Analysis of *Streptomyces* volatilomes using global molecular networking reveals the presence of metabolites with diverse biological activities

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SUPPORTING INFORMATION LIST

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Figure S2. Molecular network generated using data from cultures of 37 *Streptomyces* isolates (cosine 0.6). Each node represents one fragmentation spectrum and node size represents the summed intensity (peak area) of the ion from all samples. Nodes that have matches in GNPS spectral libraries are outlined in black. The pie charts indicate the relative abundance of each compound in the different isolate samples. The VOCs annotated by both methods (and bis(2-ethylhexyl) phthalate) are labelled and indicated with circles.
**Figure S3.** Molecular network generated using replicate cultures of the six selected *Streptomyces* isolates (cosine 0.6). Each node represents one fragmentation spectrum and node size represents the summed intensity (peak area) of the ion from all samples. Nodes that have matches in GNPS spectral libraries are outlined in black. The pie charts indicate the relative abundance of each compound in the cultures of the respective isolates grown in the different media.
Table S1. Oligonucleotide primers used for PCR amplification and DNA sequencing in the current study.

| Primer name | Sequence (5’-3’) | Annealing temperature | Purpose | Reference |
|-------------|------------------|-----------------------|---------|-----------|
| 27F         | AGAGTTTGATCCTGGCTCAG | 59                   | Amplifying 1465 bp of the 16s rDNA gene and sequencing for molecular identification | (1) |
| 1492R       | ACGGCTACCTTGTTACGACT |                      |         |           |
| 516F        | TGCCAGCAGCCGCGGTA | -                     | Sequencing 16s rDNA gene amplicons for molecular identification | (2) |
| rpoBF1      | TTCATGGACCAGAACAACC | 58                   | Amplifying 880 bp of the rpoB gene for use in phylogeny | (3) |
| rpoBR1      | CGTAGTTGTGACCCTCCC |                      |         |           |
| rpoBF2      | CCAGAACAACCGCT    | -                     | Sequencing rpoB gene amplicons for phylogeny | This Study |
| rpoBR2      | CTCCCACGGCATGAA   |                      |         |           |

+ Annealing temperatures were calculated using the NEB online Tm calculator (https://tmcalculator.neb.com/#!/main) for the Phusion system.

- means not applicable.
Table S2. Core VOCs annotated in all the 37 *Streptomyces* isolates using the MSHub/GNPS.

| Compound/VOC                                      | Retention Time (min) | Molecular Formula | Molecular Weight |
|--------------------------------------------------|----------------------|-------------------|------------------|
| **Alcohols**                                     |                      |                   |                  |
| 1-Octen-3-ol                                     | 5.46                 | C₈H₁₆O            | 128.21           |
| Cis-1,2-Cyclohexanediol                          | 11.52                | C₆H₁₂O₂           | 116.16           |
| **Esters**                                        |                      |                   |                  |
| Ethyl Undecanoate                                 | 8.54                 | C₁₃H₂₀O₂          | 214.34           |
| Carbonic Acid, Butyl 2-Ethylhexyl Ester          | 10.15                | C₁₃H₂₀O₃          | 230.34           |
| Dodecyl Formate                                   | 11.72                | C₁₃H₂₀O₂          | 214.34           |
| Methyl Para Toluane                               | 13.72                | C₉H₁₆O₂           | 150.17           |
| 2-Butenedioic Acid (Z)-, Monododecyl Ester       | 19.06                | C₁₆H₂₈O₄          | 284.39           |
| Carbonic Acid, 2,2,2-Trichloroethyl 2-Ethylhexyl Ester | 19.42              | C₁₁H₁₉Cl₃O₃       | 305.6            |
| Dodecanoic Acid, Methyl Ester                     | 19.7                 | C₁₃H₂₀O₂          | 214.34           |
| Hexanoic Acid, 2-Hexenyl Ester, (E)-              | 20.46                | C₁₂H₂₂O₂          | 198.3            |
| 3-Octyl Isovalerate                               | 21.22                | C₁₃H₂₀O₂          | 214.34           |
| 13-Methyltetradecanoic Acid Methyl Ester          | 22.1                 | C₁₆H₃₂O₂          | 256.42           |
| Allyl Hexanoate                                   | 22.37                | C₉H₁₆O₂           | 156.22           |
| Methyl Decanoate                                  | 24.22                | C₁₁H₂₂O₂          | 186.29           |
| Bis(2-Ethylhexyl) Phthalate                      | 28.42                | C₂₄H₃₈O₄          | 390.6            |
| **Hydrocarbons**                                  |                      |                   |                  |

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| Liu & Clarke et al. 2022 | Supporting Information |
|-------------------------|------------------------|
| **N-Octadecane**        | 13.22                  | C\textsubscript{18}H\textsubscript{38} | 254.5   |
| Cyclohexane, 1,2,3-Trimethyl- | 14.56                  | C\textsubscript{9}H\textsubscript{18} | 126.24  |
| Cyclopentadecane        | 17.2                   | C\textsubscript{15}H\textsubscript{30} | 210.4   |
| Cyclohexane, Tetradecyl- | 21.76                  | C\textsubscript{20}H\textsubscript{40} | 280.5   |

**Ketones**

| Pentanone (4-OH-4-Me-2-) | 5.57 | C\textsubscript{6}H\textsubscript{12}O\textsubscript{2} | 116.16  |
| 2-Tert-Butylcyclohexanone | 11.47 | C\textsubscript{10}H\textsubscript{18}O | 154.25  |
| Ethanon, 2-Chloro-1-(2,4-Dimethylphenyl)- | 11.57 | C\textsubscript{10}H\textsubscript{11}ClO | 182.64  |

**Terpenes and Terpenoids**

| Cyclohexanol, 5-Methyl-2-(1-Methylethyl)- | 12.48 | C\textsubscript{10}H\textsubscript{20}O | 156.26  |
| 1,1-Bis(4,4-Dimethyl-2,6-Dioxocyclohexyl)Ethane | 14.07 | C\textsubscript{18}H\textsubscript{26}O\textsubscript{4} | 306.4   |
| Beta-Gurjunene | 17.77 | C\textsubscript{15}H\textsubscript{24} | 204.35  |
| Cubebene (Alpha-) | 21.55 | C\textsubscript{15}H\textsubscript{24} | 204.35  |

**Diverse functional groups**

| (Z,Z)-12,15-Octadecadienoic Acid Methyl Ester | 6.04 | C\textsubscript{19}H\textsubscript{34}O\textsubscript{2} | 294.5   |
| Para-Bromo toluene | 6.25 | C\textsubscript{7}H\textsubscript{7}Br | 171.03  |
| (+)-N-Benzyl-.Alpha.-Phenethylamine | 8.46 | C\textsubscript{15}H\textsubscript{17}N | 211.3   |
| Oleic Acid | 8.74 | C\textsubscript{18}H\textsubscript{34}O\textsubscript{2} | 282.5   |
| 3-Methyl-P-Anisaldehyde | 10.29 | C\textsubscript{9}H\textsubscript{10}O\textsubscript{2} | 150.17  |
| 1,2-Benzenedicarboxaldehyde | 11.05 | C\textsubscript{8}H\textsubscript{6}O\textsubscript{2} | 134.13  |
| Docosyl Pentyl Ether | 11.96 | C\textsubscript{27}H\textsubscript{56}O | 396.7   |
| Docosanoic Anhydride | 12.19 | C\textsubscript{44}H\textsubscript{86}O\textsubscript{3} | 663.2   |
| Chemical Name                                                                 | MW   | Molecular Formula | Supporting Information |
|------------------------------------------------------------------------------|------|-------------------|------------------------|
| 3Beta-Acetoxy-20-Hydroxy-5Alpha-Cevan-6-One                                   | 13.97| C_{29}H_{45}NO_{4} | 471.7                  |
| Heptane, 3-[(Ethenyloxy)Methyl]-                                             | 16.45| C_{10}H_{20}O      | 156.26                 |
| Heptyl Tetradecyl Ether                                                      | 17.04| C_{21}H_{44}O      | 312.6                  |
| Behenyl Chloride                                                             | 18.2 | C_{22}H_{45}Cl     | 345                    |
| N-((Methylphenylamino)Methyl)Benzamide                                       | 18.38| C_{15}H_{16}N_{2}O | 240.3                  |
| 4-Benzylaminooindole                                                         | 20.3 | C_{15}H_{14}N_{2}  | 222.28                 |
| Cis-1-Chloro-9-Octadecene                                                    | 24.92| C_{18}H_{35}Cl     | 286.9                  |
| Carbonochloridic Acid, Heptyl Ester                                         | 26.67| C_{8}H_{15}ClO_{2} | 178.65                 |
| Benzoic Acid Mono-Tms                                                        | 26.8 | C_{10}H_{14}O_{2}Si| 194.3                  |
**Table S3.** Bacterially derived compounds annotated in pooled culture VOC analysis of the 37 *Streptomyces* isolates using MSHub/GNPS.

| Compound/VOC                  | Confidence in annotation | Retention time (min) | Annotated in (isolates)                                                                 |
|-------------------------------|--------------------------|----------------------|----------------------------------------------------------------------------------------|
| **Alcohols (27)**             |                          |                      |                                                                                         |
| Dihydromyrcenol               | High                     | 4.7                  | JAC33, JAC60, JAC102, JAC99, JAC47, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC17, JAC78, JAC76, JAC86 |
| 12-Bromo-1-Dodecanol          | Low                      | 5.42                 | JAC30L, JAC99, JAC90, JAC81, JAC75, JAC78, JAC96, JAC86, JAC95, JAC35, JAC88, JAC68, JAC110, JAC74L, JAC54, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC72, JAC25, JAC102, JAC87, JAC17 |
| 1-Octen-3-ol                  | High                     | 5.46                 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Octanol (2-)                  | High                     | 6.35                 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 6,10-Dimethyl-2-Undecanol     | High                     | 6.62                 | JAC33, JAC60, JAC102, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC86, JAC24 |
| 3-Hexanol, 3,5-Dimethyl-       | High                     | 8.03                 | JAC33, JAC60, JAC102, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC61A, JAC103, JAC74C, JAC48, JAC2 |
| Compound                                      | Form | PIM (Gal) |
|-----------------------------------------------|------|----------|
| 2-Decanol                                     | High | 8.26     |
| Octanol (3-)                                  | High | 9.39     |
| 1-Phenylethyl Alcohol                         | High | 10.29    |
| 2-Hexanol, 2,5-Dimethyl-,(S)-                 | High | 10.63    |
| 1-Tetradecanol                                | High | 11.29    |
| Cis-1,2-Cyclohexanediol                       | High | 11.52    |
| 1,3-Propanediol, 2-Butyl-2-Ethyl-             | High | 12.58    |
| Compound                        | Modification | Retention Time (min) |
|--------------------------------|--------------|---------------------|
| 1-Undecanol, 11-Bromo-          | High         | 12.58               |
| Hexanol                        | High         | 12.99               |
| (S)-(+)-3-Methyl-1-Pentanol     | High         | 13.09               |
| 2-Isopropyl-5-Methyl-1-Heptanol | High         | 13.66               |
| Tetrahydrolavandulol           | High         | 15.41               |
| 10-Undecen-1-ol                | High         | 17.86               |
| 12-Methyl-1-Tridecanol         | High         | 17.91               |

Supporting Information:
| Compound                          | Tier | Value  |
|----------------------------------|------|--------|
| 1-Pentadecanol                   | High | 19.1   |
| Tridecanol                       | High | 19.8   |
| Methyl 2-Hydroxydodecanoate      | Low  | 20.76  |
| Methyl (5Z,8Z,11Z,14Z)-Eicosatetraenoate | Low  | 21.85  |
| 3-Pentadecanol                   | High | 22.14  |
| 10-Methyl-1-Dodecanol            | High | 22.87  |
| Chemical Name | Concentration Level | Value |
|---------------|---------------------|-------|
| 7-Ethyl-2-Methylundecan-1-ol | Low | 28.04 |
| Aldehydes (6) | | |
| Benzeneacetaldehyde | High | 12.44 |
| Perillyl Aldehyde | Low | 13.53 |
| (Z)-11-Hexadecenal | High | 15.71 |
| Cis-9-Hexadecenal | High | 23.94 |
| Nonadecanoic Acid | Low | 24.26 |
| Compound                                                   | Level  | Value   |
|-----------------------------------------------------------|--------|---------|
| Nonanal                                                   | Low    | 28.42   |
| Esters (62)                                               |        |         |
| Cyclohexanecarboxylic Acid, 4-Methoxy-, Heptyl Ester     | Low    | 7.83    |
| Ethyl Undecanoate                                         | High   | 8.54    |
| 5-Hydroxy-3-Methoxy-2,6-Dimethyl-(6R)-((2R)-2-Methylbutyryloxy)-2,4-Cyclohexadien-1-One | Low    | 9.18    |
| Methacrylic Acid 2-Ethylhexyl Ester                      | High   | 9.61    |
| Carbonic Acid, Butyl 2-Ethylhexyl Ester                  | High   | 10.15   |

Supporting Information

AC122, JAC58, JAC72, JAC102, JAC87, JAC17, JAC24, JAC55

JAC30L, JAC99, JAC74C, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55

JAC99, JAC74C, JAC90, JAC47, JAC78, JAC96, JAC48, JAC103, JAC35, JAC88, JAC101, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC58, JAC72, JAC102, JAC87, JAC17, JAC24, JAC55

JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35

JAC30L, JAC99, JAC74C, JAC81, JAC75, JAC47, JAC78, JAC86, JAC48, JAC95, JAC103, JAC35, JAC101, JAC68, JAC45, JAC64, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55

JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC64, JAC48, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC81, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110

JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC101, JAC122, JAC1
| Compound                                      | Level | Retention Time |
|-----------------------------------------------|-------|----------------|
| Octadecyl 3-(3,5-Di-Tert-Butyl-4-             | High  | 10.21          |
| Hydroxyphenyl)Propionate                      |       |                |
| 2-Acetoxyisobutyryl Chloride                 | High  | 10.63          |
| Hexyl Acetate                                 | High  | 11.29          |
| Dodecyl Formate                               | High  | 11.72          |
| Hexyl 10-Undecenoate                          | High  | 11.85          |
| 9-Octadecenoic Acid, Methyl Ester, (E)-       | Low   | 12.94          |

Supporting Information

7,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35
JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC54,JAC31,JAC61A,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC72,JAC81,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC110,JAC24,JAC35
JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC30L,JAC76,JAC58,JAC86,JAC74L,JAC24,JAC35
JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC30L,JAC76,JAC58,JAC86,JAC74L,JAC6,JAC110,JAC24,JAC35
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JAC30L,JAC99,JAC74C,JAC90,JAC81,JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC95,JAC103,JAC35,JAC101,JAC110,JAC45,JAC33,JAC64,JAC74L,JAC54,
| Product Description                               | Level | Retention Time |
|--------------------------------------------------|-------|----------------|
| (Z)-12-Octadecenoic Acid Methyl Ester            | High  | 13.33          |
| Methyl Para Toluate                              | High  | 13.72          |
| Fumaric Acid, Dodecyl Tetradec-3-Enyl Ester      | Low   | 14.65          |
| (Z,Z)-7,11-Hexadecadienyl Acetate                | Low   | 14.73          |
| Glutaric Acid, Dec-2-Yl Dec-4-Enyl Ester         | High  | 15.41          |
| Compound                                                                 | Intensity | Retention Time | Supporting Information                                                                 |
|-------------------------------------------------------------------------|-----------|----------------|----------------------------------------------------------------------------------------|
| 1,2-Dibutyroxy-1-Ethoxyethane                                             | High      | 16.85          | JAC33, JAC60, JAC102, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC76, JAC58, JAC86, JAC24 |
| 2-Butenedioic Acid (Z)-, Monododecyl Ester                               | High      | 19.06          | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24 |
| Decan-1,10-Diol Dimethacrylate                                           | High      | 19.13          | JAC60, JAC87, JAC102, JAC96, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC61A, JAC45, JAC122, JAC17, JAC78, JAC68, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Carbonic Acid, 2,2,2-Trichloroethyl 2-Ethylhexyl Ester                  | High      | 19.42          | JAC60, JAC87, JAC102, JAC96, JAC75, JAC47, JAC31, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 2-Ethylhexyl Mercaptoacetate                                            | High      | 19.46          | JAC33, JAC60, JAC102, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC101, JAC17, JAC78, JAC72, JAC76, JAC58, JAC86, JAC24, JAC35 |
| Dodecanoic Acid, Methyl Ester                                           | High      | 19.7           | JAC33, JAC60, JAC87, JAC102, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC58, JAC86, JAC90, JAC6, JAC110, JAC24 |
| Cyanoacetic Acid, Nonyl Ester                                           | High      | 19.8           | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Compound                        | retention time (min) | elution order |
|--------------------------------|----------------------|---------------|
| Carbonic Acid, Monoamide, N-Propyl-N-Butyl, 2-Ethylhexyl Ester | High, 20.09         | JAC87, JAC102, JAC96, JAC55, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC68, JAC81, JAC30L, JAC58, JAC86, JAC24 |
| Hexanoic Acid, 2-Hexenyl Ester, (E)- | High, 20.46         | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC95, JAC25, JAC101, JAC122, JAC68, JAC72, JAC30L, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Vinyl 2-Ethylhexanoate         | High, 20.68         | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 3-Octyl Isovalerate            | High, 21.22         | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Lauryl Acetate                 | High, 21.41         | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC64, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC110, JAC24, JAC35 |
| Carbonic Acid, Isobutyl Cyclohexyl Ester | High, 21.91         | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Compound | Form | Acq. | Retention Time |
|----------|------|------|----------------|
| Hexanoic Acid, 5-Oxo-, Ethyl Ester | High | 21.91 |
| Eicosane | Low | 21.91 |
| 13-Methyltetradecanoic Acid Methyl Ester | High | 22.1 |
| Ethyl Tetradecanoate | High | 22.14 |
| Methyl Tetradecanoate | High | 22.14 |
| 2-(2-Methylpiperidino)Ethyl P-Chlorobenzoate | High | 22.28 |
| Allyl Hexanoate | High | 22.37 |
| Compound                                | Type  | Retention Time (min) | JAC Numbers |
|-----------------------------------------|-------|----------------------|-------------|
| Ethyl 3-Oxoheptanoate                   | Low   | 22.41                | JAC30L, JAC81, JAC78, JAC86, JAC68, JAC110, JAC33, JAC6, JAC60, JAC31, JAC122, JAC25, JAC102, JAC17, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 2-Methylvaleric Acid, 2-Ethylhexyl Ester | High  | 22.46                | JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Cis-3-Hexenyl 2-Ethylbutyrate           | High  | 22.65                | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Benzyl Benzoate                         | High  | 22.71                | JAC87, JAC96, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC95, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Methyl Dodecanoate                      | High  | 23.22                | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC68, JAC110, JAC45, JAC33, JAC74L, JAC54, JAC6, JAC76, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC17, JAC24, JAC55 |
| Fumaric Acid, 2-Ethylhexyl 2,2,3,3-Tetrafluoropropyl Ester | Low  | 23.78                | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, |
## Supporting Information

| Compound                                      | Level  | Mass (m/z) |
|-----------------------------------------------|--------|------------|
| Trans-2-Hexenyl 2-Ethylbutyrate               | High   | 24.14      |
| Methyl Decanoate                              | High   | 24.22      |
| Methyl Palmitate                              | High   | 24.26      |
| Isopropyl Hexadecanoate                       | High   | 25.21      |
| Isopropyl Palmitate                           | Low    | 25.21      |
| (Z)-6-Octadecenoic Acid Methyl Ester          | Low    | 25.76      |
| Compound                                      | Level | Retention Time (min) | JAC Codes |
|-----------------------------------------------|-------|----------------------|-----------|
| Carbonic Acid, Propargyl 2-Ethylhexyl Ester   | High  | 26.14                | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 1,2-Benzenedicarboxylic Acid Bis(2-Ethylhexyl) Ester | High  | 26.52                | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Eicosanebioic Acid, Dimethyl Ester            | Low   | 27.58                | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
| Bis(2-Ethylhexyl) Phthalate                   | High  | 28.42                | JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24 |
| 1,2-Benzenedicarboxylic Acid Decyl Octyl Ester | High  | 28.49                | JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Hexanedioic Acid, Bis(2-Ethylhexyl) Ester     | High  | 28.71                | JAC87, JAC88, JAC47, JAC54, JAC31, JAC61A, JAC95, JAC25, JAC101, JAC122, JAC78, JAC81, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Compound                                      | 2-ethylbutyl Ester | High | 29.13 |
|-----------------------------------------------|--------------------|------|-------|
| Succinic Acid, Monochloride                  |                    |      |       |
| Butyramide, 4-Chloro-N-Hept-2-Yl-             | Low                | 29.13|
| Ethyl 3-Acetoxybutyrate                      | High               | 29.51|
| 1,2-Benzenedicarboxylic Acid Hexyl Octyl Ester| High               | 30.29|
| Dibutyl Itaconate                            | Low                | 31.47|
| Hydrocarbons (31)                             |                    |      |       |
| Hexane, 3-Ethyl-                              | High               | 5.2  |
| Supporting Information                       |                    |      |       |
| JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 |
| JAC99,JAC74C,JAC90,JAC81,JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC95,JAC103,JAC35,JAC88,JAC101,JAC68,JAC110,JAC45,JAC33,JAC64,JAC74L,JAC54,JAC6,JAC76,JAC60,JAC122,JAC58,JAC72,JAC25,JAC102,JAC87,JAC17,JAC24,JAC55 |
| JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 |
| JAC30L,JAC90,JAC75,JAC96,JAC88,JAC68,JAC110,JAC74L,JAC54,JAC6,JAC122,JAC72,JAC25,JAC87 |
| Compound                                      | Condition | Literature |
|-----------------------------------------------|-----------|------------|
| Diisodecyl 4-Cyclohexene-1,2-Dicarboxylate    | Low       | JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110, JAC24,JAC35 |
|                                               |           | JAC30L,JAC99,JAC81,JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC95,JAC103,JAC35,JAC88, JAC101,JAC68,JAC110,JAC45,JAC33,JAC64,JAC74L,JAC54,JAC6,JAC76,JAC31,JAC122,JAC58,JAC72,JAC C25,JAC102,JAC87,JAC17,JAC24,JAC55 |
| Hexadecane                                    | High      | JAC33,JAC99,JAC75,JAC47,JAC31,JAC45,JAC64,JAC C74C,JAC48,JAC25,JAC17,JAC78,JAC68,JAC81,JAC C76,JAC58,JAC86,JAC24 |
| 1,1,4-Trimethylcyclohexane                    | High      | JAC87,JAC96,JAC88,JAC55,JAC61A,JAC95,JAC25,JAC122,JAC68,JAC76,JAC90,JAC74L,JAC6,JAC110,JAC35 |
| 1-Decene                                      | High      | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC74L,JAC6,JAC110,JAC24,JAC35 |
| Cyclohexane, 1,2,3-Trimethyl-                  | High      | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC54,JAC31,JAC61A,JAC45,JAC103,JAC48,JAC95,JAC25,JAC122,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC C6,JAC110,JAC24,JAC35 |
| 2,4,4-Trimethyl-1-Hexene                      | High      | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC35 |
| Compound                     | Mobility | Value  |
|------------------------------|----------|--------|
| N-Octadecane                 | High     | 14.56  |
| Tetracosane                  | High     | 16.01  |
| 1-Hexene, 3,5,5-Trimethyl-   | High     | 16.3   |
| Pentacosane                  | High     | 16.81  |
| Cyclohexane, Tetradecyl-     | High     | 17.2   |
| Pentane, 2,2,3,4-Tetramethyl-| High     | 17.57  |
| Compound                        | Type  | Temperature | Supporting Information |
|--------------------------------|-------|-------------|------------------------|
| (6Z,9Z)-6,9-Tricosadiene       | High  | 17.86       | JAC87, JAC96, JAC88, JAC55, JAC75, JAC54, JAC61A, JAC64, JAC95, JAC25, JAC101, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Cyclohexane, 1,2-Dimethyl-     | High  | 17.91       | JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC61A, JAC103, JAC48, JAC95, JAC25, JAC122, JAC68, JAC81, JAC74L, JAC6, JAC110 |
| (Cis/Trans)                     |       |             |                         |
| Tridecane                      | High  | 18.03       | JAC87, JAC96, JAC88, JAC55, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC74L, JAC6, JAC110, JAC35 |
| 1,19-Eicosadiene               | High  | 18.76       | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Octacosane                     | Low   | 19.13       | JAC30L, JAC90, JAC75, JAC96, JAC95, JAC35, JAC88, JAC101, JAC110, JAC74L, JAC54, JAC6, JAC122, JAC72, JAC87, JAC55 |
| 1-Heptadecene                  | High  | 19.3        | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Heptylcyclohexane              | High  | 20.14       | JAC33, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 1-Eicosene                     | High  | 20.61       | JAC33, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Compound                        | Temperature | Value  |
|--------------------------------|-------------|--------|
| Cyclopentadecane               | High        | 21.76  |
| Cyclohexane, Undecyl-          | High        | 22.56  |
| Octadecane                     | High        | 22.94  |
| Pentadecane                    | High        | 23.02  |
| Octadecane                     | High        | 25.01  |
| N-Acetyl-Alanyl-Phenylalanyl-Glycine Methylester | Low | 28.17  |

**Supporting Information**

- AC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC35
- JAC33, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC48, JAC95, JAC25, JAC122, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35
- JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35
- JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35
- JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35
- JAC87, JAC96, JAC88, JAC55, JAC75, JAC54, JAC61A, JAC103, JAC48, JAC101, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35
- JAC99, JAC81, JAC75, JAC47, JAC78, JAC96, JAC48, JAC95, JAC103, JAC35, JAC88, JAC110, JAC33, JAC64, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC55
| Liu & Clarke et al. 2022 | Supporting Information |
|-------------------------|------------------------|
| **Nonadecane** | **Low** | 28.55 |
| | | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
| **Nonacosane** | **High** | 29.22 |
| | | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| **Oct-3-Enoylamide, N-Methyl-N-(2-Ethylhexyl)-** | **Low** | 29.51 |
| | | JAC30L, JAC99, JAC75, JAC78, JAC96, JAC86, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC33, JAC74L, JAC54, JAC76, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC87, JAC17 |
| **Trans-2-Nonene** | **High** | 30.1 |
| | | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| **Ketones (19)** | | |
| **Pentanone (4-OH-4-Me-2-)** | **High** | 5.57 |
| | | JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| **2-Tridecanone** | **High** | 5.66 |
| | | JAC33, JAC60, JAC102, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC101, JAC12 |
| Compound                        | Level  | Log Kp  |
|--------------------------------|--------|---------|
| 2-Butylcyclopenanone           | High   | 9.67    |
| 2-Propyl-5,5-Dimethyl-1,3-Cyclohexanedione | High   | 10.65   |
| 1,2-Cyclopentanedione, 3-Methyl- | High   | 11.15   |
| 2-Tert-Butylcyclohexanone      | High   | 11.57   |
| Cyclohexanone, 4-(1,1-Dimethylethyl)- | High   | 12.32   |
| Ethanone, 2-Chloro-1-(2,4-Dimethylphenyl)- | High   | 16.16   |
| Compound                                | Grade | Retention Time |
|----------------------------------------|-------|----------------|
| 4'-Butoxyacetophenone                  | High  | 17.31          |
| Cyclododecanone                        | High  | 17.94          |
| 2-(1-Cyclohexenyl)Cyclohexanone        | High  | 18.93          |
| Trans-3-Nonen-2-One                    | High  | 20.57          |
| 3-Methoxyheptanophenone                | High  | 22.02          |
| 5,5-Dimethyl-1,3-Cyclohexanedione      | High  | 22.02          |

Supporting Information

JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC110, JAC35
| Compound Description                                                                 | Value  | Peak Area  |
|-------------------------------------------------------------------------------------|--------|------------|
| Tetradecanophenone                                                                  | High   | 23.05      |
| Pyrimidine, 6-Oxo-5-Acetyl-4-Hydroxy-1,6-Dihydro-                                  | High   | 27.4       |
| 2-Propanone, 1,1,1-Trichloro-                                                       | High   | 29.4       |
| (4aS,5S,8aS)-8Abeta-Formyl-5Beta-Methyl-5Alpha-(4-Methyl-3-Penteny)-3,4,4A,5,6,7,8,8A-Octahydronaphthalen-1(2H)-One | High   | 30.87      |
| Hexanal (Si-Contam)_Adms                                                           | High   | 31.2       |

**Terpenes and Terpenoids (23)**

| Compound Description       | Value  |
|----------------------------|--------|
| 2-Octene, 2,6-Dimethyl-     | High   | 7.95    |

S35
| Compound                                      | Level | Value |
|-----------------------------------------------|-------|-------|
| Perillyl Isobutyrate                          | High  | 10.08 |
| Isopulegol(Equatorial)                        | High  | 11.82 |
| 1,1-Bis(4,4-Dimethyl-2,6-Dioxocyclohexyl)Ethane | High  | 12.48 |
| Cyclohexanol, 5-Methyl-2-(1-Methylethyl)-      | High  | 14.07 |
| L-Menthol                                      | High  | 14.16 |
| (4-Isopropyl-Trans-6-Methyl-3-Cyclohexenyl)Formaldehyde 2,4-Dinitrophenylhydrazone | Low   | 15.32 |
| Compound                          | Source(s) | CI   |
|----------------------------------|-----------|------|
| (7S)-(-)-10,10-Di-Me-5-Thia-4-Azatricyclo[5.2.1.0-3,7]Dec-3-Ene-5,5-Dioxide | High      | 15.71|
| Ylangene (Alpha-)                | High      | 17.69|
| Cubebene (Alpha-)                | High      | 17.77|
| Acetic Acid, 1,7,7-Trimethyl-Bicyclo[2.2.1]Hept-2-Yl Ester           | High      | 18.23|
| Aristolochene (4,5-Di-Epi)       | High      | 18.3  |
| Sabinene                         | High      | 18.3  |
| Compound                              | Level | Retention Time |
|--------------------------------------|-------|----------------|
| Sesquiphellandrene (Beta-)          | High  | 18.51          |
| (+)-Alpha-Muurolene                  | High  | 18.59          |
| 7-Isopropenyl-1,4A-Dimethyl-3,4,5,6,7,8-Hexahydro-2-Naphthalenone | High  | 19.95          |
| 4,10-Dimethyl-7-Isopropyl-Bicyclo(4.4.0)Deca-1,4-Diene   | High  | 21.13          |
| Germacrone                           | High  | 21.18          |
| Caryophyllene (Z-)                   | High  | 21.27          |
| Eremophilene                         | High  | 21.27          |
| Compound                                      | Formulation | Category | Value |
|-----------------------------------------------|-------------|----------|-------|
| Beta-Gurjunene                                 | High        |          | 21.55 |
| 3-Isopropyl-6,10-Dimethylundecane-2-ol        | High        |          | 28.79 |
| Perfluorononanoic Acid                        | Low         |          | 31.69 |
| Diverse functional groups (139)               |             |          |       |
| Octadecyl Bromide                             | High        |          | 4.33  |
| Dramamine                                     | High        |          | 4.53  |
| Bis(2-Ethylhexyl) Hydrogen Phosphite          | Low         |          | 4.7   |

**Supporting Information**

JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC35

JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC35

JAC81, JAC75, JAC96, JAC95, JAC88, JAC68, JAC74L, JAC54, JAC61A, JAC122, JAC25

JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35

JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35

JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC25
| Compound                                      | Intensity | Value  |
|----------------------------------------------|-----------|--------|
| Behenic Amide                                 | High      | 4.86   |
| 5-Dimethylaminopyrimidine                     | Low       | 5.25   |
| 4-Chloro-2-Aminopyrimidine                    | High      | 5.33   |
| Pentadecafluoroctanoic Acid, Pentyl Ester     | High      | 5.33   |
| Oleic Anhydride                               | Low       | 5.54   |
| Hexenyl 3-Methyl Butanoate (3Z-)              | High      | 5.66   |
| Compound                                      | Level | Value | JACs  |
|----------------------------------------------|-------|-------|-------|
| Heptanone (2-)                               | High  | 5.94  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 3-Methyl-P-Anisaldehyde                       | High  | 6.04  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| (S)-3-Hydroxyisobutyric Acid                 | Low   | 6.23  | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
| (+)-N-Benzyl-.Alpha.-Phenethylamine          | High  | 6.25  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 4-Piperidinemethanamine                     | High  | 6.31  | JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Acetamide, 2-(Phenylthio)-N-Butyl-N-Ethyl-   | Low   | 6.59  | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC110, JAC24, JAC35 |
| Compound | Low | High |
|----------|-----|------|
| 1,1,3-Trimethyl-1-Silacyclo-3-Pentene | Low | 6.85 |
| Pentadecafluorooctanoic Acid, Isobutyl Ester | High | 7.11 |
| 6-Iodo-2-Picolin-5-ol | High | 7.25 |
| Pyrazine, Methoxy-, 4-Oxide | Low | 7.27 |
| 2-(4-Hydroxyphenyl)Ethanoic Acid | High | 7.32 |
| Pentadecafluorooctanoic Acid, 4-Methyl-2-Pentyl Ester | High | 7.4 |
| Compound                                           | Type  | Rf  |
|----------------------------------------------------|-------|-----|
| Acetamide, 2-(Thiophen-2-Yl)-N-Methyl-N-(3-Methylbutyl)- | Low   | 7.46|
| Pentadecafluorooctanoic Acid, 3-Methylbut-2-En-1-Yl Ester | Low   | 7.46|
| Pentadecafluorooctanoic Acid, Undec-2-En-1-Yl Ester   | High  | 7.61|
| Pentadecafluorooctanoic Acid, Dodecyl Ester        | High  | 7.79|
| Pentadecafluorooctanoic Acid, Hexyl Ester          | High  | 7.79|
| Levoglucosan                                        | High  | 7.95|
| Dotriacontyl Isobutyl Ether                        | High  | 8.36|

Supporting Information

JAC30L,JAC74C,JAC90,JAC81,JAC75,JAC47,JAC96,JAC86,JAC95,JAC88,JAC110,JAC33,JAC74L,JAC54,JAC76,JAC60,JAC31,JAC122,JAC58,JAC72,JAC25,JAC102,JAC17,JAC24,JAC55

JAC30L,JAC99,JAC74C,JAC90,JAC81,JAC75,JAC47,JAC78,JAC96,JAC48,JAC103,JAC45,JAC64,JAC74L,JAC76,JAC60,JAC122,JAC58,JAC72,JAC102,JAC17,JAC24,JAC55

JAC33,JAC60,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC74C,JAC31,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35

JAC33,JAC60,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC17,JAC78,JAC68,JAC72,JAC30L,JAC76,JAC58,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35

JAC33,JAC60,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC17,JAC78,JAC68,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35

JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC101,JAC122,JAC78,JAC68,JAC72,JAC24,JAC35
| Compound                                           | Type    | Value |
|----------------------------------------------------|---------|-------|
| 1,2-Benzenedicarboxaldehyde                        | High    | 8.46  |
| (2S)-N-Tert-Butoxycarbonyl-2-(1,4-Dimethanesulfonyloxybutyl)Pyrroloidine | Low     | 8.69  |
| (Z,Z)-12,15-Octadecadienoic Acid Methyl Ester      | High    | 8.74  |
| Arachidonic Acid                                   | High    | 8.77  |
| Perfluoro(Methylcyclohexane)                       | High    | 8.77  |
| Acetaldehyde Hexyl Isobutyl Acetal                 | High    | 8.82  |
| Compound                                                      | Level | Retention Time (min) |
|---------------------------------------------------------------|-------|----------------------|
| (5Alpha)-7,8-Didehydro-4,5-Epoxy-3-Methoxy-17-               | Low   | 9.21                 |
| Methylmorphinan-14-ol                                         |       |                      |
| 3,3-Diethylglutaric Acid                                      | High  | 9.39                 |
| Pentadecafluorooccanoic Acid, Propyl Ester                    | High  | 9.5                  |
| Tremorine                                                     | Low   | 9.5                  |
| Cresol (Ortho-)                                               | High  | 9.61                 |
| 3,6-Dimethyl-5-Oxo-1,2,3,5-Tetrahydroimidazo[1,2-A]Pyrimidine| Low   | 9.86                 |
| Compound                                                                 | Retention Time (min) | Mobility | Supporting Information |
|------------------------------------------------------------------------|----------------------|----------|------------------------|
| 4-Amino-2,2,5,5-Tetramethyl-3-Imidazoline-1-Oxyl                        | High                 | 10.03    | JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC61 A, JAC64, JAC103, JAC74 C, JAC95, JAC101, JAC102, JAC87, JAC17, JAC68, JAC76, JAC74 L, JAC110, JAC24, JAC35 |
| Benzenemethanol, 4-(1,1-Dimethylethyl)-                                 | High                 | 10.08    | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61 A, JAC45, JAC103, JAC74 C, JAC95, JAC112, JAC78, JAC68, JAC72, JAC81, JAC30 L, JAC76, JAC58, JAC86, JAC90, JAC74 L, JAC6, JAC110, JAC24, JAC35 |
| N-((Methylphenylamino)Methyl)Benzamide                                 | High                 | 10.29    | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61 A, JAC45, JAC103, JAC74 C, JAC48, JAC95, JAC25, JAC101, JAC112, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30 L, JAC76, JAC58, JAC86, JAC90, JAC74 L, JAC6, JAC110, JAC24, JAC35 |
| Ethyl 3-Methyl-5-Methylpyrrole-2-Carboxylate                           | High                 | 10.55    | JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61 A, JAC45, JAC64, JAC74 C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC68, JAC72, JAC81, JAC76, JAC58, JAC86, JAC90, JAC74 L, JAC110, JAC24, JAC35 |
| 2-Butanone, (1-Methyl-2-Propenyl)Hydrazone                             | Low                  | 10.71    | JAC30 L, JAC99, JAC74 C, JAC90, JAC81, JAC75, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74 L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61 A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
| Suberoyl Chloride                                                      | High                 | 10.77    | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61 A, JAC64, JAC95, JAC25, JAC101, JAC78, JAC68, JAC72, JAC81, JAC30 L, JAC76, JAC86, JAC90, JAC74 L, JAC110, JAC24, JAC35 |
| Compound                                           | Concentration | GI   |
|---------------------------------------------------|---------------|------|
| Pentadecafluorooctanoic Acid, Tridec-2-Yn-1-Yl Ester | Low           | 10.97|
| Oleic Acid                                        | High          | 11.05|
| 1,3-Dibenzoyl-4-Oxo-2-Thioxoimidazolidine        | High          | 11.11|
| N-.Alpha.-Benzoyl-L-Arginine                     | High          | 11.11|
| 1H,1H,2H-Perfluoro-1-Octene                      | High          | 11.15|
| Decanedioyl Dichloride                            | High          | 11.78|
| Benzeneacetic Acid, .Alpha.-Oxo-, Methyl Ester    | High          | 11.91|

Supporting Information:

- JAC30L, JAC99, JAC81, JAC75, JAC78, JAC95, JAC103, JAC35, JAC101, JAC68, JAC45, JAC33, JAC64, JAC54, JAC6, JAC76, JAC60, JAC122, JAC58, JAC72, JAC25, JAC17, JAC55
- JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35
- JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24
- JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC102, JAC87, JAC102, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35
- JAC102, JAC47, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC68, JAC81, JAC76, JAC58, JAC86, JAC90, JAC6
| Compound                                      | Phase | Retention Time |
|-----------------------------------------------|-------|----------------|
| Benzoic Acid Mono-Tms                         | High  | 11.96          |
| Carbonochloridic Acid, Heptyl Ester           | High  | 12.19          |
| 5-Trimethylsilyl-1,2,3,4-Tetrahydropyrimidine-2,4-Dione | Low   | 12.72          |
| Pentadecafluorooctanoic Acid, Octyl Ester     | Low   | 12.72          |
| Benzenamine, 2,4-Dimethoxy-                  | High  | 13.66          |
| 2,5-Dimethylbenzophenone                     | High  | 13.72          |
| Compound Name | Dilution | Retention Time (min) |
|---------------|----------|---------------------|
| O-Decylhydroxylamine | High | 13.9 |
| Para-Bromotoluene | High | 13.97 |
| 2'-Ethylpropiophenone | High | 14.16 |
| Diazene, Bis[4-(Hexyloxy)Phenyl]-, 1-Oxide | High | 14.45 |
| Pentadecafluorooctanoic Acid, 2-Ethylhexyl Ester | High | 14.65 |
| Pentadecafluorooctanoic Acid, Heptyl Ester | High | 14.84 |
| Compound                        | Level | Retention Time |
|--------------------------------|-------|----------------|
| Beta-Cyclocitral               | High  | 15.24          |
|                                |       |                |
| 1-Phenyl-1-Nonyne              | High  | 15.5           |
|                                |       |                |
| Benzene, 1,4-Bis(1-Methylethenyl)- | Low  | 15.5           |
|                                |       |                |
| Allylbenzene                   | High  | 15.75          |
|                                |       |                |
| Benzoic Acid, 2-Acetylhydrazide| High  | 15.75          |
|                                |       |                |
| Ethyl Acetophenone (P-)        | High  | 15.75          |
|                                |       |                |
| Benzenamine, 4-Bromo-3-Methyl- | Low   | 15.84          |
| Compound                                      | Location         | Support         |
|----------------------------------------------|------------------|-----------------|
| Behenyl Chloride                             | High             | 16.45           |
| Nonyl Tetradecyl Ether                       | High             | 16.58           |
| 1-Bromo-8-Tetrahydropyranloxyoctane         | High             | 16.81           |
| Benzene, 1,4-Bis(1,1-Dimethylethyl)-         | Low              | 16.97           |
| 4-Benzylaminoindole                          | High             | 17.04           |
| Methyl 6-Methyl-3-Pyridyl Ketone 4-Cyclohexylthiosemicarbazone | Low | 17.26 |
Nonalactone (Gamma-)

High 17.41

Guanidine, N,N'-Bis(2-Methylphenyl)-

High 17.86

Heptane, 3-[(Ethenyloxy)Methyl]-

High 18.2

(Z,Z,Z)-6,9,15-Octadecatrienoic Acid Methyl Ester

High 18.33

3-Ethenyl-2,5-Dibutyl-3-(4-Methyl-3-Pentenyl)Tetrahydrofuran

Low 18.33

3Beta-Acetoxy-20-Hydroxy-5Alpha-Cevan-6-One

High 18.38
| Compound                                             | Type  | Retention Time |
|------------------------------------------------------|-------|---------------|
| (Z,Z,Z)-9,12,15-Octadecatrienoic Acid Methyl Ester   | High  | 18.59         |
| Butanal, 3-Methyl-2-Methylene-, (1-Methylethyl)Hydrazone | High  | 19.1          |
| Octyltrichlorosilane                                  | Low   | 19.19         |
| 1-Chloroeicosane                                      | High  | 19.3          |
| Propanoic Acid, 2-Methyl-, 1-(1,1-Dimethylethyl)-2-Methyl-1,3-Propanediyl Ester | High  | 19.46         |
| 10-Hexyl-9-Anthracenecarbaldehyde                    | Low   | 19.54         |
| Compound                                      | Level  | Value  |
|----------------------------------------------|--------|--------|
| Benztropine                                  | Low    | 19.8   |
| Malonic Acid, Di(4-Heptyl) Ester             | High   | 19.95  |
| 4-(1-Methylethenyl)-2-Phenyl-1,3-Dioxolane   | Low    | 19.95  |
| Heptyl Tetradecyl Ether                      | High   | 20.3   |
| (Z,Z,Z)-6,9,12-Octadecatrienoic Acid Methyl Ester | High | 20.35  |
| 2(3H)-Phenanthenone, 4,4A,9,10-Tetrahydro-4A-Methyl- | Low    | 20.35  |
| Compound                                           | Type  | Retention Time | Compositions |
|----------------------------------------------------|-------|----------------|--------------|
| (Z,Z,Z)-6,9,12,15-Octadecatetraenoic Acid Methyl Ester | High  | 20.38          | JAC60, JAC102, JAC88, JAC55, JAC75, JAC74C, JAC25, JAC101, JAC122, JAC78, JAC68, JAC81, JAC90, JAC6, JAC110, JAC35 |
| 4-Tert-Butylpyrocatechol                            | High  | 20.57          | JAC60, JAC88, JAC55, JAC54, JAC61A, JAC74C, JAC48, JAC95, JAC17, JAC72, JAC74L, JAC110, JAC24 |
| 4-(Decyloxy)Benzaldehyde                            | High  | 20.87          | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC68, JAC72, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 4-Hydroxy-3-Methoxyphenylacetic Acid (2,5,6-D3,Alpha,Alpha-D2) | Low   | 20.87          | JAC74C, JAC90, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC60, JAC31, JAC58, JAC102, JAC87, JAC17, JAC24 |
| 1-Chloromethyl-3,5-Bis(1,1-Dimethylethyl)Benzene     | High  | 20.98          | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Methyl 3,4-O-Isopropylidene-Beta-D-Fucopyranoside    | High  | 21.06          | JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| 9,12-Octadecadienoyl Chloride, (Z,Z)-               | High  | 21.34          | JAC33, JAC60, JAC87, JAC88, JAC99, JAC75, JAC47, JAC54, JAC45, JAC64, JAC103, JAC95, JAC17, JAC78, JAC76, JAC86, JAC6, JAC24 |
| 5Alpha-Androst-16-En-3-One                          | Low   | 21.34          | JAC30L, JAC99, JAC74C, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC110, JAC33, JAC64, JAC54, JAC6, JAC76, JAC81, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Compound                              | Level | Value  |
|---------------------------------------|-------|--------|
| Decyl Octyl Ether                     | High  | 21.41  |
| 1,4-Dibenzoyl-2,Trans-5-Diethylpiperazine | Low   | 21.98  |
| 1,9-Dichlorononane                    | High  | 22.19  |
| 5-Bromo-2,6-Dimethyl-4-Pyrimidinamine | Low   | 22.28  |
| Cyclohexasiloxane, Dodecamethyl-      | High  | 22.71  |
| 9,12-Dioxo-5,6,7,9,12,14,15,16-Octahydro-6,15-Methanobenzo(A)Naphtho(2,3-F)Cyclodecene | Low   | 23.44  |
### Supporting Information

| Compound                                      | Type  | Retention Time |
|-----------------------------------------------|-------|----------------|
| Mevinoline                                    | Low   | 23.44          |
| (6-Bromo-(E)-1-Hexenyl)Benzene                | Low   | 23.74          |
| 5'-Chloro-2'-Methoxyacetanilide               | Low   | 23.78          |
| (Alpha,Alpha,Alpha-Trifluoro-Para-Tolyl)Acetic Acid | High  | 23.89          |
| Eicosane, 1-Iodo-                              | High  | 24.1           |
| 1-Adamantaneacetic Acid                       | High  | 24.38          |
| Butane, 1-Iodo-3-Methyl-                       | High  | 24.56          |

Supporting Information

JAC30L, JAC99, JAC74C, JAC81, JAC75, JAC48, JAC103, JAC88, JAC68, JAC45, JAC6, JAC76, JAC61A, JAC72, JAC87, JAC55

JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55

JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35

JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35

JAC33, JAC60, JAC87, JAC102, JAC96, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17
| Compound                        | Level | Value  |
|--------------------------------|-------|--------|
| 1-Iodoctane                    | High  | 24.74  |
| Cis-1-Chloro-9-Octadecene      | High  | 24.92  |
| Distearyl Thiodipropionate     | High  | 25.76  |
| Acetamide, 2-(Thiophen-2-Yl)-N-Methyl-N-Decyl- | Low   | 26.27  |
| Docosanoic Anhydride           | High  | 26.67  |
| Docosyl Pentyl Ether           | High  | 26.8   |
| Compound                                                                 | Type  | Retention Time |
|--------------------------------------------------------------------------|-------|----------------|
| Pentadecafluoroctanoic Acid, Undecyl Ester                               | High  | 26.93          |
| 11-Bromoundecanoic Acid                                                 | Low   | 27.49          |
| 2-Bromo Dodecane                                                        | High  | 27.71          |
| Maltitol                                                                | High  | 28.08          |
| Cyclobutanecarboxamide, N-Octyl-                                        | High  | 28.71          |
| 2-(3-Benzoylphenyl)Propionic Acid Trimethylsilyl Ester                   | High  | 29.04          |
| Oct-3-Enoylamine, N-Methyl-N-Pentyl-                                    | High  | 29.42          |

Supporting Information: JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC30L, JAC99, JAC74C, JAC75, JAC47, JAC48, JAC103, JAC35, JAC88, JAC101, JAC45, JAC33, JAC64, JAC6, JAC76, JAC31, JAC61A, JAC58, JAC72, JAC25, JAC17, JAC55, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC61A, JAC45, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC88, JAC99, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35.
| Compound Description                                      | Level | VOC Bin Numbers                                                                 |
|-----------------------------------------------------------|-------|---------------------------------------------------------------------------------|
| 2-Hydroxy-3-Isopropyl-5-Piperidinomethyl-2,4,6-Cycloheptatrien-1-One | Low   | 29.76 JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC78, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC54, JAC31, JAC58, JAC25, JAC55 |
| Perfluorotributylamine                                     | High  | 30.36 JAC87, JAC96, JAC88, JAC55, JAC61, JAC95, JAC25, JAC122, JAC68, JAC72, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Violuric Acid                                              | High  | 30.72 JAC87, JAC96, JAC88, JAC55, JAC61, JAC95, JAC25, JAC122, JAC68, JAC72, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Uric Acid                                                 | Low   | 31.24 JAC30L, JAC81, JAC75, JAC96, JAC95, JAC35, JAC88, JAC68, JAC110, JAC74L, JAC54, JAC6, JAC61A, JAC122, JAC72, JAC25, JAC87, JAC55 |
| 1-Octanamine, N-Methyl-                                    | High  | 31.53 JAC88, JAC55, JAC75, JAC61A, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC74L, JAC6, JAC110, JAC35 |
| Perfluoro(2-Methylpentane)                                | High  | 31.53 JAC87, JAC96, JAC88, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC30L, JAC74L, JAC6, JAC110 |
| Perfluoro-1,1-Dimethylcyclopentane                         | High  | 31.66 JAC87, JAC96, JAC88, JAC55, JAC61A, JAC95, JAC25, JAC122, JAC72, JAC81, JAC30L, JAC74L, JAC6, JAC110 |
| 1-(P-Bromobenzenesulfonyl)Piperidine                      | Low   | 31.66 JAC30L, JAC90, JAC81, JAC95, JAC88, JAC68, JAC110, JAC54, JAC72, JAC87 |
| Disulfide, Di-Tert-Dodecyl                                 | High  | 31.77 JAC87, JAC96, JAC88, JAC55, JAC75, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |

**Annotated as VocBinbase Bin Numbers (93)**

| Fiehn VocBinbase Bin #371 | Low | 4.08 JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, |
| Fiehn VocBinbase Bin #176 | High      | 4.64 |
|---------------------------|-----------|------|
|                          | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC55 |
| Fiehn VocBinbase Bin #847 | High      | 4.77 |
|                          | JAC33,JAC60,JAC87,JAC102,JAC96,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC55 |
| Fiehn VocBinbase Bin #1498 | High      | 4.86 |
|                          | JAC33,JAC60,JAC102,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC6,JAC110,JAC24,JAC55 |
| Fiehn VocBinbase Bin #1063 | High      | 4.95 |
|                          | JAC33,JAC60,JAC102,JAC88,JAC47,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC122,JAC17,JAC78,JAC72,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC55 |
| Fiehn VocBinbase Bin #387 | Low       | 4.95 |
|                          | JAC99,JAC90,JAC75,JAC47,JAC78,JAC86,JAC48,JAC95,JAC101,JAC103,JAC35,JAC88,JAC110,JAC45,JAC64,JAC74L,JAC6,JAC110,JAC24,JAC55 |
| Fiehn VocBinbase Bin #780 | Low       | 4.95 |
|                          | JAC30L,JAC99,JAC74C,JAC90,JAC81,JAC75,JAC78,JAC96,JAC86,JAC48,JAC95,JAC35,JAC88,JAC68,JAC110,JAC45,JAC33,JAC64,JAC74L,JAC54,JAC6,JAC55,
| Fiehn VocBinbase Bin #1375 | High | 5.07 |
|--------------------------|------|------|
| Supporting Information   |      |      |
| AC76, JAC60, JAC31, JAC61A, JAC122, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
| JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Fiehn VocBinbase Bin #838 | High | 5.2  |
| Supporting Information   |      |      |
| JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Fiehn VocBinbase Bin #754 | High | 5.54 |
| Supporting Information   |      |      |
| JAC60, JAC75, JAC54, JA |      |      |
| C90, JAC74L, JAC110, JAC24 |
| Fiehn VocBinbase Bin #509 | High | 5.84 |
| Supporting Information   |      |      |
| JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC35 |
| Fiehn VocBinbase Bin #37 | High | 5.84 |
| Supporting Information   |      |      |
| JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC61A, JAC103, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Fiehn VocBinbase Bin #39 | High | 6.1  |
| Supporting Information   |      |      |
| JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC61A, JAC103, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Fiehn VocBinbase Bin #1081 | High | 6.14 |
|--------------------------|------|------|
|                         |      |      |
| Fiehn VocBinbase Bin #454 | High | 6.31 |
|                         |      |      |
|                         |      |      |
| Fiehn VocBinbase Bin #467 | Low  | 6.31 |
|                         |      |      |
|                         |      |      |
| Fiehn VocBinbase Bin #888 | High | 6.75 |
|                         |      |      |
|                         |      |      |
| Fiehn VocBinbase Bin #829 | Low  | 7.14 |
|                         |      |      |
|                         |      |      |
| Fiehn VocBinbase Bin #1442 | Low  | 7.53 |
|                         |      |      |
|                         |      |      |
| Fiehn VocBinbase Bin #212 | High | 7.65 |
|                         |      |      |
|                         |      |      |
Fiehn VocBinbase Bin #518  Low  7.79  
JAC30L,JAC99,JAC81,JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC95,JAC103,JAC35,JAC88,JAC101,JAC68,JAC110,JAC45,JAC33,JAC64,JAC74L,JAC54,JAC6,JAC76,JAC60,JAC31,JAC61A,JAC122,JAC58,JAC72,JAC25,JAC87,JAC55

Fiehn VocBinbase Bin #113  Low  7.83  
JAC33,JAC60,JAC87,JAC96,JAC88,JAC55,JAC99,JAC54,JAC31,JAC61A,JAC48,JAC95,JAC25,JAC122,JAC17,JAC78,JAC68,JAC58,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC55

Fiehn VocBinbase Bin #493  High  8.38  
JAC30L,JAC99,JAC81,JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC95,JAC103,JAC35,JAC88,JAC68,JAC110,JAC45,JAC33,JAC64,JAC74L,JAC54,JAC6,JAC76,JAC60,JAC31,JAC61A,JAC122,JAC58,JAC72,JAC25,JAC102,JAC87,JAC17,JAC24,JAC55

Fiehn VocBinbase Bin #1417  Low  8.58  
JAC99,JAC90,JAC81,JAC47,JAC78,JAC96,JAC95,JAC103,JAC35,JAC64,JAC6,JAC110,JAC24,JAC55

Fiehn VocBinbase Bin #542  Low  8.58  
JAC99,JAC90,JAC81,JAC47,JAC78,JAC96,JAC95,JAC103,JAC35,JAC64,JAC6,JAC110,JAC24,JAC55

Fiehn VocBinbase Bin #1007  High  8.82  
JAC33,JAC87,JAC96,JAC88,JAC55,JAC99,JAC54,JAC31,JAC64,JAC48,JAC95,JAC25,JAC122,JAC78,JAC58,JAC90,JAC6,JAC110,JAC24,JAC35

Fiehn VocBinbase Bin #896  Low  8.88  
JAC30L,JAC99,JAC74C,JAC90,JAC81,JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC95,JAC103,JAC35,JAC64,JAC6,JAC110,JAC24,JAC88,JAC55
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Supporting Information

Fiehn VocBinbase Bin #580  High  9.21
JAC33, JAC60, JAC102, JAC55, JAC99, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC76, JAC86, JAC6, JAC24, JAC35

Fiehn VocBinbase Bin #579  High  9.29
JAC33, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC9, JAC74L, JAC6, JAC110, JAC24, JAC35

Fiehn VocBinbase Bin #226  High  9.83
JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35

Fiehn VocBinbase Bin #917  High  10.55
JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC25, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC110, JAC35

Fiehn VocBinbase Bin #1372  High  10.65
JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC47, JAC54, JAC64, JAC74C, JAC95, JAC25, JAC101, JAC122, JAC90, JAC74L, JAC6

Fiehn VocBinbase Bin #568  High  10.89
JAC33, JAC60, JAC102, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC6, JAC24, JAC35

Fiehn VocBinbase Bin #50  High  10.89
JAC33, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC
| Fiehn VocBinbase Bin #680 | High   | 12.67 |
|--------------------------|--------|-------|
| Fiehn VocBinbase Bin #846 | Low    | 13.09 |
| Fiehn VocBinbase Bin #402 | High   | 13.14 |
| Fiehn VocBinbase Bin #191 | High   | 13.72 |
| Fiehn VocBinbase Bin #352 | High   | 14.24 |
| Fiehn VocBinbase Bin #1475 | High  | 14.92 |
| Fiehn VocBinbase Bin #993 | Low    | 15.71 |

Supporting Information:

81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC30L, JAC90, JAC81, JAC75, JAC47, JAC95, JAC101, JAC68, JAC110, JAC45, JAC74L, JAC54, JAC60, JAC61A, JAC122, JAC72, JAC25, JAC102, JAC87, JAC17, JAC55, JAC33, JAC60, JAC87, JAC102, JAC88, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC30L, JAC90, JAC47, JAC78, JAC96, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC33, JAC74L,
| Bin Number                  | Type  | Value | Compounds                                                                 |
|-----------------------------|-------|-------|---------------------------------------------------------------------------|
| Fiehn VocBinbase Bin #545   | High  | 16.03 | JAC54, JAC6, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC24, JAC55 |
|                             |       |       | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47,    |
|                             |       |       | JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25,|
|                             |       |       | JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58,|
|                             |       |       | JAC6, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35                           |
| Fiehn VocBinbase Bin #1022  | High  | 16.48 | JAC33, JAC60, JAC102, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103,  |
|                             |       |       | JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC30L,|
|                             |       |       | JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35            |
| Fiehn VocBinbase Bin #1406  | Low   | 16.52 | JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, |
|                             |       |       | JAC48, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64,|
|                             |       |       | JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72,  |
|                             |       |       | JAC25, JAC102, JAC87, JAC17, JAC24, JAC35                                 |
| Fiehn VocBinbase Bin #921   | High  | 16.85 | JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54,    |
|                             |       |       | JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC101, JAC122, JAC17,|
|                             |       |       | JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L,|
|                             |       |       | JAC6, JAC110, JAC35                                                       |
| Fiehn VocBinbase Bin #524   | High  | 17.48 | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A,   |
|                             |       |       | JAC103, JAC48, JAC95, JAC101, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L,|
|                             |       |       | JAC76, JAC90, JAC74L, JAC6, JAC110, JAC35                                 |
| Fiehn VocBinbase Bin #1039  | High  | 17.52 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47,   |
|                             |       |       | JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25,|
|                             |       |       | JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L                |
| Fiehn VocBinbase Bin #1115 | High | 17.86 |
|---------------------------|------|-------|
| Fiehn VocBinbase Bin #487 | High | 18.06 |
| Fiehn VocBinbase Bin #491 | High | 18.15 |
| Fiehn VocBinbase Bin #799 | High | 18.99 |
| Fiehn VocBinbase Bin #1210 | Low  | 18.99 |
| Fiehn VocBinbase Bin #1202 | Low  | 19.1  |

S68
| Fiehn VocBinbase Bin #357 | Low | 19.37 |
|---------------------------|-----|-------|
|                          |     |       |
| JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC102, JAC87, JAC17, JAC55 |
| Fiehn VocBinbase Bin #363 | High | 19.49 |
|                          |     |       |
| JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC74C, JAC48, JAC95, JAC25, JAC17, JAC72, JAC81, JAC30L, JAC76, JAC90, JAC74L, JAC110, JAC35 |
| Fiehn VocBinbase Bin #1345 | High | 19.73 |
|                          |     |       |
| JAC30L, JAC90, JAC75, JAC96, JAC95, JAC35, JAC88, JAC101, JAC74L, JAC54, JAC61A, JAC25, JAC102, JAC87, JAC17, JAC24 |
| Fiehn VocBinbase Bin #1266 | Low | 19.73 |
|                          |     |       |
| JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC17, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC110, JAC24 |
| Fiehn VocBinbase Bin #1225 | High | 19.87 |
|                          |     |       |
| JAC33, JAC102, JAC96, JAC95, JAC35, JAC88, JAC101, JAC74L, JAC54, JAC61A, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC17, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24 |
| Fiehn VocBinbase Bin #77  | High | 20.14 |
|                          |     |       |
| JAC33, JAC102, JAC96, JAC95, JAC99, JAC75, JAC47, JAC54, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC17, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC24 |
| Fiehn VocBinbase Bin #737 | High | 20.76 |
|                          |     |       |
| JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC17, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Fiehn VocBinbase Bin #1336 | Low  | 21.31 |
|---------------------------|------|-------|
| JAC30L, JAC99, JAC74C, JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC95, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |

| Fiehn VocBinbase Bin #606 | High | 21.62 |
|---------------------------|------|-------|
| JAC33, JAC60, JAC87, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC76, JAC58, JAC86, JAC74L, JAC6, JAC24 |

| Fiehn VocBinbase Bin #1297 | High | 21.8 |
|---------------------------|------|------|
| JAC33, JAC60, JAC99, JAC75, JAC47, JAC45, JAC64, JAC103, JAC74C, JAC101, JAC17, JAC78, JAC68, JAC76, JAC58, JAC86, JAC24, JAC35 |

| Fiehn VocBinbase Bin #1091 | High | 22.49 |
|---------------------------|------|------|
| JAC33, JAC60, JAC102, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC6, JAC24, JAC35 |

| Fiehn VocBinbase Bin #749 | High | 23.05 |
|---------------------------|------|------|
| JAC33, JAC60, JAC87, JAC102, JAC55, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC74L, JAC24 |

| Fiehn VocBinbase Bin #53 | High | 24 |
|--------------------------|------|------|
| JAC33, JAC60, JAC102, JAC88, JAC99, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC101, JAC122, JAC17, JAC78, JAC68, JAC76, JAC58, JAC86, JAC90, JAC24 |

| Fiehn VocBinbase Bin #413 | High | 24.14 |
|---------------------------|------|------|
| JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Fiehn VocBinbase Bin #7   | High    | 24.33 |
|--------------------------|---------|-------|
| Fiehn VocBinbase Bin #1017 | Low    | 25.13 |
| Fiehn VocBinbase Bin #1512 | High    | 25.81 |
| Fiehn VocBinbase Bin #361 | Low    | 25.91 |
| Fiehn VocBinbase Bin #1089 | Low    | 26.58 |
| Fiehn VocBinbase Bin #1461 | High    | 26.75 |
| Fiehn VocBinbase Bin #1510 | High    | 26.85 |

| Supporting Information | JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC74C, JAC48, JAC95, JAC48, JAC95, JAC48, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
|--------------------------|---------|-------|
| Fiehn VocBinbase Bin #1017 | Low    | 25.13 |
| Fiehn VocBinbase Bin #1512 | High    | 25.81 |
| Fiehn VocBinbase Bin #361 | Low    | 25.91 |
| Fiehn VocBinbase Bin #1089 | Low    | 26.58 |
| Fiehn VocBinbase Bin #1461 | High    | 26.75 |
| Fiehn VocBinbase Bin #1510 | High    | 26.85 |

| Supporting Information | JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC74C, JAC48, JAC95, JAC48, JAC95, JAC48, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC60, JAC31, JAC61A, JAC122, JAC58, JAC72, JAC25, JAC102, JAC87, JAC17, JAC24, JAC55 |
|--------------------------|---------|-------|
| Fiehn VocBinbase Bin #1017 | Low    | 25.13 |
| Fiehn VocBinbase Bin #1512 | High    | 25.81 |
| Fiehn VocBinbase Bin #361 | Low    | 25.91 |
| Fiehn VocBinbase Bin #1089 | Low    | 26.58 |
| Fiehn VocBinbase Bin #1461 | High    | 26.75 |
| Fiehn VocBinbase Bin #1510 | High    | 26.85 |
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Supporting Information

8,JAC25,JAC101,JAC122,JAC17,JAC81,JAC30L,JAC76,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24
JAC33,JAC102,JAC96,JAC99,JAC54,JAC31,JAC61A, JAC45,JAC64,JAC103,JAC74C,JAC48,JAC25,JAC101,JAC17,JAC78,JAC72,JAC81,JAC30L,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC24,JAC35
JAC30L,JAC99,JAC74C,JAC90,JAC81,JAC75,JAC78,JAC96,JAC86,JAC48,JAC103,JAC35,JAC101,JAC68,JAC45,JAC33,JAC74L,JAC76,JAC31,JAC61A,JAC122,JAC58,JAC72,JAC25,JAC87
JAC75,JAC47,JAC78,JAC96,JAC86,JAC48,JAC103,JAC68,JAC45,JAC64,JAC54,JAC6,JAC76,JAC31,JAC122,JAC58,JAC72,JAC24
JAC99,JAC74C,JAC75,JAC47,JAC78,JAC86,JAC103,JAC35,JAC101,JAC68,JAC45,JAC64,JAC74L,JAC54,JAC31,JAC58,JAC72,JAC102,JAC17
JAC33,JAC60,JAC87,JAC102,JAC88,JAC55,JAC99,JAC47,JAC31,JAC61A,JAC64,JAC103,JAC48,JAC95,JAC101,JAC81,JAC76,JAC58,JAC74L
JAC33,JAC60,JAC102,JAC96,JAC55,JAC75,JAC47,JAC31,JAC61A,JAC64,JAC74C,JAC48,JAC95,JAC122,JAC78,JAC68,JAC72,JAC30L,JAC90,JAC74L,JAC110,JAC24,JAC35
JAC60,JAC102,JAC96,JAC47,JAC54,JAC45,JAC64,JAC74C,JAC101,JAC68,JAC81,JAC76,JAC86,JAC74L,JAC110,JAC35
JAC74C,JAC90,JAC81,JAC75,JAC78,JAC86,JAC48,JAC95,JAC103,JAC35,JAC88,JAC101,JAC68,JAC45,JAC33,JAC76,JAC60,JAC61A,JAC122,JAC58,JAC72,JAC102,JAC17,JAC24,JAC55
| Fiehn VocBinbase Bin # | Level | Value | Supporting Information |
|------------------------|-------|-------|------------------------|
| #1494                  | High  | 29.26 | JAC102, JAC88, JAC55, JAC99, JAC75, JAC31, JAC45, JAC103, JAC74C, JAC48, JAC101, JAC122, JAC17, JAC68, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC6, JAC110 |
| #899                   | Low   | 29.26 | JAC90, JAC81, JAC75, JAC47, JAC78, JAC96, JAC86, JAC48, JAC103, JAC35, JAC88, JAC101, JAC68, JAC110, JAC45, JAC33, JAC64, JAC74L, JAC54, JAC6, JAC76, JAC31, JAC58, JAC87, JAC17, JAC24, JAC55 |
| #1224                  | High  | 29.35 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| #1168                  | High  | 29.58 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| #863                   | High  | 29.76 | JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC61A, JAC122, JAC72, JAC25, JAC17, JAC24, JAC55 |
| #1500                  | Low   | 29.76 | JAC87, JAC96, JAC54, JAC61A, JAC95, JAC68, JAC72, JAC81, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Fiehn VocBinbase Bin # | Level | Value | Compounds Present |
|------------------------|-------|-------|-------------------|
| #1506                  | High  | 30.59 | JAC87, JAC96, JAC88, JAC55, JAC75, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| #1038                  | High  | 30.69 | JAC87, JAC96, JAC88, JAC55, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC30L, JAC90, JAC74L, JAC110, JAC35 |
| #494                   | High  | 31.49 | JAC87, JAC96, JAC88, JAC55, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| #809                   | High  | 31.88 | JAC87, JAC96, JAC88, JAC75, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC72, JAC81, JAC30L, JAC90, JAC74L, JAC6, JAC110 |
Table S4. VOCs annotated with high confidence in the pooled culture screen using MSHub/GNPS.

| Compound/VOC* | Retention time (min) | Annotated in (isolates) | Reported in plants | Reported in Streptomyces |
|---------------|----------------------|-------------------------|-------------------|-------------------------|
| **Alcohols**  |                      |                         |                   |                         |
| Dihydromyrcenol | 4.7                  | JAC33, JAC60, JAC102, JAC99, JAC47, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC17, JAC78, JAC76, JAC86, JAC87, JAC96, JAC88, JAC55, JAC54, JAC95 | Yes | Yes |
| 1-Octen-3-ol | 5.46                  | JAC101, JAC122, JAC68, JAC90, JAC74L, JAC6, JAC110, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Octanol (2-) | 6.35                  | JAC33, JAC60, JAC102, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC24, JAC33, JAC60, JAC102, JAC88, JAC55, JAC97, JAC47, JAC31, JAC61A, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC24 | Yes | Yes |
| 6,10-Dimethyl-2-Undecanol | 6.62 | Yes | No |
| 3-Hexanol, 3,5-Dimethyl- | 8.03 | Yes | No |
| 2-Decanol | 8.26                  | Yes | Yes |
| Octanol (3-) | 9.39                  | Yes | Yes |
| Compound                        | Log P  | JAC Codes                                                                 | Supporting Information |
|--------------------------------|--------|---------------------------------------------------------------------------|------------------------|
| 1-Phenylethyl Alcohol          | 10.29  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC48, JAC9 5, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                    |
| 2-Hexanol, 2,5-Dimethyl-, (S)-  | 10.63  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                    |
| 1-Tetradecanol                 | 11.29  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC48, JAC95, JAC101, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC110 | Yes                    |
| Cis-1,2-Cyclohexanediol        | 11.52  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC4C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC6, JAC110, JAC24, JAC35 | Yes                    |
| 1,3-Propanediol, 2-Butyl-2-Ethyl- | 12.58  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC4C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                    |
| 1-Undecanol, 11-Bromo-         | 12.58  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC103, JAC74C, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                    |
| Compound                              | RRT  |
|--------------------------------------|------|
| Hexanol                              | 12.99 |
| (S)-(+-)-3-Methyl-1-Pentanol         | 13.09 |
| 2-Isopropyl-5-Methyl-1-Heptanol      | 13.66 |
| Tetrahydrolavandulol                 | 15.41 |
| 10-Undecen-1-ol                      | 17.86 |
| 12-Methyl-1-Tridecanol               | 17.91 |

Supporting Information

| Compound                              | RRT  |
|--------------------------------------|------|
| Hexanol                              | Yes  |
| (S)-(+-)-3-Methyl-1-Pentanol         | Yes  |
| 2-Isopropyl-5-Methyl-1-Heptanol      | Yes  |
| Tetrahydrolavandulol                 | Yes  |
| 10-Undecen-1-ol                      | No   |
| 12-Methyl-1-Tridecanol               | Yes  |

S77
| Aldehyde/Alcohol        | % RSD | Supporting Information |
|-------------------------|-------|------------------------|
| 1-Pentadecanol          | 19.1  | Yes                    |
| Tridecanol              | 19.8  | Yes                    |
| 3-Pentadecanol          | 22.14 | Yes                    |
| 10-Methyl-1-Dodecanol   | 22.87 | No                     |
| Aldehydes               |       |                        |
| Benzeneacetaldehyde     | 12.44 | Yes                    |

S78
| Compound                                                                 | Value  | JAC Numbers                                      | Supporting Information |
|-------------------------------------------------------------------------|--------|-------------------------------------------------|------------------------|
| **(Z)-11-Hexadecenal**                                                  | 15.71  | JAC60, JAC102, JAC99, JAC47, JAC31, JAC45, JAC45, JAC64, JAC25, JAC101, JAC17, JAC78, JAC72, JAC81, JAC58, JAC24 | No                      |
| **Cis-9-Hexadecenal**                                                   | 23.94  | JAC33, JAC60, JAC87, JAC102, JAC88, JAC99, JAC75, JAC47, JAC31, JAC61, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC76, JAC58, JAC86, JAC6, JAC110, JAC24, JAC35 | Yes                     |
| **Esters**                                                              |        |                                                 |                        |
| Ethyl Undecanoate                                                       | 8.54   | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No                      |
| Methacrylic Acid 2-Ethylhexyl Ester                                    | 9.61   | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC45, JAC64, JAC48, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC81, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110 | No                      |
| Carbonic Acid, Butyl 2-Ethylhexyl Ester                                | 10.15  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No                      |
| Octadecyl 3-(3,5-Di-Tert-Butyl-4-Hydroxyphenyl)Propionate              | 10.21  | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC110, JAC24, JAC35 | No                      |
| Compound                                      | Weight | JAC33, JAC60, JAC87, JAC102, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC45, JAC64, JAC103, JAC74, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC74L, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC101, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes     | No      |
| Acetoxyisobutyryl Chloride                    | 10.63  | Yes     | No      |
| Hexyl Acetate                                 | 11.29  | Yes     | No      |
| Dodecyl Formate                               | 11.72  | Yes     | No      |
| Hexyl 10-Undecenoate                          | 11.85  | No      | No      |
| (Z)-12-Octadecenoic Acid Methyl Ester         | 13.33  | Yes     | Yes     |
| Compound | Molecular Formula | Molar Mass | JAC Codes | Support | Supporting Information |
|----------|------------------|------------|-----------|---------|------------------------|
| Methyl Para Toluate | C8H10O | 13.72 | JAC33, JAC102, JAC88, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC81, JAC76, JAC58, JAC86, JAC74L, JAC6, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Glutaric Acid, Dec-2-Yl Dec-4-Enyl Ester | C8H16O2 | 15.41 | JAC33, JAC60, JAC102, JAC99, JAC75, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| 1,2-Dibutyroxy-1-Ethoxyethane | C22H44O4 | 16.85 | JAC33, JAC60, JAC102, JAC96, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC76, JAC58, JAC86, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC76, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24 | No | No |
| 2-Butenedioic Acid (Z)-, Monododecyl Ester | C22H44O4 | 19.06 | JAC33, JAC60, JAC102, JAC96, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC74L, JAC6, JAC110, JAC35 | Yes | No |
| Decan-1,10-Diol Dimethacrylate | C22H44O4 | 19.13 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC55, JAC99, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC74L, JAC6, JAC110, JAC35, JAC60, JAC87, JAC102, JAC96, JAC47, JAC31, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35 | No | No |
| Carbonic Acid, 2,2,2-Trichloroethyl 2-Ethylhexyl Ester | C22H44O4 | 19.42 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC55, JAC99, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC60, JAC87, JAC102, JAC96, JAC47, JAC31, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Compound                                      | TAU | JACs                                                                 |
| ----------------------------------------------|-----|----------------------------------------------------------------------|
| 2-Ethylhexyl Mercaptoacetate                  | 19.46 | JAC33, JAC60, JAC102, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC101, JAC17, JAC78, JAC72, JAC76, JAC58, JAC86, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JA C61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC4 8, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| Dodecanoic Acid, Methyl Ester                | 19.7 | Yes                                                                  |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
| Cyanoacetic Acid, Nonyl Ester                | 19.8 | No                                                                    |
|                                               |     | No                                                                    |
| Carbonic Acid, Monoamide, N-Propyl-N-Butyl-, 2-Ethylhexyl Ester | 20.09 | Yes                                                                   |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
| Hexanoic Acid, 2-Hexenyl Ester, (E)-         | 20.46 | Yes                                                                   |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
| Vinyl 2-Ethylhexanoate                        | 20.68 | No                                                                    |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
| 3-Octyl Isovalerate                           | 21.22 | Yes                                                                   |
|                                               |     | No                                                                    |
|                                               |     | No                                                                    |
| Substance                                      | Retention Time (min) | JAC Numbers               | Supporting Information |
|-----------------------------------------------|----------------------|---------------------------|------------------------|
| Lauryl Acetate                                | 21.41                | C31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC9, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | No |
| Carbonic Acid, Isobutyl Cyclohexyl Ester      | 21.91                | C31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Hexanoic Acid, 5-Oxo-, Ethyl Ester            | 21.91                | C31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| 13-Methyltetradecanoic Acid Methyl Ester      | 22.1                 | C31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Ethyl Tetradecanoate                          | 22.14                | C31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Methyl Tetradecanoate                         | 22.14                | C31, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Compound | % GC | JCs Present | JCs Absent |
|----------|-----|-------------|------------|
| 2-(2-Methylpiperidino)Ethylp-Chlorobenzoate | 22.28 | JAC17, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC6, JAC110, JAC24, JAC35, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC81, JAC58, JAC86, JAC6, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Allyl Hexanoate | 22.37 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| 2-Methylvaleric Acid, 2-Ethylhexyl Ester | 22.46 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Cis-3-Hexenyl 2-Ethylbutyrate | 22.65 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Benzyl Benzoate | 22.71 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Compound                                      | Retention Time | Supporting Information |
|-----------------------------------------------|----------------|------------------------|
| Methyl Dodecanoate_Repeat                      | 23.22          | No                     |
| Trans-2-Hexenyl 2-Ethylbutyrate               | 24.14          | No                     |
| Methyl Decanoate                              | 24.22          | Yes                    |
| Methyl Palmitate                              | 24.26          | Yes                    |
| Isopropyl Hexadecanoate                       | 25.21          | Yes                    |
| Carbonic Acid, Propargyl 2-Ethylhexyl Ester   | 26.14          | No                     |
| Compound | Molecular Formula | Retention Time (min) | Yes | No |
|----------|------------------|---------------------|-----|----|
| 1,2-Benzenedicarboxylic Acid Bis(2-Ethylhexyl) Ester | 0L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35,JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC44,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | 26.52 | Yes | No |
| Bis(2-Ethylhexyl) Phthalate | JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | 28.42 | Yes | Yes |
| 1,2-Benzenedicarboxylic Acid Decyl Octyl Ester | JAC87,JAC88,JAC47,JAC54,JAC31,JAC6,JAC10,JAC24,JAC35 | 28.49 | No | No |
| Hexanedioic Acid, Bis(2-Ethylhexyl) Ester | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC78,JAC81,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | 28.71 | Yes | Yes |
| Succinic Acid, Monochloride 2-Ethylbutyl Ester | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC78,JAC81,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | 29.13 | No | No |
| Ethyl 3-Acetoxybutyrate | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC78,JAC81,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | 29.51 | Yes | Yes |
| Compound                        | R²  | No. of JACs | Supporting Information |
|--------------------------------|-----|------------|------------------------|
| **1,2-Benzenedicarboxylic Acid Hexyl Octyl Ester** | 30.29 | No | No |
| **Hydrocarbons**               |     |            |                        |
| Hexane, 3-Ethyl-               | 5.2 | No         | No                     |
| Hexadecane                     | 12.1| Yes        | No                     |
| 1,1,4-Trimethylcyclohexane     | 12.62 | Yes | Yes |
| 1-Decene                       | 12.94 | Yes | Yes |
| Cyclohexane, 1,2,3-Trimethyl-   | 13.22 | Yes | Yes |
| Substance                        | 2,4,4-Trimethyl-1-Hexene | N-Octadecane | Tetracosane | 1-Hexene, 3,5,5-Trimethyl- | Pentacosane |
|---------------------------------|--------------------------|--------------|-------------|---------------------------|-------------|
|                                 | 13.57                    | 14.56        | 16.01       | 16.3                      | 16.81       |
| No                              | No                       | Yes          | Yes         | No                        | Yes         |
| C61A, JAC45, JAC103, JAC48, JAC95, JAC2, JAC122, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35, JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC75, JAC54, JAC61A, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35, JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35.
| Compound                        | Delta T (°C) | Yes | No  | Yes | No  |
|--------------------------------|--------------|-----|-----|-----|-----|
| Cyclohexane, Tetradecyl-       | 17.2         | Yes | No  |
| Pentane, 2,2,3,4-Tetramethyl-  | 17.57        | Yes | No  |
| (6Z,9Z)-6,9-Tricosadiene       | 17.86        | No  | No  |
| Cyclohexane, 1,2-Dimethyl- (Cis/Trans) | 17.91       | No  | No  |
| Tridecane                      | 18.03        | Yes | Yes |
| 1,19-Eicosadiene               | 18.76        | Yes | Yes |
| Compound                     | Retention Time | Peaks Present |
|------------------------------|----------------|---------------|
| 1-Heptadecene                | 19.3           | Yes, Yes      |
| Heptylcyclohexane            | 20.14          | Yes, No       |
| 1-Eicosene                   | 20.61          | Yes, Yes      |
| Cyclopentadecane             | 21.76          | Yes, Yes      |
| Cyclohexane, Undecyl-        | 22.56          | Yes, No       |
| Octadecane                   | 22.94          | Yes, Yes      |
| Compound               | Retention Time (min) | Response to Pentadecane | Response to Octadecane | Response to Nonacosane | Response to Trans-2-Nonene | Response to Ketones  |
|------------------------|----------------------|--------------------------|-------------------------|------------------------|---------------------------|----------------------|
| Pentadecane            | 23.02                | Yes                      | Yes                     | Yes                    | Yes                       | Yes                  |
| Octadecane             | 25.01                | Yes                      | Yes                     | Yes                    | Yes                       | Yes                  |
| Nonacosane             | 29.22                | Yes                      | Yes                     | Yes                    | No                        | Yes                  |
| Trans-2-Nonene         | 30.1                 | No                       | No                      | No                     | No                        | No                   |
| Ketones                |                      |                          |                         |                         |                           |                      |
| Pentanone (4-OH-4-Me-2-) | 5.57                | Yes                      | Yes                     |                         |                           | Yes                  |
| Compound                               | pKa  | Yes  | No  |
|----------------------------------------|------|------|-----|
| 2-Tridecanone                          | 5.66 | Yes  | Yes |
| 2-Butylcyclopenanone                   | 9.67 | Yes  | Yes |
| 2-Propyl-5,5-Dimethyl-1,3-Cyclohexanedione | 10.65 | No   | No  |
| 1,2-Cyclopentanedione, 3-Methyl-       | 11.15 | Yes  | Yes |
| 2-Tert-Butylcyclohexanone              | 11.57 | No   | No  |
| Cyclohexanone, 4-(1,1-Dimethylethyl)-  | 12.32 | No   | No  |
| Compound                                      | Retention Time | Detected in JAC  | Detected in C30L |
|-----------------------------------------------|----------------|------------------|------------------|
| **Ethanone, 2-Chloro-1-(2,4-Dimethylphenyl)-**| 16.16          | No               | No               |
| 4'-Butoxyacetophenone                         | 17.31          | No               | No               |
| Cyclododecanone                               | 17.94          | Yes              | Yes              |
| 2-(1-Cyclohexenyl)Cyclohexanone               | 18.93          | Yes              | No               |
| Trans-3-Nonen-2-One                           | 20.57          | Yes              | Yes              |
| Compound                          | MW  | Yes/No |
|----------------------------------|-----|--------|
| 3-Methoxyheptanophenone          | 22.02 | Yes/No |
| 5,5-Dimethyl-1,3-Cyclohexanodione | 22.02 | Yes/No |
| Tetradecanophenone               | 23.05 | No/No  |
| Pyrimidine, 6-Oxo-5-Acetyl-4-Hydroxy-1,6-Dihydro- | 27.4 | No/No  |
| 2-Propanone, 1,1,1-Trichloro-     | 29.4 | Yes/No |
| Hexanal (Si-Contam)_Adms        | 31.2 | Yes/Yes|
| Terpenes and Terpenoids                          | Supporting Information |
|-------------------------------------------------|------------------------|
| **2-Octene, 2,6-Dimethyl-**                     | **7.95**               |
| JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | Yes | No |
| **Perillyl Isobutyrate**                        | **10.08**              |
| JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | No | No |
| **Isopulegol(Equatorial)**                      | **11.82**              |
| JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | Yes | Yes |
| **1,1-Bis(4,4-Dimethyl-2,6-Dioxocyclohexyl)Ethan e** | **12.48**              |
| JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC75,JAC47,JAC54,JAC61A,JAC45,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC58,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | No | No |
| Compound                           | LogP  | JAC Entries                                                                 | Supporting Information |
|-----------------------------------|-------|-----------------------------------------------------------------------------|------------------------|
| Cyclohexanol, 5-Methyl-2-(1-Methylethyl)- | 14.07 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC74L, JAC6, JAC110, JAC54, JAC110, JAC24, JAC35, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC48, JAC25, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| L-Menthol                         | 14.16 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC48, JAC25, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC48, JAC25, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| (7S)-(-)-10,10-Di-Me-5-Thia-4-Azatricyclo[5.2.1.0^3,7]Dec-3-Ene-5,5-Dioxide | 15.71 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Ylangene (Alpha-)                | 17.69 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Cubebe (Alpha-)                  | 17.77 | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Acetic Acid, 1,7,7-Trimethyl-     | 18.23 | JAC33, JAC60, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | No |
| Compound                              | Retention Time | Supporting Information |
|---------------------------------------|----------------|------------------------|
| Bicyclo[2.2.1]Hept-2-Yl Ester         |                |                        |
| Aristolochene (4,5-Di-Epi)            | 18.3           | Yes                    |
| Sabinene                              | 18.3           | Yes                    |
| Sesquiphellandrene (Beta-)            | 18.51          | Yes                    |
| (+)-Alpha-Muurolene                   | 18.59          | Yes                    |
| 7-Isopropenyl-1,4A-Dimethyl-3,4,5,6,7,8-Hexahydro-2-Naphthalenone | 19.95          | Yes                    |
| 4,10-Dimethyl-7-Isopropyl-            | 21.13          | No                     |
| Compound                  | Mass (Da) | Yes/No | Supporting Information |
|---------------------------|-----------|--------|------------------------|
| Bicyclo(4.4.0)Deca-1,4-Diene |           |        |                        |
| Germacrone                | 21.18     | Yes    | Yes                    |
| Caryophyllene (Z-)        | 21.27     | Yes    | Yes                    |
| Eremophilene              | 21.27     | Yes    | Yes                    |
| Beta-Gurjunene            | 21.55     | Yes    | Yes                    |
| 3-Isopropyl-6,10-Dimethylundecane-2-ol | 28.79 | No     | No                     |
| Diverse functional groups | Octadecyl Bromide | Dramamine | Behenic Amide | 4-Chloro-2-Aminopyrimidine | Pentadecafluorooctanoic Acid, Pentyl Ester | Hexenyl 3-Methyl Butanoate (3Z-) |
|--------------------------|-------------------|-----------|---------------|---------------------------|----------------------------------------|-----------------------------|
|                          | 4.33              | 4.53      | 4.86          | 5.33                      | 5.33                                   | 5.66                        |
|                          | JAC33,JAC60,JAC87,JAC102,JAC96,JAC88,JAC55,JAC99,JAC75,JAC54,JAC31,JAC61A,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC58,JAC86,JAC90,JAC6,JAC110,JAC24,JAC35 | Yes | No | Yes | Yes | No | No | Yes | No |

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| Compound                                      | Log P | Supporting Information |
|------------------------------------------------|-------|------------------------|
| Heptanone (2-)                                | 5.94  | Yes                    |
| 3-Methyl-P-Anisaldehyde                       | 6.04  | Yes                    |
| (+)-N-Benzyl-Alpha.-Phenethylylamine          | 6.25  | Yes                    |
| 4-Piperidinemethanamine                       | 6.31  | No                     |
| Pentadecafluorooctanoic Acid, Isobutyl Ester  | 7.11  | No                     |
| Supporting Information                                      | 6-Iodo-2-Picolin-5-ol | 2-(4-Hydroxyphenyl)Ethanoic Acid | Pentadecafluorooctanoic Acid, 4-Methyl-2-Pentyl Ester | Pentadecafluorooctanoic Acid, Undec-2-En-1-Yl Ester | Pentadecafluorooctanoic Acid, Dodecyl Ester | Pentadecafluorooctanoic Acid, Hexyl Ester | Levoglucosan |
|-------------------------------------------------------------|----------------------|----------------------------------|------------------------------------------------------|--------------------------------------------------|----------------------------------------|----------------------------------------|-------------|
| 7.25                                                        | JAC87,JAC96,JAC88,JAC55,JAC75,JAC4 4,JAC31,JAC61A,JAC103,JAC48,JAC95,JAC25,JAC122,JAC68,JAC72,JAC81,JAC30L,JAC86,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | No                               | No                                                  | No                                               | Yes                                                  | No                                                  | Yes         |
| 7.32                                                        | JAC33,JAC60,JAC102,JAC96,JAC99,JAC47,JAC31,JAC45,JAC64,JAC74C,JAC48,JAC101,JAC17,JAC78,JAC76,JAC58,JAC8 6,JAC24 | Yes                              | No                                                  | No                                               | No                                                  | No                                                  | Yes         |
| 7.4                                                         | JAC33,JAC60,JAC102,JAC88,JAC55,JAC 99,JAC75,JAC54,JAC45,JAC64,JAC74C,JAC95,JAC25,JAC101,JAC122,JAC17,JAC 78,JAC68,JAC72,JAC81,JAC74L,JAC110,JAC24,JAC35 | No                               | No                                                  | No                                               | No                                                  | No                                                  | Yes         |
| 7.61                                                        | JAC33,JAC60,JAC102,JAC96,JAC98,JAC8 8,JAC55,JAC99,JAC75,JAC47,JAC54,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC7 4C,JAC48,JAC95,JAC25,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | No                               | No                                                  | No                                               | No                                                  | No                                                  | Yes         |
| 7.79                                                        | JAC33,JAC60,JAC102,JAC96,JAC88,JAC5 5,JAC99,JAC75,JAC47,JAC54,JAC31,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC2 5,JAC101,JAC122,JAC17,JAC78,JAC68,JAC72,JAC81,JAC30L,JAC76,JAC58,JAC8 6,JAC90,JAC74L,JAC6,JAC110,JAC24,JAC35 | Yes                              | No                                                  | No                                               | No                                                  | No                                                  | Yes         |
| 7.79                                                        | JAC33,JAC60,JAC102,JAC96,JAC88,JAC 47,JAC31,JAC61A,JAC45,JAC64,JAC103,JAC74C,JAC48,JAC95,JAC25,JAC17,JAC 78,JAC72,JAC30L,JAC76,JAC58,JAC90,JAC24,JAC35 | No                               | No                                                  | No                                               | No                                                  | No                                                  | Yes         |
| 7.95                                                        | JAC33,JAC60,JAC102,JAC96,JAC88,JAC5 88,JAC55,JAC99,JAC54,JAC31,JAC61A,JAC6,JAC110,JAC24,JAC35 | Yes                              | Yes                                                  | Yes                                               | Yes                                                  | Yes                                                  | Yes         |
| Name                                                        | TIC  | Supported in Binary ^a^ | Supported in Matrix ^a^ |
|--------------------------------------------------------------|------|-------------------------|-------------------------|
| Dotriacontyl Isobutyl Ether                                 | 8.36 | Yes                     | Yes                     |
| 1,2-Benzenedicarboxaldehyde                                 | 8.46 | Yes                     | Yes                     |
| (Z,Z)-12,15-Octadecadienoic Acid Methyl Ester               | 8.74 | Yes                     | No                      |
| Arachidonic Acid                                            | 8.77 | Yes                     | Yes                     |
| Perfluoro(Methylcyclohexane)                                | 8.77 | Yes                     | Yes                     |
| Compound                                      | log D Value | JAC Entries                                                                 | Supporting Information |
|-----------------------------------------------|-------------|------------------------------------------------------------------------------|------------------------|
| Acetaldehyde Hexyl Isobutyl Acetal            | 8.82        | AC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No                     |
|                                               |             | JAC33, JAC60, JAC87, JAC102, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC45, JAC103, JAC48, JAC95, JAC22, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35 | No                     |
|                                               |             | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC22, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No                     |
| 3,3-Diethylglutaric Acid                      | 9.39        | JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC25, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                   |
|                                               |             | JAC33, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC25, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                   |
| Pentadecafluorooctanoic Acid, Propyl Ester    | 9.5         | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC25, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No                     |
|                                               |             | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC103, JAC74C, JAC48, JAC25, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No                     |
| Cresol (Ortho-)                               | 9.61        | JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes                   |
| 4-Amino-2,2,5,5-Tetramethyl-3-Imidazoline-1-Oxyl | 10.03    | JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC64, JAC103, JAC74C, JAC95, JAC101, JAC122, JAC17, JAC68, JAC76, JAC74L, JAC110, JAC24, JAC35 | No                     |
| Benzenemethanol, 4-(1,1-Dimethylethyl)-        | 10.08       | JAC96, JAC88, JAC55, JAC99, JAC47, JAC54, JAC31, JAC64, JAC103, JAC74C, JAC95, JAC101, JAC122, JAC17, JAC68, JAC76, JAC74L, JAC110, JAC24, JAC35 | Yes                   |
| Compound                                      | R-value | Supporting Information |
|-----------------------------------------------|---------|------------------------|
| N-((Methylphenylamino)Methyl)Benzamide         | 10.29   | No                     |
| Ethyl 3-Methyl-5-Methylpyrrole-2-Carboxylate  | 10.55   | Yes                    |
| Suberoyl Chloride                             | 10.77   | Yes                    |
| Oleic Acid                                    | 11.05   | Yes                    |
| 1,3-Dibenzoyl-4-Oxo-2-Thioxoimidazolidine     | 11.11   | No                     |
| Chemical Name                        | LogP | Supporting Information |
|------------------------------------|------|------------------------|
| N-Alpha-Benzyol-L-Arginine         | 11.11| Yes                    |
| 1H,1H,2H-Perfluoro-1-Octene        | 11.15| Yes                    |
| Decanedioyl Dichloride             | 11.78| Yes                    |
| Benzeneacetic Acid, Alpha-Oxo-, Methyl Ester | 11.91| No                     |
| Benzoic Acid Mono-Tms              | 11.96| Yes                    |
| Carbonochloridic Acid, Heptyl Ester| 12.19| Yes                    |

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| Substance                          | IC₅₀ (μM) | JAC Numbers                                                                 | Supporting Information |
|-----------------------------------|----------|-----------------------------------------------------------------------------|------------------------|
| Benzenamine, 2,4-Dimethoxy-       | 13.66    | JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC60, JAC87, JAC96, JAC99, JAC47, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC110, JAC35, JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC103, JAC74C, JAC48, JAC95, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35 | No | No |
| 2,5-Dimethylbenzophenone          | 13.72    | JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC81, JAC30L, JAC76, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC35 | Yes | Yes |
| O-Decylhydroxylamine              | 13.9     | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Para-Bromotoluene                 | 13.97    | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| 2'-Ethylpropiophenone             | 14.16    | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC25, JAC101, JAC17, JAC78, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC6, JAC110, JAC24 | Yes | No |
| Compound | Retention Time | Peaks Detected |
|----------|---------------|----------------|
| Diazene, Bis[4-(Hexyloxy)Phenyl]-1-Oxide | 14.45 | No | No |
| Pentadecafluoroctanoic Acid, 2-Ethylhexyl Ester | 14.65 | No | No |
| Pentadecafluoroctanoic Acid, Heptyl Ester | 14.84 | No | No |
| Beta-Cyclocitral | 15.24 | Yes | Yes |
| 1-Phenyl-1-Nonyne | 15.5 | Yes | No |
| Allylbenzene | 15.75 | Yes | Yes |

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Supporting Information

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| Compound                      | Mass (amu) | JACs Present | JACs Absent |
|-------------------------------|------------|--------------|-------------|
| **Benzoic Acid, 2-Acetylhydrazide** | 15.75      | No           | No          |
|                               |            | JAC87, JAC96, JAC55, JAC54, JAC71, JAC8, JAC6, JAC110, JAC35 |                      |
| **Ethyl Acetophenone (P-)**   | 15.75      | Yes          | No          |
|                               |            | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC90, JAC74L, JAC6, JAC110, JAC35 |                      |
| **Behenyl Chloride**          | 16.45      | Yes          | No          |
|                               |            | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC78, JAC68, JAC72, JAC30L, JAC76, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |                      |
| **Nonyl Tetradecyl Ether**    | 16.58      | No           | No          |
|                               |            | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC48, JAC95, JAC25, JAC122, JAC78, JAC68, JAC81, JAC30L, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |                      |
| **1-Bromo-8-Tetrahydropyranloxyoctane** | 16.81 | No           | No          |
|                               |            | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |                      |
| Name                                                                 | R Value | JAC Samples |
|----------------------------------------------------------------------|---------|-------------|
| 4-Benzylaminoindole                                                  | 17.04   | Yes         |
| Nonalactone (Gamma-)                                                | 17.41   | Yes         |
| Guanidine, N,N'-Bis(2-Methylphenyl)-                                | 17.86   | No          |
| Heptane, 3-[(Ethenyloxy)Methyl]-                                    | 18.2    | Yes         |
| (Z,Z,Z)-6,9,15-Octadecatrienoic Acid Methyl Ester                    | 18.33   | Yes         |
| 3Beta-Acetoxy-20-Hydroxy-5Alpha-Cevan-6-One                          | 18.38   | No          |
| Compound Description                                      | Value  | JAC Numbers | Supporting Information |
|------------------------------------------------------------|--------|-------------|------------------------|
| (Z,Z,Z)-9,12,15-Octadecatrienoic Acid Methyl Ester         | 18.59  | JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35, JAC33, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC95, JAC25, JAC122, JAC17, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Butanal, 3-Methyl-2-Methylene-, (1-Methylethyl)Hydrazone   | 19.1   | JAC33, JAC87, JAC102, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC81, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC10, JAC24, JAC35 | No | No |
| 1-Chloroeicosane                                           | 19.3   | JAC33, JAC60, JAC102, JAC96, JAC88, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC6, JAC110, JAC24, JAC35 | Yes | Yes |
| Propanoic Acid, 2-Methyl-, 1-(1,1-Dimethylethyl)-2-Methyl-1,3-Propanediyl Ester | 19.46  | JAC33, JAC60, JAC87, JAC88, JAC55, JAC99, JAC75, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes | No |
| Malonic Acid, Di(4-Heptyl) Ester                          | 19.95  | JAC33, JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No | No |
| Substance                                                                 | Molar Mass | JACs Present                                      | Supporting Information |
|--------------------------------------------------------------------------|------------|--------------------------------------------------|------------------------|
| Heptyl Tetradecyl Ether                                                 | 20.3       | JAC33, JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes, No |
| (Z,Z,Z)-6,9,12-Octadecatrienoic Acid Methyl Ester                       | 20.35      | JAC60, JAC102, JAC99, JAC47, JAC45, JAC74C, JAC48, JAC101, JAC17, JAC72, JAC6, JAC86, JAC110, JAC24 | Yes, No |
| (Z,Z,Z,Z)-6,9,12,15-Octadecatetraenoic Acid Methyl Ester                | 20.38      | JAC60, JAC88, JAC55, JAC74C, JAC25, JAC101, JAC122, JAC78, JAC68, JAC81, JAC90, JAC6, JAC110, JAC35 | Yes, No |
| 4-Tert-Butylpyrocatechol                                                 | 20.57      | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC6, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes, Yes |
| 4-(Decyloxy)Benzaldehyde                                                | 20.87      | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC122, JAC6, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | Yes, No |
| 1-Chloromethyl-3,5-Bis(1,1-Dimethylethyl)Benzene                        | 20.98      | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61A, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No, No |
| Methyl 3,4-O-Isopropylidene-Beta-D-Fucopyranoside                       | 21.06      | JAC60, JAC87, JAC96, JAC88, JAC55, JAC99, JAC75, JAC31, JAC45, JAC64, JAC103, JAC74C, JAC48, JAC95, JAC25, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 | No, No |
| Chemical Name                        | log P | JAC33 | JAC60 | JAC87 | JAC88 | JAC99 | JAC75 | JAC47 | JAC54 | JAC64 | JAC103 | JAC95 | JAC25 | JAC68 | JAC72 | JAC81 | JAC30L | JAC76 | JAC58 | JAC86 | JAC90 | JAC74L | JAC6 | JAC110 | JAC35 |
|-------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|--------|-------|-------|
| 9,12-Octadecadienoyl Chloride, (Z,Z)- | 21.34 | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   |
| Decyl Octyl Ether                   | 21.41 | No    | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   |
| 1,9-Dichlorononane                  | 22.19 | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   |
| Cyclohexasiloxane, Dodecamethyl-    | 22.71 | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   |
| (Alpha,Alpha,Alpha-Trifluoro-Para-Tolyl)Acetic Acid | 23.89 | No    | No    | No    | No    | No    | No    | No    | No    | No    | No     | No    | No    | No    | No    | No    | No     | No    | No    | No    | No    | No     | No    | No    |
| Eicosane, 1-Iodo-                   | 24.1  | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   | Yes   | Yes   | Yes    | Yes   | Yes   |
| Compound                                | Response | Methane  |
|-----------------------------------------|----------|---------|
| 1-Adamantaneacetic Acid                 | Yes      | Yes     |
| Butane, 1-Iodo-3-Methyl-                | Yes      | Yes     |
| 1-Iodoctane                            | Yes      | Yes     |
| Cis-1-Chloro-9-Octadecene               | Yes      | Yes     |
| Distearyl Thiodipropionate              | Yes      | Yes     |
| Docosanoic Anhydride                    | Yes      | Yes     |
| Compound                                    | Retention Time (min) | Analysis No. | PE Analysis No. |
|---------------------------------------------|----------------------|--------------|-----------------|
| **Docosyl Pentyl Ether**                    | 26.8                 | No           | No              |
| **Pentadecafluoroocanoic Acid, Undecyl Ester** | 26.93                | No           | No              |
| **2-Bromo Dodecane**                        | 27.71                | Yes          | Yes             |
| **Maltitol**                                | 28.08                | Yes          | Yes             |
| **Cyclobutanecarboxamide, N-Octyl-**        | 28.71                | No           | No              |
| **2-(3-Benzyolphenyl)Propionic Acid Trimethylsilyl Ester** | 29.04                | No           | No              |
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| Supporting Information |
|------------------------|
| Oct-3-Enoylamide, N-Methyl-N-Pentyl- | 29.42 |
| JAC60, JAC87, JAC102, JAC96, JAC88, JAC55, JAC99, JAC75, JAC47, JAC54, JAC31, JAC61, JAC45, JAC64, JAC74C, JAC48, JAC95, JAC25, JAC101, JAC122, JAC17, JAC78, JAC68, JAC72, JAC81, JAC30L, JAC76, JAC58, JAC86, JAC90, JAC74L, JAC6, JAC110, JAC24, JAC35 |
| JAC87, JAC96, JAC88, JAC55, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC6, JAC110, JAC35 |
| No | No |
| Perfluorotributylamine | 30.36 |
| JAC87, JAC96, JAC55, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC6, JAC110, JAC35 |
| Yes | Yes |
| Violuric Acid | 30.72 |
| JAC87, JAC96, JAC55, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC74L, JAC6, JAC110, JAC35 |
| Yes | Yes |
| 1-Octanamine, N-Methyl- | 31.53 |
| JAC87, JAC96, JAC88, JAC75, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC74L, JAC6, JAC110, JAC35 |
| No | No |
| Perfluoro(2-Methylpentane) | 31.53 |
| JAC87, JAC96, JAC88, JAC75, JAC54, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC74L, JAC6, JAC110 |
| Yes | No |
| Perfluoro-1,1-Dimethycyclopentane | 31.66 |
| JAC87, JAC96, JAC88, JAC55, JAC61A, JAC95, JAC25, JAC122, JAC72, JAC81, JAC30L, JAC74L, JAC6, JAC110 |
| Yes | Yes |
| Disulfide, Di-Tert-Dodecyl | 31.77 |
| JAC87, JAC96, JAC88, JAC55, JAC75, JAC5, JAC61A, JAC95, JAC25, JAC122, JAC68, JAC72, JAC81, JAC30L, JAC90, JAC74L, JAC6, JAC110, JAC35 |
| Yes | No |

* VOCs have not been reported from *Streptomyces* previously are highlighted in bold.
Table S5. Bacterially derived compounds annotated in pooled culture VOC analysis of the 37 *Streptomyces* isolates using the conventional method.

| VOC                                         | Retention Time (min) | Confidence in annotation | Annotated in (isolates)          |
|---------------------------------------------|----------------------|--------------------------|----------------------------------|
| **Alcohols (28)**                           |                      |                          |                                  |
| 3-Pentanol, 3-methyl-                       | 4.036                | Unknown                  | JAC99, JAC48                     |
| (S)-3,4-Dimethylpentanol                    | 4.129                | Unknown                  | JAC122                           |
| 2-Buten-1-ol, 2-methyl-                     | 4.316                | Unknown                  | JAC74C                           |
| Cyclopentanol, 1-methyl-                    | 4.676                | Low                      | JAC99, JAC103, JAC76, JAC48       |
| meso-3,4-Hexanediol                         | 4.724                | Unknown                  | JAC30L                           |
| (S)-3,4-Dimethylpentanol                    | 4.744                | Unknown                  | JAC87                            |
| 2-Methyl-2,3-pentanediol                    | 4.757                | Unknown                  | JAC17                            |
| 2-Hexanol                                   | 4.766                | Unknown                  | JAC88                            |
| DL-2,3-Butanediol                           | 4.798                | High                     | JAC17, JAC47                     |
| DL-2,3-Butanediol                           | 4.798                | Unknown                  | JAC103                           |
| 1-Hexanol                                   | 6.223                | High                     | JAC60, JAC61A                    |
| 4-Octanol, 2-methyl-                        | 6.918                | Unknown                  | JAC99                            |
| Ether, 3-butenyl propyl                     | 7.524                | Unknown                  | JAC6, JAC88, JAC55               |
| 1-Octen-3-ol                                | 8.963                | High                     | JAC74C                           |
| 3-Octanol                                   | 9.342                | Unknown                  | JAC122                           |
| (S)-3-Ethyl-4-methylpentanol                | 9.462                | Unknown                  | JAC25, JAC88, JAC61A             |
| Benzyl alcohol                              | 10.29                | High                     | JAC17, JAC58, JAC25, JAC122, JAC30L |
| Compound                                      | Octanol | JAC Numbers         |
|-----------------------------------------------|---------|---------------------|
| 1-Octanol                                     | 11.282  | High JAC99, JAC101, JAC64 |
| DL-4,5-Octanediol                             | 11.475  | Unknown JAC17      |
| 1-Octanol, 2-butyl-                           | 12.098  | Unknown JAC35      |
| Phenylethyl Alcohol                           | 12.432  | High JAC17, JAC31, JAC86, JAC101, JAC33, JAC58, JAC74C, JAC25, JAC110, JAC74L, JAC30L |
| trans-1,10-Dimethyl-trans-9-decalinol         | 18.385  | Unknown JAC24, JAC60, JAC58, JAC45 |
| 5,10-Pentadecadiyn-1-ol                       | 18.969  | Unknown JAC81      |
| 1-Dodecanol                                   | 19.054  | High JAC68         |
| 5,10-Pentadecadiyn-1-ol                       | 21.247  | Unknown JAC76, JAC90 |
| 1- Allyl-cyclohexane-1,2-diol                 | 21.544  | Unknown JAC81      |
| Cyclohexanol, 1-ethyl-2,2-dimethyl-6-methylene-| 22.219  | Unknown JAC81      |
| 5,10-Pentadecadiyn-1-ol, (Z,Z)                | 25.467  | Unknown JAC102     |

**Aldehydes (4)**

| Aldehyde                                      | Octanol | JAC Numbers         |
|-----------------------------------------------|---------|---------------------|
| Acetamidoacetaldehyde                         | 7.523   | Unknown JAC110, JAC74L |
| (1,2,2-trimethyl-3-cyclopent-1-yl)acetaldehyde| 15.315  | Unknown JAC81      |
| Phenylacetaldehyde N-methyl-N-formylhydrazone| 16.707  | Unknown JAC25      |
| Dodecanal                                     | 18.199  | Unknown JAC24, JAC33 |

**Esters (17)**

| Esters                                        | Octanol | JAC Numbers         |
|-----------------------------------------------|---------|---------------------|
| Propanedioic acid, (bromomethyl)methyl-, bis(1,1-dimethylethyl) ester | 4.019   | Unknown JAC61A     |
| Compound Description                                                                 | Retention Time (min) | Identification | Supporting Information |
|-------------------------------------------------------------------------------------|----------------------|----------------|------------------------|
| Propanoic acid, 2-methyl-, 2-ethyl-1-propyl-1,3-propanediyl ester                   | 4.273                | Unknown        | JAC64                  |
| Butanoic acid, 2-methyl-, methyl ester                                               | 4.359                | Unknown        | JAC45, JAC47           |
| Propanoic acid, 2,2-dimethyl-, 2,4-dinitrophenyl ester                               | 4.361                | Unknown        | JAC60, JAC64           |
| Sulfurous acid, isobutyl pentyl ester                                               | 4.485                | Unknown        | JAC103                 |
| Methyl 2-methoxypropenoate                                                           | 4.824                | Unknown        | JAC30L                 |
| Propanoic acid, 2,2-dimethyl-, 2,4-dinitrophenyl ester                               | 5.488                | Unknown        | JAC45                  |
| 2-Butenoic acid, 2-methyl-, methyl ester                                             | 6.158                | Unknown        | JAC74C                 |
| Vinyl butyrate                                                                      | 6.751                | Unknown        | JAC61A                 |
| Carbonic acid, bis(1-methylethyl) ester                                             | 6.791                | Unknown        | JAC33                  |
| Methyl 2-methylhexanoate                                                             | 8.537                | High           | JAC45, JAC64           |
| Formic acid, heptyl ester                                                           | 8.714                | Unknown        | JAC99                  |
| Propanoic acid, 3-chloro-, 4-formylphenyl ester                                      | 10.547               | Unknown        | JAC54                  |
| Formic acid, 2-ethylhexyl ester                                                      | 11.49                | Unknown        | JAC99, JAC101, JAC64   |
| 6-Octen-1-ol, 3,7-dimethyl-, formate                                                | 15.123               | Unknown        | JAC74C                 |
| 2,4-Furandicarboxylic acid, dimethyl ester                                          | 17.364               | High           | JAC74C                 |
| n-Heptyl methylphosphonofluoridate                                                   | 18.818               | Unknown        | JAC78, JAC95           |
| n-Hexyl methylphosphonofluoridate                                                   | 18.841               | Unknown        | JAC86                  |
| Dodecanoic acid, methyl ester                                                       | 19.695               | High           | JAC35                  |
| Benzoic acid, 4-ethoxy-, ethyl ester                                                | 19.728               | Unknown        | JAC88                  |
| Compound                                                                 | Retention Time | Mass Spectrum | Original JAC | Note          |
|-------------------------------------------------------------------------|----------------|---------------|---------------|---------------|
| Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester      | 20.535         | High          | JAC122        |               |
| Hexanethioic acid, S-methyl ester                                       | 21.058         | Unknown       | JAC81         |               |
| Methyl tetradecanoate                                                   | 22.094         | High          | JAC35, JAC110, JAC74L |          |
| Hexanedioic acid, mono(2-ethylhexyl)ester                               | 28.637         | Unknown       | JAC81         |               |
| Phthalic acid, di(hept-3-yl) ester                                      | 30.506         | Unknown       | JAC81         |               |
| **Hydrocarbons (30)**                                                   |                |               |               |               |
| Cyclohexane, 1,1,2-trimethyl-                                           | 6.691          | Low           | JAC99         |               |
| 4-Octene, 2,3,7-trimethyl-, [S-(E)]-                                    | 9.601          | Unknown       | JAC25         |               |
| 4-Nonene, 3-methyl-, (Z)-                                              | 10.026         | Unknown       | JAC31         |               |
| Cyclopropane, 1-butyl-2-(2-methylpropyl)-                               | 10.337         | Unknown       | JAC87         |               |
| 6-Dodecene, (E)-                                                       | 12.024         | Unknown       | JAC87         |               |
| Undecane                                                                | 12.099         | High          | JAC95, JAC6, JAC122 |          |
| Bicyclo[3.2.0]hepta-2,6-diene                                           | 12.4           | Unknown       | JAC90         |               |
| Cyclopropane, pentyl-                                                  | 12.917         | High          | JAC99, JAC101 |               |
| Cyclopropane, 1-butyl-2-(2-methylpropyl)-                               | 13.103         | Unknown       | JAC86         |               |
| 1,3-Methanopentalene, octahydro-                                       | 14.053         | Unknown       | JAC45, JAC64  |               |
| Dodecane                                                                | 14.56          | High          | JAC95, JAC6, JAC122, JAC68 |          |
| 3-Hexadecene, (Z)-                                                     | 16.299         | Unknown       | JAC122        |               |
| 1-Tridecene                                                             | 16.3           | Unknown       | JAC6          |               |
| 6-Tridecene, (Z)-                                                      | 16.301         | Unknown       | JAC95, JAC68  |               |
| Tricyclo[4.1.0.0(2,7)]heptane                                          | 16.311         | Unknown       | JAC47         |               |
| Compound                                              | Retention Time | Intensity | JAC    |
|-------------------------------------------------------|----------------|-----------|--------|
| Heptylcyclohexane                                     | 17.204         | High      | JAC95, JAC6, JAC122, JAC68 |
| 1,4-Dimethyladamantane                                | 18.726         | Unknown   | JAC95  |
| 3-Heptyne, 5-methyl-                                  | 18.726         | Unknown   | JAC25, JAC81 |
| Cyclopentane, nonyl-                                  | 18.755         | Unknown   | JAC95, JAC6, JAC122 |
| 4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-, [1S-(1.alpha.,4.alpha.,7.alpha.)]-trans,trans- and trans,cis-1,8-Dimethylspiro[5.5]undecane | 18.95          | Unknown   | JAC86  |
| 7-Tetradecene                                         | 19.307         | Low       | JAC35  |
| 6-Tridecane                                           | 19.307         | Unknown   | JAC88  |
| n-Heptadecylcyclohexane                              | 20.143         | Unknown   | JAC95, JAC6, JAC122, JAC68 |
| Cetene                                                | 20.633         | High      | JAC47  |
| 3,4-Nonadien-6-yne, 5-ethyl-3-methyl-1-Nonadecene     | 21.482         | Unknown   | JAC81  |
| 10-Heneicosene (c,t)                                  | 21.758         | Unknown   | JAC25  |
| Cyclohexene, 1,5,5-trimethyl-6-(2-propenylidene)-     | 21.921         | Unknown   | JAC81  |
| 5,6-Decadien-3-yne, 5,7-diethyl-                      | 24.274         | Unknown   | JAC35  |

**Ketones (14)**

| Compound                                                | Retention Time | Intensity | JAC    |
|---------------------------------------------------------|----------------|-----------|--------|
| Cyclobutanone, 2,3-dimethyl-, trans-                    | 4.061          | Unknown   | JAC88, JAC30L |
| 2-Hexanone, 6-methoxy-                                  | 4.29           | Unknown   | JAC6   |
| 3-Hexanone                                              | 4.493          | Low       | JAC99, JAC76, JAC48, JAC6 |
| Compound                                                   | Retention Time | Identity   | Source(s)       |
|------------------------------------------------------------|----------------|------------|-----------------|
| 2-Hexanone                                                 | 4.523          | Unknown    | JAC6            |
| 2-Hydroxy-3-pentanone                                      | 4.856          | Unknown    | JAC88, JAC30L   |
| 3-Hexanone, 5-methyl-                                       | 5.486          | Low        | JAC64           |
| (R)-(+)-3-Methylcyclopentanone                             | 5.742          | High       | JAC6            |
| Butanedioic acid, phenyl-                                  | 6.733          | Unknown    | JAC88           |
| 3-Octanone                                                 | 9.038          | High       | JAC122          |
| 2-Hydroxy-5-ethyl-5-methylcyclopent-2-en-1-one             | 15.944         | Unknown    | JAC81           |
| Bicyclo[3.2.0]hept-2-en-6-one, 7-chloro-2H-Benzocyclohepten-2-one, decahydro-4a-methyl-, trans- | 19.147         | Unknown    | JAC25           |
| Dichlorphen, O,O'-bis(4-fluoro-2-trifluoromethylbenzoyl)-  | 19.496         | Unknown    | JAC61A          |
| Benzoic acid, 3-fluoro-, 2-oxo-2-phenylethyl ester         | 21.976         | Unknown    | JAC25           |

**Terpene and terpenoid (27)**

| Compound                                                   | Retention Time | Identity   | Source(s)       |
|------------------------------------------------------------|----------------|------------|-----------------|
| Tricyclo[2.2.1.0(1,4)]heptan-2-one, 6-nitro-2-Methyl-2-bornene | 9.615          | Unknown    | JAC58           |
| Tricyclo[3.2.1.0(2,4)]octane, 8-methylene-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)- | 10.075         | Unknown    | JAC35           |
| 2-Methylisoborneol                                          | 14.38          | High       | JAC102, JAC99, JAC31, JAC101, JAC60, JAC78, JAC25, JAC72, JAC55, JAC54, JAC61A, JAC90 |
| (2S,4R)-p-Mentha-[1(7),8]-diene 2-hydroperoxide            | 15.292         | Unknown    | JAC86           |
| Compound                                                                 | MW   | Level    | JAC Numbers |
|------------------------------------------------------------------------|------|----------|-------------|
| Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-                | 15.528 | Unknown  | JAC122      |
| 2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester                      | 16.82 | High     | JAC74C      |
| 1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-, (4aS-cis)- | 18.341 | High     | JAC102      |
| Geosmin                                                                | 18.356 | High     | JAC102, JAC31, JAC86, JAC101, JAC33, JAC76, JAC47, JAC64, JAC78, JAC74C, JAC25, JAC95, JAC35, JAC88, JAC55, JAC110, JAC74L, JAC54, JAC61A, JAC75, JAC90, JAC87, JAC81 |
| 1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane | 18.507 | Unknown  | JAC81       |
| Dodecane, 2,6,10-trimethyl-                                            | 18.875 | Low      | JAC6, JAC68, JA95 |
| 1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylene)-, [S-(E,E)]- | 19.27 | High     | JAC25, JAC81 |
| Cyclohexanemethanol, 4-ethenyl-.alpha..alpha..4-trimethyl-3-(1-methylene)-, [1R-(1.alpha.,3.alpha.,4.beta.)]- | 20.162 | High     | JAC74C      |
| Cyclohexanol, 4-ethyl-4-methyl-3-(1-methylene)-, (1.alpha.,3.alpha.,4.beta.)- | 20.279 | Unknown  | JAC87       |
| 2,7-Octadiene-1,6-diol, 2,6-dimethyl-, (E)-                           | 20.454 | Unknown  | JAC81       |
| Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylene)-     | 20.502 | Unknown  | JAC25       |
| Dihydro-cis-.alpha.-copaene-8-ol                                       | 20.549 | Unknown  | JAC24, JAC86, JAC95, JAC87 |
| Compound Description                                                                 | Retention Time | Elution | JAC Codes                          |
|-------------------------------------------------------------------------------------|----------------|---------|------------------------------------|
| epicycubenol                                                                         | 21.128         | High    | JAC25, JAC95, JAC90, JAC87         |
| 1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1R-(1.alpha.,4.beta.,4a.beta.,8a.beta.])- (Cadinol) | 21.182         | High    | JAC17, JAC102, JAC24, JAC86        |
| Alloaromadendrene                                                                    | 21.265         | Low     | JAC88, JAC75, JAC87                |
| Dihydro-cis-alpha-copaene-8-ol                                                       | 21.267         | Unknown | JAC95                              |
| cubenol                                                                             | 21.277         | High    | JAC47, JAC25, JAC110, JAC74L, JAC81|
| 2-Naphthalenemethanol, decahydro-α,α,4a-trimethyl-8-methylene- [2R-(2α,4aa,8aβ)]- | 21.32          | High    | JAC86, JAC101, JAC33, JAC76, JAC74C|
| 7-epi-alpha-selinene                                                                 | 21.544         | Low     | JAC95, JAC87                       |
| 7-epi-alpha-eudesmol                                                                 | 21.599         | Low     | JAC86                              |
| 10-epi-gamma-Eudesmol                                                                | 21.655         | Low     | JAC31                              |
| **Diverse functional groups (43)**                                                  |                |         |                                    |
| Butane, 2-azido-2,3,3-trimethyl-                                                    | 4.022          | Unknown | JAC72, JAC75, JAC81                |
| t-Butyl cyclopentaneperoxycarboxylate                                              | 4.026          | Unknown | JAC96                              |
| t-Butyl cyclopentaneperoxycarboxylate                                              | 4.057          | Unknown | JAC96                              |
| 1-n-Butoxy-2,3-dimethylidiaziridine                                                | 4.065          | Unknown | JAC75                              |
| 1-Heptene, 3-methoxy-                                                               | 4.268          | Unknown | JAC74C                             |
| Toluene                                                                              | 4.322          | Low     | JAC103                             |
| (2,3,3-Trimethyloxiranyl)methanol                                                  | 4.714          | Unknown | JAC88                              |
| 2-Furanmethanol                                                                     | 5.826          | Unknown | JAC30L                             |
| Hexanenitrile                                                                       | 6.403          | High    | JAC60, JAC78, JAC61A               |
| Chemical Name                                                                 | Retention Time | Detection Level | Supporting Information |
|------------------------------------------------------------------------------|----------------|-----------------|------------------------|
| Pyrazine, 2,5-dimethyl-                                                      | 7.23           | High            | JAC17, JAC24, JAC31, JAC33, JAC47, JAC64, JAC78, JAC74C, JAC25, JAC35, JAC96, JAC110, JAC74L, JAC61A, JAC30L, JAC87, JAC81 |
| 1,6:3,4-Dianhydro-2-deoxy-.beta.-d-ribo-hexopyranose                        | 8.253          | Unknown         | JAC88                  |
| Dimethyl trisulfide                                                          | 8.636          | Unknown         | JAC90                  |
| 3(2H)-Thiophenone, dihydro-2-methyl-                                         | 9.139          | Unknown         | JAC96                  |
| Ethanol, 2-(2-ethoxyethoxy)-                                                | 9.425          | High            | JAC17                  |
| 6-Azabicyclo[3,2,0]heptan-7-one                                              | 10.079         | Unknown         | JAC61A                 |
| Benzoyl bromide                                                             | 11.954         | Unknown         | JAC86, JAC76           |
| Hydrazine, (phenylmethyl)-                                                  | 12.396         | Unknown         | JAC55                  |
| Iron, tricarbonyl[(2,3,4,5-eta.)-2,4-cycloheptadien-1-ol]-                 | 13.856         | Unknown         | JAC45                  |
| Benzene, (iodomethyl)-                                                      | 13.969         | Unknown         | JAC30L                 |
| Benzene, [(methylsulfonyl)methyl]-                                          | 14.023         | Unknown         | JAC58                  |
| Iron, tricarbonyl[(2,3,4,5-eta.)-2,4-cycloheptadien-1-ol]-                 | 14.818         | Unknown         | JAC45                  |
| Sydnone, 3-(phenylmethyl)-                                                  | 14.82          | Unknown         | JAC64                  |
| Benzothiazole                                                               | 15.082         | Unknown         | JAC61A                 |
| Tricyclo[3.3.1.1(3,7)]decanone, 4-iodo-, (1.alpha.,3.beta.,4.beta.,5.alpha.,7.beta.)- | 15.236         | Unknown         | JAC25, JAC81           |
| Phenol, 4-[2-(methylamino)ethyl]-                                           | 15.317         | Unknown         | JAC25                  |
| (3R,2E)-2-(Hexadec-15-ynylidene)-3-hydroxy-4-methylenebutanolide           | 18.654         | Unknown         | JAC81                  |
| Compound Description | Retention Time (min) | Identification | Source |
|----------------------|---------------------|----------------|--------|
| Cyclobutaneacetonitrile, 1-methyl-2-(1-methylethylidene)- | 18.78 | Unknown | JAC86 |
| Pyrrol-2(5H)-one, 4-acetyl-3-hydroxy-5-(3-nitrophenyl)-1-[2-(1-piperazinyl)ethyl]- | 18.795 | Unknown | JAC87 |
| 3-Isopropoxy-1,1,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane | 18.96 | Unknown | JAC87 |
| tert-Butyl 3-methylbutyl disulfide | 18.977 | Unknown | JAC33 |
| 1-Hexyl-2-nitrocyclohexane | 20.947 | Unknown | JAC74C |
| β-Vatirenene | 21.177 | Unknown | JAC72, JAC75, JAC81 |
| 10-Methylundecan-4-olide | 21.22 | Low | JAC74C |
| 10-Methyldodecan-5-olide | 22.831 | Low | JAC45 |
| 1-Nitrosoadamantane | 24.376 | Unknown | JAC35 |
Table S6. VOCs annotated with high confidence in the pooled culture screen using conventional method.

| VOCs*          | Retention time (min) | Annotated in (isolates)                  | Reported in plants | Reported in Streptomyces |
|----------------|----------------------|------------------------------------------|--------------------|--------------------------|
| **Alcohols**   |                      |                                          |                    |                          |
| DL-2,3-Butanediol | 4.798               | JAC17, JAC47                             | No                 | No                       |
| 1-Hexanol      | 6.223                | JAC60, JAC61A                            | Yes                | Yes                      |
| 1-Octen-3-ol   | 8.963                | JAC74C                                   | Yes                | No                       |
| Benzyl alcohol | 10.29                | JAC17, JAC58, JAC25, JAC122, JAC30L       | Yes                | Yes                      |
| 1-Octanol      | 11.282               | JAC99, JAC101, JAC64, JAC17, JAC31, JAC86, JAC101, JAC17, JAC30L | Yes | Yes |
| Phenylethyl Alcohol | 12.432          | JAC33, JAC58, JAC74C, JAC25, JAC110, JAC74L, JAC30L | Yes | Yes |
| 1-Dodecanol    | 19.054               | JAC68                                    | No                 | No                       |
| **Esters**     |                      |                                          |                    |                          |
| Methyl 2-methylhexanoate | 8.537       | JAC45, JAC64                             | No                 | No                       |
| 2,4-Furandicarboxylic acid, dimethyl ester | 17.364 | JAC74C | No | No |
| Dodecanoic acid, methyl ester | 19.695 | JAC35 | Yes | Yes |
| Pentanoic acid, 2,2,4-trimethyl-3-carboxisopropyl, isobutyl ester | 20.535 | JAC122 | No | No |
| Methyl tetradecanoate | 22.094 | JAC35, JAC110, JAC74L | Yes | No |
| **Hydrocarbons** |                      |                                          |                    |                          |
| Undecane       | 12.099               | JAC95, JAC6, JAC122                      | Yes                | No                       |
| Cyclopropane, pentyl- | 12.917       | JAC99, JAC101                           | Yes                | No                       |
| Dodecane       | 14.56                | JAC95, JAC6, JAC122, JAC68               | Yes                | Yes                      |
| Heptylcyclohexane | 17.204           | JAC95, JAC6, JAC122, JAC68               | Yes                | No                       |
| Cetene         | 20.633               | JAC47                                    | No                 | No                       |
| **Ketones**    |                      |                                          |                    |                          |
| (R)-(+)-3-Methylcyclopentanone | 5.742  | JAC6 | No | No |
| 3-Octanone     | 9.038                | JAC122                                   | No                 | No                       |
| Terpenes and terpenoids                                                                 | Supporting Information                                                                 |
|----------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|
| 2-Methyl-2-bornene                                                                      | JAC25                                                                                  | No | Yes |
| 2-Methylisoborneol                                                                      | JAC102, JAC99, JAC31, JAC101, JAC60, JAC78, JAC25, JAC72, JAC55, JAC54, JAC61A, JAC90 | No | Yes |
| **2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester**                                   |                                                                                        | No | No |
| 1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene- (4aS-cis)- |                                                                                        | Yes | Yes |
| Geosmin                                                                                |                                                                                        | No | Yes |
| 1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [S-(E,E)]-                |                                                                                        | Yes | Yes |
| Cyclohexanemethanol, 4-ethenyl-alpha...alpha..4-trimethyl-3-(1-methylethenyl)-, [1R-(1.alpha.,3.alpha.,4.beta.)]- |                                                                                        | No | Yes |
| Epi-cubenol                                                                            |                                                                                        | No | Yes |
| 1-Naphthalenol, 1,2,3,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1R-(1.alpha.,4.beta.,4a.beta.,8a.beta.)] - (Cadinol) |                                                                                        | Yes | No |
| Cubenol                                                                                |                                                                                        | Yes | Yes |
| 2-Naphthalenemethanol, decahydro-\(\alpha,\alpha,4a\)-trimethyl-8-methylene-, [2R-(2\(\alpha,\alpha,8\beta\)])- |                                                                                        | Yes | Yes |

**Diverse functional groups**
| VOC                          | Retention Time (min) | Strains                                      | Supporting Information |
|------------------------------|----------------------|----------------------------------------------|-------------------------|
| Hexanenitrile                | 6.403                | JAC60, JAC78, JAC61A                        | No                      |
| Pyrazine, 2,5-dimethyl-      | 7.23                 | JAC17, JAC24, JAC31, JAC33, JAC47, JAC64, JAC78, JAC74C, JAC25, JAC35, JAC96, JAC110, JAC74L, JAC61A, JAC30L, JAC87, JAC81 | No                      |
| Ethanol, 2-(2-ethoxyethoxy)- | 9.425                | JAC17                                        | No                      |

* VOCs have not been reported from *Streptomyces* previously are highlighted in bold.
**Table S7.** Bacterially derived compounds annotated in replicate VOC analysis of the six selected *Streptomyces* isolates using the MShub/GNPS. VOCs annotated during both the pooled culture screen and the replicated analysis are shown in bold and labelled with an asterisk*.

| Compound/VOC                                      | Retention time (min) | Annotated in (isolates)                  | Media              |
|--------------------------------------------------|-----------------------|------------------------------------------|--------------------|
| Benzaldehyde, 3-Methoxy-4-(Phenylmethoxy)-        | 4.25                  | JAC95, JAC25, JAC45                     | YMS, Synthetic, SFM|
| 2,4-Heptanedione, 6-Methyl-                        | 4.52                  | JAC25, JAC74C                           | SFM, YMS, Synthetic|
| Hexenyl Butanoate (3Z-)                            | 4.62                  | JAC74C, JAC60, JAC81, JAC25             | SFM, Synthetic, YMS|
| Hexenyl Isobutanoate (3Z-)                         | 4.62                  | JAC81, JAC95, JAC25                     | YMS, Synthetic, SFM|
| **Octanol (2-)**                                  |                       |                                          |                    |
| Nonacosane*                                       | 5.2                   | JAC45, JAC60, JAC81, JAC60, JAC95       | YMS, Synthetic, SFM|
| Triacontane                                       | 5.2                   | JAC60, JAC25                            | Synthetic, SFM, YMS|
| **1-Butanol**                                     |                       |                                          |                    |
| Nonane, 2,2,4,4,6,8,8-Heptamethyl-                 | 5.48                  | JAC60, JAC25                            | Synthetic, SFM, YMS|
| 4-Piperidinone, 2,2,6,6-Tetramethyl-               | 5.53                  | JAC60, JAC74C, JAC25, JAC95             | Synthetic, SFM, YMS|
| **Pentanone (4-OH-4-Me-2-)**                      | 5.53                  | JAC81, JAC74C                          | YMS, Synthetic, SFM|
| Hexenyl 3-Methyl Butanoate (3Z-)*                 | 5.65                  | JAC81, JAC95, JAC25                     | YMS, Synthetic, SFM|
| Cyclohexanone, 2,6-Dimethyl-                       | 5.75                  | JAC74C, JAC25, JAC81                    | SFM, Synthetic, YMS|
| **Pentadecafluoroctanoic Acid, 2-Methylpent-3-Yl Ester** | 5.93                  | JAC60, JAC25, JAC74C, JAC95, JAC45      | Synthetic, SFM, YMS|
| Nonadecanoic Acid Methyl Ester                    | 5.93                  | JAC95, JAC60                            | YMS, Synthetic     |
| Benzenemethanamine, N-Phenyl-                     | 6.03                  | JAC74C, JAC95, JAC25, JAC45             | SFM, Synthetic, YMS|
| Silane, Trichlororooctadecyl-                     | 6.1                   | JAC25, JAC95                            | SFM, YMS, Synthetic|
| **1-Hexanol**                                     |                       |                                          |                    |
| 1-Ethylpentyl Acetate                              | 6.22                  | JAC60, JAC95, JAC81                     | Synthetic, SFM, YMS|
| **1-Hexanethiol**                                 | 6.29                  | JAC60, JAC95                            | Synthetic, SFM, YMS|
| Compound                                                                 | Retention Time | JAC | Notes                      |
|------------------------------------------------------------------------|----------------|-----|----------------------------|
| N-Trimethylsilylphenylacetylglucose Trimethylsilyl Ester               | 6.33           | JAC60 | Synthetic, SFM, YMS          |
| **Carbonic Acid, Monoamide, N-Hexadecyl-, Allyl Ester**               | 6.59           | JAC45 | YMS, Synthetic, SFM          |
| Nonanol                                                                | 6.62           | JAC60, JAC95, JAC74C | Synthetic, SFM, YMS          |
| 2,4-Dimethylcyclopentanone                                             | 6.62           | JAC74C, JAC25 | SFM, Synthetic, YMS          |
| **Hexyl Acetate**                                                      | 6.62           | JAC95 | YMS, Synthetic, YMS          |
| Butanamide, N,N-Diethyl-3-Oxo-1H-Inden-1-One, 2,3-Dihydro-            | 6.73           | JAC74C, JAC25 | SFM, Synthetic, YMS          |
| **Benzyl Chloride**                                                    | 6.96           | JAC45, JAC60, JAC81, JAC95 | SFM, Synthetic, YMS          |
| Ethylene Glycol Monoisobutyl Ether                                    | 7.01           | JAC74C, JAC25, JAC95, JAC81 | SFM, Synthetic, YMS          |
| **2-Propyl-5,5-Dimethyl-1,3-Cyclohexanediene**                        | 7.14           | JAC74C, JAC60, JAC95, JAC81, JAC45 | SFM, Synthetic, YMS          |
| 2-Butyrylfuran                                                        | 7.14           | JAC95, JAC45 | YMS, Synthetic, SFM          |
| **Pentadecafluoroctanoic Acid, 3-Methylbut-2-Yl Ester**               | 7.29           | JAC74C, JAC25 | SFM, Synthetic, YMS          |
| Cyclohexanol Acetate (Trans-2-Tert-Butyl)                             | 7.4            | JAC45 | YMS, Synthetic, SFM          |
| Vinyl 10-Undecenoate                                                  | 7.4            | JAC74C, JAC81 | SFM, Synthetic, YMS          |
| Cyclopentadecanolide                                                  | 7.4            | JAC95, JAC45 | YMS, Synthetic, SFM          |
| Thujene (Alpha-)                                                      | 7.78           | JAC45 | YMS, Synthetic, SFM          |
| Octyl P-Toluene sulfonate                                             | 7.95           | JAC74C, JAC95 | YMS, Synthetic, YMS          |
| 1-Hexanol, 4-Methyl- (S)-                                             | 8.02           | JAC45 | YMS, Synthetic, SFM          |
| **9-Octadecenoic Acid, Methyl Ester, (E)**                            | 8.12           | JAC95, JAC81, JAC45 | YMS, Synthetic, SFM          |
| ((5-Isopropyl-2-Methylcyclohexyl)Sulfonylmethyl)Benzene                | 8.26           | JAC74C, JAC25 | SFM, Synthetic, YMS          |
| **Cis-1-Chloro-9-Octadecene**                                         | 8.37           | JAC45, JAC74C | Synthetic, SFM               |
| Oleic Anhydride                                                       | 8.38           | JAC60, JAC74C, JAC25 | Synthetic, SFM, YMS          |
| N,N’-Bis(4,5-Dihydro-3-Furoyl)-M-Phenylenediamine                     | 8.54           | JAC60, JAC81 | Synthetic, SFM, YMS          |
| 1-Heptanol                                                            | 8.66           | JAC60, JAC95, JAC45 | Synthetic, SFM, YMS          |
| Substance                                                   | pIC50 | JACs                          | Source               |
|--------------------------------------------------------------|-------|-------------------------------|----------------------|
| Cimetidine                                                  | 8.73  | JAC45                         | YMS, Synthetic, SFM  |
| Hexanoic Acid                                               | 8.79  | JAC25                         | Synthetic, YMS       |
| **Benztropine**                                            | 8.79  | JAC81                         | YMS, Synthetic, SFM  |
| **10-Methyl-1-Dodecanol**                                   | 8.85  | JAC25, JAC45, JAC74C, JAC60,  | SFM, Synthetic, YMS  |
|                                                            |       | JAC81                         |                      |
| N,N’-(M-Phenylene)Dibenzamide                               | 8.87  | JAC45, JAC95                  | YMS, Synthetic, SFM  |
| 1-Undecanol                                                 | 8.92  | JAC95, JAC25,                 | YMS, Synthetic, SFM  |
| 10-Hydroxydecanoic Acid                                     | 8.93  | JAC60, JAC74C                 | Synthetic, SFM, YMS  |
| **7-Ethyl-2-Methylundecan-1-ol**                            | 8.93  | JAC74C, JAC25                 | SFM, Synthetic       |
| Ethyl 3-(6-Methoxy-3-Methyl-2-Benzofuranyl)-3-(P-Methoxyphenyl)Propionate | 9.02  | JAC25, JAC81, JAC95           | SFM, YMS, Synthetic  |
| **1-Octanol**                                               | 9.04  | JAC25, JAC95                  | SFM, YMS, Synthetic  |
| Cyanoacetic Acid, Heptyl Ester                              | 9.13  | JAC45, JAC45                  | YMS, Synthetic, SFM  |
| Heptane, 2-Chloro-                                          | 9.13  | JAC60, JAC25, JAC74C, JAC95,  | Synthetic, SFM, YMS  |
|                                                            |       | JAC45                         |                      |
| Pentyl Furan (2-)                                           | 9.18  | JAC60, JAC95, JAC45, , JAC25  | Synthetic, SFM, YMS  |
| Propylene Glycol                                            | 9.21  | JAC45, JAC81, JAC74C          | YMS, Synthetic, SFM  |
| **3,3-Diethylglutaric Acid**                                | 9.4   | JAC60, JAC25, JAC95, JAC81,   | Synthetic, SFM, YMS  |
|                                                            |       | JAC45, JAC74C                 |                      |
| Tetradeacne                                                 | 9.47  | JAC25, JAC95                  | SFM, YMS, Synthetic  |
| Cetotiamine                                                 | 9.47  | JAC60, JAC95, JAC81           | Synthetic, YMS       |
| 3-Amino-4,5,6,7,8,9-Hexahydrocyclooct(C)Isoxazole          | 9.5   | JAC45                         | YMS, Synthetic, SFM  |
| 4,5-Dimethyl-2-Propyloxazole                                | 9.62  | JAC25                         | SFM, YMS, Synthetic  |
| 2,2,5-Trimethyl-1-Phenyl-4-Hexen-1-ol                      | 9.62  | JAC60, JAC25                  | Synthetic, SFM, YMS  |
| S,S’-(Thiodi-P-Phenylene) Bis(2-Methyl-2-Propenethioate)   | 9.62  | JAC74C, JAC45                 | SFM, Synthetic, YMS  |
| **2-Butylcyclopentanone**                                   | 9.67  | JAC60, JAC74C, JAC81          | Synthetic, SFM, YMS  |
| 2-Piperidinoethyl 3,5-Dichlorobenzoate                     | 9.71  | JAC60, JAC45                  | Synthetic, SFM, YMS  |
| Nonadienal (2E, 6Z)                                         | 9.82  | JAC60                         | Synthetic, SFM, YMS  |
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| Chemical Name                                      | Retention Time | JAC Samples | Supporting Information |
|----------------------------------------------------|----------------|-------------|------------------------|
| 1,3-Propanediol, 2-Butyl-2-Ethyl-*                 | 9.84           | JAC25, JAC45, JAC74C, JAC60, JAC95, JAC81 | YMS, Synthetic, SFM, Synthetic, YMS |
| Methacrylic Acid 2-Ethylhexyl Ester                | 9.84           | JAC74C, JAC25, JAC95 | YMS, Synthetic, SFM, Synthetic, YMS |
| Pentadecafluorooctanoic Acid, Heptyl Ester*        | 9.84           | JAC95, JAC74C, JAC25, JAC45, JAC60 | YMS, Synthetic, SFM, Synthetic, YMS |
| Bulnesene (Alpha-)                                 | 9.97           | JAC60, JAC45, JAC81, JAC95, JAC25 | Synthetic, SFM, YMS |
| (S)-(−)-(4-Isopropenyl-1-Cyclohexenyl)Methanol     | 10.07          | JAC60, JAC95, JAC81 | Synthetic, SFM, YMS |
| (S)-(+)−5-Methyl-1-Heptanol                        | 10.14          | JAC60, JAC45, JAC74C, JAC25, JAC95 | Synthetic, SFM, YMS |
| Geraniol                                           | 10.21          | JAC25, JAC45 | SFM, YMS, Synthetic |
| Cresol (Ortho-)*                                   | 10.27          | JAC95, JAC45, JAC25 | YMS, Synthetic, SFM, Synthetic, YMS |
| Benzyl Alcohol*                                    | 10.3           | JAC60, JAC25 | SFM, YMS |
| 4-Nitrobenzyl Alcohol                              | 10.31          | JAC95 | YMS, Synthetic, SFM, YMS |
| N-((Methylphenylamino)Methyl)Benzamide*            | 10.31          | JAC95 | YMS, Synthetic, SFM, YMS |
| Cis-1,2-Cyclohexanediol*                           | 10.43          | JAC60, JAC74C, JAC25, JAC95, JAC81, JAC45 | Synthetic, SFM, YMS |
| Fumaric Acid, 3-Fluorophenyl Tetradecyl Ester      | 10.53          | JAC60, JAC25 | Synthetic, SFM, YMS |
| N-Tetracosanol-1                                   | 10.53          | JAC74C, JAC81, JAC45 | SFM, Synthetic, YMS |
| 1-Methylbutyl Acetoacetate                        | 10.58          | JAC60, JAC25 | Synthetic, SFM, YMS |
| 3,4-Epoxy Mentane                                  | 10.77          | JAC60, JAC74C, JAC45 | Synthetic, SFM, YMS |
| Heptane, 2,3-Dimethyl-                             | 10.85          | JAC60, JAC25 | Synthetic, SFM, YMS |
| Pentadecane, 2,6,10,14-Tetramethyl-                | 10.85          | JAC74C, JAC95 | SFM, Synthetic, YMS |
| Cyclopentadecane*                                  | 10.89          | JAC74C, JAC81 | Synthetic, SFM, YMS |
| Dodecane*                                          | 11             | JAC60, JAC25, JAC95, JAC74C | Synthetic, SFM, YMS |
| Pentadecane*                                       | 11             | JAC74C, JAC45, JAC60, JAC95 | SFM, Synthetic, YMS |
| Oleic Acid*                                        | 11.05          | JAC74C, JAC25, JAC95, JAC81, JAC45 | Synthetic, SFM, YMS |
| Acetophenone                                       | 11.09          | JAC74C, JAC81, JAC45, JAC25 | SFM, Synthetic, YMS |
| Benzamide, N-(2′-Ethylphenyl)-                     | 11.1           | JAC95, JAC60 | YMS, Synthetic, SFM |
| Compound                                      | Retention Time | Peaks Present                                      | Supporting Information |
|----------------------------------------------|----------------|---------------------------------------------------|-------------------------|
| Decylamine, N-allyl-                         | 11.25          | JAC60, JAC74C, JAC25, JAC81                       | Synthetic, SFM, YMS     |
| 1-Tetradecanol*                              | 11.29          | JAC60, JAC74C, JAC25, JAC45, JAC95                | Synthetic, SFM, YMS     |
| Methyl P-Aminosalicylate                     | 11.38          | JAC60, JAC81                                       | Synthetic, SFM, YMS     |
| 12-Methyl-1-Tetradecanol                    | 11.42          | JAC60, JAC25, JAC81                               | Synthetic, SFM, YMS     |
| 7-Tetradecene*                               | 11.61          | JAC60, JAC74C, JAC95, JAC25                      | Synthetic, SFM, YMS     |
| 18-Nonadecenoic Acid                         | 11.72          | JAC60, JAC95                                      | Synthetic, SFM, YMS     |
| Dodecyl Formate*                             | 11.72          | JAC74C, JAC25, JAC81                              | SFM, Synthetic, YMS     |
| Octane, 2,3-Dichloro-S-Benzoyl-N-(O-Hydroxybenzylidene)Thiohydroxylamine | 11.86          | JAC60, JAC95, JAC25, JAC81                        | Synthetic, SFM, YMS     |
| Methyl Benzoate                              | 11.89          | JAC74C, JAC45, JAC25                             | SFM, Synthetic, YMS     |
| Hexahydro-2H-Pyrido(1,2-A)Pyrazin-3(4H)-One  | 11.96          | JAC60, JAC74C, JAC95, JAC25, JAC81, JAC45         | Synthetic, SFM, YMS     |
| Undecane*                                    | 12.01          | JAC81                                            | YMS, Synthetic, SFM     |
| L-Proline, N-(Cyclopentylcarbonyl)-, Undecyl Ester | 12.01          | JAC81, JAC45                                     | YMS, Synthetic, SFM     |
| Linalool                                     | 12.05          | JAC74C, JAC95, JAC81                              | SFM, Synthetic, YMS     |
| Camphene_Adms                                | 12.05          | JAC81, JAC74C                                    | YMS, Synthetic, SFM     |
| Dodecyl Octyl Ether                          | 12.09          | JAC25, JAC45, JAC95, JAC74C                      | SFM, YMS, Synthetic     |
| 2,3-Dihydroxy-3,7,11,15-Tetramethylhexadecan-1-ol Nitrate | 12.09          | JAC60, JAC74C                                    | Synthetic, SFM, YMS     |
| 3,5,5-Trimethylhexanol                        | 12.19          | JAC45, JAC95                                      | YMS, Synthetic, SFM     |
| 1,1,4-Trimethylcyclohexane*                  | 12.19          | JAC60, JAC81, JAC95                              | Synthetic, SFM, YMS     |
| 2-Propanoic Acid, 2-Methyl-, 1,2-Ethanediyl Ester | 12.35          | JAC60, JAC25                                      | Synthetic, SFM, YMS     |
| Didodecylphosphine Oxide                     | 12.41          | JAC74C, JAC25, JAC81                              | SFM, Synthetic, YMS     |
| Cyclopentanecarboxamide, N-(Cyclopentylcarbonyl)-N-Isobutyl- | 12.42          | JAC74C, JAC25, JAC81                              | Synthetic, SFM          |
| Phenyl Ethyl Alcohol*                        | 12.42          | JAC45, JAC25, JAC95                              | YMS, Synthetic, SFM     |
| Heptane, 1,1’-Oxybis-                        | 12.44          | JAC60, JAC74C, JAC25, JAC95                      | Synthetic, SFM, YMS     |
| Compound                                      | Retention Time | Sources                        | Notes                  |
|-----------------------------------------------|----------------|--------------------------------|------------------------|
| 2-Tert-Butylcyclohexanone*                    | 12.85          | JAC60, JAC74C, JAC95, JAC81, JAC45 | Synthetic, SFM, YMS    |
| Propanoic Acid, 2-Methyl-, 2-Methypentyl Ester | 12.93          | JAC60, JAC95, JAC81             | Synthetic, SFM, YMS    |
| Tartaric Acid-Tetra-Tms                       | 13             | JAC25, JAC60                    | SFM, YMS, Synthetic    |
| 2-Heptylfuran                                 | 13             | JAC95                          | YMS, Synthetic, SFM    |
| Cyclopentasiloxane, Decamethyl-2-Heptenoic Acid | 13.08          | JAC60, JAC95, JAC81            | Synthetic, SFM, YMS    |
| Cyclodecanone                                 | 13.22          | JAC81, JAC95, JAC25, JAC45     | SFM, Synthetic, YMS    |
| Tricosane                                     | 13.28          | JAC81                          | YMS, Synthetic, SFM    |
| 2,3-Dimethyl-3-Heptene, (Z)-                  | 13.41          | JAC25, JAC45                   | SFM, YMS, Synthetic    |
| 1-Methoxy-2-Methylbenzene                     | 13.48          | JAC45                          | YMS, Synthetic, SFM    |
| 2,4,4-Trimethyl-1-Hexene*                     | 13.57          | JAC60, JAC45                   | Synthetic, SFM, YMS    |
| Docosyl Pentyl Ether*                         | 13.69          | JAC74C, JAC25                  | SFM, Synthetic, YMS    |
| Cyclohexanol, 5-Methyl-2-(1-Methylethyl)-*    | 14.07          | JAC60, JAC74C, JAC25, JAC95, JAC45 | Synthetic, SFM, YMS |
| Cyclohexane, 2-Chloro-4-Methyl-1-(1-Methylethyl)-, [1S-(1.Alpha.,2.Beta.,4.Beta.)]- | 14.16          | JAC60, JAC95, JAC45            | Synthetic, SFM, YMS    |
| 2-Methylisoborneol*                           | 14.35          | JAC60                          | Synthetic, SFM, YMS    |
| Bornyl Pentanoate                             | 14.44          | JAC81                          | YMS, Synthetic, SFM    |
| N-Octadecane*                                 | 14.56          | JAC60, JAC81                   | Synthetic, SFM, YMS    |
| (Z)-2-Tridecen-1-ol                           | 14.65          | JAC60                          | Synthetic, SFM, YMS    |
| Tridecanal                                    | 14.65          | JAC81                          | YMS, Synthetic, SFM    |
| P-Benzylxoxybenzaldehyde                      | 14.79          | JAC25, JAC74C                  | Synthetic, YMS         |
| Semicarbazone                                 |                |                                |                        |
| 1-Chloroeicosane*                             | 14.83          | JAC25, JAC45, JAC74C           | SFM, YMS, Synthetic    |
| Ethanone, 2-Chloro-1-(2,4-Dimethylphenyl)-*   | 14.88          | JAC95, JAC81                   | Synthetic, SFM         |
| P-Methoxybenzylazidoformate                   | 14.95          | JAC60, JAC45, JAC74C           | Synthetic, SFM, YMS    |
| 2-(1-Cyclohexenyl)Cyclohexanone*              | 15.23          | JAC74C, JAC81, JAC95           | SFM, Synthetic, YMS    |
| Compound                                                                 | RRT  | Reference                  | Supplier       |
|-------------------------------------------------------------------------|------|----------------------------|----------------|
| Carbonic Acid, Monoamide, N-Isobutyl-, 2-Methoxyethyl Ester Cyclohexanecarboxylic Acid, 1-Phenyl-Calamenene (Cis-) | 15.38| JAC25, JAC81               | SFM, Synthetic |
| (2-Hydroxy-4,5-Dimethylbenzoyl)Formic Acid Phthalic Acid Dipropyl Ester Bis(3-Methoxybenzyl) Ether                  | 15.49| JAC74C, JAC95, JAC45, JAC25 | SFM, Synthetic, YMS |
| (7S)-(−)-10,10-Di-Me-5-Thia-4-Azatricyclo[5.2.1.03,7]Dec-3-Ene-5,5-Dioxide* | 15.58| JAC45                       | YMS, Synthetic, SFM |
| Ethyl Acetophenone (P-)*                                                | 15.75| JAC74C, JAC81, JAC95, JAC45, JAC25 | SFM, Synthetic, YMS |
| 3,4-Dimethylbenzophenone                                                | 15.84| JAC74C, JAC45               | SFM, Synthetic, YMS |
| Gamma-Linolenic Acid                                                   | 15.84| JAC81                       | Synthetic, SFM  |
| 1-Hexanol, 5-Methyl-2-(1-Methylethyl)-Pentadecafluoroctanoic Acid, 2-Ethylhexyl Ester* | 15.93| JAC95, JAC81               | YMS, Synthetic, SFM |
| (Z,Z,Z)-6,9,15-Octadecatrienoic Acid Methyl Ester*                      | 16.02| JAC60, JAC74C, JAC25, JAC81 | Synthetic, YMS  |
| 2′-Ethylpropiophenone*                                                 | 16.15| JAC25, JAC74C, JAC81, JAC95, JAC45 | SFM, YMS, Synthetic |
| Benzoic Acid, Heptyl Ester                                              | 16.19| JAC81                       | YMS, Synthetic, SFM |
| 4-N-Dodecylresorcinol                                                   | 16.19| JAC81, JAC60                | Synthetic, SFM  |
| 4-Tert-Butylphenyl Acetate                                              | 16.26| JAC81, JAC95                | YMS, Synthetic, SFM |
| Tridecanol*                                                             | 16.3  | JAC81                       | YMS, Synthetic, SFM |
| 3,4-Dimethylbenzoic Acid                                               | 16.36| JAC25                       | SFM, Synthetic  |
| Trimethylsilyl Ester                                                   | 16.36| JAC25                       | YMS, SFM        |
| 4-Formyl-2-Methoxytropone                                              | 16.36| JAC25                       | YMS, SFM        |
| N,N′-(4-Methyl-M-Phenylene)Bisacetamide                                 | 16.64| JAC95, JAC60                | YMS, Synthetic, SFM |
| Decyl Heptyl Ether                                                      | 16.81| JAC25, JAC74C, JAC95        | SFM, YMS, Synthetic |
| Chemical Name                        | Retention Time | JAC Codes                     |
|-------------------------------------|----------------|--------------------------------|
| Hexane, 3,3-Dimethyl-               | 17.11          | JAC25, JAC74C                 |
| Phenethyl Acetate                   | 17.37          | JAC74C                        |
| 4’-Ethylpropiophenone               | 17.4           | JAC25, JAC74C                 |
| **Cubebeene (Alpha-)**              | 17.77          | JAC95, JAC81                  |
| **Caryophyllene (Z-)**              | 17.93          | JAC95, JAC81, JAC25           |
| Guaiadiene (6,9-)                   | 18.05          | JAC60, JAC74C, JAC81, JAC95,  |
|                                     |                | JAC45, JAC25, JAC74C          |
| Gamma-Muurolene                     | 18.05          | JAC74C, JAC25, JAC95, JAC81   |
| Ibuprofen                           | 18.23          | JAC25, JAC74C, JAC60, JAC45   |
| (1S,2E,4E,7E,11E)-10-Oxocembre-2,4,7,11-Tetraene | 18.23 | JAC95 |
| Longifolene                          | 18.3           | JAC74C, JAC60, JAC45, JAC95   |
| 5,9,13,17-Tetramethyl 4,8,12,16-Octadecatetraenoic Acid | 18.5 | JAC25 |
| 5-Acetylsalicylamide                | 18.5           | JAC25, JAC60, JAC95           |
| 2,6,10,15,19,23-Pentamethyl-2,6,18,22-Tetracosatetraen-10,15-Diol | 18.51 | JAC74C, JAC45 |
| Beta-Caryophyllene                  | 18.51          | JAC81                         |
| 1-Ethyl-Trans-2-Butenyl 2,4,6-Trimethylbenzoate, (+/-)- | 18.76 | JAC25, JAC74C, JAC60, JAC81 |
| Eicosyl Isobutyl Ether              | 18.86          | JAC60, JAC81                  |
| 2,6-Di-Tert-Butyl-1,4-Benzquinone   | 18.93          | JAC74C, JAC45, JAC60, JAC45   |
| 2,5-Dimethoxy-alpha-Methyl-Benzeneethanamine | 18.99 | JAC95 |
| **Carbonic Acid, 2,2,2-Trichloroethyl 2-Ethylhexyl Ester** | 19.06 | JAC81, JAC95 |
| Cyclodecane                         | 19.13          | JAC25, JAC74C, JAC60, JAC95,  |
|                                     |                | JAC45                         |
| **Eicosane**                        | 19.26          | JAC60, JAC25                  |
| Bis(2-Ethylhexyl)Hydrogen Phosphate | 19.63          | JAC81                         |
| Liguloxide                          | 19.7           | JAC81, JAC95                  |
| **Octadecane**                      | 19.85          | JAC25, JAC60, JAC81           |
| **Nonadecane**                      | 19.86          | JAC74C, JAC81                 |
| Compound                                                                 | Retention Time | JAC Codes |
|------------------------------------------------------------------------|----------------|-----------|
| Malonic Acid, Di(4-Heptyl) Ester*                                      | 20.09          | JAC25, JAC60, JAC95, JAC45 |
| Heptylcyclohexane*                                                     | 20.14          | JAC81     |
| 3,7-Dimethyl-6-Octenyl 3-Methylbutyrate                                | 20.3           | JAC45     |
| Diethyl Phthalate                                                      | 20.54          | JAC25, JAC74C, JAC81, JAC45 | SFM, YMS, Synthetic |
| 2H-Pyran-2-One, Tetrahydro-6-Nonyl-Benzophenone                        | 21.06          | JAC81, JAC25 | YMS, Synthetic, SFM |
| Androstane-1,4-diene                                                  | 21.12          | JAC74C, JAC60, JAC45 | SFM, Synthetic, YMS |
| Cyclopentanecarboxylic Acid, 1-(4-Methylphenyl)-(1S,3S,4R)-(+-)-Methyl (R)-P-Toluenesulfinate | 21.31          | JAC45, JAC74C, JAC60, JAC25, JAC95, JAC81 | YMS, Synthetic, SFM |
| 1-Pentadecene                                                        | 21.59          | JAC25, JAC60, JAC45 | SFM, YMS, Synthetic |
| Triacontane, 1-Iodo-                                                   | 21.85          | JAC25, JAC74C, JAC95, JAC60, JAC81 | SFM, YMS, Synthetic |
| Benzoic Acid, 2-Ethylhexyl Ester                                       | 21.97          | JAC60, JAC95 | Synthetic, SFM, YMS |
| Methyl Tetradecanoate*                                                 | 22.09          | JAC60, JAC81, JAC95 | Synthetic, SFM, YMS |
| Tris(Trimethylsiloxy)Ethylene                                          | 22.23          | JAC25, JAC74C, JAC45, JAC95 | SFM, YMS |
| 7-Methoxy-2,5-Dimethyl-1,2,3,4-Tetrahydropyrimido(1,6-A)Indole         | 22.41          | JAC60, JAC81, JAC45 | Synthetic, SFM, YMS |
| Hexanoic Acid, 2-Hexenyl Ester, (E)-*                                  | 22.65          | JAC81     | YMS, Synthetic, SFM |
| Benzene, 1-Methoxy-3-Undecyl-Octadecanol                               | 22.67          | JAC45     | Synthetic, SFM |
| 13-Methyltetradecanoic Acid Methyl Ester*                              | 23.17          | JAC95, JAC60 | YMS, Synthetic, SFM |
| Diisobutyl Phthalate                                                  | 23.57          | JAC60, JAC95, JAC81 | Synthetic, SFM, YMS |
| 2-Pentadecanoine                                                      | 23.98          | JAC25     | YMS |
| Methyl Palmitate*                                                     | 24.21          | JAC60, JAC25, JAC95, JAC81 | Synthetic, SFM, YMS |
| 15-Methylhexadecanoic Acid Methyl Ester                                | 24.31          | JAC60, JAC25 | Synthetic, SFM, YMS |
| Fumaric Acid, 2,4,4-Trimethylpentyl 3-Methylbut-2-En-1-Yl Ester        | 24.69          | JAC45, JAC25 | YMS, Synthetic, SFM |
| Compound Description                                                                 | Retention Time (min) | JAC Numbers |
|-------------------------------------------------------------------------------------|----------------------|-------------|
| Disulfide, Di-Tert-Dodecyl*                                                          | 25.01                | JAC74C, JAC45 |
| L-Arginine                                                                           | 25.1                 | JAC25       |
| N-(O-Chlorophenyl)-4,5-Dihydro-3-Furamid                                             | 25.44                | JAC60       |
| Pyridoxamine                                                                        | 25.5                 | JAC25, JAC60 |
| 2,4,6-Tris(Trimethylsiloxy)Benzoic Acid Trimethylsilyl Ester                         | 25.99                | JAC60, JAC74C |
| 1,2-Benzenedicarboxylic Acid 2-Ethylhexylmethyl Ester                              | 26.14                | JAC60, JAC81, JAC95 |
| 1-Bromo-8-Tetrahydropyranoxyoctane*                                                 | 26.21                | JAC25, JAC81, 74C |
| Benzene-1,2,4,5-Tetraarboxylic Acid Tetra(Trimethylsilyl) Ester                     | 26.34                | JAC74C, JAC45 |
| 2-(3-Benzoylphenyl)Propionic Acid Trimethylsilyl Ester*                              | 26.39                | JAC60, JAC81 |
| Octahydro-2H-Quinolizine                                                             | 26.43                | JAC60       |
| Undecane*                                                                           | 26.49                | JAC25, JAC45, JAC60, JAC74C |
| Tetracosane*                                                                         | 27.23                | JAC25, JAC74C, JAC60, JAC81, JAC95 |
| 3-Methyladipic Acid Di-Tms                                                           | 27.44                | JAC25       |
| Heptacosane*                                                                         | 27.53                | JAC81, JAC25 |
| 2,3,4-Tris(Trimethylsiloxy)Benzoic Acid Trimethylsilyl Ester                         | 28.06                | JAC25, JAC74C, JAC60, JAC81 |
| Behenic Amide*                                                                       | 28.27                | JAC81       |
| Hexacosane, 1-Iodo-                                                                  | 28.49                | JAC74C, JAC25, JAC95, JAC81 |
| Butyl Hexacosyl Ether                                                                | 29.06                | JAC45       |
| Diamyl Phthalate                                                                     | 29.29                | JAC74C, JAC81 |
| 1,2-Benzenedicarboxylic Acid, Bis(2-Methylpropyl) Ester                            | 29.31                | JAC45       |
| Butoxycarbonylmethyl Butyl Phthalate                                                 | 29.35                | JAC25       |
| 3-Ethyl-2,6,10-Trimethylundecane                                                     | 29.57                | JAC25       |
| Hexanamide, 6-Bromo-N-Hept-2-Yl-                                                    | 29.94                | JAC74C, JAC95, JAC60, JAC45 |
| Compound                                                                 | TIC (%) | JAC25, JAC45, JAC74C, JAC60, JAC95, JAC81 | SFM, YMS, Synthetic, YMS, SFM, Synthetic |
|-------------------------------------------------------------------------|---------|---------------------------------|-------------------------------------|
| 1,2-Benzenedicarboxylic Acid Bis(2-Ethylhexyl) Ester*                  | 30.59   |                                 |                                     |
| Dodecyl Nonyl Ether                                                     | 31.11   | JAC25                           | YMS, SFM, Synthetic, YMS            |
| N-(Aminocarbonyl)-2-Bromo-2-Ethyl-Butanamide Carbromal                  | 31.17   | JAC74C, JAC25                   | Synthetic, YMS                      |
| 3-Isopropyl-6,10-Dimethylundecane-2-ol*                                 | 31.78   | JAC25                           | SFM, YMS, Synthetic                 |
**Table S8.** Bacterially derived compounds annotated in replicate VOC analysis of the six selected *Streptomyces* isolates using the conventional method. VOCs annotated during both the pooled culture screen and the replicated analysis are shown in bold and labelled with an asterisk*.

| Compound/VOC                                      | Retention time (min) | Annotated in (isolates) | Media     |
|--------------------------------------------------|----------------------|-------------------------|-----------|
| 2-Furanol, tetrahydro-2-methyl-                  | 4.02                 | JAC81, JAC95            | synthetic |
| Pyrimidine-2,4(1H,3H)-dione, 5-amino-6-nitroso-  | 4.021                | JAC25                   | SFM       |
| Tetrahydrofuran, 2-propyl-                       | 4.024                | JAC74C                  | synthetic |
| Benzene, (propoxymethyl)-                        | 4.231                | JAC45                   | SFM       |
| Diacetyl sulphide                                | 4.313                | JAC45                   | YMS       |
| **Butanoic acid, 2-methyl-, methyl ester**       | 4.314                | JAC45, JAC60            | SFM, synthetic |
| Cyclobutanone, 2-methyl-                         | 4.562                | JAC45                   | SFM       |
| Acetamide, N,N'-ethylenebis(N-nitro-             | 4.579                | JAC81                   | YMS       |
| 2-Methyl-2,3-pentanediol*                        | 4.72                 | JAC60, JAC25            | YMS, SFM  |
| 1,8-Nonanediol, 8-methyl-                        | 4.722                | JAC25, JAC60            | YMS       |
| **2-Hydroxy-3-pentanone**                        | 4.854                | JAC95, JAC60            | YMS       |
| 4-Methyl-2,4-bis(4'-trimethylsilyloxyphenyl)pentene-1 | 4.862               | JAC60                   | synthetic |
| Hexane, 3,4-bis(1,1-dimethyl)-2,2,5,5-tetramethyl-| 4.864               | JAC95                   | SFM       |
| Sulfurous acid, cyclohexylmethyl heptadecyl ester| 4.923                | JAC25                   | YMS       |
| Propanoic acid, 2-methyl-, anhydride              | 5.111                | JAC95                   | YMS       |
| 1,6:3,4-Dianhydro-2-deoxy- beta.-d-ribo-hexopyranose | 5.499               | JAC25                   | YMS       |
| Butanoic acid, 3-methyl-                         | 5.582                | JAC95                   | synthetic |
| Butanoic acid, 3-methyl-                         | 5.634                | JAC95                   | synthetic |
| **Butane, 2-azido-2,3,3-trimethyl-**             | 5.683                | JAC95                   | synthetic |
| Compound                                           | Retention Time | Detector | Notes                      |
|----------------------------------------------------|----------------|----------|----------------------------|
| Butanoic acid, 3-methyl-                           | 6.112          | JAC74C   | YMS                        |
| 1-Hexanol*                                         | 6.197          | JAC60    | synthetic                  |
| (S)-3,4-Dimethylpentanol*                          | 6.257          | JAC95    | YMS                        |
| Butanedioic acid, phenyl-*                         | 6.73           | JAC60    | synthetic                  |
| Hexanoic acid, 5-methyl-, methyl ester             | 9.322          | JAC60    | SFM                        |
| Benzyl alcohol*                                    | 10.269         | JAC95    | SFM                        |
| Pyrazine, 2-methyl-5-(1-methylethyl)-              | 10.541         | JAC95    | YMS                        |
| Benzoic acid, methyl ester                         | 11.889         | JAC95    | SFM                        |
| Phenylethyl Alcohol*                               | 12.393         | JAC95, JAC60 | SFM, YMS                |
| Bicyclo[3.2.0]hepta-2,6-diene*                     | 12.398         | JAC95    | YMS                        |
| 4-Acetylbenzoic acid                               | 14.294         | JAC95    | YMS                        |
| 2-Methylisoborneol*                                | 14.348         | JAC60, JAC25 | SFM, synthetic, YMS        |
| 1H-Indene, 1-ethylideneoctahydro-7a-methyl-, cis-  | 15.234         | JAC60, JAC25, JAC95, JAC81, JAC74C | SFM, synthetic, YMS        |
| 1H-Indene, 1-ethylideneoctahydro-7a-methyl-, (1Z,3αα,7αβ)- | 15.316         | JAC25, JAC95, JAC81 | SFM, synthetic          |
| 1H-Indene, 1-ethylideneoctahydro-7a-methyl-, (1E,3αα,7αβ)- | 15.626         | JAC81    | SFM                        |
| (1,2,2-trimethyl-3-cyclopenten-1-yl)acetaldehyde* | 15.711         | JAC25, JAC95, JAC81 | SFM                        |
| Phenol, 4-[2-(methylamino)ethyl]-*                 | 15.712         | JAC74C   | YMS                        |
| 2-Hydroxy-5-ethyl-5-methylcyclopent-2-en-1-one*    | 15.94          | JAC81    | SFM                        |
| Decane, 3-bromo-                                   | 16.709         | JAC74C   | SFM                        |
| 2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester | 16.772         | JAC74C   | YMS                        |
| 1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethenyl)-, [S-(Z,E)]- | 17.933         | JAC95, JAC74C | SFM, YMS                |
| Compound                                                                 | Retention Time | Source          |
|--------------------------------------------------------------------------|----------------|-----------------|
| Geosmin*                                                                 | 18.331         | JAC60, JAC25, JAC95, JAC81, JAC74C |
| 1-Methylene-2-b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane* | 18.421         | JAC95, JAC81    |
| 1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylenepicene, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-4,4-Dimethyl-3-(3-methylbut-3-enylidene)-2-methylenecyclo[4.1.0]heptane | 18.506         | JAC81          |
| 2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane          | 18.724         | JAC81          |
| 3-Heptyne, 5-methyl-*                                                    | 18.729         | JAC95          |
| 2H-Pyran-2-one, 6-hexyltetrahydro-5,6-Decadien-3-yne, 5,7-diethyl-        | 18.811         | JAC81          |
| Cadina-1(10),6,8-triene                                                  | 18.812         | JAC81          |
| 2R-Acetoxy methyl-1,3,3-trimethyl-4t-(3-methyl-2-butene-1-yl)-1t-cyclohexanol | 18.918         | JAC81          |
| 3-Isopropoxy-1,1,7,7,7-hexamethylyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane* | 18.965         | JAC81          |
| 2,3,4-Trifluorobenzoic acid, 2,6-dimethylnon-1-en-3-yne-5-yl ester        | 18.967         | JAC81          |
| Cyclobutaneacetonitrile, 1-methyl-2-(1-methylethylidene)-                 | 19.031         | JAC74C         |
| 1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)],[S-(E,E)]-*  | 19.273         | JAC25, JAC95, JAC81, JAC74C |
| Acetic acid, (dodecahydro-7-hydroxy-1,4b,8,8-tetramethyl-10-oxo-2(1H)-phenanthrenylidene)-2-(dimethylamino)ethyl ester | 19.482         | JAC81          |
| 2H-3,9a-Methano-1-benzoexpin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.,9a.alpha.)]-photocitral B | 19.699         | JAC81          |
| Cyclohexanol, 4-ethyl-4-methyl-3-(1-methylethyl)-, (1.alpha.,3.beta.,4.alpha.)- | 19.704         | JAC95          |
| 1-Hexyl-2-nitrocyclohexane*                                              | 19.803         | JAC95          |
| Hexacosane                                                               | 19.854         | JAC95          |
| Cyclobutaneacetonitrile, 1-methyl-2-(1-methylethylidene)-                | 19.855         | JAC95          |

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| Compound                                                                 | Retention Time (min) | Supporting Information |
|--------------------------------------------------------------------------|----------------------|------------------------|
| 1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethenyl)-, [S-(Z,E)]-        | 20.109               | JAC74C, YMS             |
| Hexane, 2,3-dimethyl-                                                    | 20.282               | JAC95, SFM              |
| 5-Hepten-3-one, 5-ethyl-2-methyl-                                        | 20.451               | JAC81, SFM              |
| Caryophyllenyl alcohol                                                  | 20.523               | JAC95, SFM              |
| Diethyl Phthalate                                                       | 20.523               | JAC25, JAC81, JAC74C, YMS |
| Ethaneperoxoic acid, 1-cyano-1-[2-(2-phenyl,1,3-dioxolan-2-yl)ethyl]pentyl ester | 20.523               | JAC74C, YMS             |
| 6,7-Dodecanedione                                                       | 21.056               | JAC81, SFM              |
| 2(5H)-Furanone, 5-(bromomethyl)-5-phenyl-                               | 21.06                | JAC81, SFM              |
| **5,6-Decadien-3-yne, 5,7-diethyl-**                                     | 21.126               | JAC25, synthetic        |
| Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-*    | 21.128               | JAC25, SFM, YMS         |
| cis-muurola-3,5-diene                                                  | 21.129               | JAC25, SFM              |
| .alfa.-Copaene                                                          | 21.13                | JAC95, SFM              |
| **10-Methylundecan-4-olide**                                            | 21.155               | JAC74C, Synthetic, YMS  |
| 1-Phenyl-2-methyl-oct-1-ene                                             | 21.177               | JAC81, SFM, synthetic, YMS |
| **Dihydro-cis-.alpha.-copaene-8-ol**                                    | 21.263               | JAC81, JAC25, JAC95, SFM |
| Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethyl)-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]- | 21.268               | JAC95, SFM              |
| **Phenylacetaldehyde N-methyl-N-formylhydrazone**                       | 21.391               | JAC95, YMS              |
| 7-epi-.alpha.-eudesmol*                                                | 21.547               | JAC95, SFM              |
| 1-Methyl-4-isopropyl-cyclohexyl 2-hydroperfluorobutanoate               | 21.836               | JAC45, YMS              |
| Cyclohexanol, 1,3,3-trimethyl-2-(3-methyl-2-methylene-3-butenyldiene)-, (Z)-2,5-Octadiyne, 4,4-diethyl- | 21.836               | JAC60, YMS              |
| **Cyclohexanol, 1-ethyl-2,2-dimethyl-6-methylene-**                     | 22.103               | JAC81, SFM              |
| Heptacosane                                                             | 25.901               | JAC25, YMS              |

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| Liu & Clarke et al. 2022 | Hexadecanoic acid, 15-methyl-, methyl ester | 26.128 | JAC25 | YMS |
|------------------------|------------------------------------------|--------|-------|-----|
| 1-Hexyl-2-nitrocyclohexane | 27.638 | JAC25 | YMS |
| **Hexanedioic acid, bis(2-ethylhexyl) ester** | 28.636 | JAC25 | YMS |
Table S9. Web links for MSHub/GNPS jobs generated in this study.

| Job                                                      | Web link                                                                 |
|----------------------------------------------------------|--------------------------------------------------------------------------|
| MSHub for pooled culture VOCs analysis of the 37 *Streptomyces* isolates | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=8aa14b90160d482aa19de0cd20558038 |
| GNPS library search for the 37 *Streptomyces* isolates (annotatio cosine score 0.5) | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=2fccfed64f1047009283bb6904104202 |
| GNPS library search for the 37 *Streptomyces* isolates (annotatio cosine score 0.65) | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=b47661ec7ae84c1bae3c90b6e9c56764 |
| MSHub for replicate VOCs analysis of JAC25               | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=9fefb239a3514a638afefaf3a88aa6ba |
| GNPS library search for JAC25                            | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=3b476735d4684a3b9e09f7e95f8416eb |
| MSHub for replicate VOCs analysis of JAC45               | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=659ab3212752409fa093221e05203ff4 |
| GNPS library search for JAC45                            | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=e0a436259d6d430090d59af66976c134 |
| MSHub for replicate VOCs analysis of JAC60               | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=c8f70167c87e4384968c47cccbd386b9 |
| GNPS library search for JAC60                            | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=8f88689b27d7a74b29dd3c44408b728 |
| MSHub for replicate VOCs analysis of JAC74C               | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=595aff5b193a439583b8b14f48eb3bd0 |
| GNPS library search for JAC74C                            | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=17f939cdb9934ec1934e2a6d91e4e277 |
| MSHub for replicate VOCs analysis of JAC81               | https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=ca387e87543a4b72aa642069db5868cb |
REFERENCES

1. Shi W, Li M, Wei G, Tian R, Li C, Wang B, Lin R, Shi C, Chi X, Zhou B, Gao Z. 2019. The occurrence of potato common scab correlates with the community composition and function of the geocaulosphere soil microbiome. Microbiome 7:14.

2. Nagashima K, Hisada T, Sato M, Mochizuki J. 2003. Application of new primer-enzyme combinations to terminal restriction fragment length polymorphism profiling of bacterial populations in human feces. Appl Environ Microbiol 69:1251–1262.

3. Guo Y, Zheng W, Rong X, Huang Y. 2008. A multilocus phylogeny of the *Streptomyces griseus* 16S rRNA gene clade: Use of multilocus sequence analysis for streptomycete systematics. Int J Syst Evol Microbiol 58:149–159.