Compounds detected and concentration (µg/mg**)** in butanol *Artemisia afra* extracts from three vendors by GC×GC-TOF-MS for the identified and unidentified compounds

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Sample name** | **Mass** | **Mean RT (s)** | ***A. afra* from vendor A** (µg/mg sample**)** | ***A. afra* from vendor B** (µg/mg sample**)** | ***A. afra* from vendor C** (µg/mg sample**)** |
| **Metabolite name** |
| 3-Phenyl butyric acid (IS) | 118 | 1193 | 0.049 | 0.046 | 0.046 |
| Cyclohexene, 2-ethenyl-1,3,3-trimethyl- | 135 | 359 | 0.061 | 0.049 | 0.055 |
| 2,2-Dichloroethyl methyl ether | 61 | 360 | 0.142 | 0.163 | 0.134 |
| **3,3,6-Trimethyl-1,4-heptadien-6-ol#** | 59 | 365 | 0.368 | 0.320 | 0.383 |
| 3,3,6-Trimethyl-1,4-heptadien-6-ol | 59 | 366 | 0.155 | 0.047 | 0.179 |
| Analyte 5 | 61 | 368 | 0.026 | 0 | 0.228 |
| **Glycerin#** | 61 | 371 | 0.288 | 0 | 0 |
| Analyte 7 | 72 | 377 | 0.030 | 0.026 | 0.018 |
| Cyclohexene, 1-methoxy- | 97 | 382 | 0.057 | 0.023 | 0.055 |
| à-Phellandrene | 93 | 389 | 0.071 | 0.049 | 0.059 |
| à-Phellandrene | 93 | 389 | 0.035 | 0.033 | 0.035 |
| **2H-Tetrazole, 2-methyl-#** | 56 | 398 | 0.049 | 0 | 0 |
| Cyclohexene, 1-methyl-4-(1-methylethylidene)- | 93 | 404 | 0.057 | 0.069 | 0.054 |
| 1-Butanol, 3-methoxy- | 59 | 413 | 0.074 | 0.065 | 0.101 |
| **o-Cymene#** | 119 | 419 | 0.303 | 0.187 | 0.189 |
| **Pyridine#** | 52 | 417.5 | 0 | 2.041 | 1.698 |
| Benzene, 1-methyl-3-(1-methylethyl)- | 119 | 416 | 0.381 | 0.325 | 0.369 |
| Analyte 17 | 112 | 419 | 0.026 | 0.018 | 0.014 |
| Cyclohexene, 3-methyl-6-(1-methylethyl)- | 95 | 422 | 0.140 | 0.070 | 0.115 |
| 2,5-Furandione, 3,4-dimethyl- | 54 | 425 | 0.031 | 0.018 | 0.028 |
| trans-2,7-Dimethyl-4,6-octadien-2-ol | 59 | 425 | 0.295 | 0.239 | 0.347 |
| á-Phellandrene | 93 | 428 | 0.061 | 0.048 | 0.053 |
| Eucalyptol | 81 | 431 | 0.032 | 0.023 | 0.030 |
| 2(3H)-Furanone, 5-ethenyldihydro-5-methyl- | 111 | 437 | 0.049 | 0.039 | 0.051 |
| 1-Cyclohexene-1-acetaldehyde, à,2-dimethyl- | 81 | 437 | 0.015 | 0.013 | 0.038 |
| Binapacryl\* | 83 | 470 | 1.436 | 0.859 | 1.335 |
| ç-Terpinene | 93 | 473 | 0.073 | 0.046 | 0.059 |
| Analyte 27 | 75 | 485 | 0.037 | 0.110 | 0.058 |
| Ethyl 4-(ethyloxy)-2-oxobut-3-enoate | 99 | 491 | 0.027 | 0.025 | 0.026 |
| p-Cresol | 107 | 494 | 0.030 | 0.019 | 0.029 |
| 3,5-Hexadien-2-ol, 2-methyl- | 69 | 497 | 0.564 | 0.510 | 0.544 |
| Tricyclo[4.1.0.0(2,7)]heptane | 79 | 500 | 0.046 | 0.033 | 0.042 |
| 1,5-Heptadien-4-ol, 3,3,6-trimethyl- | 85 | 509 | 0.443 | 0.368 | 0.487 |
| Benzene, 1-methyl-4-(1-methylethenyl)- | 117 | 530 | 0.210 | 0.178 | 0.200 |
| tert-Butyl N-hydroxycarbamate | 57 | 539 | 0.056 | 0.041 | 0.053 |
| 3,7-Octadiene-2,6-diol, 2,6-dimethyl- | 71 | 550 | 0.054 | 0.059 | 0.033 |
| o-Menthan-8-ol | 59 | 557 | 0.159 | 0.142 | 0.063 |
| 3-Penten-2-one, 3,4-dimethyl-\*\* | 69 | 560 | 4.126 | 3.597 | 4.234 |
| **Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-#\*** | 81 | 560 | 0.888 | 0 | 1.062 |
| Levoglucosenone | 68 | 566 | 0.032 | 0.029 | 0.026 |
| Phenylethyl Alcohol | 91 | 572 | 0.035 | 0.031 | 0.046 |
| 4-Ethyl-2-hexynal | 67 | 572 | 0.035 | 0.028 | 0.053 |
| Analyte 42 | 73 | 578 | 0.084 | 0.046 | 0.105 |
| Analyte 43 | 69 | 578 | 0.060 | 0.050 | 0.061 |
| Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-, [1S-(1à,4á,5à)]- | 81 | 581 | 0.098 | 0.053 | 0.105 |
| Analyte 45 | 59 | 581 | 0.046 | 0.043 | 0.036 |
| 4-(Trimethylsilyoxy)-3-penten-2-one | 157 | 584 | 0.280 | 0.219 | 0.310 |
| 2-Butene, 2,3-dimethyl- | 84 | 587 | 0.063 | 0.046 | 0.057 |
| 1-Hexene, 4,5-dimethyl- | 71 | 587 | 0.055 | 0.041 | 0.059 |
| Analyte 49 | 59 | 587 | 0.057 | 0.053 | 0.054 |
| 3-Hexanol, 2,3-dimethyl- | 87 | 587 | 0.040 | 0.024 | 0.034 |
| Cyclohexanone, 2-ethyl- | 55 | 596 | 0.052 | 0.044 | 0.052 |
| 2-Butene, 2,3-dimethyl- | 69 | 599 | 0.190 | 0.167 | 0.175 |
| Cyclopropanemethanol, à,à-dimethyl-2-methylene- | 72 | 605 | 0.107 | 0.110 | 0.102 |
| 2,6-Dimethoxyamphetamine | 152 | 611 | 0.125 | 0.132 | 0.117 |
| Cyclobutane, methylene- | 68 | 614 | 0.043 | 0.040 | 0.050 |
| Analyte 56 | 83 | 617 | 0.077 | 0.086 | 0.081 |
| Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)- | 83 | 620 | 0.032 | 0.025 | 0.033 |
| **Bicyclo[3.1.1]heptan-3-ol, 6,6-dimethyl-2-methylene-, [1S-(1à,3à,5à)]-#** | 92 | 626 | 0.076 | 0.062 | 0.080 |
| 4,4-Dimethyl-non-5-enal | 69 | 626 | 0.316 | 0.272 | 0.341 |
| 5-Isopropenyl-3,3-dimethyl-dihydrofuran-2-one | 95 | 632 | 0.024 | 0.017 | 0.023 |
| **Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-#\*\*\*** | 95 | 638 | 13.381 | 12.009 | 14.853 |
| Analyte 62 | 100 | 647 | 0.027 | 0.020 | 0.015 |
| 1,3,8-p-Menthatriene | 119 | 650 | 0.016 | 0.015 | 0.014 |
| Cyclobutane-1,1-dicarboxamide, N,N'-di-benzoyloxy- | 105 | 650 | 0.018 | 0.016 | 0.017 |
| Bicyclo[2.2.1]heptan-2-ol, 2,3,3-trimethyl- | 71 | 653 | 0.044 | 0.043 | 0.045 |
| Cyclohexene, 3-methyl- | 96 | 656 | 0.051 | 0.044 | 0.053 |
| Octa-3,5-diene-2,7-dione, 4,5-dihydroxy- | 85 | 665 | 0.077 | 0.066 | 0.079 |
| Pinocarvone | 53 | 665 | 0.322 | 0.298 | 0.311 |
| Cyclohexene, 3-methyl-1-(trimethylsilyloxy)- | 73 | 668 | 0.112 | 0.083 | 0.130 |
| Octanoic acid | 60 | 670 | 0.035 | 0.015 | 0.036 |
| 2,2,5-Trimethyl-hex-4-enoic acid | 69 | 671 | 0.064 | 0.057 | 0.068 |
| Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- | 73 | 674 | 0.079 | 0.101 | 0.064 |
| **7-Octen-2-ol, 2-methyl-6-methylene-#** | 59 | 680 | 0.067 | 0 | 0.072 |
| 6-Nonynoic acid, methyl ester | 59 | 683 | 0.078 | 0.114 | 0.083 |
| endo-Borneol\* | 95 | 683 | 2.290 | 2.232 | 2.360 |
| **2-(1-Cyclopent-1-enyl-1-methylethyl)cyclopentanone#** | 109 | 683 | 0.033 | 0 | 0.063 |
| Butane, 2,3-dimethyl- | 71 | 692 | 0.058 | 0.060 | 0.057 |
| Trimethylsilyl 2-acetoxyacetate | 75 | 692 | 0.325 | 0.317 | 0.311 |
| Santolina triene | 93 | 698 | 0.038 | 0.036 | 0.037 |
| Bicyclo[2.2.1]heptane-2,5-diol, 1,7,7-trimethyl-, (2-endo,5-exo)- | 85 | 701 | 0.090 | 0.079 | 0.086 |
| Analyte 81 | 67 | 701 | 0.079 | 0.071 | 0.084 |
| 3-Cyclohexene-1-methanol | 79 | 707 | 0.068 | 0.050 | 0.062 |
| Ethanone, 1-(3-methylphenyl)- | 119 | 707 | 0.111 | 0.079 | 0.084 |
| Benzenemethanol, à,à,4-trimethyl- | 135 | 710 | 0.084 | 0.079 | 0.083 |
| 6-Methyl-hept-2-en-4-ol | 71 | 713 | 0.033 | 0.031 | 0.032 |
| Analyte 86 | 70 | 713 | 0.043 | 0.040 | 0.046 |
| Analyte 87 | 155 | 713 | 0.064 | 0.059 | 0.063 |
| 1,2-Dimethyldiaziridine | 71 | 716 | 0.275 | 0.274 | 0.267 |
| Butane, 1,2,3-tris(trimethylsiloxy)- | 117 | 719 | 0.199 | 0.218 | 0.188 |
| Analyte 90 | 58 | 725 | 0.042 | 0.029 | 0.042 |
| à-Terpineol | 91 | 728 | 0.039 | 0.032 | 0.037 |
| N-1H-Tetrazol-5-ylacetamide | 127 | 731 | 0.150 | 0.150 | 0.150 |
| **p-Mentha-1,5-dien-8-ol#** | 59 | 731 | 0.046 | 0 | 0.042 |
| Nona-3,5-dien-2-ol | 85 | 737 | 0.049 | 0.033 | 0.049 |
| trans-Crotyl alcohol, trimethylsilyl ether | 73 | 739 | 0.126 | 0.120 | 0.132 |
| 2-Hexanone, 3-methyl- | 72 | 739 | 0.061 | 0.061 | 0.062 |
| Analyte 97 | 71 | 746 | 0.019 | 0.015 | 0.017 |
| 3,3,6-Trimethyl-1,4-heptadien-6-ol | 139 | 746 | 0.033 | 0.037 | 0.035 |
| Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1S)- | 107 | 752 | 0.030 | 0.025 | 0.030 |
| Analyte 100 | 111 | 755 | 0.208 | 0.194 | 0.212 |
| **2-Hexanone, 3-methyl-#** | 72 | 761 | 0.236 | 0.241 | 0.261 |
| Analyte 102 | 59 | 764 | 0.094 | 0.116 | 0.098 |
| Phenol, 4-ethenyl-, acetate | 120 | 767 | 0.032 | 0.038 | 0.033 |
| Analyte 104 | 59 | 770 | 0.025 | 0 | 0.024 |
| Analyte 105 | 82 | 776 | 0.138 | 0.145 | 0.145 |
| Octan-2-one, 3,6-dimethyl- | 58 | 779 | 0.066 | 0.061 | 0.060 |
| 5-Hydroxymethylfurfural | 97 | 782 | 0.184 | 0.185 | 0.165 |
| Silane, trimethyl(2-phenylethoxy)- | 103 | 782 | 0.016 | 0.012 | 0.017 |
| Phenol, 3-(1-methylethyl)- | 121 | 782 | 0.036 | 0.025 | 0.036 |
| **Borneol, trimethylsilyl ether#\*** | 95 | 785 | 1.056 | 0.943 | 1.148 |
| 2,5-Dimethyl-[1,3]dioxane-4-carboxaldehyde | 71 | 788 | 0.017 | 0.019 | 0.037 |
| 2-Oxabicyclo[2.2.2]octan-6-ol, 1,3,3-trimethyl- | 108 | 788 | 0.045 | 0.044 | 0.043 |
| 1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl- | 139 | 797 | 0.024 | 0.024 | 0.023 |
| Propennitrile, 3-ethoxy-2-(2-thienylmethylsulfonyl)- | 97 | 797 | 0.100 | 0.084 | 0.096 |
| Analyte 115 | 59 | 806 | 0.741 | 0.719 | 0.731 |
| Analyte 116 | 82 | 807 | 1.614 | 1.718 | 1.730 |
| Analyte 117 | 75 | 809 | 0.157 | 0.158 | 0.152 |
| Benzeneacetic acid | 91 | 821 | 0.207 | 0.197 | 0.207 |
| Analyte 119 | 70 | 827 | 0.075 | 0.066 | 0.073 |
| 2-Cyclohexen-1-one, 2-methyl-5-(1-methylethyl)-, (S)- | 82 | 833 | 0.047 | 0.024 | 0.044 |
| **Butane, 1,1-dibutoxy-#** | 57 | 839 | 0.410 | 0.298 | 0.372 |
| 2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)- | 82 | 842 | 0.077 | 0.062 | 0.079 |
| Carvenone | 95 | 848 | 0.045 | 0.038 | 0.062 |
| 1-Penten-1-one, 2-methyl- | 69 | 857 | 0.112 | 0.096 | 0.112 |
| Analyte 125 | 73 | 860 | 0.107 | 0.085 | 0.117 |
| Nonanoic acid | 60 | 863 | 0.050 | 0.049 | 0.040 |
| Analyte 127 | 97 | 863 | 0.119 | 0.105 | 0.130 |
| 1,7-Octadiene-3,6-diol, 2,6-dimethyl- | 67 | 876 | 0.045 | 0.032 | 0.044 |
| Analyte 129 | 109 | 881 | 0.015 | 0.018 | 0.014 |
| **Glycerol, tris(trimethylsilyl) ether#** | 73 | 884 | 0.360 | 0.319 | 0.321 |
| Analyte 131 | 73 | 884 | 0.043 | 0.090 | 0.036 |
| Analyte 132 | 73 | 890 | 0.062 | 0.060 | 0.065 |
| Analyte 133 | 73 | 896 | 0.074 | 0.071 | 0.084 |
| Analyte 134 | 97 | 896 | 0.036 | 0.038 | 0.040 |
| Bornyl acetate | 93 | 902 | 0.026 | 0.017 | 0.029 |
| Cyclopropanemethanol, à,à-dimethyl-2-methylene- | 59 | 903 | 0.732 | 0.767 | 0.748 |
| 1,7,7-Trimethylbicyclo[2.2.1]hept-5-en-2-one | 93 | 908 | 0.047 | 0.027 | 0.042 |
| Analyte 138 | 59 | 908 | 0.036 | 0.036 | 0.036 |
| Analyte 139 | 70 | 908 | 0.023 | 0.024 | 0.025 |
| Thymol | 135 | 912 | 0.032 | 0.123 | 0.028 |
| Analyte 141 | 139 | 914 | 0.043 | 0.045 | 0.043 |
| Analyte 142 | 143 | 914 | 0.597 | 0.507 | 0.553 |
| p-Cymen-7-ol | 105 | 914 | 0.041 | 0.041 | 0.038 |
| Benzeneacetic acid, trimethylsilyl ester | 73 | 920 | 0.114 | 0.100 | 0.108 |
| 4-Hexen-3-ol, 2,5-dimethyl- | 85 | 920 | 0.133 | 0.135 | 0.132 |
| Analyte 146 | 71 | 923 | 0.058 | 0 | 0.051 |
| Phenol, 2-methyl-5-(1-methylethyl)- | 135 | 929 | 0.313 | 0.262 | 0.302 |
| 1,3-Dimethyl-1-cyclohexene | 95 | 929 | 0.088 | 0.084 | 0.093 |
| 4-Hexen-3-ol, 2,5-dimethyl- | 85 | 932 | 0.194 | 0.202 | 0.198 |
| Analyte 150 | 85 | 935 | 0.237 | 0.225 | 0.238 |
| Analyte 151 | 74 | 958 | 0.092 | 0.072 | 0.084 |
| **Bicyclo[2.2.1]heptane-2-carboxylic acid, 3,3-dimethyl-#** | 67 | 959 | 0.320 | 0.314 | 0.309 |
| Pentenoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester | 73 | 962 | 0.029 | 0.055 | 0.051 |
| 1-Nonen-4-ol | 55 | 966 | 0.058 | 0.148 | 0.130 |
| Analyte 155 | 155 | 971 | 0.218 | 0.212 | 0.225 |
| 4-Nitrosophenyl-á-phenylpropionate | 91 | 989 | 0.031 | 0.026 | 0.025 |
| 1,5-Heptadien-4-ol, 3,3,6-trimethyl- | 85 | 1001 | 0.104 | 0.100 | 0.104 |
| Analyte 158 | 73 | 1007 | 0.166 | 0.153 | 0.169 |
| Analyte 159 | 67 | 1013 | 0.065 | 0.061 | 0.066 |
| Analyte 160 | 73 | 1016 | 0.045 | 0.032 | 0.053 |
| Analyte 161 | 107 | 1019 | 0.026 | 0.029 | 0.025 |
| 1,2-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)- | 71 | 1019 | 0.051 | 0.048 | 0.052 |
| Analyte 163 | 70 | 1019 | 0.058 | 0.063 | 0.062 |
| Butane-1,1-dicarbonitrile, 1-cyclohexyl-3-methyl- | 83 | 1022 | 0.037 | 0.039 | 0.037 |
| Analyte 165 | 70 | 1025 | 0.032 | 0.029 | 0.031 |
| à-Cubebene | 105 | 1026 | 0.034 | 0.013 | 0.031 |
| Analyte 167 | 126 | 1025 | 0.023 | 0.011 | 0.024 |
| 3-Cyclohexene-1-methanol, 2-hydroxy-à,à,4-trimethyl- | 59 | 1028 | 0.133 | 0.142 | 0.129 |
| Ethosuximide | 113 | 1031 | 0.120 | 0.117 | 0.115 |
| 4-Acetylanisole | 135 | 1034 | 0.070 | 0.044 | 0.065 |
| **Ethanedioic acid, dibutyl ester#** | 57 | 1043 | 0.278 | 0.175 | 0.257 |
| Analyte 172 | 59 | 1043 | 0.124 | 0.138 | 0.135 |
| 1,6-Octadiene, 3,7-dimethyl- | 81 | 1046 | 0.330 | 0.308 | 0.334 |
| Analyte 174 | 73 | 1049 | 0.036 | 0.037 | 0.052 |
| Analyte 175 | 144 | 1049 | 0.143 | 0.128 | 0.141 |
| Analyte 176 | 73 | 1052 | 0.066 | 0.072 | 0.065 |
| Analyte 177 | 73 | 1058 | 0.036 | 0.033 | 0.038 |
| Analyte 178 | 143 | 1061 | 0.057 | 0.053 | 0.055 |
| Analyte 179 | 59 | 1061 | 0.049 | 0.055 | 0.049 |
| Allyl o-tolyl ether | 105 | 1067 | 0.054 | 0.061 | 0.054 |
| 2,3,4-Trimethyl-hex-3-enal | 111 | 1076 | 0.020 | 0.018 | 0.020 |
| Analyte 182 | 143 | 1076 | 0.041 | 0.031 | 0.042 |
| Analyte 183 | 83 | 1082 | 0.041 | 0.097 | 0.036 |
| 1,3,3,4-Tetramethyl-2-oxabicyclo[2.2.0]hexane | 55 | 1085 | 0.010 | 0.031 | 0.040 |
| Analyte 185 | 73 | 1085 | 0.204 | 0.198 | 0.199 |
| Hydroxy-à-terpenyl acetate | 59 | 1085 | 0.062 | 0.079 | 0.073 |
| Analyte 187 | 73 | 1094 | 0.072 | 0.065 | 0.069 |
| Analyte 188 | 100 | 1097 | 0.032 | 0.020 | 0.032 |
| 2H-Pyran-3-ol, tetrahydro-3-methyl-6-propyl-, acetate | 69 | 1100 | 0.029 | 0.026 | 0.054 |
| Bicyclo[2.2.2]octane-1,4-diol, monoacetate | 109 | 1105 | 0.075 | 0.074 | 0.078 |
| Analyte 191 | 73 | 1109 | 0.089 | 0.096 | 0.109 |
| Analyte 192 | 73 | 1112 | 0.065 | 0.057 | 0.053 |
| Analyte 193 | 73 | 1115 | 0.088 | 0.131 | 0.156 |
| trans-3(10)-Caren-2-ol | 109 | 1115 | 0.026 | 0.022 | 0.034 |
| **5-Hepten-2-one, 6-methyl-#\*** | 108 | 1118 | 0.926 | 0.861 | 0.941 |
| 3-Cyclohexene-1-methanol, 2-hydroxy-à,à,4-trimethyl- | 59 | 1121 | 0.066 | 0.074 | 0.071 |
| Analyte 197 | 155 | 1124 | 0.057 | 0.070 | 0.050 |
| **Bicyclo[3.2.0]heptan-2-one, 5-formylmethyl-6-hydroxy-3,3-dimethyl-6-vinyl-#** | 107 | 1127 | 0.019 | 0.018 | 0.028 |
| Analyte 199 | 71 | 1130 | 0.061 | 0.055 | 0.081 |
| **Binapacryl#** | 83 | 1136 | 0.187 | 0.168 | 0.183 |
| Analyte 201 | 96 | 1139 | 0.113 | 0.132 | 0.114 |
| (t-Butyldimethylsilyl)[3-methyl-3-(4-methyl-pent-3-enyl)-oxiran-2-yl]-methanone | 73 | 1145 | 0.040 | 0.030 | 0.028 |
| Analyte 203 | 108 | 1145 | 0.049 | 0.047 | 0.047 |
| Analyte 204 | 59 | 1154 | 0.086 | 0.089 | 0.085 |
| Analyte 205 | 73 | 1163 | 0.103 | 0.100 | 0.107 |
| Analyte 206 | 73 | 1166 | 0.089 | 0.096 | 0.088 |
| 1-Hydroxymethyl-2-methyl-1-cyclohexene | 95 | 1169 | 0.048 | 0.043 | 0.042 |
| Analyte 208 | 59 | 1172 | 0.021 | 0 | 0 |
| 8-Hydroxycarvotanacetone | 59 | 1175 | 0.192 | 0.198 | 0.148 |
| Analyte 210 | 96 | 1175 | 0.053 | 0.051 | 0.060 |
| Analyte 211 | 83 | 1181 | 0.043 | 0.036 | 0.042 |
| Analyte 212 | 75 | 1181 | 0.080 | 0.106 | 0.105 |
| Analyte 213 | 83 | 1184 | 0.021 | 0.022 | 0.022 |
| Analyte 214 | 73 | 1187 | 0.135 | 0.148 | 0.139 |
| Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene | 141 | 1190 | 0.077 | 0.065 | 0.069 |
| Benzaldehyde, 2-hydroxy-4-methyl- | 136 | 1196 | 0.127 | 0.182 | 0.152 |
| Pinonic acid | 83 | 1192 | 0.041 | 0.023 | 0.044 |
| **Acetophenone, 4'-hydroxy-#** | 121 | 1196 | 0.750 | 0.759 | 0.727 |
| 1,8-Cyclopentadecadiyne | 105 | 1226 | 0.032 | 0.019 | 0.030 |
| 1-Methyl-2-trimethylsilyloxycyclohexene | 108 | 1238 | 0.032 | 0.033 | 0.029 |
| Analyte 222 | 93 | 1244 | 0.039 | 0.024 | 0.026 |
| Acetophenone, 4'-(trimethylsiloxy)- | 193 | 1247 | 0.210 | 0.183 | 0.198 |
| Analyte 224 | 73 | 1253 | 0.029 | 0.030 | 0.028 |
| Analyte 225 | 73 | 1259 | 0.054 | 0.051 | 0.050 |
| Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)- | 161 | 1259 | 0.040 | 0.028 | 0.038 |
| Analyte 227 | 75 | 1268 | 0.061 | 0.070 | 0.059 |
| Apocynin | 151 | 1274 | 0.053 | 0.050 | 0.051 |
| Analyte 229 | 72 | 1274 | 0.018 | 0.017 | 0.018 |
| p-Menthane-1,2,3-triol | 112 | 1277 | 0.048 | 0.050 | 0.057 |
| **D-Allose#\*** | 60 | 1280 | 1.844 | 2.076 | 1.842 |
| Analyte 232 | 109 | 1283 | 0.294 | 0.319 | 0.309 |
| Analyte 233 | 129 | 1286 | 0.081 | 0.084 | 0.085 |
| L-2-Aminobutyric acid, N-dimethylaminomethylene-, butyl ester | 113 | 1298 | 0.018 | 0.020 | 0.018 |
| Analyte 235 | 161 | 1304 | 0.033 | 0.016 | 0.017 |
| 1,8-Nonadiene, 2-methyl-5,7-dimethylene- | 91 | 1304 | 0.030 | 0.029 | 0.048 |
| Propanoic acid, 2-oxo-, trimethylsilyl ester | 73 | 1304 | 0.166 | 0.169 | 0.164 |
| 2-Oxabicyclo[2.2.2]octan-6-ol, 1,3,3-trimethyl-, acetate | 71 | 1313 | 0.055 | 0.055 | 0.057 |
| Benzoic acid, 4-hydroxy- | 121 | 1321 | 0.129 | 0.110 | 0.095 |
| Analyte 240 | 59 | 1328 | 0.025 | 0.021 | 0.022 |
| Methyl 4-O-methyl-d-arabinopyranoside | 87 | 1327 | 0.541 | 0.654 | 0.567 |
| Analyte 242 | 169 | 1331 | 0.011 | 0 | 0.010 |
| Analyte 243 | 181 | 1337 | 0.027 | 0.030 | 0.032 |
| Analyte 244 | 58 | 1338 | 0.038 | 0.048 | 0.036 |
| Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)- | 119 | 1343 | 0.106 | 0.090 | 0.091 |
| Analyte 246 | 134 | 1349 | 0.037 | 0.050 | 0.032 |
| **trans-calamenene#** | 159 | 1349 | 0.282 | 0.222 | 0.241 |
| Analyte 248 | 73 | 1352 | 0.088 | 0.068 | 0.121 |
| Benzoic acid, 4-acetyloxy-, trimethylsilyl ester | 195 | 1356 | 0.059 | 0.050 | 0.057 |
| 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl- | 111 | 1358 | 0.075 | 0.072 | 0.069 |
| Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)- | 119 | 1367 | 0.077 | 0.070 | 0.073 |
| Analyte 252 | 73 | 1373 | 0.101 | 0.086 | 0.097 |
| Analyte 253 | 73 | 1373 | 0.073 | 0.071 | 0.069 |
| à-Calacorene | 157 | 1382 | 0.119 | 0.106 | 0.108 |
| Propanoic acid, 2-methyl-, trimethylsilyl ester | 73 | 1382 | 0.060 | 0.064 | 0.056 |
| Analyte 256 | 73 | 1388 | 0.068 | 0.044 | 0.034 |
| Naphthalene, 1,6-dimethyl- | 141 | 1400 | 0.196 | 0.172 | 0.188 |
| 3-Hydroxy-4-methoxybenzoic acid | 168 | 1403 | 0.016 | 0.014 | 0.005 |
| Analyte 259 | 59 | 1412 | 0.021 | 0.024 | 0.022 |
| Dodecanoic acid | 60 | 1415 | 0.014 | 0.015 | 0.014 |
| Fumaric acid, 4-chlorophenyl ethyl ester | 127 | 1421 | 0.189 | 0.199 | 0.175 |
| **(-)-Spathulenol#** | 91 | 1445 | 0.298 | 0.325 | 0.304 |
| Analyte 263 | 73 | 1445 | 0.035 | 0.034 | 0.032 |
| Analyte 264 | 75 | 1449 | 0.112 | 0.104 | 0.125 |
| Caryophyllene oxide | 79 | 1454 | 0.083 | 0.088 | 0.100 |
| Analyte 266 | 73 | 1460 | 0.111 | 0.102 | 0.100 |
| 1,6-Anhydro-á-D-glucofuranose | 73 | 1462 | 0.142 | 0.186 | 0.168 |
| Benzoic acid, 4-hydroxy-, tert.-butyldimethylsilyl ester | 195 | 1466 | 0.133 | 0.147 | 0.114 |
| Analyte 269 | 73 | 1475 | 0.070 | 0.043 | 0.066 |
| Analyte 270 | 58 | 1475 | 0.119 | 0.113 | 0.115 |
| Analyte 271 | 87 | 1481 | 0.032 | 0.035 | 0.032 |
| Analyte 272 | 75 | 1484 | 0.041 | 0.047 | 0.051 |
| Analyte 273 | 98 | 1489 | 0.250 | 0.241 | 0.253 |
| Analyte 274 | 73 | 1491 | 0.087 | 0.100 | 0.096 |
| Analyte 275 | 73 | 1493 | 0.081 | 0.097 | 0.086 |
| 2-Isopropylidene-3-methylhexa-3,5-dienal | 91 | 1499 | 0.026 | 0.023 | 0.026 |
| Azelaic acid | 55 | 1523 | 0.029 | 0.022 | 0.021 |
| **Benzoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester#** | 73 | 1526 | 0.134 | 0.100 | 0.128 |
| Ethyl 2-(methylamino)-1-phenyl-3-cyclohexene-1-carboxylate | 83 | 1526 | 0.208 | 0.191 | 0.205 |
| Analyte 280 | 87 | 1529 | 0.154 | 0.168 | 0.149 |
| Analyte 281 | 73 | 1535 | 0.040 | 0.026 | 0.036 |
| Analyte 282 | 113 | 1535 | 0.052 | 0.054 | 0.049 |
| **Myo-Inositol, 4-C-methyl-#\*\*** | 87 | 1531 | 2.487 | 3.261 | 2.563 |
| Analyte 284 | 73 | 1541 | 0.071 | 0.063 | 0.104 |
| Naphthalene, 1,4,5-trimethyl- | 155 | 1544 | 0.026 | 0.016 | 0.016 |
| Methyl 10,12-octadecadiynoate | 91 | 1541 | 0.096 | 0.079 | 0.096 |
| Aromadendrene oxide-(1) | 91 | 1550 | 0.063 | 0.032 | 0.062 |
| 3-(Methylthio)benzoic acid, trimethylsilyl ester | 225 | 1550 | 0.075 | 0.077 | 0.078 |
| Cyclohexanecarboxaldehyde, 6-methyl-3-(1-methylethyl)-2-oxo-1-(3-oxobutyl)- | 55 | 1553 | 0.055 | 0.017 | 0.049 |
| à-Cadinol | 95 | 1559 | 0.117 | 0.125 | 0.130 |
| 2-Propenoic acid, 3-(4-hydroxyphenyl)-, methyl ester | 147 | 1567 | 0.033 | 0.015 | 0.035 |
| 1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis- | 81 | 1574 | 0.021 | 0.017 | 0.019 |
| cis-Z-à-Bisabolene epoxide | 81 | 1580 | 0.016 | 0.015 | 0.013 |
| Analyte 294 | 73 | 1579 | 0.131 | 0.177 | 0.150 |
| 2,3,4,5-Tetrahydro-1H,1'H-[2,2']bipyrrolyl-5-carbonitrile | 106 | 1580 | 0.037 | 0.044 | 0.039 |
| Ethanone, 1-(2,3-dihydro-1H-inden-5-yl)- | 145 | 1592 | 0.028 | 0.034 | 0.026 |
| 1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethylidene)-, [1R-(1à,4aá,8aà)]- | 67 | 1595 | 0.189 | 0.178 | 0.182 |
| Analyte 298 | 73 | 1598 | 0.078 | 0.078 | 0.074 |
| 4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane | 91 | 1610 | 0.047 | 0.046 | 0.048 |
| Analyte 300 | 75 | 1610 | 0.082 | 0.104 | 0.091 |
| 11-Hexadecyn-1-ol | 96 | 1617 | 0.055 | 0.062 | 0.056 |
| Analyte 302 | 75 | 1621 | 0.305 | 0.400 | 0.334 |
| Analyte 303 | 75 | 1634 | 0.108 | 0.138 | 0.116 |
| Analyte 304 | 75 | 1640 | 0.051 | 0.032 | 0.053 |
| Benzeneacetic acid, 4-hydroxy-3-methoxy-, methyl ester | 137 | 1677 | 0.011 | 0.019 | 0.013 |
| Analyte 306 | 73 | 1679 | 0.151 | 0.184 | 0.178 |
| Isoaromadendrene epoxide | 93 | 1685 | 0.025 | 0.016 | 0.027 |
| Analyte 308 | 100 | 1691 | 0.089 | 0.103 | 0.090 |
| Ethyl 6,9,12-hexadecatrienoate | 79 | 1697 | 0.032 | 0.028 | 0.030 |
| Chamazulene | 169 | 1700 | 0.050 | 0.050 | 0.049 |
| 1-Cyclopentylethanol, trimethylsilyl ether | 73 | 1703 | 0.102 | 0.093 | 0.103 |
| 1-Cyclohexanone, 2-methyl-2-(3-methyl-2-oxobutyl) | 153 | 1706 | 0.118 | 0.130 | 0.117 |
| Analyte 313 | 73 | 1712 | 0.160 | 0.174 | 0.165 |
| Analyte 314 | 100 | 1718 | 0.142 | 0.169 | 0.153 |
| 2-Propenoic acid, 3-(4-hydroxyphenyl)-, methyl ester | 147 | 1727 | 0.077 | 0.066 | 0.074 |
| Analyte 316 | 99 | 1730 | 0.018 | 0.020 | 0.019 |
| Analyte 317 | 73 | 1736 | 0.100 | 0.148 | 0.125 |
| Carbonic acid, butyl 3-methylphenyl ester | 108 | 1739 | 0.054 | 0.017 | 0.057 |
| Tetradecanoic acid | 60 | 1745 | 0.111 | 0.110 | 0.105 |
| Analyte 320 | 74 | 1748 | 0.017 | 0.014 | 0.016 |
| Analyte 321 | 73 | 1754 | 0.345 | 0.297 | 0.338 |
| Analyte 322 | 99 | 1766 | 0.024 | 0.017 | 0.018 |
| 4,4'-Dimethylbiphenyl | 182 | 1776 | 0.055 | 0.060 | 0.051 |
| Aromadendrene oxide-(2) | 91 | 1778 | 0.051 | 0.029 | 0.033 |
| Cyclohexanone, 5-methyl-2-(1-methylethylidene)- | 109 | 1778 | 0.054 | 0.028 | 0.048 |
| Analyte 326 | 73 | 1781 | 0.040 | 0.044 | 0.040 |
| Naphthalene, 1-(chloromethyl)-2-methyl- | 153 | 1793 | 0.036 | 0.024 | 0.033 |
| Isoaromadendrene epoxide | 93 | 1793 | 0.080 | 0.071 | 0.086 |
| Analyte 329 | 109 | 1796 | 0.046 | 0.040 | 0.044 |
| 3-Hydroxy-4,4-dimethyl-3-(1-methyl-3-oxobut-1-enyl)cycloheptanone | 112 | 1808 | 0.061 | 0.061 | 0.062 |
| Analyte 331 | 232 | 1814 | 0.028 | 0.017 | 0.026 |
| **Isoaromadendrene epoxide#** | 71 | 1820 | 0.164 | 0.185 | 0.186 |
| Pentanoic acid, 3-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester | 73 | 1829 | 0.042 | 0.046 | 0.047 |
| **cis-Z-à-Bisabolene epoxide#** | 55 | 1829 | 0.059 | 0.029 | 0 |
| Analyte 335 | 73 | 1838 | 0.020 | 0.028 | 0.024 |
| Analyte 336 | 73 | 1841 | 0.026 | 0.046 | 0.021 |
| Cyclopent-2-ene-1-carboxylic acid, 2,3-dimethyl-1-ethyl-, ethyl ester | 123 | 1841 | 0.021 | 0.020 | 0.019 |
| 1,3-Benzodioxin-4-one,4a,5-dimethylperhydro-2-(1,1-dimethylethyl) | 110 | 1850 | 0.026 | 0.026 | 0.023 |
| Analyte 339 | 109 | 1857 | 0.043 | 0.016 | 0.040 |
| 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester | 208 | 1862 | 0.014 | 0.015 | 0.015 |
| Analyte 341 | 113 | 1862 | 0.022 | 0.018 | 0.015 |
| Analyte 342 | 100 | 1862 | 0.096 | 0.113 | 0.092 |
| 3-Octadecyne | 68 | 1868 | 0.069 | 0.081 | 0.071 |
| 1H-Imidazole-4-ethanamine, á,á-dimethyl- | 110 | 1868 | 0.028 | 0.027 | 0.026 |
| Analyte 345 | 100 | 1871 | 0.028 | 0.037 | 0.033 |
| 2-Pentadecanone, 6,10,14-trimethyl- | 58 | 1874 | 0.062 | 0.047 | 0.060 |
| Tetradecanoic acid, trimethylsilyl ester | 117 | 1886 | 0.116 | 0.121 | 0.121 |
| 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | 149 | 1898 | 0.030 | 0.023 | 0.028 |
| Pentadecanoic acid | 60 | 1901 | 0.036 | 0.038 | 0.034 |
| Analyte 350 | 87 | 1904 | 0.080 | 0.095 | 0.079 |
| Aromadendrene oxide-(2) | 91 | 1903 | 0.027 | 0.018 | 0.046 |
| 3,7,11,15-Tetramethyl-2-hexadecen-1-ol | 81 | 1907 | 0.022 | 0.017 | 0.015 |
| Analyte 353 | 109 | 1919 | 0.055 | 0.052 | 0.047 |
| Analyte 354 | 73 | 1928 | 0.074 | 0.093 | 0.082 |
| 3,7,11,15-Tetramethyl-2-hexadecen-1-ol | 81 | 1934 | 0.029 | 0.024 | 0.031 |
| Analyte 356 | 97 | 1955 | 0.018 | 0.022 | 0.020 |
| Bicyclo[3.2.0]heptan-2-one, 6-hydroxy-5-methyl-6-vinyl- | 97 | 1961 | 0.043 | 0.049 | 0.042 |
| Undecanone, 2-methyl oxime | 87 | 1967 | 0.054 | 0.069 | 0.056 |
| 10,12-Tricosadiynoic acid, trimethylsilyl ester | 73 | 1967 | 0.143 | 0.153 | 0.177 |
| Undecanone, 2-methyl oxime | 87 | 1991 | 0.152 | 0.199 | 0.150 |
| Isoaromadendrene epoxide | 71 | 1997 | 0.129 | 0.144 | 0.138 |
| Hexadecanoic acid, methyl ester | 74 | 2000 | 0.027 | 0.032 | 0.026 |
| Analyte 363 | 81 | 2012 | 0.073 | 0.082 | 0.079 |
| **Scopoletin#\*** | 192 | 2031 | 1.690 | 1.865 | 1.744 |
| n-Pentadecanoic acid, trimethylsilyl ester | 117 | 2033 | 0.034 | 0.039 | 0.038 |
| Dibutyl phthalate | 149 | 2039 | 0.349 | 0.387 | 0.365 |
| **n-Hexadecanoic acid#\*\*** | 60 | 2053 | 2.456 | 2.467 | 2.418 |
| 4-Biphenyl methyl carbinol | 183 | 2057 | 0.039 | 0.024 | 0.036 |
| Butyl myristate | 56 | 2087 | 0.020 | 0.029 | 0.018 |
| Scopoletin, trimethylsilyl ether | 234 | 2144 | 0.063 | 0.100 | 0.069 |
| Cyclopropanol, 2,2-dimethyl-3-(2-phenylethynyl)- | 171 | 2153 | 0.191 | 0.183 | 0.176 |
| Indan, 1-benzylidenehexahydro-7a-methyl-, cis- | 91 | 2159 | 0.065 | 0.047 | 0.064 |
| 1,3-Dioxolane, 2-(3-bromo-5,5,5-trichloro-2,2-dimethylpentyl)- | 73 | 2159 | 0.058 | 0.078 | 0.068 |
| Hexadecanoic acid, trimethylsilyl ester\* | 117 | 2172 | 1.035 | 1.304 | 1.194 |
| Heptadecanoic acid | 60 | 2190 | 0.045 | 0.047 | 0.047 |
| Analyte 376 | 222 | 2209 | 0.271 | 0.321 | 0.296 |
| Analyte 377 | 207 | 2213 | 0.017 | 0.016 | 0.019 |
| Analyte 378 | 65 | 2258 | 0.020 | 0.017 | 0.022 |
| 2H-1-Benzopyran-2-one, 6,7-dimethoxy-4-methyl- | 220 | 2267 | 0.070 | 0.071 | 0.073 |
| 9,12-Octadecadienoic acid (Z,Z)- | 67 | 2285 | 0.509 | 0.609 | 0.612 |
| 9,12,15-Octadecatrienal | 79 | 2291 | 0.142 | 0.173 | 0.182 |
| cis-Vaccenic acid | 55 | 2294 | 0.610 | 0.650 | 0.682 |
| 7-Methoxy-3,4-dihydro-1(2H)-phenanthrenone | 155 | 2312 | 0.065 | 0.060 | 0.061 |
| Octadecanoic acid | 60 | 2327 | 0.499 | 0.538 | 0.489 |
| Analyte 385 | 170 | 2330 | 0.072 | 0.065 | 0.072 |
| Silane, [(3,7,11,15-tetramethyl-2-hexadecenyl)oxy]trimethyl- | 143 | 2345 | 0.022 | 0.029 | 0.025 |
| Hexadecanoic acid, butyl ester | 56 | 2360 | 0.190 | 0.373 | 0.178 |
| Preg-4-en-3-one, 17à-hydroxy-17á-cyano- | 53 | 2381 | 0.044 | 0.024 | 0.044 |
| 9,12-Octadecadienoic acid (Z,Z)-, trimethylsilyl ester | 75 | 2390 | 0.051 | 0.073 | 0.059 |
| Oleic acid, trimethylsilyl ester | 75 | 2399 | 0.052 | 0.071 | 0.067 |
| Analyte 391 | 123 | 2402 | 0.055 | 0.032 | 0.051 |
| Analyte 392 | 91 | 2408 | 0.075 | 0.096 | 0.070 |
| Octadecanoic acid, trimethylsilyl ester | 117 | 2435 | 0.042 | 0.052 | 0.040 |
| Preg-4-en-3-one, 17à-hydroxy-17á-cyano- | 97 | 2438 | 0.016 | 0.032 | 0.020 |
| Analyte 395 | 207 | 2441 | 0.039 | 0.025 | 0.037 |
| 3-Methyl-2-butenoic acid, tridec-2-ynyl ester | 83 | 2441 | 0.022 | 0.022 | 0.023 |
| Analyte 397 | 87 | 2453 | 0.072 | 0.085 | 0.086 |
| Analyte 398 | 191 | 2462 | 0.156 | 0.127 | 0.134 |
| Analyte 399 | 191 | 2471 | 0 | 0.021 | 0.027 |
| Analyte 400 | 106 | 2474 | 0.025 | 0.035 | 0.040 |
| Analyte 401 | 100 | 2474 | 0.022 | 0.025 | 0.020 |
| Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl- | 205 | 2492 | 0.057 | 0.044 | 0.058 |
| Analyte 403 | 173 | 2501 | 0.020 | 0.020 | 0.030 |
| Cyclodeca[b]furan-2,9(3H,4H)-dione, 4-(acetyloxy)-3a,7,8,10,11,11a-hexahydro-6-methyl-3,10-bis(methylene)-, [3ar-(3ar\*,4R\*,5E,11as\*)]- | 91 | 2504 | 0.515 | 0.578 | 0.566 |
| Methyl 7,11,14-eicosatrienoate | 95 | 2507 | 0.076 | 0.082 | 0.083 |
| Analyte 406 | 191 | 2513 | 0.095 | 0.108 | 0.095 |
| **5-Benzofuranacetic acid, 6-ethenyl-2,4,5,6,7,7a-hexahydro-3,6-dimethyl-à-methylene-2-oxo-, methyl ester#\*** | 120 | 2516 | 1.151 | 1.344 | 1.330 |
| 2-[4-methyl-6-(2,6,6-trimethylcyclohex-1-enyl)hexa-1,3,5-trienyl]cyclohex-1-en-1-carboxaldehyde | 71 | 2558 | 0.040 | 0.042 | 0.037 |
| 4,8,12,16-Tetramethylheptadecan-4-olide | 99 | 2561 | 0.091 | 0.085 | 0.085 |
| 9,12-Octadecadienoic acid, methyl ester, (E,E)- | 67 | 2570 | 0.021 | 0.058 | 0.031 |
| cis-Vaccenic acid | 55 | 2579 | 0.027 | 0.053 | 0.034 |
| Eicosanoic acid | 60 | 2582 | 0.078 | 0.079 | 0.074 |
| Phenol, 2-[5-(2-furanyl)pyrazol-3-yl]-5-methyl- | 240 | 2609 | 0.017 | 0.017 | 0.014 |
| Octadecanoic acid, butyl ester | 56 | 2612 | 0.075 | 0.109 | 0.071 |
| 4-Undecene, 3-methyl-, (E)- | 55 | 2612 | 0.073 | 0.049 | 0.057 |
| 2-[4-methyl-6-(2,6,6-trimethylcyclohex-1-enyl)hexa-1,3,5-trienyl]cyclohex-1-en-1-carboxaldehyde | 98 | 2624 | 0.053 | 0.070 | 0.058 |
| Analyte 417 | 228 | 2648 | 0.025 | 0.023 | 0.028 |
| Analyte 418 | 98 | 2657 | 0.095 | 0.114 | 0.098 |
| Analyte 419 | 260 | 2705 | 0.037 | 0.039 | 0.039 |
| Analyte 420 | 69 | 2714 | 0.093 | 0.087 | 0.093 |
| 1-Docosene | 55 | 2738 | 0.055 | 0.054 | 0.046 |
| Analyte 422 | 258 | 2765 | 0.038 | 0.025 | 0.026 |
| Cyclopropanecarboxyllic acid, tridec-2-ynyl ester | 69 | 2777 | 0.023 | 0.017 | 0.020 |
| Analyte 424 | 111 | 2777 | 0.048 | 0.051 | 0.051 |
| Bis(2-ethylhexyl) phthalate | 149 | 2777 | 0.064 | 0.057 | 0.056 |
| 1-Docosanol, trimethylsilyl ether | 75 | 2804 | 0.072 | 0.077 | 0.066 |
| Docosanoic acid | 60 | 2819 | 0.056 | 0.057 | 0.056 |
| **Ingol 12-acetate#** | 111 | 2831 | 0.539 | 0.530 | 0.558 |
| Analyte 429 | 129 | 2892 | 0.049 | 0.063 | 0.062 |
| (S)-8,8-Dimethyl-2-oxo-7,8-dihydro-2H,6H-pyrano(3,2-g)chromen-7-yl 3-methyl-2-butenoate | 83 | 2912 | 0.891 | 0.925 | 0.888 |
| Gitoxigenin | 147 | 2949 | 0.190 | 0.195 | 0.197 |
| 1-Docosene | 57 | 2967 | 0.013 | 0.016 | 0.007 |
| Analyte 433 | 71 | 3002 | 0.059 | 0.057 | 0.065 |
| Tetracosan-1-ol trimethylsilyl ether | 75 | 3020 | 0.026 | 0.031 | 0.028 |
| Tetracosanoic acid | 60 | 3041 | 0.019 | 0.019 | 0.020 |
| Analyte 436 | 71 | 3046 | 0.125 | 0.145 | 0.139 |
| Analyte 437 | 81 | 3083 | 0.030 | 0.027 | 0.036 |
| **1-Cyclohexyl-5-(4-methoxy-benzyl)-pyrimidine-2,4,6(1H,3H,5H)-trione#** | 121 | 3098 | 0.250 | 0.260 | 0.255 |
| 4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-(4-methoxyphenyl)- | 298 | 3197 | 0.258 | 0.247 | 0.254 |
| 7-((5R,8R,8aS)-8-Methyloctahydroindolizin-5-yl)heptan-2-ol | 138 | 3209 | 0.045 | 0.046 | 0.041 |
| Analyte 441 | 244 | 3245 | 0.113 | 0.099 | 0.099 |

Internal standard added: 50 µl (50 µg/mL); Samples: 2.5 µg added per sample. Relative concentrations of the metabolites were calculated as: detected area of metabolite / detected area of internal standards x 2.5 µg. Compound name were identified using in-house mass spectral libraries (NIST). Key: RT: Retention Time (s), #Compounds with known antimicrobial activity, \*\*\*Compounds with highest concentration (12 – 15 µg/mg sample), \*\*Compounds with second highest concentration (2.4 – 5.0 µg/mg sample), \*Compound with third highest concentration (0.85 – 2.0 µg/mg sample)