**Table 1.** Mean normalized chromatographic peak areas, retention times, match factor and reverse match factor for the volatile organic compounds identified in Vespa velutina hornets and in their external cover of the nest, extracted in hexane and in the mixture acetone:methanol (50:50).

| | | | | Hornets | | | | | | | | External cover of the nest | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | Hexane | | | | AcMeOH | | | | Hexane | | | | AcMeOH | | | |
| **Compounds** | **RT** | **MF** | **RMF** | **Nest 1** | **Nest 2** | **Nest 3** | **Nest 4** | **Nest 1** | **Nest 2** | **Nest 3** | **Nest 4** | **Nest 1** | **Nest 2** | **Nest 3** | **Nest 4** | **Nest 1** | **Nest 2** | **Nest 3** | **Nest 4** |
| (-)-Globulol | 15.549 | 88.3 | 88.7 | | | | | | | | | 31095 | | | | 710584 | | | |
| (+-)-4-Amino-4,5-dihydro-2(3H)-furanone | 4.787 | 70 | 71.5 | | | | | 1418802 | 876219 | 451565 | 1187065 | | | | | | | | |
| 1-(3-(Cyclohexylamino)propyl)guanidine | 13.062 | 58.8 | 60.1 | | | | | 93824 | 129128 | 15689 | 116657 | | | | | | | | |
| 1,3,5-Pentanetriol, 3-methyl- | 11.045 | 72.5 | 73.2 | | | | | | | | | | | | | | | | 378864 |
| 1,7,7-Trimethyl-3-phenethylidenebicyclo[2.2.1]heptan-2-one | 26.577 | 70.2 | 74.2 | | | | | | | | | | | | | 10930 | 196033 | 165413 | 256403 |
| 1,7-Dimethyl-4-(1-methylethyl)cyclodecane | 9.468 | 77.4 | 82.3 | 14454 | 13465 | 12998 | 20117 | | | | | | | | | | | | |
| 10-Heneicosene (c,t) | 18.052 | 78.7 | 82 | | | | | | | | | 12001 | 16417 | 27753 | 27635 | | | | |
| 10-Methylnonadecane | 10.111 | 81.7 | 83.9 | 21223 | 21527 | 25537 | 31530 | | | | | | | | | | | | |
| 11,14,17-Eicosatrienoic acid, methyl ester | 35.305 | 78 | 83.8 | 1943232 | 2469365 | 1289596 | 1684425 | 2327317 | 960908 | 735694 | 899090 | | | | | | | | |
| 11-Methylnonacosane | 34.133 | 77.6 | 82.5 | | | | | 400733 | 244281 | 152914 | 285534 | | | | | | | | |
| 11-Methylpentacosane | 31.821 | 8.62 | 9.33 | | | | | 1358010 | 919739 | 533168 | 1061981 | | | | 227314 | | 1331630 | 2313024 | |
| 11-Octadecenoic acid, methyl ester | 24.776 | 9.06 | 9.12 | | | | | 2171981 | 49859707 | 33857890 | 25505077 | | | | | | 1106612 | 876499 | 979809 |
| 13-Docosen-1-ol, (Z)- | 34.730 | 76.9 | 79.7 | | | | | | 1007879 | 672178 | 498146 | | | | | | | | |
| 13-Docosenamide, (Z)- | 34.239 | 81.7 | 85.5 | | | | | | | | | | | | | | 2441697 | 2464001 | 3205536 |
| 13-Heptadecyn-1-ol | 23.338 | 78.8 | 79 | | | | | | | | | | | | | 132642 | 258622 | 385878 | |
| 13-Methylheptacosane | 34.125 | 89.3 | 90.7 | 311900 | 556278 | 372955 | 586918 | 2955791 | 1429189 | 858912 | 2136606 | | | | | | | | |
| 1-Butanamine, 2-methyl-N-(2-methylbutylidene)- | 7.468 | 86.1 | 89.4 | | | | | 753631 | 453629 | 410315 | 603622 | | | | | | | | |
| 1-Decanol, 2-hexyl- | 11.392 | 7.17 | 7.18 | 157277 | 178706 | 194767 | 236413 | | | | | 33804 | 30487 | 37416 | 35408 | | | | |
| 1-Decanol, 2-octyl- | 18.944 | 78.9 | 79 | 501638 | 570876 | 692333 | 844523 | | | | | | | | | | | | |
| 1-Docosene | 14.919 | 81.2 | 82.1 | 381035 | 445193 | 523643 | 618200 | | | | | | | | | | | | |
| 1-Dodecanol, 2-hexyl- | 18.720 | 76.9 | 77.1 | | | | | | | | | 50872 | 61847 | 62850 | 56898 | | | | |
| 1-Dodecanol, 2-methyl-, (S)- | 13.582 | 71.3 | 72.6 | 78110 | 87917 | 102548 | 121180 | | | | | | | | | | | | |
| 1-Dodecanol, 2-octyl- | 31.119 | 84.1 | 85.9 | 353737 | 409583 | 496236 | 612853 | | | | | | | | | | | | |

SUPPLEMENTARY MATERIAL

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-Dodecanol, 3,7,11-trimethyl- | 8.555 | 7.93 | 8.17 | 13706 | 11592 | 11726 | 16745 | | | | | | | | | 199747 | 169395 | 232400 | 399434 |
| 1H-Azepine, 1-acetylhexahydro- | 7.865 | 72.8 | 75.7 | | | | | | | | | | | | | | | | 2358266 |
| 1-Heptacosanol | 33.986 | 8.46 | 8.61 | 132875 | 158486 | 98331 | 256545 | | | | | | | | | 726496 | 1742937 | 1824465 | 1086451 |
| 1-Heptene, 2,6,6-trimethyl- | 5.138 | 76.1 | 79.2 | 28679 | 19043 | 28685 | 40556 | | | | | | | | | | | | |
| 1-Hexadecanol, 3,7,11,15-tetramethyl- | 15.105 | 80 | 80.3 | 428893 | 494584 | 595062 | 694733 | | | | | | | | | | | | |
| 1-Hexanol, 2-ethyl- | 3.286 | 78.8 | 82.6 | | | | | | | | | 671081 | | | | | | | |
| 1H-Pyrazole, 3,5-bis(1,1-dimethylethyl)- | 11.667 | 71.4 | 73.4 | | | | | 377489 | 399541 | 47989 | 734414 | | | | | | | | |
| 1-Nonadecene | 18.369 | 7.99 | 8 | 334809 | 386577 | 475272 | 572579 | | | | | 22283 | 26775 | 26559 | 25488 | | | | |
| 1-Octadecene | 14.631 | 84.1 | 84.8 | 323695 | 362609 | 430577 | 508668 | | | | | | | | | | | | |
| 1-Octanol, 2,2-dimethyl- | 10.504 | 83.9 | 84.2 | 159258 | 163021 | 140501 | 225064 | | | | | | | | | | | | |
| 1-Octanol, 2-butyl- | 10.449 | 81.7 | 85.6 | 44833 | 48900 | 47857 | 60913 | | | | | | | | | | | | |
| 1-Octene, 3,7-dimethyl- | 7.738 | 80 | 85.3 | 17785 | 15345 | 17335 | 25492 | | | | | | | | | | | | |
| 1-Pentanol, 2-methyl- | 7.967 | 75.6 | 76.9 | 49652 | | | | | | | | | | | | | | | |
| 1-Tetracosene | 11.151 | 76.2 | 79.3 | 577490 | 631826 | 689464 | 827726 | | | | | | | | | | | | |
| 1-Undecene, 8-methyl- | 10.855 | 83.4 | 85.6 | 83516 | 96690 | 101004 | 113014 | | | | | | | | | | | | |
| 2-(2-Methyl-propenyl)-cyclohexanone oxime | 11.629 | 69.8 | 74 | | | | | 94918 | 107763 | 35644 | 247437 | | | | | | | | |
| 2,2,4-Trimethyl-3-(3,8,12,16-tetramethyl-heptadeca-3,7,11,15-tetraenyl)-cyclohexanol | 34.556 | 80.3 | 81.8 | | | | | | | | | | | | | 509145 | | | |
| 2,2,7,7-Tetramethyloctane | 9.180 | 79.2 | 90.5 | 121109 | 102213 | 95359 | 150081 | | | | | | | | | | | | |
| 2,2-Dimethyl-4-octenal | 7.514 | 62.2 | 62.6 | | | | | 334660 | 245582 | 60464 | 348198 | | | | | | | | |
| 2,2'-Trimethylenebis-1,3-dioxolane | 11.371 | 72.3 | 77.5 | | | | | 2754128 | 2290144 | 580002 | 4067610 | | | | | | | | |
| 2,3-Dimethyldecane | 8.111 | 77.2 | 79.2 | 33991 | 29520 | 30141 | 44294 | | | | | | | | | | | | |
| 2,4-Dimethyl-1-heptene | 4.470 | 94.6 | 96.3 | 928100 | 743883 | 897241 | 1301480 | | | | | | | | | | | | |
| 2,4-Dimethyldodecane | 10.517 | 83.5 | 84 | 101405 | 99175 | 128532 | 141446 | | | | | | | | | | | | |
| 2,6,10-Trimethyltridecane | 10.462 | 87.2 | 88.1 | 206554 | 191557 | 176919 | 289259 | | | | | | | | | | | | |
| 2,6-Dimethyldecane | 8.191 | 86.9 | 88.1 | 193260 | 183038 | 176072 | 266962 | | | | | | | | | | | | |
| 2-Cyclohexen-1-one, 3,6-dimethyl-6-(1-methylethyl)- | 8.614 | 76.2 | 76.7 | | | | | 288989 | 279574 | 56118 | 328524 | | | | | | | | |
| 2-Cyclopenten-1-one, 2,3-dimethyl- | 8.229 | 82.1 | 85.5 | | | | | 578339 | 657870 | 117352 | 1366191 | | | | | | | | |
| 2-Diethylamino-4-phenylthiooct-2-ene nitrile | 14.259 | 70.8 | 79.7 | | | | | 90442 | 199548 | 4173 | 410843 | | | | | | | | |
| 2-Hexyl-1-octanol | 14.923 | 7.46 | 8.1 | 235069 | 276508 | 325035 | 382367 | | | | | 72972 | 60438 | 84458 | 92440 | | | | |
| 2-Isopropyl-5-methyl-1-heptanol | 18.230 | 78.2 | 79.8 | 120205 | 136526 | 177597 | 201682 | | | | | | | | | | | | |

SUPPLEMENTARY MATERIAL

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-Methyl-1-undecanol | 8.635 | 79.6 | 82.3 | 18480 | 16518 | 16430 | 24544 | | | | | | | | | | | | |
| 2-Methyl-E-7-hexadecene | 13.752 | 73.2 | 74.3 | 88087 | 100627 | 117562 | 137536 | | | | | | | | | | | | |
| 2-Methylheptacosane | 34.002 | 79.8 | 86.8 | | | | | | 327660 | 211606 | 374968 | | | | | | | | |
| 2-methyloctacosane | 17.147 | 83 | 83 | 70121 | 86084 | 124131 | 113098 | | | | | | | | | | | | |
| 2-Methyl-Z-4-tetradecene | 26.848 | 80.5 | 81.7 | | 290951 | 366774 | 449326 | | | | | | | | | | | | |
| 2-Pentanone, 4-amino-4-methyl- | 5.218 | 90.6 | 90.6 | | | | | 29720799 | 37358546 | | 34300070 | | | | | | | | |
| 2-Pentanone, 4-hydroxy-4-methyl- | 4.926 | 91.6 | 92.7 | | | | | 92202734 | 64780711 | 25763391 | | | | | | | | | |
| 2-Pentanone, 4-methoxy-4-methyl- | 5.201 | 9.5 | 9.7 | | | | | 171854 | 2785485 | | 3031796 | | | | | 2687702 | 1029527 | 2622737 | 22516444 |
| 2-Pentenoic acid, 4-oxo-, methyl ester, (Z)- | 6.491 | 67.9 | 87.9 | | | | | | | | | | | | | 242673 | 591540 | 325770 | 962123 |
| 2-Propen-1-amine, N,N-bis(1-methylethyl)- | 8.115 | 78.4 | 78.8 | | | | | 559527 | 727111 | 237442 | 2108390 | | | | | | | | |
| 3,3-Dimethyl-tetrahydro-pyrrolo[1,2-c]thiazol-1-one | 6.368 | 77.9 | 80.6 | | | | | 787958 | 396981 | 81798 | 520728 | | | | | | | | |
| 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl- | 7.895 | 68.8 | 69.9 | | | | | 193034 | 259186 | 48447 | 316680 | | | | | | | | |
| 3-Hexanethiol | 4.694 | 86 | 86.8 | | | | 46766 | | | | | | | | | | | | |
| 3-Methylheptacosane | 33.990 | 83.8 | 90.9 | | | | | | | | | 201796 | 98282 | 412129 | 648987 | | | | |
| 3-Methylhexacosane | 33.152 | 75.3 | 86.9 | | | | | | | | | | | | | | | | |
| 3-Methylpentacosane | 32.138 | 92.4 | 96.6 | 853526 | 1363389 | 825797 | 1907448 | 193558 | 2098733 | 1213673 | 1913304 | | | | | | | | |
| 3-Octanol, 2-methyl- | 9.946 | 68.9 | 73.3 | | | | | 2197686 | 1780207 | 428401 | 2495869 | | | | | | | | |
| 3-Octanol, 3-methyl- | 9.189 | 68.7 | 73.4 | | | | | 202338 | 232477 | 74619 | 280110 | | | | | | | | |
| 3-Penten-2-one, 4-methyl- | 3.827 | 9.27 | 9.28 | | | | | 2788364 | 19860216 | 16212994 | 35000233 | | | | | | | | 5078357 |
| 3-Trifluoroacetoxytetradecane | 11.219 | 72.8 | 77.5 | | | | | | | | | | | | | 122782 | 117696 | 396340 | 362245 |
| 4(1H)-Quinolinone, octahydro-1-methyl- | 9.083 | 68.2 | 72.1 | | | | | 192741 | 247635 | 25740 | 255762 | | | | | | | | |
| 4,4-Dipropylheptane | 9.574 | 81.6 | 85.1 | 23803 | 22782 | 22252 | 30695 | | | | | | | | | | | | |
| 4H-Cyclopropa[5',6']benz[1',2':7,8]azuleno[5,6-b]oxiren-4-one, 8-(acetyloxy)-1,1a,1b,1c,2a,3,3a,6a,6b,7,8,8a-dodecahydro-3a,6b,8a-trihydroxy-2a-(hydroxymethyl)-1,1,5,7-tetramethyl-, [1ar-(1aα,1bβ,1cα,2aα,3aβ,6aα,6bα,7α,8β,8aα)]- | 28.564 | 78.4 | 78.6 | | | | | | | | | | | | | | 585526 | | |
| 4-Heptanol, acetate | 5.755 | 75.4 | 79.6 | | | | | 1397548 | 2967408 | 659226 | 2709957 | | | | | | | | |
| 4-Piperidinone, 2,2,6,6-tetramethyl- | 8.144 | 89.3 | 90 | | | | | 18355 | 632290 | 211380 | 480815 | | | | | 235350 | | | 5152816 |

SUPPLEMENTARY MATERIAL

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a:1',2'-d]pyrazine | 22.365 | 70.7 | 79.7 | | | | | 304142 | 258039 | 126645 | 194398 | | | | | | | | |
| 5,8,11,14,17-Eicosapentaenoic acid, methyl ester, (all-Z)- | 27.520 | 93.2 | 93.3 | 217515 | 514754 | 444427 | 183269 | 43349 | 761543 | 345958 | 293140 | | | | | | | | |
| 5,8,11,14-Eicosatetraenoic acid, methyl ester, (all-Z)- | 27.410 | 92.5 | 92.8 | | | | | 44635 | 222674 | 109051 | 73097 | | | | | | | | |
| 5-Ethyl-1-nonene | 7.819 | 77.6 | 81.9 | 332366 | 257338 | 353061 | 635520 | | | | | | | | | | | | |
| 5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-one, 4,9,9a-tris(acetyloxy)-3-[(acetyloxy)methyl]-1,1a,1b,4,4a,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl- | 33.859 | 76.8 | 77.2 | | | | | | | | | | | | | | 462367 | 815183 | |
| 5-Hepten-2-one, 6-methyl- | 6.918 | 76.2 | 78.3 | | | | | 584093 | 390291 | 159215 | 487837 | | | | | | | | |
| 5-Methyl-2-propyl-1,4,4a,5,6,7,8,8a-octahydroquinoline | 13.735 | 68.4 | 82.1 | | | | | 649654 | 659489 | 48972 | 1450126 | | | | | | | | |
| 5-Undecene, (E)- | 7.180 | 84 | 84.6 | 38038 | 32888 | 33808 | 49382 | | | | | | | | | | | | |
| 7,10,13-Eicosatrienoic acid, methyl ester | 34.941 | 75.5 | 79 | | | | | | | | | | | | | | 1197295 | 1811843 | |
| 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | 21.591 | 83.8 | 85.4 | | | | | | | | | | | | | 211762 | 201771 | 397618 | 375845 |
| 7-Hexadecenoic acid, methyl ester, (Z)- | 21.122 | 91 | 91 | | | | | 39402 | 2226945 | 1853935 | 1077265 | | | | | | | | |
| 7-Isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene | 24.162 | 77.7 | 86 | | | | | | | | | | | | | | 175350 | 184780 | 88112 |
| 7-Tetradecene, (E)- | 10.339 | 78.9 | 79.1 | 103330 | 100538 | 105243 | 141197 | | | | | | | | | | | | |
| 9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol, (3β,5Z,7E)- | 30.738 | 70.5 | 74.8 | | | | | | | | | | | | | | 278697 | 494612 | 453839 |
| 9,12,15-Octadecatrien-1-ol, (Z,Z,Z)- | 34.954 | 75.9 | 82.6 | 2185273 | 2384637 | 1657703 | 2154515 | 2712321 | 1310656 | 888486 | 1367927 | | | | | | | | |
| 9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)- | 24.784 | 80.4 | 82.9 | | | | | | | | | | | | | 31742 | 241168 | 216093 | 363777 |
| 9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester | 33.347 | 77.3 | 78.2 | | | | | | | | | | | | | 507549 | 1218456 | 1531774 | |
| 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- | 25.249 | 9.05 | 9.11 | | | | | 11812951 | 5985791 | 3061130 | 2469011 | | | | | | 192645 | 208297 | 270802 |
| 9,12-Octadecadienoic acid (Z,Z)- | 25.393 | 86.5 | 89.1 | | | | | | | | | | | | | 145019 | 1092431 | 642227 | 1359374 |
| 9,12-Octadecadienoic acid (Z,Z)-, methyl ester | 24.708 | 9.55 | 9.55 | 2263303 | 2780529 | 3273502 | 1539970 | 5699987 | 2563882 | 2024662 | 1918607 | | | | | 138409 | 1257853 | 1163067 | 1365252 |
| 9-Hexadecenoic acid | 22.822 | 74.1 | 75.1 | | | | | | | | | | | | | | 138772 | 250582 | |
| 9-Hexadecenoic acid, methyl ester, (Z)- | 21.080 | 92.9 | 92.9 | 795666 | 1022643 | 1192754 | 331591 | 15380 | 692728 | 341151 | 153069 | | | | | | | | |
| 9-Octadecenamide, (Z)- | 26.053 | 8.21 | 8.72 | 670076 | 1105158 | 1436253 | 1679039 | | 501772 | | 309785 | | | | | 8787706 | 7029597 | 10910971 | 23483469 |
| 9-Octadecenamide, N,N-dimethyl- | 30.222 | 62.7 | 74.4 | | | | | | | | | | | | | 250804 | 161637 | 247168 | 279991 |
| 9-Octadecenoic acid (Z)-, methyl ester | 24.763 | 93.5 | 93.6 | 10891208 | 13657712 | 13440994 | 6956717 | 24684382 | 10488492 | 6095273 | 5431988 | | | | | | | | |

SUPPLEMENTARY MATERIAL

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Acetamide, N-methyl-N-[4-[2-acetoxymethyl-1-pyrrolidyl]-2-butynyl]- | 25.008 | 71.3 | 74.3 | | | | | | | | | | | | | | 472785 | 85895 | |
| Acetic acid n-octadecyl ester | 26.628 | 89.9 | 93 | | | | | | | | | 224045 | | | 298530 | 868787 | 1104860 | 1631059 | 1808485 |
| Acetic acid, 3,7,11,15-tetramethyl-hexadecyl ester | 23.181 | 80 | 80.1 | 94506 | | | | | | | | | | | | | | | |
| Androst-5,7-dien-3-ol-17-one | 28.306 | 76.4 | 79.5 | | | | | | | | | | | | | | 160528 | 103368 | 67906 |
| Behenic alcohol | 31.114 | 7.95 | 8.31 | | | | | | | 156889 | 269026 | | | | | 261952 | 206312 | 338776 | 298601 |
| Benzenamine, N,N-dimethyl-4-[[(1-methylethyl)imino]methyl]- | 10.893 | 74.8 | 83 | | | | | 174108 | 189932 | 20188 | 319220 | | | | | | | | |
| Benzene, 1,3-bis(1,1-dimethylethyl)- | 10.491 | 9.23 | 9.34 | | 88893 | 53706 | | | | | | | | | | 26194 | 49517 | 311731 | 232071 |
| Benzoic acid, 2,4-dihydroxy-3,6-dimethyl-, methyl ester | 18.107 | 80.4 | 84.3 | | | | | | | | | | | | | 44001 | 2386017 | 142051 | 493724 |
| Betulin | 35.926 | 74.2 | 74.5 | | | | | | | | | | | | | 213314 | 669726 | 2315007 | 760797 |
| Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)- | 9.240 | 72.3 | 76.9 | | | | | | | | | | | | | | 246676 | 113839 | 197785 |
| Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl- | 9.671 | 75.6 | 78.8 | | | | | | | | | | | | | 11610 | 79227 | 207705 | 162109 |
| Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl- | 9.882 | 76.3 | 81.4 | | | | | | | | | | | | | | 129794 | 297564 | 184680 |
| Biotin | 15.130 | 63.9 | 64.4 | | | | | 124175 | 38201 | 93244 | 36735 | | | | | | | | |
| Butane, 2,2-dimethyl- | 3.345 | 81.5 | 85.3 | | | | | | | | | 1644081 | | | | | | | |
| Butyl tetratriacontyl ether | 11.570 | 70.7 | 71 | 62425 | 59082 | 50742 | 92692 | | | | | | | | | | | | |
| Butylated Hydroxytoluene | 14.276 | 76.9 | 79 | | | | | | | | | | | | | 241388 | 63535 | 203468 | 468905 |
| Cholest-5-en-3-ol, 24-propylidene-, (3β)- | 32.924 | 82.7 | 87.4 | | | | | 70055 | 236651 | 163154 | 97090 | | | | | | | | |
| cis-11-Eicosenoic acid | 28.099 | 80.6 | 82.9 | | | | | 378391 | 341139 | 207524 | 248320 | | | | | | | | |
| cis-13-Eicosenoic acid | 33.322 | 73.3 | 77.1 | | | | | | 203443 | 163986 | 229821 | | | | | | | | |
| Cyclohexane, 1,2,3,4,5,6-hexaethyl- | 12.267 | 73.8 | 75.7 | 48165 | 45902 | 40063 | 77108 | | | | | | | | | | | | |
| Cyclohexane, methyl- | 3.510 | 90.1 | 91.8 | | | | | | | | | 479173 | | | | | | | |
| Cyclohexanespiro-5'-(2',4',4'-trimethyl-2'-oxazoline) | 8.258 | 70.2 | 74.3 | | | | | 279760 | 390821 | 99490 | 652334 | | | | | | | | |
| Cyclopropa[3,4]cyclohepta[1,2-a]naphthalene, 1,1a,1b,2,3,7b,8,9,10,10a-decahydro-5-methoxy-10-methylene- | 24.031 | 70.7 | 72.9 | | | | | | | | | | | | | 8403 | 109567 | 93447 | 114961 |
| Decane, 2,3,5,8-tetramethyl- | 13.451 | 85.9 | 87.6 | 214607 | 237103 | 281654 | 318081 | | | | | | | | | | | | |
| Decane, 2,6,8-trimethyl- | 10.250 | 72.9 | 77.3 | 68811 | 72367 | 74108 | 105079 | | | | | | | | | | | | |
| Decane, 2-methyl- | 10.242 | 85.2 | 87.1 | 139327 | 130236 | 143399 | 196900 | | | | | | | | | | | | |
| Decane, 3,8-dimethyl- | 9.553 | 81 | 81.8 | 40384 | 37481 | 36199 | 56461 | | | | | | | | | | | | |

SUPPLEMENTARY MATERIAL

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Decane, 4-methyl- | 7.024 | 82.7 | 82.8 | 56598 | 48310 | 49030 | 90698 | | | | | | | | | | | | |
| Decane, 5-ethyl-5-methyl- | 13.747 | 78.7 | 79.5 | 278158 | 317478 | 384510 | 432622 | | | | | | | | | | | | |
| Decane, 5-methyl- | 6.986 | 83.1 | 83.1 | 91504 | | 82370 | 121217 | | | | | | | | | | | | |
| Dehydroabietic acid | 30.611 | 92.5 | 96.8 | | | | | | | | | | | | | 22587 | 6682450 | 546848 | 3304800 |
| Diethyl Phthalate | 16.077 | 96.8 | 96.9 | | | | | 3021127 | 2019801 | 1722296 | 6501281 | | | | | | | | |
| D-Mannitol, 1,2:5,6-bis-O-(1-methylethylidene)- | 16.306 | 74.6 | 80.4 | | | | | | | | | | | | | | 972846 | 276210 | 75032 |
| Docosane | 26.327 | 87.6 | 89.9 | | | | | | | | | | | | | | | | |
| Docosane, 11-decyl- | 31.871 | 83.3 | 84.4 | | | | | | 247884 | 160281 | 264779 | | | | | | | | |
| Docosane, 5-butyl- | 33.918 | 76.5 | 79.1 | 273671 | 485489 | 264545 | | | | | | | | | | | | | |
| Docosane, 7-hexyl- | 32.040 | 77.4 | 81.6 | | | | | 286130 | 157294 | 108116 | 227900 | | | | | | | | |
| Docosyl octyl ether | 22.044 | 79.7 | 80.7 | 205161 | 230859 | 302127 | 318522 | | | | | | | | | | | | |
| Dodecane | 7.620 | 83.2 | 83.9 | 102367 | 87691 | 89139 | 133871 | | | | | | | | | | | | |
| Dodecane, 2,2,11,11-tetramethyl- | 12.576 | 75 | 76.1 | 74388 | 74121 | 66857 | 114129 | | | | | | | | | | | | |
| Dodecane, 2,6,10-trimethyl- | 10.026 | 85.5 | 86.9 | 275362 | 252343 | 231228 | 384624 | | | | | | | | | | | | |
| Dodecane, 2,6,11-trimethyl- | 10.356 | 80.4 | 80.4 | 231726 | 209859 | 182924 | 353100 | | | | | 27964 | | 57790 | 30854 | 575820 | 515647 | 1110588 | 1003716 |
| Dodecane, 4,6-dimethyl- | 10.149 | 87.2 | 87.5 | 235524 | 223975 | 250742 | 326744 | | | | | | | | | | | | |
| Dodecanoic acid | 15.549 | 87.8 | 92.1 | | | | | 471130 | 108677 | 255157 | 169130 | | | | | | | | |
| Dodecanoic acid, methyl ester | 14.458 | 88.8 | 89.5 | 33659 | 105600 | 84812 | | | | | | | | | | | | | |
| Dotriacontane | 34.375 | 79.4 | 82.9 | | | | | | | | | | | | | | | | |
| E-14-Hexadecenal | 11.274 | 81.8 | 81.8 | 1436433 | 1548804 | 1708573 | 2058657 | | | | | | | | | | | | |
| Eicosane | 22.835 | 84.8 | 84.8 | | | | | | | | | | | | 177981 | | | | |
| Eicosane, 2-methyl- | 17.511 | 79.7 | 82.3 | | | | | | | | | 22406 | 19994 | 46036 | 57402 | | | | |
| Eicosanoic acid, methyl ester | 35.783 | 61.6 | 66.4 | | | | | 243733 | 92815 | 74874 | 47141 | | | | | | | | |
| Eicosen-1-ol, cis-9- | 29.017 | 80.6 | 86.5 | | | | | 75604 | 666793 | 500151 | 356841 | | | | | | | | |
| Ethanol, 2-(9-octadecenyloxy)-, (Z)- | 33.144 | 82.2 | 85.4 | | | | | 964282 | 487074 | 343662 | 538949 | | | | | 269169 | 311461 | 603836 | 225211 |
| Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1α,2β,4aα,4bβ,10β)- | 26.433 | 77 | 77 | | | | | | | | | | | | | | 624935 | 144647 | 584285 |
| Heneicosane | 32.484 | 75.1 | 77 | 88717 | 108969 | 157476 | 142562 | | 1392498 | 871883 | 1411393 | | | | | 369883 | 372771 | 425764 | 366994 |
| Heptacos-1-ene | 24.708 | 81 | 87.2 | | | | | | 2079126 | 2148014 | 6467931 | | | | | | | | |
| Heptacosane | 33.178 | 92.3 | 94.2 | | | | 694043 | | 1563661 | 1156204 | 1980272 | | 1006350 | | 730959 | 2195879 | 2001661 | 5240263 | 2764914 |
| Heptadecane, 2,6,10,15-tetramethyl- | 34.197 | 8.61 | 9.15 | 183291 | 172845 | 159328 | 272464 | | | | | | | | | | | | |

SUPPLEMENTARY MATERIAL

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Heptadecane, 2,6-dimethyl- | 11.929 | 86.2 | 86.4 | 26060 | 23310 | 24453 | 35800 | | | | | | | | | | | | |
| Heptadecanoic acid, 16-methyl-, methyl ester | 9.481 | 84.2 | 86.7 | | | | | | | | | | | | | | 339508 | 346157 | 244730 |
| Heptadecanoic acid, methyl ester | 25.190 | 79.2 | 85.4 | 58848 | 88827 | 75380 | 30992 | 184996 | 60536 | 49601 | 50140 | | | | | | | | |
| Heptadecanoic acid, methyl ester | 23.486 | 80.2 | 80.5 | | | | | | | | | | | | | | | | |
| Heptane, 2,2,3,3,5,6,6-heptamethyl- | 10.318 | 77.4 | 79.6 | 92847 | 90979 | 104081 | 134667 | | | | | | | | | | | | |
| Heptane, 2,4,6-trimethyl- | 6.284 | 83.2 | 90.1 | 35283 | 31744 | 33313 | 50032 | | | | | | | | | | | | |
| Heptane, 2,4-dimethyl- | 4.254 | 87.6 | 88.2 | 110524 | 96882 | 108621 | 171915 | | | | | | | | | | | | |
| Heptane, 3-ethyl- | 6.089 | 86.1 | 90.9 | 49168 | | 45543 | | | | | | | | | | | | | |
| Hexacosane | 32.565 | 9.2 | 9.39 | 1286196 | 1485320 | 1557323 | 2173229 | 1298579 | 370382 | 281158 | 774057 | | | | | 3323470 | 2899128 | 4409168 | 2662114 |
| Hexacosane, 9-octyl- | 34.112 | 79.4 | 79.9 | | | | | | | | | | | | | 1221259 | 3218139 | 7350625 | 2633021 |
| Hexadecanamide | 26.340 | 86.1 | 86.5 | 843216 | 1487893 | 1747582 | 2073082 | 2092381 | 2118393 | 2275930 | 3194217 | | | | | | | | |
| Hexadecane | 10.876 | 85.5 | 87.2 | 109161 | 114802 | 135820 | 156586 | | | | | | | | | | | | |
| Hexadecane, 2,6,10,14-tetramethyl- | 17.266 | 84.7 | 84.7 | 113544 | 138588 | 183707 | 182304 | | | | | | | | | | | | |
| Hexadecane, 2,6,11,15-tetramethyl- | 18.462 | 85.8 | 86.7 | 328082 | 388095 | 562808 | 522951 | | | | | 28216 | 15563 | 44355 | 26565 | | | | |
| Hexadecane, 2-methyl- | 17.105 | 83.3 | 83.5 | 131732 | 146340 | 179607 | 221226 | | | | | | | | | | | | |
| Hexadecane, 7,9-dimethyl- | 14.014 | 74 | 75.2 | 87644 | 103783 | 148218 | 134035 | | | | | | | | | | | | |
| Hexadecane, 7-methyl- | 12.107 | 84.3 | 85.8 | 106279 | 102318 | 94758 | 159307 | | | | | | | | | | | | |
| Hexadecanoic acid, 10-hydroxy-, methyl ester | 28.991 | 77.9 | 81.5 | | | | | 711103 | 244249 | 20096 | 110800 | | | | | | | | |
| Hexadecanoic acid, 14-methyl-, methyl ester | 23.346 | 87.7 | 90.7 | | | | | 169069 | 190695 | 124260 | 90977 | | | | | | | | |
| Hexadecanoic acid, 2-methylpropyl ester | 25.600 | 8.5 | 8.68 | | 145090 | 275993 | | | | | | 302288 | 204748 | 331821 | 327712 | 527391 | 936038 | 1468563 | 1710162 |
| Hexadecanoic acid, butyl ester | 26.323 | 9 | 9 | | | 558768 | | | | | | 1128195 | 720244 | 1501633 | 2348539 | | 3480520 | 7828046 | 6088819 |
| Hexadecanoic acid, methyl ester | 21.668 | 9.5 | 9.51 | 2574101 | 3749773 | 4284011 | 1253197 | | 9876993 | 6179221 | 5589231 | | | | | 166600 | 916156 | 704895 | 584097 |
| Hexatriacontane | 35.889 | 9.09 | 9.3 | 705601 | 540765 | | | | | | | 373032 | 744570 | 690395 | 1332109 | | | | |
| Isopinocarveol | 8.825 | 71.3 | 83.4 | | | | | | | | | | | | | | 112540 | 345054 | 115521 |
| Methyl 6-oxoheptanoate | 11.747 | 71.6 | 72.5 | | | | | | | | | | | | | 189965 | 131299 | 405585 | 378579 |
| Methyl dehydroabietate | 28.983 | 82.4 | 90.1 | | | | | | | | | | | | | | 853601 | | 744182 |
| Methyl eicosa-5,8,11,14,17-pentaenoate | 28.032 | 93.4 | 93.5 | | | | | 1182632 | 449176 | 384106 | 262728 | | | | | | | | |
| Methyl stearate | 25.220 | 94.3 | 94.6 | 1574971 | 2160644 | 2015908 | 802678 | 430259 | 6451116 | 4760208 | 2907691 | | | | | | | | |
| Methyl tetradecanoate | 17.794 | 93.9 | 94.2 | 83633 | 162169 | 175123 | 44652 | 25608 | 1118018 | 785543 | 173926 | | | | | | | | |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| N-[3-[N-Aziridyl]propylidene]tetrahydrofurfurylamine | 8.791 | 72.4 | 73.7 | | | | | 597263 | | | | | | | | | | | |
| Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1α,7β,8aα)]- | 13.244 | 86.9 | 90.2 | | | | | | | | | | | | | 286960 | | | |
| n-Hexadecanoic acid | 22.535 | 9.41 | 9.5 | 2763547 | 4863693 | 6137051 | 3397869 | | | | | | | | | 2107795 | 2088321 | 1605868 | 2629030 |
| Nonadecane | 13.528 | 8.41 | 8.73 | 110208 | 126059 | 161763 | 168061 | | | | | | | | 290873 | | | | |
| Nonane, 3-methyl-5-propyl- | 11.629 | 83.1 | 83.9 | 573119 | 529186 | 445324 | 853049 | | | | | | | | | | | | |
| Norgestrel, trimethylsilyl ether | 25.338 | 67 | 70.6 | | | | | | | | | | | | | 153738 | 234368 | 368590 | 542387 |
| n-Tridecan-1-ol | 11.388 | 80.2 | 82.4 | 335376 | 303788 | 251181 | 317214 | | | | | | | | | | | | |
| Octacosane | 33.588 | 9.29 | 9.47 | 6566352 | 8564873 | 7194995 | 12424069 | 444857 | 226671 | | | | | | | 1499091 | 3858543 | 9971084 | 4756552 |
| Octacosanol | 34.734 | 90.5 | 92.1 | | | | | | | 874373 | 2227718 | | | | | | | | |
| Octadecanal, 2-bromo- | 32.548 | 68.6 | 69.1 | | | | | 165957 | 100672 | 80926 | 99199 | | | | | | | | |
| Octadecanamide | 30.015 | 84 | 84.7 | | | | | 462353 | 668557 | 583013 | 1071758 | | | | | | | | |
| Octadecane | 16.449 | 83.2 | 83.6 | 63055 | 62917 | 89880 | 82057 | | | | | | | | | | | | |
| Octadecane, 1-iodo- | 32.320 | 83.8 | 87.5 | 593623 | 897973 | 611302 | 1294137 | | | | | | | | | | | | |
| Octadecane, 2-methyl- | 15.435 | 84.4 | 86.3 | 33865 | 42303 | 51981 | 54054 | | | | | | | | | | | | |
| Octadecane, 3-ethyl-5-(2-ethylbutyl)- | 34.155 | 7.79 | 7.94 | | | | | | 314320 | | | | | | | 1410108 | 2057182 | 3320729 | 1514101 |
| Octadecane, 6-methyl- | 14.661 | 70.6 | 76.7 | | | | | | | | | | | | | 211054 | 171145 | 550288 | 687231 |
| Octadecanoic acid | 26.074 | 9.06 | 9.09 | 1950162 | 3156641 | 3769478 | 1929503 | 12652639 | 6852821 | 7841293 | 6796254 | | | | | | 663582 | | |
| Octadecanoic acid, 2-methylpropyl ester | 29.562 | 89.3 | 92.1 | | | | | | | | | 293276 | | 1036765 | | | 2385565 | 4993125 | 4451408 |
| Octadecanoic acid, butyl ester | 29.668 | 8.66 | 8.67 | 268389 | 240974 | 429443 | | | | | | 605755 | 491427 | 942100 | 1224976 | 2353748 | 1772618 | 3279468 | 2793244 |
| Octane, 2,3,3-trimethyl- | 11.625 | 77.5 | 78.7 | 82952 | 82553 | 79304 | 129511 | | | | | | | | | | | | |
| Octane, 3,3-dimethyl- | 6.897 | 83.6 | 85.1 | 651815 | 617186 | 554123 | 871085 | | | | | | | | | | | | |
| Octane, 5-ethyl-2-methyl- | 7.531 | 85.2 | 85.5 | 145531 | 127157 | 131971 | 193714 | | | | | | | | | | | | |
| Octanenitrile, 2-methylene- | 8.381 | 65.3 | 66.5 | | | | | 1214490 | 1478709 | 237666 | 1811659 | | | | | | | | |
| Octanoic acid, 7-oxo- | 8.347 | 70.6 | 71.3 | | | | | | | | | | | | | 212016 | | | 1320508 |
| Octatriacontyl pentafluoropropionate | 35.047 | 79.3 | 81.8 | 233004 | 223159 | | 361793 | | | | | | | | | | | | |
| Octyl tetracosyl ether | 23.131 | 79.8 | 81.2 | 295198 | 303153 | 403177 | 464457 | | | | | | | | | | | | |
| Oleic Acid | 28.099 | 80.4 | 82.7 | | | | | 537754 | 471725 | 289777 | | | | | | | | | |
| Oleic acid, eicosyl ester | 35.427 | 71.3 | 72.1 | | | | | | | | | | | | | 467702 | 798390 | 1233556 | 1141886 |
| Oxalic acid, 2-ethylhexyl pentyl ester | 5.814 | 68.3 | 72.7 | | | | | 1337114 | 810727 | 381852 | 1315597 | | | | | | | | |
| Oxazole, 5-ethyl-2-methyl-4-benzoyl- | 15.193 | 65.9 | 66 | | | | | 302128 | 313477 | 52495 | 322916 | | | | | | | | |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Palmitoleic acid | 22.086 | 92.8 | 93 | 646855 | 1047631 | 1163892 | 373679 | | | | | | | | | | | | |
| Pentacos-1-ene | 19.393 | 7.86 | 8.24 | 387178 | 415497 | 511209 | 636014 | | | | | 11758 | 6797 | 14897 | 14066 | | | | |
| Pentacosane | 31.406 | 91.3 | 92.9 | 1790366 | 2890583 | 1746364 | 3437076 | 4234766 | 3182024 | 1391663 | 3816088 | | | | | | | | |
| Pentacosane, 13-undecyl- | 33.787 | 7.38 | 7.53 | | | | | 97292 | 394809 | 218614 | 352345 | | | | | 160523 | 327105 | 610002 | |
| Pentadecane | 11.561 | 86.2 | 86.9 | 253325 | 304894 | 409994 | 388727 | | | | | | | | | | | | |
| Pentadecane, 2,6,10-trimethyl- | 12.056 | 83.9 | 84 | 224195 | 206711 | 181208 | 333190 | | | | | | | | | | | | |
| Pentadecane, 3-methyl- | 12.238 | 84.5 | 85.9 | 123152 | 116552 | 105553 | 188434 | | | | | | | | | | | | |
| Pentatriacontene | 34.878 | 8.39 | 8.4 | | | | | 1246088 | | 569576 | 1308199 | | | | | | | 632289 | |
| Phenol, 2,4-bis(1-methyl-1-phenylethyl)- | 31.601 | 93.2 | 93.4 | 788172 | 843771 | 1543717 | 1304998 | | | | | | | | | | | | |
| Phenol, 2-methyl-5-(1,2,2-trimethylcyclopentyl)-, (S)- | 19.206 | 81.9 | 90.9 | | | | | | | | | | | | | 128787 | 299762 | 263577 | 379583 |
| Phorone | 8.694 | 90.7 | 92 | | | | | 796644 | 776269 | 111428 | 946969 | | | | | | | | |
| Pimaric acid | 28.915 | 76.3 | 83.6 | | | | | | | | | | | | | | 983580 | | |
| Piperidine, 1-(1-methylpentyl)- | 10.567 | 75 | 75.8 | | | | | 3059035 | 3567858 | 499498 | 1912415 | | | | | | | | |
| Piperidine, 1,4-dimethyl- | 5.835 | 69.8 | 70.3 | | | | | 9778816 | 5032082 | 2195087 | 10213265 | | | | | | | | |
| Piperonyl butoxide | 30.002 | 76.6 | 80 | | | | | 10649 | 18605 | 7362 | 92983 | | | | | | | | |
| Podocarpa-8,11,13-triene-7β,13-diol, 14-isopropyl- | 28.649 | 82.4 | 86.1 | | | | | | | | | | | | | | 51815 | 736349 | |
| Propane, 1,2-dibromo- | 4.681 | 84.2 | 90.5 | 296531 | 201181 | 171645 | 382138 | | | | | | | | | | | | |
| Propanoic acid, 2,2-dimethyl-, hexyl ester | 4.191 | 70.4 | 75.3 | 54269 | 46158 | 53560 | 80891 | | | | | | | | | | | | |
| Pyridine, 2,4,6-trimethyl- | 6.914 | 71.8 | 80 | | | | | 309603 | 436507 | 151052 | 810600 | | | | | | | | |
| Pyrrole, 1-methyl-3-(1,1-dimethylethyl)- | 6.516 | 79.9 | 86.6 | | | | | 3152527 | 4207997 | 1211017 | 7602377 | | | | | | | | |
| Pyrrolidine, 1,1'-methylenebis- | 8.423 | 73.1 | 86.3 | | | | | 599226 | 631110 | 144827 | 433169 | | | | | | | | |
| Squalene | 34.434 | 78.7 | 89.9 | | | | | | | | | | | 170295 | 117960 | | | | |
| Sulfurous acid, 2-ethylhexyl nonyl ester | 9.147 | 82.4 | 84.2 | 118565 | 98915 | 88555 | 143712 | | | | | | | | | | | | |
| Sulfurous acid, dodecyl 2-ethylhexyl ester | 11.697 | 80 | 85.4 | 64671 | 60829 | 51919 | 96055 | | | | | | | | | | | | |
| Tetracosane, 3-ethyl- | 29.626 | 92.3 | 93.9 | 165988 | 287147 | 169271 | 332012 | | | | | | | | | | | | |
| Tetradecanamide | 22.661 | 87.9 | 88.7 | 195217 | 453822 | 551216 | 436023 | 502033 | 641708 | 623577 | 1149742 | | | | | | | | |
| Tetradecane | 12.601 | 91.8 | 94.1 | 33083 | | 83992 | 50618 | | | | | | | | | | | | |
| Tetradecane, 2,6,10-trimethyl- | 22.213 | 83.5 | 85.4 | | | | | | | | | 136934 | 86275 | 75389 | 169119 | 213371 | 231795 | 451068 | 562699 |
| Tetradecane, 3-methyl- | 10.914 | 81.7 | 83 | 131695 | 120315 | 104575 | 192927 | | | | | | | | | | | | |
| Tetradecane, 4,11-dimethyl- | 13.138 | 83.7 | 84.9 | 20896 | 31707 | 68920 | 33279 | | | | | | | | | | | | |

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| Tetradecane, 4-methyl- | 10.191 | 81.1 | 82.7 | 36411 | 34003 | 33658 | 51986 | | | | | | | | | | | | |
| Tetradecane, 6,9-dimethyl- | 10.610 | 82.1 | 82.1 | 411340 | 382893 | 348687 | 588625 | | | | | | | | | | | | |
| Tetradecanoic acid | 18.547 | 93.2 | 93.6 | | | | | 58572 | 727418 | 394478 | 143696 | | | | | | | | |
| Tetratetracontane | 35.335 | 8.41 | 8.48 | 248875 | 424772 | 279499 | 458627 | | | | | | | | | 482555 | 923339 | 1504235 | 827306 |
| trans-13-Octadecenoic acid | 25.478 | 90.8 | 91.4 | | | | | | | | | | | | | 118800 | 1671618 | 788109 | 1837555 |
| Trichloroacetic acid, hexadecyl ester | 14.475 | 80.8 | 81.3 | 183072 | 212292 | 276558 | 307506 | | | | | | | | | | | | |
| Tricosane | 35.335 | 8.41 | 8.48 | 645217 | 961695 | 1677109 | 703454 | | | | | 1430738 | | | | | | | |
| Tridecane, 3-methyl- | 11.895 | 82.4 | 83.9 | 191539 | 177798 | 154364 | 290761 | | | | | | | | | | | | |
| Tridecane, 6-propyl- | 12.157 | 79.6 | 79.9 | 201175 | 184499 | 154020 | 304612 | | | | | | | | | | | | |
| Tridecane, 7-propyl- | 12.990 | 79 | 79.2 | 46931 | 45054 | 46149 | 70957 | | | | | | | | | | | | |
| Tridecanoic acid, methyl ester | 17.989 | 78.3 | 78.8 | 222733 | 426836 | 460913 | 107123 | | | | | | | | | | | | |
| Tropidine, 2-acetyl-8-demethyl- | 8.115 | 66.5 | 68.5 | | | | | | | | | | | | | 154455 | | | 2448588 |
| Undecane | 8.229 | 88.2 | 90.4 | | | | | | | | | | | | | | 465065 | 656960 | 827750 |
| Undecane, 2-methyl- | 11.066 | 83.4 | 83.9 | 91823 | 104013 | 133087 | 133058 | | | | | | | | | | | | |
| Undecane, 3,8-dimethyl- | 17.832 | 74.4 | 76.9 | 91246 | 105495 | 137544 | 154236 | | | | | | | | | | | | |
| Undecane, 3-ethyl- | 9.350 | 79.5 | 81 | 38811 | 33953 | 33762 | 49807 | | | | | | | | | | | | |
| Undecane, 3-methyl- | 9.980 | 81 | 82.4 | 141689 | 129342 | 122181 | 197620 | | | | | | | | | | | | |
| Undecane, 4,8-dimethyl- | 9.832 | 86.1 | 86.3 | 68315 | 68908 | 72316 | 96808 | | | | | | | | | | | | |
| Undecane, 4-methyl- | 8.385 | 81 | 81 | 65217 | 59209 | 61285 | 91789 | | | | | | | | | | | | |
| Z-12-Pentacosene | 31.021 | 93.1 | 93.6 | 518709 | 466436 | 802976 | 2304501 | | 459201 | 521787 | 1954514 | | | | | | | | |
| β-D-Glucopyranose, 4-O-β-D-galactopyranosyl- | 11.603 | 74.8 | 76.3 | | | | | | | | | | | | | 690136 | 484081 | 1088146 | 997244 |
| β-Pimaric acid | 27.955 | 72.2 | 73.4 | | | | | | | | | | | | | | 431758 | 176272 | 173456 |
| β-Sitosterol | 34.709 | 85.2 | 88.5 | | | | | | | | | 134575 | 199833 | 233868 | 158444 | 564931 | 2297148 | 2078929 | 2550039 |
| γ-Elemene | 14.141 | 75.2 | 80.7 | | | | | | | | | | | | | | | | |
| γ-Linolenic acid, methyl ester | 24.420 | 88.4 | 88.6 | 29097 | 65198 | 56903 | | | | | | | | | | | | | |

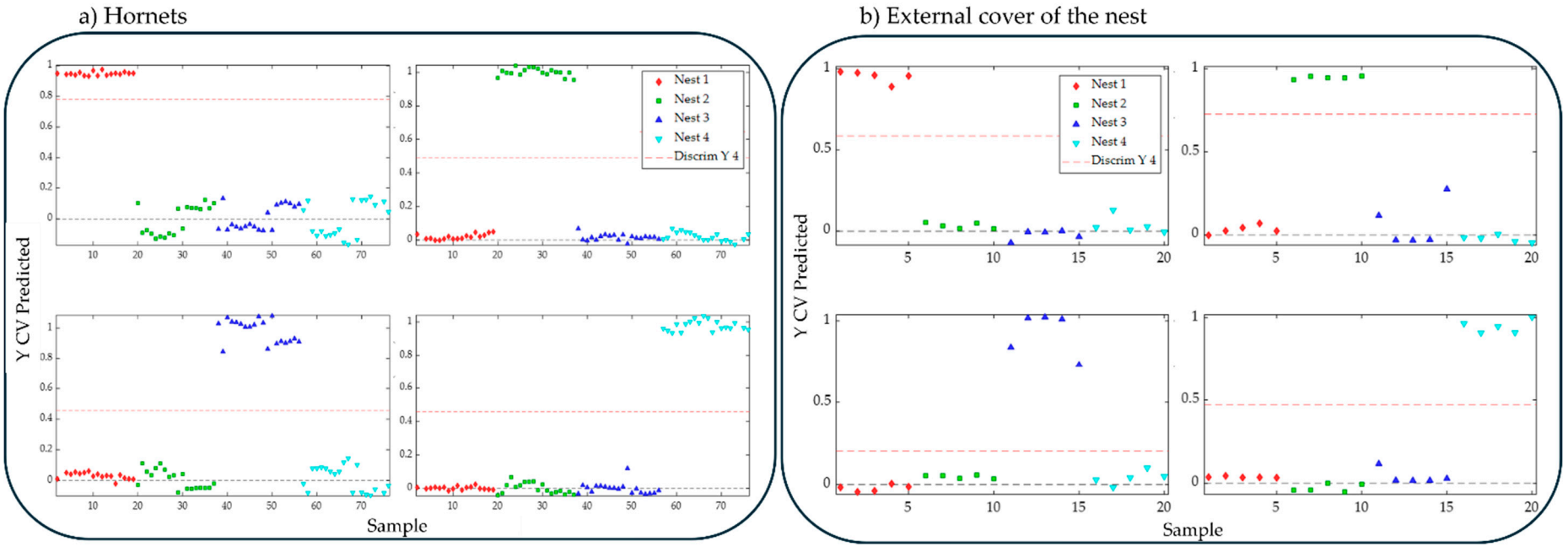



**Figure 1.** Predicted Y-values for the hornet and the external cover of the nests samples with the location of the different colonies as discriminant classes for the CV: nest 1 – Ajangiz (red), nests 2 and 3 – Amorebieta (green and dark blue) and nest 4 – Leioa (light blue). The red line is the classification threshold.