyl-2-tridecanone | 1557 | | + |
| | 11-Methyl-2-tridecanone | 1567 | | ++ |
| | Hexadecane | 1596 | + | ++ |
| | Lenthionine | 1623 | | + |
| | Cyclosiloxane | 1669 | | ++ |
| an | 2-Pentadecanone | 1695 | | ++ |
| ao | Hexathiepane | 1707 | | ++ |

| | | | |
|----|------------------------------|------|------|
| ap | 14-Methyl-2-pentadecanone | 1760 | ++ |
| | Octadecane | 1796 | ++ |
| | m/z: 253, 268, 185, 171, 85 | 1800 | + |
| | m/z: 229, 145, 159, 161, 119 | 1802 | ++ |
| * | m/z: 157, 143, 185, 270 | 1857 | + |
| * | Bis(2-methylpropyl)phthalat* | 1866 | ++ |
| | Heptadecen-2-on | 1874 | ++ |
| | Nonadecan | 1896 | ++ |
| * | Di-2-pyridinylethanedion* | 1906 | ++ |
| * | Dibutylphthalat* | 1961 | + |
| | m/z: 239, 183, 253, 268 | 1988 | + |
| | Eicosane | 1995 | ++ |
| aq | Octasulfur | 2025 | ++++ |

^{a)}Peak in chromatogram, ^{b)}Abundance relative to the largest peak in the total ion chromatogram: + 0 – 0.5%; ++ 0.5 – 10%; +++ 10 – 30%; +++++ 30 – 100%, ^{c)}not determined, *) artifact, grey shading – also identified in medium.

Figure S2C Total ion chromatogram and compounds identified of *B. subtilis* headspace.

Largest peaks are indicated with a letter which corresponds with the list of compounds below.



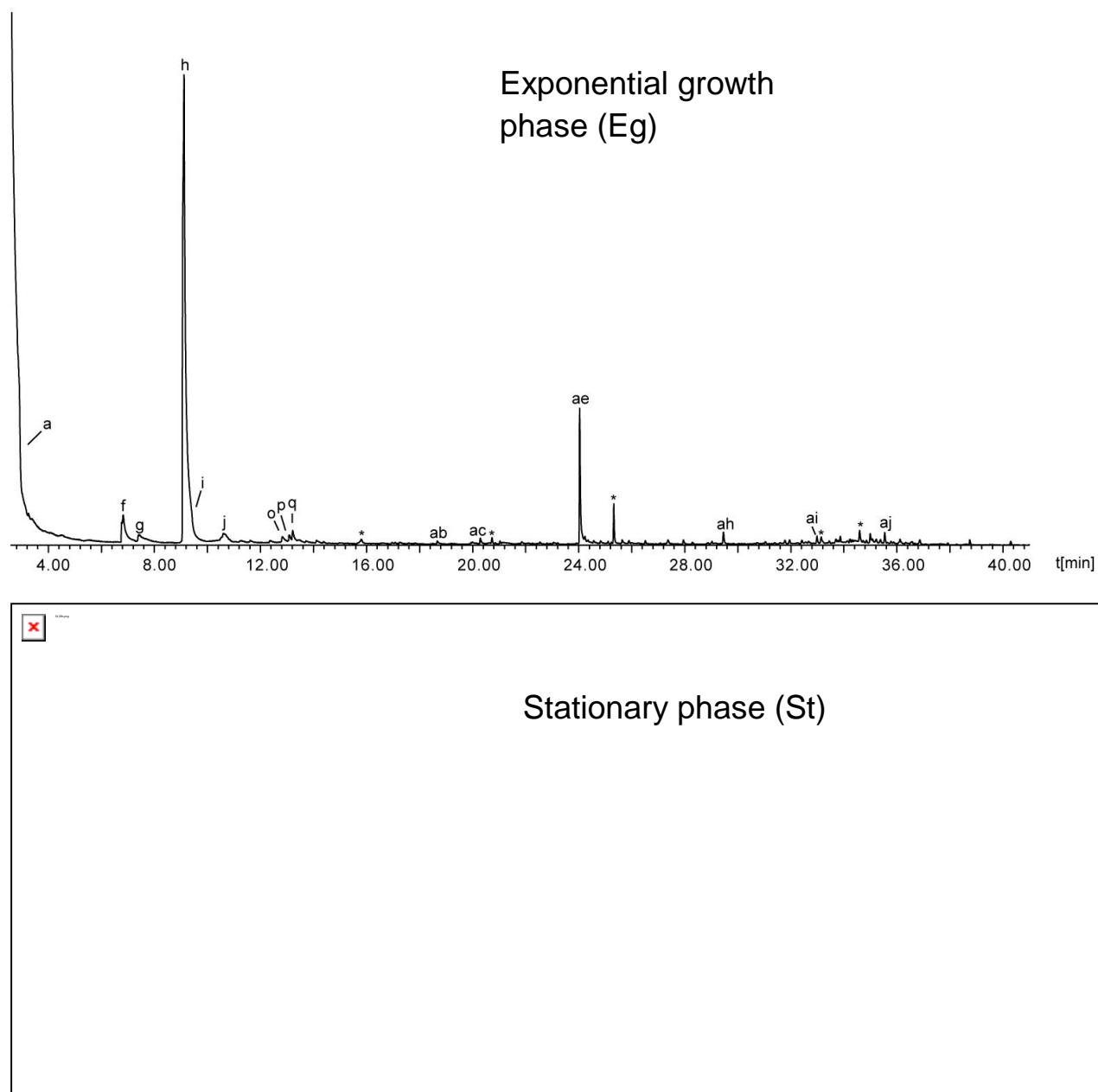
| GC ^{a)} | Compound | Retention index ^{b)} | Intensity | |
|------------------|--------------------|-------------------------------|-----------|------|
| | | | A | B |
| a | Acetoin | n.e. ^{c)} | ++ | ++ |
| b | 3-Methyl-1-butanol | n.e. | | ++ |
| c | Dimethyldisulfide | n.e. | | ++ |
| d | Toluol | n.e. | ++++ | |
| e | Butylacetate | 826 | +++ | ++++ |
| f | m/z: 88, 43, 55 | 854 | | +++ |
| g | Cyclohexanone | 901 | +++ | |

| | | | |
|----|--|------|------|
| h | 3-(Acetoxy)-2-butanone | 903 | ++ |
| i | 2,5-Dimethylpyrazine | 915 | +++ |
| j | 2-Hydroxy-3-heptanon or isomere | 947 | ++ |
| k | 3-Hydroxy-2-heptanon or isomere | 952 | ++ |
| l | Butylisobutyrate | 958 | ++ |
| m | Benzaldehyde | 963 | ++++ |
| n | Dimethyltrisulfide | 968 | ++++ |
| o | Trimethylpyrazine | 999 | ++ |
| p | 2-Acetylthiazol | 1016 | ++ |
| q | 2-Ethyl-1-hexanol* | 1029 | +++ |
| | Ethyl-2-isopropyl-2-butenoate | 1042 | ++ |
| r | Butyl-2-methylbutanoate | 1042 | ++ |
| s | Pyrazine, M: 136 | 1050 | ++ |
| t | Acetophenone | 1063 | ++ |
| u | 2-Ethyl-3,6-dimethylpyrazine | 1075 | ++ |
| | Pyrazine, M: 136 | 1082 | + |
| v | 2-Methoxyphenol | 1087 | ++ |
| | Ethylbenzenediol | 1090 | + |
| w | m/z: 43, 123, 101, 138 | 1111 | + |
| | m/z: 132, 67, 99, 53, 39 | 1139 | + |
| | m/z: 97, 59, 140 | 1150 | + |
| | Pyrazine, M: 150 | 1151 | + |
| | 2,6-Di(1-Methylethyl)pyrazine | 1153 | + |
| * | Siloxane | 1156 | + |
| x | Unknown, MW: 150 | 1170 | ++ |
| | Naphthalene | 1176 | + |
| y | Tetrathiolane | 1187 | + |
| z | Dimethyl-(2-methylpropyl)-Pyrazine M=164 | 1196 | ++ |
| aa | Dimethyltetrasulfide | 1208 | +++ |
| ab | 2-Butyl-3,6-dimethylpyrazine | 1253 | ++ |
| ac | Isobornylacetate | 1285 | ++ |
| | 2-Undecanone | 1292 | + |
| | Pyrazine | 1302 | + |
| ad | 2,5-Dimethyl-3-(3-methylbutyl)-pyrazine | 1313 | ++ |
| * | Siloxane | 1329 | + |
| | m/z: 138, 95, 83, 193, 57 | 1340 | + |
| * | Unknown | 1371 | + |
| | m/z: 91, 71, 99, 117, 55 | 1379 | + |
| | Pyrazine | 1388 | + |
| | m/z: 113, 192, 45, 136, | 1390 | + |
| | m/z: 71, 117, 43 | 1428 | ++ |
| ae | Isobutyl-2-phenylacetate | 1432 | ++ |
| af | Pentathiane | 1437 | ++ |
| * | Unknown | 1442 | ++ |
| ag | Dimethylpentasulfide | 1455 | ++ |
| * | Unknown | 1465 | ++ |
| * | Cyclohexadien-1,4-dion-Derivate | 1470 | + |
| ah | 5-Methyl-2-phenyl-2-hexenal | 1488 | + |
| | Pentadecane | 1498 | + |
| * | Cyclosiloxane | 1499 | + |

| | | | | | |
|----|---|-----------------------------------|------|----|------|
| | * | 2,4-Bis(1,1-dimethylethyl)-phenol | 1509 | ++ | ++ |
| ai | | Hexadecane | 1596 | ++ | |
| | * | Cyclosiloxane | 1669 | + | |
| aj | | 2-Pentadecanone | 1695 | | ++ |
| ak | | Hexathiepane | 1707 | | ++ |
| | | 14-Methyl-2-pentadecanone | 1760 | + | |
| | * | Unknown | 1763 | + | |
| | | 13-Methyl-2-pentadecanone | 1771 | + | |
| | | Methyl-13-methyltetradecanoat | 1786 | + | |
| | * | Unknown | 1829 | + | |
| | * | Bis(2-methylpropyl)phthalate | 1866 | ++ | + |
| | * | Dibutylphthalate | 1961 | ++ | |
| | | m/z: 239, 183, 253, 268 | 1988 | + | |
| al | | Octasulfur | 2025 | | ++++ |
| | | m/z: 237, 195, 241, 221, 252 | 2058 | + | |
| | | Dodecanoic acid ethylester | 2099 | + | |
| am | | m/z: 149, 91, 121, 79 | 2253 | ++ | |

^{a)}Peak in chromatogram, ^{b)}Abundance relative to the largest peak in the total ion chromatogram: + 0 – 0.5%; ++ 0.5 – 10%; +++ 10 – 30%; +++++ 30 – 100%, ^{c)}not determined, *) artifact, grey shading – also identified in medium.

Figure S2D Total ion chromatogram of *S. epidermidis* headspace and compounds identified



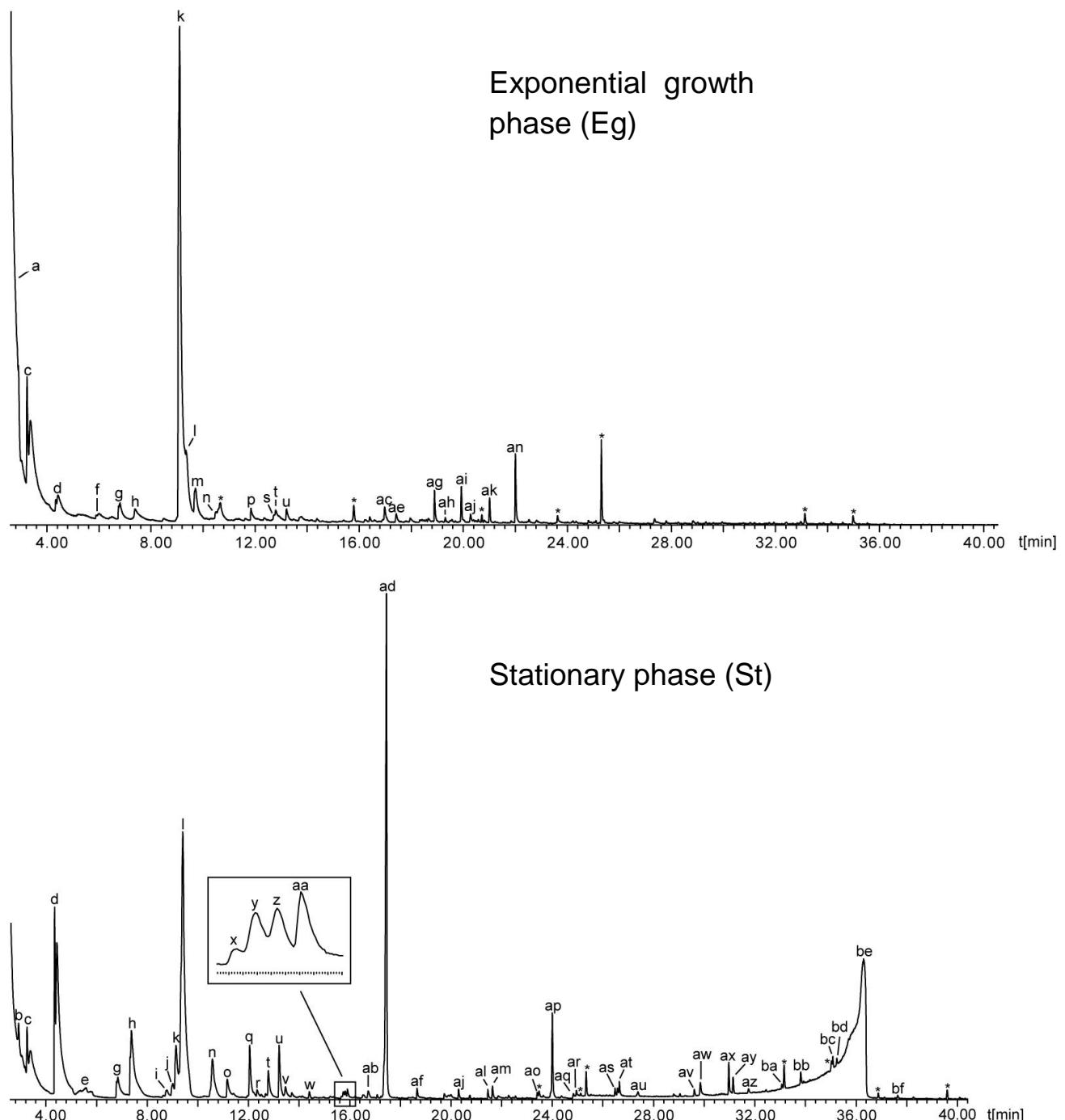
| GC ^{a)} | Compound ^{b)} | Retention index ^{c)} | Intensity | |
|------------------|------------------------|-------------------------------|-----------|------|
| | | | A | B |
| a | 1-Butanol | n.e. ^{c)} | +++ | |
| b | Acetoin | n.e. | +++ | |
| c | 3-Methyl-1-butanol | n.e. | +++ | |
| d | Dimethyldisulfide | n.e. | +++ | |
| e | Butylacetate | 826 | ++++ | |
| f | Cyclohexanone | 901 | ++ | ++ |
| g | 2,5-Dimethylpyrazine | 915 | ++ | +++ |
| h | Benzaldehyde | 963 | ++++ | ++++ |
| i | Dimethyltrisulfide | 968 | +++ | ++++ |

| | | | | |
|----|---|------|----|-----|
| | Butylbutyrate | 997 | + | ++ |
| j | Trimethylpyrazine | 999 | + | ++ |
| k | 2-Acetylthiazol | 1016 | | ++ |
| l | 2-Ethyl-1-hexanol* | 1029 | | ++ |
| | Ethyl 2-isopropyl-2-butenoate | 1042 | | + |
| m | Butyl-2-methylbutanoate | 1042 | | ++ |
| n | Pyrazine, M: 136 | 1050 | + | ++ |
| | S-Methyl-methanthiosulphonate | 1062 | | + |
| o | Acetophenone | 1063 | ++ | ++ |
| p | 5-Nonanone | 1073 | ++ | + |
| q | 2-Ethyl-3,6-dimethylpyrazine | 1075 | ++ | ++ |
| r | Pyrazine, M: 136 | 1082 | | ++ |
| s | Ethylbenzenediol | 1090 | + | ++ |
| | Nonanal | 1104 | + | + |
| t | m/z: 43, 123, 101, 138 | 1111 | + | ++ |
| u | Phenylacetonitril | 1138 | | + |
| v | Pyrazine, M: 150 | 1151 | | + |
| w | 2,6-Di(1-Methylethyl)pyrazine | 1153 | | ++ |
| x | 8-Methyl-2-nonanone | 1155 | | ++ |
| * | Silanol | 1156 | + | ++ |
| | 7-Methyl-2-nonanone | 1160 | | + |
| | Pyrazine, M=164 | 1193 | + | |
| y | Dimethyl-(2-methylpropyl)-Pyrazine | 1196 | + | ++ |
| z | Decanal | 1201 | | ++ |
| aa | Dimethyltetrasulfide | 1208 | | +++ |
| ab | 2-Butyl-3,6-dimethylpyrazine | 1253 | + | ++ |
| | α-Ethylidenebenzeneacetaldehyd e | 1272 | | + |
| | 2-Undecanone | 1292 | | + |
| | Indol | 1294 | | + |
| | m/z: 57, 143, 87, 69, 159 | 1301 | + | |
| | Pyrazine | 1302 | + | + |
| | m/z: 57, 143, 87, 159, 69 | 1303 | | + |
| ac | 2,5-Dimethyl-3-(3-methylbutyl)-pyrazine | 1313 | + | ++ |
| | m/z: 138, 95, 83, 193, 57 | 1340 | ++ | |
| | 10-Methyl-2-undecanone | 1359 | | + |
| | 9-Methyl-2-undecanone | 1363 | | + |
| | Pyrazine | 1388 | | + |
| | Tetradecane | 1397 | + | + |
| | Sesquiterpen: Cadina-1,4-dien | 1420 | | + |
| ad | Dimethylpentasulfide | 1455 | | ++ |
| ae | 6-Pentyl-2H-Pyran-2-on* | 1456 | | ++ |
| | Cyclohexadien-1,4-dion-derivate* | 1470 | + | + |
| | 5-Methyl-2-phenyl-2-hexenal | 1488 | + | ++ |
| | 2-Tridecanone | 1496 | | + |
| * | Cyclosiloxane | 1499 | + | + |
| | 2,4-Bis(1,1-dimethylethyl)-phenol | 1509 | ++ | ++ |
| | Dodecanoic acidmethylester | 1530 | + | ++ |
| | m/z: 159, 202, 129, 131 | 1535 | + | |
| | 12-Methyl-2-tridecanone | 1557 | | + |
| | m/z: 193, 55, 222, 95, 43 | 1562 | + | |

| | | | |
|----|---|--------------|----|
| af | m/z: 69, 93, 41, 107, 71 11-Methyl-2-tridecanone | 1563 1567 | + |
| ag | m/z: 107, 163, 56, 79, 41 Hexadecane | 1586 1596 | + |
| * | Unknown | 1598 | + |
| | Cyclosiloxane | 1669 | + |
| ah | m/z: 109, 135, 82, 123, 93 2-Pentadecanone | 1692 1695 | + |
| | Hexathiepane | 1707 | + |
| | 14-Methyl-2-pentadecanone | 1760 | + |
| | m/z: 253, 268, 185, 171, 85 | 1800 | + |
| | m/z: 229, 145, 159, 161, 119 | 1802 | + |
| ai | m/z: 143, 157, 270, 185, 200 * Bis(2-methylpropyl)phthalate* | 1861 1866 | ++ |
| | m/z: 119, 105, 272, 204, 91 | 1884 | + |
| | m/z: 145, 160, 270, 95, 106 | 1905 | ++ |
| | m/z: 160, 145, 270, 95, 105 | 1943 | ++ |
| | m/z: 243, 91, 258, 147, 133 | 1950 | + |
| | m/z: 243, 91, 119, 161, 105 | 1968 | + |
| | m/z: 256, 157, 131, 143, 118 | 1975 | + |
| aj | m/z: 239, 183, 253, 268 2-Octadecanone | 1988 2004 | ++ |
| ak | Octasulfur | 2025 | ++ |
| | m/z: 197, 282, 254, 239, 141 | 2121 | + |
| | Diterpene | 2168 | ++ |
| | m/z: 231, 246, 108, 121, 81 | 2211 | + |
| | m/z: 121, 91, 79, 105, 93 | 2257 | + |
| al | m/z: 149, 91, 121, 79, 243 | 2257 | ++ |

a) Peak in chromatogram, b) Artefacts, c)Abundance relative to the largest peak in the total ion chromatogram: + 0 – 0.5%; ++ 0.5 – 10%; +++ 10 – 30%; +++++ 30 – 100%, d) not determined

Figure S2E Total ion chromatogram of *B. epidermidis* headspace and compounds identified



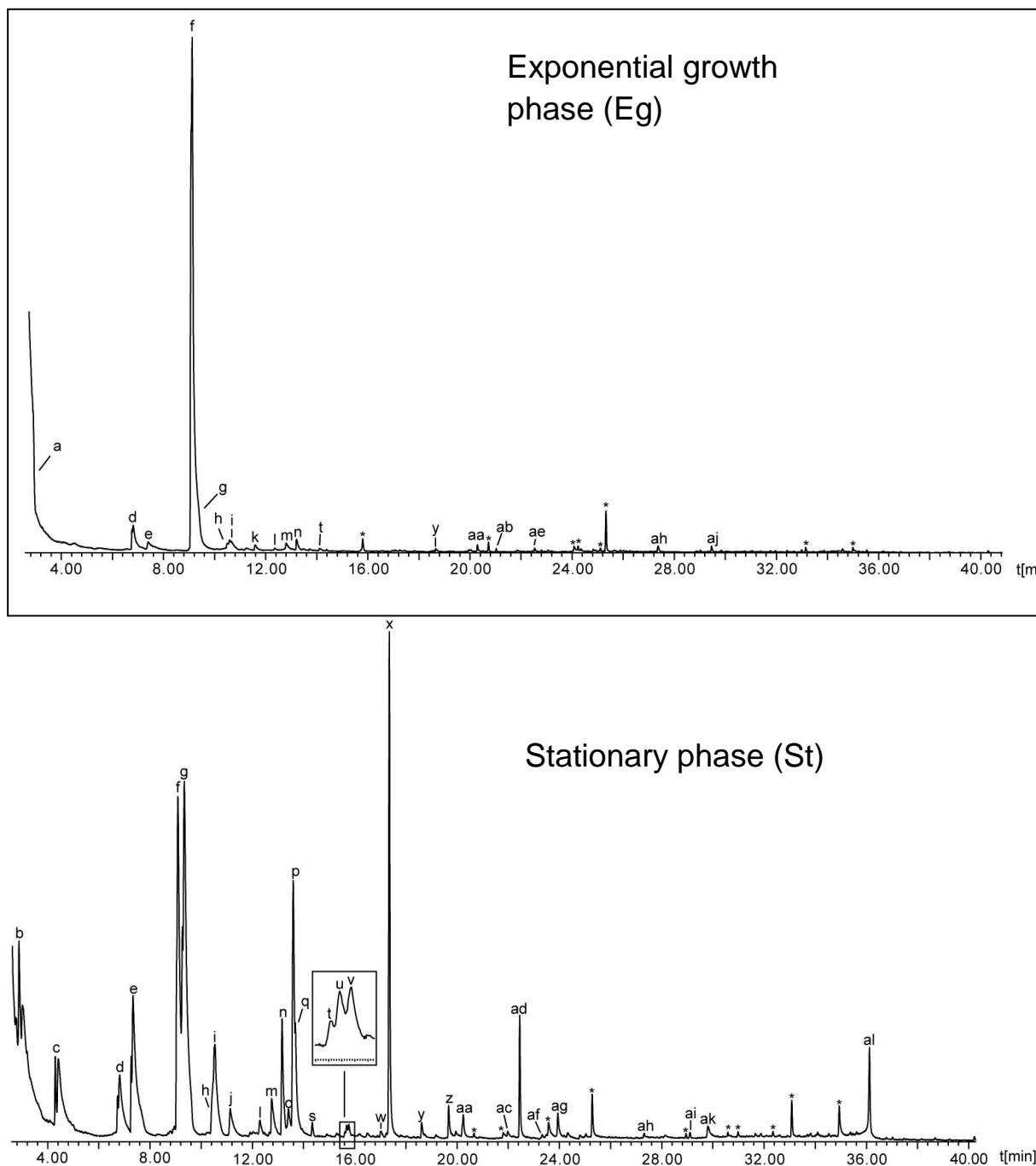
| GC ^{a)} | Compound ^{b)} | Retention index ^{c)} | Intensity | |
|------------------|------------------------|-------------------------------|-----------|------|
| | | | A | B |
| a | 1-Butanol | n.e. ^{c)} | ++ | |
| b | Dimethyldisulfide | n.e. | | ++ |
| c | Toluol | n.e. | +++ | +++ |
| d | Butylacetate | 826 | ++ | ++++ |
| e | 3-Methylbutanoic acid | 863 | | ++ |
| f | Xylool | 872 | + | |

| | | | | |
|----|--|------|------|------|
| g | Cyclohexanone | 901 | ++ | ++ |
| h | 2,5-Dimethylpyrazine | 915 | ++ | +++ |
| i | 3-Hydroxy-2-heptanon or isomere | 952 | | ++ |
| j | Butylisobutyrate | 958 | | ++ |
| k | Benzaldehyde | 963 | ++++ | ++ |
| l | Dimethyltrisulfide | 968 | +++ | ++++ |
| m | 1,2-Dithiolane | 978 | ++ | |
| n | Trimethylpyrazine | 999 | ++ | ++ |
| * | Cyclosiloxan | 1003 | ++ | |
| o | 2-Acetylthiazole | 1016 | | ++ |
| p | 2,3-Dimethyl-2-cyclopenten-1-one | 1037 | ++ | |
| q | Butyl-2-methylbutanoate | 1042 | | ++ |
| r | Pyrazine, M: 136 | 1050 | + | ++ |
| s | S-Methyl-methanthiosulphonate | 1062 | ++ | |
| t | Acetophenone | 1063 | ++ | ++ |
| u | 2-Ethyl-3,6-dimethylpyrazine | 1075 | ++ | ++ |
| v | Pyrazine, M: 136 | 1082 | | ++ |
| | Ethylbenzenediol | 1090 | | + |
| | m/z: 43, 123, 101, 138 | 1111 | + | ++ |
| x | Pyrazine, M: 150 | 1151 | | + |
| y | 2,6-Di(1-Methylethyl)pyrazine | 1153 | | ++ |
| z | Pyrazine, M: 150 | 1155 | | + |
| * | Silanolane | 1156 | + | |
| aa | 7-Methyl-2-nonanone | 1160 | | + |
| ab | Tetrathiolane | 1187 | | ++ |
| ac | Sulfur compound | 1195 | ++ | |
| | Dimethyl-(2-methylpropyl)-pyrazine M=164 | 1196 | | + |
| ad | Dimethyltetrasulfide | 1208 | | ++++ |
| ae | Indan Derivate | 1210 | ++ | |
| af | 2-Butyl-3,6-dimethylpyrazine | 1253 | + | ++ |
| ag | 1-Chlorodecane | 1263 | ++ | |
| ah | 3-Methyldodecane | 1279 | + | |
| | 2-Undecanone | 1292 | | + |
| | Indol | 1294 | | + |
| ai | m/z: 57, 143, 87, 69, 159 | 1301 | ++ | |
| | Pyrazine | 1302 | | + |
| aj | 2,5-Dimethyl-3-(3-methylbutyl)-pyrazine | 1313 | ++ | ++ |
| ak | m/z: 138, 95, 83, 193, 57 | 1340 | ++ | |
| al | 10-Methyl-2-undecanone | 1359 | | ++ |
| am | 9-Methyl-2-undecanone | 1363 | | ++ |
| an | m/z: 91, 71, 99, 117, 55 | 1379 | ++ | |
| | Pyrazine | 1388 | | + |
| | m/z: 113, 192, 45, 136 | 1390 | | + |
| | Tetradecane | 1397 | + | + |
| | Isobutyl-2-phenylacetate | 1432 | | + |
| ao | Pentathiane | 1437 | | ++ |
| * | Unknown | 1442 | ++ | |
| ap | Dimethylpentasulfide | 1455 | | ++ |
| | Hexasulfur | 1487 | + | + |
| aq | 5-Methyl-2-phenyl-2-hexenal | 1488 | + | + |

| | | | |
|----|-----------------------------------|------|------|
| ar | 2-Tridecanone | 1496 | + |
| * | 2,4-Bis(1,1-dimethylethyl)-phenol | 1509 | ++ |
| as | 12-Methyl-2-tridecanone | 1557 | ++ |
| at | 11-Methyl-2-tridecanone | 1567 | ++ |
| au | Hexadecane | 1596 | + |
| | m/z: 71, 43, 139, 224, 97 | 1609 | + |
| | 13-Methyl-2-tetradecanone | 1662 | + |
| av | 2-Pentadecanone | 1695 | ++ |
| aw | Hexathiepane | 1707 | ++ |
| ax | 14-Methyl-2-pentadecanone | 1760 | ++ |
| ay | 13-Methyl-2-pentadecanone | 1771 | ++ |
| az | 2-Hexadecanone | 1800 | ++ |
| ba | 15-Methyl-2-hexadecanone | 1865 | ++ |
| * | Bis(2-methylpropyl)phthalat | 1866 | ++ |
| bb | 2-Heptadecanone | 1902 | ++ |
| | m/z: 160, 145, 270, 95, 105 | 1943 | + |
| * | Dibutylphthalat | 1961 | ++ |
| bc | 16-Methyl-2-heptadecanone | 1968 | ++ |
| bd | 15-Methyl-2-heptadecanone | 1976 | ++ |
| | m/z: 239, 183, 253, 268 | 1988 | + |
| | 2-Octadecanone | 2004 | + |
| be | Octasulfur | 2025 | ++++ |
| bf | 2-Nonadecanone | 2105 | + |
| * | Cyclosiloxan | 2217 | + |

a) Peak in chromatogram, b) Artefacts, c) Abundance relative to the largest peak in the total ion chromatogram: + 0 – 0.5%; ++ 0.5 – 10%; +++ 10 – 30%; +++++ 30 – 100%, d) not determined

Figure S2F Total ion chromatogram of *P. aeruginosa* headspace and compounds identified



| GC ^{a)} | Compound ^{b)} | Retention index ^{c)} | Intensity A | Intensity B |
|------------------|------------------------|-------------------------------|-------------|-------------|
| a | 1-Butanol | n.e. ^{c)} | ++ | |
| b | Dimethyldisulfide | n.e. | | +++ |
| c | Butylacetate | 826 | | +++ |
| d | Cyclohexanone | 901 | ++ | +++ |
| e | 2,5-Dimethylpyrazine | 915 | ++ | ++++ |
| | Butylisobutyrate | 958 | | + |
| f | Benzaldehyde | 963 | ++++ | ++++ |

| | | | | |
|----|---|------|-----|------|
| g | Dimethyltrisulfide | 968 | +++ | ++++ |
| h | Butylbutyrate | 997 | ++ | ++ |
| i | Trimethylpyrazine | 999 | ++ | ++++ |
| j | 2-Acetylthiazole | 1016 | | ++ |
| k | 2-Ethyl-1-hexanol | 1029 | ++ | |
| l | Pyrazine, M: 136 | 1050 | ++ | ++ |
| m | Acetophenone | 1063 | ++ | ++ |
| n | 2-Ethyl-3,6-dimethylpyrazine | 1075 | ++ | +++ |
| o | Pyrazine, M: 136 | 1082 | + | ++ |
| p | 1-Undecene | 1088 | | ++++ |
| q | Methylbenzoate | 1091 | | +++ |
| r | Nonanal | 1104 | + | |
| s | m/z: 43, 123, 101, 138 | 1111 | | ++ |
| t | Pyrazine, M: 150 | 1151 | | + |
| u | 2,6-Di(1-Methylethyl)pyrazine | 1153 | | + |
| v | Pyrazine, M: 150 | 1155 | | + |
| * | Silanol | 1156 | ++ | |
| w | Pyrazine, M=164 | 1193 | + | |
| | Dimethyl-(2-methylpropyl)-pyrazin M=164 | 1196 | | + |
| x | Decanal | 1201 | + | |
| | Dimethyltetrasulfide | 1208 | | ++++ |
| | 2-Butyl-3,6-dimethylpyrazine | 1253 | + | ++ |
| z | 2-Undecanone | 1292 | | ++ |
| | m/z: 57, 143, 87, 69, 159 | 1301 | + | |
| | Pyrazine | 1302 | + | |
| aa | 2,5-Dimethyl-3-(3-methylbutyl)-pyrazine | 1313 | ++ | ++ |
| | m/z: 69, 43, 85, 111,154 | 1321 | + | |
| ab | m/z: 138, 95, 83, 193, 57 | 1340 | + | |
| ac | Nerylmethylthioether | 1379 | | + |
| ad | Geranyl methylthioether | 1396 | | +++ |
| ae | Tetradecan | 1397 | + | |
| af | Diphenylmethane | 1430 | | + |
| ag | Dimethylpentasulfid | 1455 | | ++ |
| * | Cyclohexadien-1,4-dion-Derivat | 1470 | + | + |
| | 5-Methyl-2-phenyl-2-hexenal | 1488 | + | |
| * | Cyclosiloxane | 1499 | + | |
| * | 2,4-Bis(1,1-dimethylethyl)-phenol | 1509 | ++ | ++ |
| ah | Hexadecane | 1596 | ++ | + |
| ai | Hydrocarbon | 1677 | | + |
| aj | m/z: 109, 82, 135, 121, 150 | 1692 | | + |
| ak | Hexathiepan | 1707 | | + |
| | m/z: 229, 145, 159, 161,119 | 1802 | + | |
| | m/z: 157, 143, 185, 270 | 1857 | + | |
| * | Bis(2-methylpropyl)phthalat | 1866 | ++ | |
| | m/z: 145, 160, 270, 95, 106 | 1905 | + | |
| | m/z: 160, 145, 270, 95, 105 | 1943 | + | |
| * | Dibutylphthalat | 1961 | + | ++ |
| al | Octasulfur | 2025 | + | +++ |

a) Peak in chromatogram, b) Artefacts, c)Abundance relative to the largest peak in the total ion chromatogram: + 0 – 0.5%; ++ 0.5 – 10%; +++ 10 – 30%; +++++ 30 – 100%, d) not determined