Table S1. A total of 324 volatile organic compounds (VOCs) were measured in the breath of participants using TD-GCMS.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Variable | VOC\_GROUP | VOC\_NAME | Mol Weight (amu) | CAS Number |
| A\_1 | VSC | Methanethiol | 48.003 | 000074-93-1 |
| A\_2 | VSC | Dimethyl disulfide | 93.991 | 000624-92-0 |
| A\_3 | VSC | Dimethy sulfide | 62.019 | 000075-18-3 |
| A\_4 | VSC | Sulfur dioxide | 63.962 | 007446-09-5 |
| A\_5 | VSC | Carbon disulfide | 75.944 | 000075-15-0 |
| A\_6 | VSC | Methyl propenyl sulfide (E) | 88.035 | 042848-06-6 |
| A\_7 | VSC | Methyl propenyl sulfide (Z) | 88.035 | 052195-40-1 |
| A\_8 | VSC | Allyl methyl sulfide | 88.035 | 010152-76-8 |
| A\_9 | VSC | Methyl propyl sulfide | 90.05 | 003877-15-4 |
| A\_10 | VSC | Dimethyl sulfone | 94.009 | 000067-71-0 |
| A\_11 | VSC | Allyl Isothiocyanate | 99.014 | 000057-06-7 |
| A\_12 | VSC | Dimethyl Sulfoxide | 78.014 | 000067-68-5 |
| A\_13 | VSC | 4-Methylaminophenol sulfate | 221.0357 | 000055-55-0 |
| A\_14 | VSC | Allyl sulfide | 114.05 | 000592-88-1 |
| A\_15 | VSC | 2-Methyltetrahydrothiophene | 102.05 | 001795-09-1 |
| A\_16 | VSC | (2E)-2-butenyl methyl sulfide | 102.05 | 032931-14-9 |
| A\_17 | VSC | Allyl methyl disulfide | 120.007 | 002179-58-0 |
| A\_18 | VSC | 2-Aminoethyl hydrogen sulfate | 141.01 | 000926-39-6 |
| A\_19 | VSC | 2,4-Dimethylheptane | 128.157 | 002213-23-2 |
| A\_20 | VSC | 3-Sulfo-L-alanine | 169.005 | 000498-40-8 |
| A\_21 | Ketones | Acetone | 58.042 | 000067-64-1 |
| A\_22 | Ketones | Methyl vinyl ketone | 70.042 | 000078-94-4 |
| A\_23 | Ketones | 2-Butanone | 72.058 | 000078-93-3 |
| A\_24 | Ketones | 2-Heptanone | 114.104 | 000110-43-0 |
| A\_25 | Ketones | 3-Heptanone | 114.104 | 000106-35-4 |
| A\_26 | Ketones | 2,3-Butanedione | 86.037 | 000431-03-8 |
| A\_27 | Ketones | Dihydro-2(3H)-furanone | 86.037 | 000096-48-0 |
| A\_28 | Ketones | 2-Pentanone | 86.073 | 000107-87-9 |
| A\_29 | Ketones | Methyl isopropyl ketone | 86.073 | 000563-80-4 |
| A\_30 | Ketones | Acetoin | 88.052 | 000513-86-0 |
| A\_31 | Ketones | Cyclohexanone | 98.073 | 000108-94-1 |
| A\_32 | Ketones | Piperidinone | 99.068 | 027154-43-4 |
| A\_33 | Ketones | 2-Methylpropyl methyl ketone | 100.089 | 000108-10-1 |
| A\_34 | Ketones | 4-Heptanone | 114.104 | 000123-19-3 |
| A\_35 | Ketones | Acetophenone | 120.058 | 000098-86-2 |
| A\_36 | Ketones | D-Carvone | 150.105 | 002244-16-8 |
| A\_37 | Ketones | (+)-Isodihydoarvone | 152.12 | 006909-25-7 |
| A\_38 | Ketones | 2-Isopropylidene-5-methylcyclohexanone | 152.12 | 015932-80-6 |
| A\_39 | Ketones | trans-Dihydrocarvone | 152.12 | 005948-04-9 |
| A\_40 | Ketones | Menthone | 154.136 | 000089-80-5 |
| A\_41 | Ketones | 5-Methyl-2-(1-methylethyl)-, (2S-cis)-cyclohexanone | 154.135 | 010458-14-7 |
| A\_42 | Ketones | l-Menthone | 154.136 | 014073-97-3 |
| A\_43 | Ketones | 6-Methylphenanthridine | 193.089 | 003955-65-5 |
| A\_44 | Ketones | 2-Methyl-3-hexanone | 114.104 | 007379-12-6 |
| A\_45 | Ketones | (2R,5R)-2-Isopropyl-5-methylcyclohexanon | 154.249 | 005146-52-1 |
| A\_46 | Alcohol | Ethanol | 46.042 | 000064-17-5 |
| A\_47 | Alcohol | 1-propanol | 60.058 | 000071-23-8 |
| A\_48 | Alcohol | 2-Propanol | 60.058 | 000067-63-0 |
| A\_49 | Alcohol | 1,2-Ethanediol | 62.037 | 000107-21-1 |
| A\_50 | Alcohol | Acetol | 74.037 | 000116-09-6 |
| A\_51 | Alcohol | 1-Butanol | 74.073 | 000071-36-3 |
| A\_52 | Alcohol | 2-Methyl-2-propanol | 74.073 | 000075-65-0 |
| A\_53 | Alcohol | 2-Butanol | 74.073 | 000078-92-2 |
| A\_54 | Alcohol | 2-Methylpropyl alcohol | 74.073 | 000078-83-1 |
| A\_55 | Alcohol | Isobutenylcarbinol | 86.073 | 000763-32-6 |
| A\_56 | Alcohol | 3-Octanol | 130.136 | 000589-98-0 |
| A\_57 | Alcohol | 3-Pentanol | 88.089 | 000584-02-1 |
| A\_58 | Alcohol | 2-Methyl-2-butanol | 88.089 | 000075-85-4 |
| A\_59 | Alcohol | 2,3-Butanediol | 90.068 | 000513-85-9 |
| A\_60 | Alcohol | 1,3-Butanediol | 90.068 | 000107-88-0 |
| A\_61 | Alcohol | 1-Methoxy-2-propanol | 90.068 | 000107-98-2 |
| A\_62 | Alcohol | Phenol | 94.042 | 000108-95-2 |
| A\_63 | Alcohol | 3-Methoxybutanol | 104.084 | 002517-43-3 |
| A\_64 | Alcohol | 1,2-Propanediol | 106.063 | 000623-39-2 |
| A\_65 | Alcohol | Benzenemethanol | 108.058 | 000100-51-6 |
| A\_66 | Alcohol | 2,3-Dimethyl-2,3-butanediol | 118.099 | 000076-09-5 |
| A\_67 | Alcohol | 2-Ethyl-1-Hexanol | 130.136 | 000104-76-7 |
| A\_68 | Alcohol | 2-Phenyl-2-propanol | 136.089 | 000617-94-7 |
| A\_69 | Alcohol | 2-Phenoxy-ethanol | 138.068 | 000122-99-6 |
| A\_70 | Alcohol | (2,5-Dimethyltetrahydro-2H-pyran-2-yl)methanol | 144.115 | 054004-46-5 |
| A\_71 | Alcohol | 2,6-Dimethyl-4-heptanol | 144.151 | 000108-82-7 |
| A\_72 | Alcohol | 2,5-Dimethyl-2,5-hexanediol | 146.131 | 000110-03-2 |
| A\_73 | Alcohol | 2-(4-Methyl-3-cyclohexen-1-yl)-2-propanol | 154.136 | 000098-55-5 |
| A\_74 | Alcohol | Menthol | 156.151 | 001490-04-6 |
| A\_75 | Alcohol | (+-)-Isomenthol | 156.151 | 023283-97-8 |
| A\_76 | Alcohol | Cis-1,3,trans-1,4-Menthol | 156.151 | 000089-78-1 |
| A\_77 | Alcohol | Trans-1,3,trans-1,4-Menthol | 156.151 | 000491-01-0 |
| A\_78 | Alcohol | L-(-)-Menthol | 156.151 | 002216-51-5 |
| A\_79 | Alcohol | Menthol, (.+-.)- | 156.151 | 015356-70-4 |
| A\_80 | Alcohol | 3-Allyl-2-methoxyphenol | 164.084 | 001941-12-4 |
| A\_81 | Alcohol | 4-Nonylphenol | 220.183 | 000104-40-5 |
| A\_82 | Alcohol | (S)-1,3-Butanediol | 90.068 | 024621-61-2 |
| A\_83 | Alcohol | 2-Butoxy-ethanol | 118.17 | 000111-76-2 |
| A\_84 | Alcohol | Cyclohexanol | 100.089 | 000108-93-0 |
| A\_85 | Alcohol | 2-(2-Ethoxyethoxy)-ethanol | 134.094 | 000111-90-0 |
| A\_86 | Alcohol | 2-Methyldecane | 156.31 | 006975-98-0 |
| A\_87 | Alcohol | 1-(1,5-Dimethylhexyl)-4-methylcyclohexanol | 226.23 | 024945-44-6 |
| A\_88 | Alcohol | 3,7-Dimethyl-1,6-octadien-3-ol | 154.136 | 000078-70-6 |
| A\_89 | Halo-Hydrocarbons | Dichloroethene | 95.953 | 000156-59-2 |
| A\_90 | Halo-Hydrocarbons | Ethane, 1,1-difluoro- | 66.028 | 000075-37-6 |
| A\_91 | Halo-Hydrocarbons | Dichloro-, radical ion(1+) methane | 83.953 | 058165-12-1 |
| A\_92 | Halo-Hydrocarbons | Methylene chloride | 83.953 | 000075-09-2 |
| A\_93 | Halo-Hydrocarbons | 1,2-Dichloro- ethane | 97.969 | 000107-06-2 |
| A\_94 | Halo-Hydrocarbons | 1-Chloro-1,1-difluoro- ethane | 99.989 | 000075-68-3 |
| A\_95 | Halo-Hydrocarbons | 1,2-Dichloro- propane | 111.985 | 000078-87-5 |
| A\_96 | Halo-Hydrocarbons | Chloroform | 117.914 | 000067-66-3 |
| A\_97 | Halo-Hydrocarbons | (Z)-1,2-Dichloro- ethylene | 152.12 | 000076-22-2 |
| A\_98 | Halo-Hydrocarbons | Bromodichloro- methane | 161.864 | 000075-27-4 |
| A\_99 | Halo-Hydrocarbons | (E)-1,2-Dichloroethylene | 95.953 | 000156-60-5 |
| A\_100 | Halo-Hydrocarbons | Trichloroethene | 129.914 | 000079-01-6 |
| A\_101 | Halo-Hydrocarbons | Dibromo(chloro)methane | 205.813 | 000124-48-1 |
| A\_102 | Halo-Hydrocarbons | Iodomethane | 141.928 | 000074-88-4 |
| A\_103 | Halo-Hydrocarbons | Tetrachloroethene | 163.876 | 000127-18-4 |
| A\_104 | Halo-Hydrocarbons | Chlorobenzene | 112.008 | 000108-90-7 |
| A\_105 | Alkenes | 1,2-Pentadiene | 68.063 | 000591-95-7 |
| A\_106 | Alkenes | 3-Methyl-1,2-butadiene | 68.063 | 000598-25-4 |
| A\_107 | Alkenes | 2-Methyl-1,3-cyclopentadiene | 80.063 | 003727-31-9 |
| A\_108 | Alkenes | 1-Pentene | 70.078 | 000109-67-1 |
| A\_109 | Alkenes | 2-Methyl-1-pentene | 84.094 | 000763-29-1 |
| A\_110 | Alkenes | 4-Methyl-1-pentene | 84.094 | 000691-37-2 |
| A\_111 | Alkenes | 1-Hexene | 84.094 | 000592-41-6 |
| A\_112 | Alkenes | (3Z)-3-Methyl-3-hexene | 98.11 | 004914-89-0 |
| A\_113 | Alkenes | 3-Methyl-3-hexene | 98.11 | 000692-24-0 |
| A\_114 | Alkenes | 3-Methylene-1-vinylcyclopentene | 106.078 | 061142-07-2 |
| A\_115 | Alkenes | 4-Methyl-3-heptene | 112.125 | 004485-16-9 |
| A\_116 | Alkenes | 1-Octene | 112.125 | 000111-66-0 |
| A\_117 | Alkenes | 2,4-dimethyl-1-heptene | 126.141 | 019549-87-2 |
| A\_118 | Alkyne | 2-Pentyne | 68.063 | 000627-21-4 |
| A\_119 | Alkane | 1,1-Diethoxyethane | 118.099 | 000105-57-7 |
| A\_120 | Alkane | 3-Ethyl-5-(2-ethylbutyl)octadecane | 366.423 | 055282-12-7 |
| A\_121 | Alkane | 3-Methylnonane | 142.172 | 005911-04-6 |
| A\_122 | Alkane | Dimethylmethane | 44.063 | 000074-98-6 |
| A\_123 | Alkane | Butane | 58.078 | 000106-97-8 |
| A\_124 | Alkane | Methylcyclobutane | 70.078 | 000598-61-8 |
| A\_125 | Alkane | Diethyl ether | 74.073 | 000060-29-7 |
| A\_126 | Alkane | Cyclohexane | 84.094 | 000110-82-7 |
| A\_127 | Alkane | 1,2,4-trimethylcyclohexane | 126.141 | 002234-75-5 |
| A\_128 | Alkane | 4-Methyl nonane | 142.172 | 017301-94-9 |
| A\_129 | Alkane | 2,3-Dimethylbutane | 86.11 | 000079-29-8 |
| A\_130 | Alkane | 2-Methyl pentane | 86.11 | 000107-83-5 |
| A\_131 | Alkane | Hexane | 86.11 | 000110-54-3 |
| A\_132 | Alkane | Methylcyclohexane | 98.11 | 000108-87-2 |
| A\_133 | Alkane | 2,4-Dimethylpentane | 100.125 | 000108-08-7 |
| A\_134 | Alkane | Heptane | 100.125 | 000142-82-5 |
| A\_135 | Alkane | 3-Methyl-hexane | 100.125 | 000589-34-4 |
| A\_136 | Alkane | 2-Methylhexane | 100.125 | 000591-76-4 |
| A\_137 | Alkane | Cyclopentane | 70.078 | 000287-92-3 |
| A\_138 | Alkane | Propylcyclopentane | 112.125 | 002040-96-2 |
| A\_139 | Alkane | Ethylcyclohexane | 112.125 | 001678-91-7 |
| A\_140 | Alkane | 4-Methylheptane | 114.141 | 000589-53-7 |
| A\_141 | Alkane | 2-Methylheptane | 114.141 | 000592-27-8 |
| A\_142 | Alkane | Octane | 114.141 | 000111-65-9 |
| A\_143 | Alkane | 1,2-Diethoxyethane | 118.099 | 000629-14-1 |
| A\_144 | Alkane | 2,2,3,3-Tetramethylpentane | 128.157 | 007154-79-2 |
| A\_145 | Alkane | 2,3,4-Trimethylhexane | 128.157 | 000921-47-1 |
| A\_146 | Alkane | 4-Methyloctane | 128.157 | 002216-34-4 |
| A\_147 | Alkane | n-Nonane | 128.157 | 000111-84-2 |
| A\_148 | Alkane | 3,5-Dimethyloctane | 142.172 | 015869-93-9 |
| A\_149 | Alkane | 2-Methylnonane | 142.172 | 000871-83-0 |
| A\_150 | Alkane | 2,6-Dimethyloctane | 142.172 | 002051-30-1 |
| A\_151 | Alkane | 2,5-Dimethyloctane | 142.172 | 015869-89-3 |
| A\_152 | Alkane | Decane | 142.172 | 000124-18-5 |
| A\_153 | Alkane | 5-Ethyl-2-methyl- octane | 156.188 | 062016-18-6 |
| A\_154 | Alkane | Undecane | 156.188 | 001120-21-4 |
| A\_155 | Alkane | 3,7-Dimethyl-decane | 170.204 | 017312-54-8 |
| A\_156 | Alkane | 5-Methylundecane | 170.204 | 001632-70-8 |
| A\_157 | Alkane | 4-Ethyldecane | 170.204 | 001636-44-8 |
| A\_158 | Alkane | 3,6-Dimethyldecane | 170.204 | 017312-53-7 |
| A\_159 | Alkane | Heptane, 2,2,4,6,6-pentamethyl- | 170.204 | 013475-82-6 |
| A\_160 | Alkane | Dodecane | 170.204 | 000112-40-3 |
| A\_161 | Alkane | 2,6,7-Trimethyldecane | 184.219 | 062108-25-2 |
| A\_162 | Alkane | 2,6,6-Trimethyl-decane | 184.219 | 062108-24-1 |
| A\_163 | Alkane | 3,6-Dimethylundecane | 184.219 | 017301-28-9 |
| A\_164 | Alkane | Tridecane | 184.219 | 000629-50-5 |
| A\_165 | Alkane | 3-Methyltridecane | 198.235 | 006418-41-3 |
| A\_166 | Alkane | Tetradecane | 198.235 | 000629-59-4 |
| A\_167 | Alkane | 1,2,3,4,4a,5,8,9,12,12a-Decahydro-1,4-methanobenzocyclodecene | 202.172 | 074708-73-9 |
| A\_168 | Alkane | 2,7,10-Trimethyldodecane | 212.25 | 074645-98-0 |
| A\_169 | Alkane | Pentadecane | 212.25 | 000629-62-9 |
| A\_170 | Alkane | 2,6,11-Trimethyldodecane | 212.25 | 031295-56-4 |
| A\_171 | Alkane | 2,6,10-Trimethyldodecane | 212.25 | 003891-98-3 |
| A\_172 | Alkane | Hexadecan | 226.266 | 000544-76-3 |
| A\_173 | Alkane | 2,2,3,3,6,8,8-heptamethylnonane | 226.44 | \*(CID21107818) |
| A\_174 | Alkane | 2,2,11,11-Tetramethyldodecane | 226.266 | 127204-12-0 |
| A\_175 | Alkane | 2,2,4,4,6,8,8-Heptamethylnonane | 226.266 | 004390-04-9 |
| A\_176 | Alkane | 8-Methylheptadecane | 254.297 | 013287-23-5 |
| A\_177 | Alkane | Octadecane | 254.297 | 000593-45-3 |
| A\_178 | Alkane | Nonadecane | 268.313 | 000629-92-5 |
| A\_179 | Alkane | Icosane | 282.329 | 000112-95-8 |
| A\_180 | Alkane | 2,6,10,14-Tetramethylhexadecane | 282.329 | 000638-36-8 |
| A\_181 | Alkane | Docosane | 310.36 | 000629-97-0 |
| A\_182 | Alkane | Isopentane | 72.093 | 000078-78-4 |
| A\_183 | Alkane | (2Z)-3-Methyl-2-hexene | 98.11 | 010574-36-4 |
| A\_184 | Alkane | Tetracosane | 338.391 | 000646-31-1 |
| A\_185 | Alkane | Heneicosane | 296.344 | 000629-94-7 |
| A\_186 | Alkane | Tricosane | 324.376 | 000638-67-5 |
| A\_187 | Terpens | Isoprene | 68.062 | 000078-79-5 |
| A\_188 | Terpens | 3-methylene-6-(1-methylethyl)-cyclohexene | 136.125 | 000555-10-2 |
| A\_189 | Terpens | p-Cymene | 134.11 | 000099-87-6 |
| A\_190 | Terpens | Camphene | 136.125 | 000079-92-5 |
| A\_191 | Terpens | (+)-Sabinene | 136.125 | 003387-41-5 |
| A\_192 | Terpens | γ-Terpinene | 136.125 | 000099-85-4 |
| A\_193 | Terpens | L-Limonene | 136.125 | 005989-54-8 |
| A\_194 | Terpens | 1-Methyl-4-(1-methylethylidene)- cyclohexene | 136.125 | 000586-62-9 |
| A\_195 | Terpens | (R)-Limonene | 136.125 | 005989-27-5 |
| A\_196 | Terpens | Myrcene | 136.125 | 000123-35-3 |
| A\_197 | Terpens | 3-Carene | 136.125 | 013466-78-9 |
| A\_198 | Terpens | 2-Pinene | 136.125 | 000080-56-8 |
| A\_199 | Terpens | (+)-beta-Pinene | 136.125 | 000127-91-3 |
| A\_200 | Terpens | (+)-Alpha-Pinene | 136.125 | 007785-70-8 |
| A\_201 | Terpens | D-Sylvestrene | 136.125 | 000499-03-6 |
| A\_202 | Terpens | (-)-Alpha-Pinene | 136.125 | 007785-26-4 |
| A\_203 | Terpens | (-)-beta-Pinene | 136.125 | 018172-67-3 |
| A\_204 | Terpens | 1-Methyl-4-(1-methylethylidene)- cyclohexane | 138.141 | 001124-27-2 |
| A\_205 | Terpens | 1-Isobutylcyclohexene | 138.141 | 003983-03-7 |
| A\_206 | Terpens | Bornane | 138.141 | 000464-15-3 |
| A\_207 | Terpens | Carane | 138.141 | 000554-59-6 |
| A\_208 | Terpens | Carane, (1S,3S,6R)-(-)- | 138.141 | 002778-68-9 |
| A\_209 | Aromatics | 1,3,5-Trimethylbenzene | 120.094 | 000108-67-8 |
| A\_210 | Aromatics | o-Cymene | 134.11 | 000527-84-4 |
| A\_211 | Aromatics | m-Cymene | 134.11 | 000535-77-3 |
| A\_212 | Aromatics | Benzene | 78.047 | 000071-43-2 |
| A\_213 | Aromatics | Toluene | 92.063 | 000108-88-3 |
| A\_214 | Aromatics | Benzoic acid | 122.037 | 000065-85-0 |
| A\_215 | Aromatics | Ethylbenzene | 106.078 | 000100-41-4 |
| A\_216 | Aromatics | Styrene | 104.063 | 000100-42-5 |
| A\_217 | Aromatics | (2-Methyl-1-propenyl)benzene | 132.094 | 000768-49-0 |
| A\_218 | Aromatics | 2-Butenyl-benzene | 132.094 | 001560-06-1 |
| A\_219 | Aromatics | p-Xylene | 106.078 | 000106-42-3 |
| A\_220 | Aromatics | Xylene | 106.078 | 001330-20-7 |
| A\_221 | Aromatics | o-Xylene | 106.078 | 000095-47-6 |
| A\_222 | Aromatics | m-Xylene | 106.078 | 000108-38-3 |
| A\_223 | Aromatics | (1-Methylethyl)-benzene | 120.094 | 000098-82-8 |
| A\_224 | Aromatics | Alpha-methylstyrene | 118.078 | 000098-83-9 |
| A\_225 | Aromatics | 1-Ethyl-3-methylbenzene | 120.094 | 000620-14-4 |
| A\_226 | Aromatics | 1,2,3-Trimethylbenzene | 120.094 | 000526-73-8 |
| A\_227 | Aromatics | Naphthalene | 128.063 | 000091-20-3 |
| A\_228 | Aromatics | Azulene | 128.063 | 000275-51-4 |
| A\_229 | Aromatics | 1,2,3,5-tetramethylbenzene | 134.11 | 000527-53-7 |
| A\_230 | Aromatics | 2-Ethyl-1,4-dimethylbenzene | 134.11 | 001758-88-9 |
| A\_231 | Aromatics | 4-Ethyl-1,2-dimethylbenzene | 134.11 | 000934-80-5 |
| A\_232 | Aromatics | 1-Ethyl-2,3-dimethylbenzene | 134.11 | 000933-98-2 |
| A\_233 | Aromatics | Phthalic anhydride | 148.016 | 000085-44-9 |
| A\_234 | Aromatics | 1-Methoxy-4-[(1E)-1-propen-1-yl]benzene | 148.089 | 000104-46-1 |
| A\_235 | Acetate | Acetic acid, methyl ester | 74.037 | 000079-20-9 |
| A\_236 | Acetate | Formic acid, ethyl ester | 74.037 | 000109-94-4 |
| A\_237 | Acetate | Acetic acid ethenyl ester | 86.037 | 000108-05-4 |
| A\_238 | Acetate | sopropenyl formate | 86.037 | 032978-00-0 |
| A\_239 | Acetate | Acetic acid ethyl ester | 88.052 | 000141-78-6 |
| A\_240 | Acetate | Acetic acid, butyl ester | 116.084 | 000123-86-4 |
| A\_241 | Acetate | Methyl 2-hydroxy-2-methylpropanoate | 118.063 | 002110-78-3 |
| A\_242 | Acetate | 1-Butanol, 3-methyl-, acetate | 130.099 | 000123-92-2 |
| A\_243 | Acetate | Methyl 3-hydroxy-3-methylbutanoate | 132.079 | 006149-45-7 |
| A\_244 | Acetate | Ethyl 2-hydroxy-2-methylpropanoate | 132.079 | 000080-55-7 |
| A\_245 | Acetate | 1,2,3-Propanetriol, monoacetate | 134.058 | 000106-61-6 |
| A\_246 | Acetate | Acetic acid, hexyl ester | 144.115 | 000142-92-7 |
| A\_247 | Acetate | Acetic acid, phenylmethyl ester | 150.068 | 000140-11-4 |
| A\_248 | Acetate | Methyl 2-hydroxybenzoate | 152.047 | 000119-36-8 |
| A\_249 | Acetate | 2-Hydroxy-1,3-propanediyl diacetate | 176.068 | 000105-70-4 |
| A\_250 | Acetate | 3-Hydroxy-1,2-propanediyl diacetate | 176.068 | 025395-31-7 |
| A\_251 | Acetate | 2-Ethylhexyl acrylate | 184.146 | 000103-11-7 |
| A\_252 | Acetate | 3,7-Dimethyl-1,6-octadien-3-yl acetate | 196.146 | 000115-95-7 |
| A\_253 | Acetate | Isobornyl acetate | 196.146 | 000125-12-2 |
| A\_254 | Acetate | 2-Isopropyl-5-methylcyclohexyl acetate | 198.162 | 002230-87-7 |
| A\_255 | Acetate | 3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate | 216.173 | 074367-34-3 |
| A\_256 | Acetate | 1,2,3-Propanetriol, triacetate | 218.079 | 000102-76-1 |
| A\_257 | Acetate | Citronellylisovalerate | 240.209 | 068922-10-1 |
| A\_258 | Acetate | Isopropyl myristate | 270.256 | 000110-27-0 |
| A\_259 | Acetate | 1,4-Dioxane | 88.052 | 000123-91-1 |
| A\_260 | Acid | Acetic acid | 60.021 | 000064-19-7 |
| A\_261 | Acid | Propanoic acid | 74.037 | 000079-09-4 |
| A\_262 | Acid | Butanoic acid | 88.053 | 000107-92-6 |
| A\_263 | Acid | 2-Methylpropanoic acid | 88.053 | 000079-31-2 |
| A\_264 | Acid | 3-Methylbutanoic acid | 102.068 | 000503-74-2 |
| A\_265 | Acid | 2-Methylbutanoic acid | 102.068 | 000116-53-0 |
| A\_266 | Acid | Acetonic acid | 104.047 | 000594-61-6 |
| A\_267 | Acid | 3-Methyl pentanoic acid | 116.084 | 000105-43-1 |
| A\_268 | Acid | (N-(-2-Acetamido))-2-aminoethanesulfonic acid | 182.036 | 007365-82-4 |
| A\_269 | Furan | (2R,5S)-2,5-Dimethyltetrahydrofuran | 100.089 | 001003-38-9 |
| A\_270 | Furan | 2,2,5,5-Tetramethyltetrahydrofuran | 128.12 | 015045-43-9 |
| A\_271 | Furan | 3,6-Dimethyl-4,5,6,7-tetrahydro-1-benzofuran | 150.104 | 000494-90-6 |
| A\_272 | steroid | (14beta)-pregnane | 288.282 | 016396-79-5 |
| A\_273 | Aldehyde | Acetaldehyde | 44.026 | 000075-07-0 |
| A\_274 | Aldehyde | Methacrolein | 70.042 | 000078-85-3 |
| A\_275 | Aldehyde | 2-Butenal | 70.042 | 004170-30-3 |
| A\_276 | Aldehyde | 3-methyl-2-Butenal | 84.058 | 000107-86-8 |
| A\_277 | Aldehyde | 2-Furaldehyde | 96.021 | 000098-01-1 |
| A\_278 | Aldehyde | Hexanal | 100.089 | 000066-25-1 |
| A\_279 | Aldehyde | Benzaldehyde | 106.042 | 000100-52-7 |
| A\_280 | Aldehyde | Heptanal | 114.104 | 000111-71-7 |
| A\_281 | Aldehyde | Octanal | 128.12 | 000124-13-0 |
| A\_282 | Aldehyde | Nonanal | 142.136 | 000124-19-6 |
| A\_283 | Aldehyde | (2Z)-3,7-Dimethyl-2,6-octadienal | 152.12 | 000106-26-3 |
| A\_284 | Aldehyde | Decanal | 156.151 | 000112-31-2 |
| A\_285 | Other | Dimethylselenide | 109.963 | 000593-79-3 |
| A\_286 | Other | Methyl isopropyl ether | 74.073 | 000598-53-8 |
| A\_287 | Nitrogen | Pyridine | 79.042 | 000110-86-1 |
| A\_288 | Nitrogen | Indole | 117.058 | 000120-72-9 |
| A\_289 | Nitrogen | Acetonitrile | 41.027 | 000075-05-8 |
| A\_290 | Nitrogen | 1,2-Dimethylhydrazine | 60.069 | 000540-73-8 |
| A\_291 | Nitrogen | Nitromethane | 61.016 | 000075-52-5 |
| A\_292 | Nitrogen | 1-(1-Pyrrolidinyl)-1-icosanone | 365.366 | \*(ChemSpider ID:29760013) |
| A\_293 | Nitrogen | 1-(1-Pyrrolidinyl)-1-docosanone | 393.397 | \*(ChemSpider ID:29760063) |
| A\_294 | Other | Ethylene oxide | 44.026 | 000075-21-8 |
| A\_295 | Other | 1-Methoxy-2-methylpropane | 88.089 | 000625-44-5 |
| A\_296 | Other | (1S)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one | 152.12 | 000464-48-2 |
| A\_297 | Other | 1,8-Cineol | 154.136 | 000470-82-6 |
| A\_298 | Other | n-Heptyl methylphosphonofluoridate | 196.103 | 162085-82-7 |
| A\_299 | Other | Sevoflurane | 200.007 | 028523-86-6 |
| A\_300 | Other | 4-[5-(2-Methoxyphenyl)-1,3,4-oxadiazol-2-yl]pyridine | 253.085 | \*(CID706995) |
| A\_301 | Other | Cyclohexanone, 2-methyl-5-(1-methylethenyl)-, trans- | 152.12 | 005524-05-0 |
| A\_302 | Other | Propanethioic acid, 2-methyl-, S-ethyl ester | 132.061 | 002432-50-0 |
| A\_303 | Other | Thiosulfuric acid S-[2-[[5-[O-tolyloxy]pentyl]amino]propyl ester | 347.123 | \*(CID548547) |
| Excluded | Siloxane | Trimethylsilanol | 90.05 | 001066-40-6 |
| Excluded | Siloxane | Dimethyl(1,1,2-trimethylpropyl)silanol | 160.128 | 055644-10-5 |
| Excluded | Siloxane | Benzeneethanamine, N-[(pentafluorophenyl)methylene]-.beta.,4-bis[(trimethylsilyl)oxy] | 475.6 | 055429-85-1 |
| Excluded | Siloxane | 5,5,10,10-Tetramethyl-5,10-dihydrosilanthrene | 268.11 | 033022-24-1 |
| Excluded | Siloxane | Trimethyl(2-trimethylsilyloxyethylsulfanyl)silane | 222.093 | 078921-31-0 |
| Excluded | Siloxane | Methyl [(trimethylsilyl)oxy](4-[(trimethylsilyl)oxy]phenyl)acetate | 326.137 | 055334-40-2 |
| Excluded | Siloxane | Benzeneacetic acid, .alpha.,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester | 384.161 | 037148-64-4 |
| Excluded | Siloxane | alpha,4-Bis[(trimethylsilyl)oxy]benzeneacetic acid ethyl ester | 340.153 | \*(CID622432) |
| Excluded | Siloxane | m-Hydroxymandelic acid, tris(trimethylsilyl)- | 384.161 | 068595-69-7 |
| Excluded | Siloxane | Difluoro(dimethyl)silane | 96.02 | 000353-66-2 |
| Excluded | Siloxane | Hexamethyl disiloxane | 162.09 | 000107-46-0 |
| Excluded | Siloxane | 1,1,3,3,5,5-hexamethyltrisiloxane | 208.077 | 001189-93-1 |
| Excluded | Siloxane | 2,2,4,4,6,6-Hexamethyl-1,3,5,2,4,6-trioxatrisilinane | 222.056 | 000541-05-9 |
| Excluded | Siloxane | 2,4,6,8-tetramethyl-1,3,5,7,2,4,6,8-tetraoxatetrasilocane | 240.013 | 002370-88-9 |
| Excluded | Siloxane | 2,2,4,4,6,6,8,8-Octamethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane | 296.075 | 000556-67-2 |
| Excluded | Siloxane | Decamethyltetrasiloxane | 310.127 | 000141-62-8 |
| Excluded | Siloxane | Methyltris(trimethylsiloxy)silane | 310.127 | 017928-28-8 |
| Excluded | Siloxane | 3,3-Diisopropoxy-1,1,1,5,5,5-hexamethyltrisiloxane | 324.161 | 018082-56-9 |
| Excluded | Siloxane | 1-(4-Trimethylsilyloxyphenyl)-2-trimethylsilylaminoethanol trimethylsilyl ether | 339.169 | \*(CID91739849) |
| Excluded | Siloxane | 1,1,3,3,5,5,7,7,9,9-Decamethylpentasiloxane | 356.115 | 000995-83-5 |
| Excluded | Siloxane | p-Trimethylsilyloxyphenyl-bis(trimethylsilyloxy)ethane | 370.182 | \*(CID622436) |

Abbreviations: VSC, Volatile sulfur compound; TD-GCMS, Thermal desorption gas chromatography mass spectrometry

Table S2. Fifty-eight breath volatile organic compounds (VOCs) and two clinical variables were significantly different between patients with chronic kidney disease (non-dialysis CKD + hemodialysis) and normal healthy control groups in the *t*-test.

|  |  |  |  |
| --- | --- | --- | --- |
| INDEP\_VAR\_NAME | p value | EQ\_VAR\_PVAL | INDEP\_VAR |
| Cyclohexanone | 0.0000 | 0.0010 | A\_31 |
| Acetophenone | 0.0000 | 0.0238 | A\_35 |
| 1,2-Dichloro-ethane | 0.0000 | 0.0008 | A\_93 |
| Heptane | 0.0000 | 0.9624 | A\_134 |
| Decane | 0.0000 | 0.3326 | A\_152 |
| m-Xylene | 0.0000 | 0.8969 | A\_222 |
| Acetic acid ethyl ester | 0.0000 | 0.0241 | A\_239 |
| Nonanal | 0.0000 | 0.0000 | A\_282 |
| AGE | 0.0001 | 0.0096 |  |
| Trichloroethene | 0.0001 | 0.9999 | A\_100 |
| n-Nonane | 0.0004 | 0.1102 | A\_147 |
| Sulfur dioxide | 0.0006 | 0.0025 | A\_4 |
| 2-Methylpentane | 0.0011 | 0.0219 | A\_130 |
| p-Xylene | 0.0011 | 0.0001 | A\_219 |
| Azulene | 0.0014 | 0.0001 | A\_228 |
| 3-Heptanone | 0.0015 | 0.0040 | A\_25 |
| 4-Methylnonane | 0.0016 | 0.0000 | A\_128 |
| 2-Ethyl-1-Hexanol | 0.0021 | 0.0000 | A\_67 |
| Systolic blood pressure | 0.0030 | 0.2315 |  |
| Ethylcyclohexane | 0.0032 | 0.0000 | A\_139 |
| 2-Hydroxy-1,3-propanediyl diacetate | 0.0033 | 0.0000 | A\_249 |
| Propylcyclopentane | 0.0047 | 0.0000 | A\_138 |
| Methanethiol | 0.0049 | 0.0000 | A\_1 |
| Nonadecane | 0.0055 | 0.0000 | A\_178 |
| 3-Pentanol | 0.0077 | 0.0000 | A\_57 |
| 3-Hydroxy-1,2-propanediyl diacetate | 0.0082 | 0.0000 | A\_250 |
| Menthol | 0.0090 | 0.0000 | A\_74 |
| Acetone | 0.0102 | 0.2735 | A\_21 |
| 2-Butanone | 0.0113 | 0.0170 | A\_23 |
| Dihydro-2(3H)-furanone | 0.0116 | 0.5507 | A\_27 |
| Hexadecan | 0.0116 | 0.0000 | A\_172 |
| Phenol | 0.0119 | 0.0000 | A\_62 |
| Octanal | 0.0134 | 0.4196 | A\_281 |
| (1-Methylethyl)-benzene | 0.0139 | 0.0108 | A\_223 |
| 4-Methylheptane | 0.0158 | 0.0000 | A\_140 |
| 2-Butanol | 0.0169 | 0.0000 | A\_53 |
| (14beta)-pregnane | 0.0180 | 0.0000 | A\_272 |
| Ethylene oxide | 0.0216 | 0.9437 | A\_294 |
| 3-Sulfo-L-alanine | 0.0238 | 0.0361 | A\_20 |
| 2,5-Dimethyloctane | 0.0280 | 0.0000 | A\_151 |
| 3-Methyl pentanoic acid | 0.0281 | 0.0000 | A\_267 |
| Pentadecane | 0.0297 | 0.0000 | A\_169 |
| (2R,5S)-2,5-Dimethyltetrahydrofuran | 0.0297 | 0.0000 | A\_269 |
| 2-Phenoxy-ethanol | 0.0316 | 0.0000 | A\_69 |
| Allyl Isothiocyanate | 0.0325 | 0.0000 | A\_11 |
| Octadecane | 0.0325 | 0.0000 | A\_177 |
| Chloroform | 0.0341 | 0.0000 | A\_96 |
| Isoprene | 0.0341 | 0.0000 | A\_187 |
| Ethanol | 0.0343 | 0.2734 | A\_46 |
| 2-Pentanone | 0.0372 | 0.0000 | A\_28 |
| 2,4-dimethyl-1-heptene | 0.0374 | 0.0000 | A\_117 |
| 3-Methylene-1-vinylcyclopentene | 0.0391 | 0.0000 | A\_114 |
| 3-Carene | 0.0423 | 0.0004 | A\_197 |
| Methyl isopropyl ketone | 0.0435 | 0.0000 | A\_29 |
| 2-Methylheptane | 0.0439 | 0.3700 | A\_141 |
| Acetic acid, butyl ester | 0.0465 | 0.0106 | A\_240 |
| Nitromethane | 0.0477 | 0.0000 | A\_291 |
| (Z)-1,2-Dichloro- ethylene | 0.0485 | 0.0209 | A\_97 |
| 1-Methyl-4-(1-methylethylidene)- cyclohexane | 0.0486 | 0.0000 | A\_204 |
| (-)-beta-Pinene | 0.0493 | 0.8214 | A\_203 |

Table S3. Training/test set analysis:100 randomly repeated samplings (training vs. test set) and logistic regression multivariate modeling with the training set, with an average accuracy of 0.714.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| ITER  NUM | Accuracy | CASE  0\_0 | CASE  0\_1 | CASE  1\_0 | CASE  1\_1 | AIC | MODEL |
| 1 | 0.6923 | 4 | 1 | 3 | 5 | 10 | A\_130 + A\_215 + A\_222 + A\_239 |
| 2 | 0.9167 | 3 | 1 | 0 | 8 | 14 | AGE + A\_187 + A\_100 + A\_134 + A\_178 + A\_221 |
| 3 | 0.7692 | 4 | 1 | 2 | 6 | 10 | AGE + A\_31 + A\_130 + A\_239 |
| 4 | 0.5833 | 1 | 3 | 2 | 6 | 14 | PE\_SBP + A\_21 + A\_35 + A\_187 + A\_285 + A\_177 |
| 5 | 0.7692 | 4 | 1 | 2 | 6 | 12 | AGE + A\_27 + A\_67 + A\_279 + A\_299 |
| 6 | 0.5833 | 3 | 1 | 4 | 4 | 12 | A\_27 + A\_93 + A\_152 + A\_215 + A\_279 |
| 7 | 0.5385 | 2 | 3 | 3 | 5 | 12 | AGE + A\_31 + A\_93 + A\_142 + A\_154 |
| 8 | 0.7500 | 3 | 1 | 2 | 6 | 8 | AGE + A\_152 + A\_228 |
| 9 | 0.5385 | 2 | 3 | 3 | 5 | 10 | AGE + PE\_SBP + A\_4 + A\_177 |
| 10 | 0.8333 | 2 | 2 | 0 | 8 | 12 | AGE + A\_93 + A\_100 + A\_130 + A\_196 |
| 11 | 0.4615 | 4 | 1 | 6 | 2 | 10 | A\_17 + A\_222 + A\_239 + A\_281 |
| 12 | 0.8333 | 3 | 1 | 1 | 7 | 10 | AGE + A\_31 + A\_147 + A\_154 |
| 13 | 0.6154 | 1 | 4 | 1 | 7 | 12 | A\_35 + A\_130 + A\_178 + A\_198 + A\_213 |
| 14 | 0.7500 | 2 | 2 | 1 | 7 | 12 | AGE + A\_27 + A\_209 + A\_130 + A\_299 |
| 15 | 0.6923 | 3 | 2 | 2 | 6 | 10 | AGE + PE\_SBP + A\_4 + A\_31 |
| 16 | 0.7500 | 3 | 1 | 2 | 6 | 10 | A\_35 + A\_62 + A\_130 + A\_239 |
| 17 | 0.7692 | 3 | 2 | 1 | 7 | 14 | A\_25 + A\_35 + A\_130 + A\_215 + A\_222 + A\_239 |
| 18 | 0.6364 | 2 | 1 | 3 | 5 | 14 | AGE + PE\_SBP + A\_100 + A\_147 + A\_150 + A\_215 |
| 19 | 0.6923 | 2 | 3 | 1 | 7 | 8 | A\_130 + A\_134 + A\_239 |
| 20 | 0.7273 | 3 | 0 | 3 | 5 | 10 | AGE + PE\_SBP + A\_31 + A\_130 |
| 21 | 0.9167 | 3 | 1 | 0 | 8 | 14 | AGE + PE\_SBP + A\_62 + A\_134 + A\_154 + A\_239 |
| 22 | 0.5000 | 1 | 3 | 3 | 5 | 8 | AGE + PE\_SBP + A\_130 |
| 23 | 0.8462 | 5 | 0 | 2 | 6 | 14 | AGE + A\_31 + A\_130 + A\_134 + A\_152 + A\_239 |
| 24 | 0.6667 | 3 | 1 | 3 | 5 | 12 | A\_35 + A\_93 + A\_130 + A\_239 + A\_299 |
| 25 | 0.8462 | 5 | 0 | 2 | 6 | 12 | AGE + A\_31 + A\_130 + A\_215 + A\_239 |
| 26 | 0.7500 | 3 | 1 | 2 | 6 | 8 | AGE + PE\_SBP + A\_147 |
| 27 | 0.6923 | 3 | 2 | 2 | 6 | 10 | AGE + PE\_SBP + A\_100 + A\_130 |
| 28 | 0.7500 | 3 | 1 | 2 | 6 | 14 | AGE + A\_28 + A\_187 + A\_130 + A\_134 + A\_239 |
| 29 | 0.6923 | 3 | 2 | 2 | 6 | 12 | AGE + A\_31 + A\_121 + A\_134 + A\_154 |
| 30 | 0.9167 | 4 | 0 | 1 | 7 | 16 | A\_25 + A\_35 + A\_130 + A\_134 + A\_141 + A\_152 + A\_239 |
| 31 | 0.6154 | 3 | 2 | 3 | 5 | 20 | A\_27 + A\_28 + A\_31 + A\_25 + A\_62 + A\_93 + A\_152 + A\_222 + A\_239 |
| 32 | 0.6667 | 2 | 2 | 2 | 6 | 12 | AGE + A\_31 + A\_25 + A\_121 + A\_139 |
| 33 | 0.6154 | 3 | 2 | 3 | 5 | 10 | A\_31 + A\_93 + A\_130 + A\_239 |
| 34 | 0.5833 | 2 | 2 | 3 | 5 | 10 | AGE + A\_31 + A\_130 + A\_215 |
| 35 | 0.6154 | 3 | 2 | 3 | 5 | 8 | AGE + A\_93 + A\_134 |
| 36 | 0.5833 | 2 | 2 | 3 | 5 | 10 | A\_35 + A\_130 + A\_134 + A\_152 |
| 37 | 0.5385 | 3 | 2 | 4 | 4 | 10 | PE\_SBP + A\_150 + A\_177 + A\_281 |
| 38 | 0.7500 | 3 | 1 | 2 | 6 | 12 | AGE + A\_31 + A\_134 + A\_152 + A\_239 |
| 39 | 0.5385 | 3 | 2 | 4 | 4 | 10 | A\_31 + A\_35 + A\_285 + A\_281 |
| 40 | 0.5833 | 2 | 2 | 3 | 5 | 8 | A\_35 + A\_130 + A\_203 |
| 41 | 0.8462 | 4 | 1 | 1 | 7 | 10 | AGE + PE\_SBP + A\_134 + A\_239 |
| 42 | 0.9167 | 3 | 1 | 0 | 8 | 14 | AGE + A\_67 + A\_130 + A\_134 + A\_152 + A\_279 |
| 43 | 0.6923 | 2 | 3 | 1 | 7 | 10 | AGE + A\_27 + A\_62 + A\_130 |
| 44 | 0.5000 | 2 | 2 | 4 | 4 | 10 | AGE + A\_67 + A\_130 + A\_161 |
| 45 | 0.6923 | 2 | 3 | 1 | 7 | 10 | AGE + A\_62 + A\_130 + A\_142 |
| 46 | 0.9091 | 2 | 1 | 0 | 8 | 12 | AGE + PE\_SBP + A\_67 + A\_134 + A\_239 |
| 47 | 0.9231 | 5 | 0 | 1 | 7 | 12 | AGE + A\_31 + A\_134 + A\_154 + A\_239 |
| 48 | 0.8333 | 3 | 1 | 1 | 7 | 12 | A\_31 + A\_130 + A\_285 + A\_177 + A\_196 |
| 49 | 0.4615 | 2 | 3 | 4 | 4 | 12 | A\_4 + A\_25 + A\_203 + A\_221 + A\_222 |
| 50 | 0.7500 | 1 | 3 | 0 | 8 | 14 | AGE + PE\_SBP + A\_35 + A\_100 + A\_134 + A\_239 |
| 51 | 0.9167 | 3 | 1 | 0 | 8 | 14 | AGE + PE\_SBP + A\_31 + A\_134 + A\_147 + A\_239 |
| 52 | 0.6667 | 2 | 2 | 2 | 6 | 12 | AGE + A\_31 + A\_130 + A\_147 + A\_154 |
| 53 | 0.6923 | 4 | 1 | 3 | 5 | 8 | AGE + A\_31 + A\_130 |
| 54 | 0.9167 | 4 | 0 | 1 | 7 | 14 | AGE + PE\_SBP + A\_31 + A\_134 + A\_147 + A\_239 |
| 55 | 0.9091 | 2 | 1 | 0 | 8 | 14 | AGE + PE\_SBP + A\_31 + A\_152 + A\_154 + A\_198 |
| 56 | 0.8333 | 4 | 0 | 2 | 6 | 12 | AGE + PE\_SBP + A\_67 + A\_228 + A\_239 |
| 57 | 0.7692 | 2 | 3 | 0 | 8 | 8 | AGE + A\_130 + A\_134 |
| 58 | 0.9167 | 4 | 0 | 1 | 7 | 12 | A\_62 + A\_130 + A\_150 + A\_177 + A\_239 |
| 59 | 0.6923 | 3 | 2 | 2 | 6 | 10 | A\_147 + A\_154 + A\_213 + A\_279 |
| 60 | 0.6667 | 2 | 2 | 2 | 6 | 12 | A\_35 + A\_46 + A\_93 + A\_130 + A\_222 |
| 61 | 0.7692 | 2 | 3 | 0 | 8 | 12 | A\_17 + A\_25 + A\_93 + A\_215 + A\_222 |
| 62 | 0.4167 | 0 | 4 | 3 | 5 | 12 | A\_62 + A\_178 + A\_222 + A\_273 + A\_281 |
| 63 | 0.6923 | 3 | 2 | 2 | 6 | 12 | PE\_SBP + A\_121 + A\_130 + A\_141 + A\_239 |
| 64 | 0.8182 | 1 | 2 | 0 | 8 | 10 | AGE + PE\_SBP + A\_31 + A\_239 |
| 65 | 0.6154 | 4 | 1 | 4 | 4 | 8 | AGE + A\_31 + A\_299 |
| 66 | 0.5833 | 3 | 1 | 4 | 4 | 16 | PE\_SBP + A\_28 + A\_62 + A\_93 + A\_141 + A\_177 + A\_260 |
| 67 | 0.7273 | 1 | 2 | 1 | 7 | 12 | PE\_SBP + A\_31 + A\_134 + A\_154 + A\_239 |
| 68 | 0.5833 | 2 | 2 | 3 | 5 | 14 | A\_4 + A\_31 + A\_93 + A\_134 + A\_203 + A\_20 |
| 69 | 0.6154 | 2 | 3 | 2 | 6 | 16 | PE\_SBP + A\_27 + A\_25 + A\_35 + A\_187 + A\_178 + A\_219 |
| 70 | 0.6667 | 2 | 2 | 2 | 6 | 10 | AGE + A\_35 + A\_130 + A\_299 |
| 71 | 0.8333 | 4 | 0 | 2 | 6 | 16 | PE\_SBP + A\_23 + A\_62 + A\_100 + A\_177 + A\_197 + A\_213 |
| 72 | 0.8333 | 4 | 0 | 2 | 6 | 14 | AGE + A\_31 + A\_93 + A\_100 + A\_130 + A\_178 |
| 73 | 0.6923 | 3 | 2 | 2 | 6 | 10 | AGE + A\_35 + A\_130 + A\_299 |
| 74 | 0.8333 | 3 | 1 | 1 | 7 | 14 | AGE + A\_100 + A\_130 + A\_177 + A\_215 + A\_222 |
| 75 | 0.7692 | 3 | 2 | 1 | 7 | 14 | AGE + A\_31 + A\_121 + A\_152 + A\_154 + A\_198 |
| 76 | 0.6667 | 4 | 0 | 4 | 4 | 12 | AGE + PE\_SBP + A\_31 + A\_25 + A\_152 |
| 77 | 0.6667 | 1 | 3 | 1 | 7 | 12 | PE\_SBP + A\_31 + A\_25 + A\_154 + A\_178 |
| 78 | 0.8333 | 3 | 1 | 1 | 7 | 10 | A\_31 + A\_130 + A\_285 + A\_177 |
| 79 | 0.8462 | 5 | 0 | 2 | 6 | 12 | AGE + A\_31 + A\_25 + A\_130 + A\_215 |
| 80 | 0.8333 | 3 | 1 | 1 | 7 | 12 | AGE + A\_31 + A\_215 + A\_222 + A\_239 |
| 81 | 0.6923 | 2 | 3 | 1 | 7 | 12 | AGE + A\_25 + A\_35 + A\_147 + A\_239 |
| 82 | 0.9167 | 3 | 1 | 0 | 8 | 12 | AGE + A\_67 + A\_100 + A\_130 + A\_134 |
| 83 | 0.3846 | 4 | 1 | 7 | 1 | 10 | A\_130 + A\_177 + A\_219 + A\_281 |
| 84 | 0.5455 | 2 | 1 | 4 | 4 | 12 | AGE + PE\_SBP + A\_31 + A\_147 + A\_222 |
| 85 | 0.8462 | 3 | 2 | 0 | 8 | 14 | A\_31 + A\_35 + A\_130 + A\_134 + A\_152 + A\_239 |
| 86 | 0.5833 | 1 | 3 | 2 | 6 | 14 | A\_28 + A\_35 + A\_62 + A\_169 + A\_20 + A\_299 |
| 87 | 0.7692 | 3 | 2 | 1 | 7 | 14 | A\_31 + A\_40 + A\_130 + A\_215 + A\_222 + A\_239 |
| 88 | 0.8333 | 2 | 2 | 0 | 8 | 12 | A\_31 + A\_130 + A\_215 + A\_222 + A\_239 |
| 89 | 0.8333 | 3 | 1 | 1 | 7 | 12 | AGE + PE\_SBP + A\_31 + A\_100 + A\_239 |
| 90 | 0.5833 | 1 | 3 | 2 | 6 | 16 | PE\_SBP + A\_28 + A\_121 + A\_100 + A\_134 + A\_178 + A\_233 |
| 91 | 0.5000 | 1 | 3 | 3 | 5 | 12 | AGE + PE\_SBP + A\_141 + A\_142 + A\_279 |
| 92 | 0.5833 | 2 | 2 | 3 | 5 | 12 | AGE + A\_4 + A\_130 + A\_198 + A\_222 |
| 93 | 0.7692 | 4 | 1 | 2 | 6 | 16 | AGE + A\_25 + A\_35 + A\_134 + A\_215 + A\_239 + A\_299 |
| 94 | 0.7000 | 2 | 0 | 3 | 5 | 12 | AGE + PE\_SBP + A\_134 + A\_154 + A\_239 |
| 95 | 0.7692 | 3 | 2 | 1 | 7 | 12 | AGE + A\_31 + A\_130 + A\_178 + A\_196 |
| 96 | 0.5833 | 3 | 1 | 4 | 4 | 10 | A\_62 + A\_130 + A\_150 + A\_239 |
| 97 | 0.7692 | 3 | 2 | 1 | 7 | 14 | PE\_SBP + A\_16 + A\_134 + A\_141 + A\_152 + A\_239 |
| 98 | 0.8333 | 3 | 1 | 1 | 7 | 14 | A\_31 + A\_130 + A\_215 + A\_222 + A\_239 + A\_299 |
| 99 | 0.8462 | 5 | 0 | 2 | 6 | 12 | AGE + A\_31 + A\_93 + A\_130 + A\_239 |
| 100 | 0.6667 | 4 | 0 | 4 | 4 | 14 | AGE + A\_25 + A\_215 + A\_221 + A\_222 + A\_239 |

AIC, Akaike Information Criterion

Table S4. Significant continuous variables were selected from the first step of multivariate analysis through a hundred-times repeated training and test sets. The variables are listed in order of frequency as shown in Table S3.

|  |  |  |  |
| --- | --- | --- | --- |
| Name of VOC or clinical variable | VOC group | Frequency | VOC\_variable |
| Age |  | 60 |  |
| 2-Methyl pentane | Alkane | 47 | A\_130 |
| Cyclohexanone | Ketones | 40 | A\_31 |
| Acetic acid ethyl ester | Acetate | 39 | A\_239 |
| Systolic blood pressure |  | 31 |  |
| Heptane | Alkane | 26 | A\_134 |
| Acetophenone | Ketones | 18 | A\_35 |
| m-Xylene | Aromatics | 16 | A\_222 |
| Ethylbenzene | Aromatics | 15 | A\_215 |
| 1,2-Dichloro-ethane | Halo-Hydrocarbons | 13 | A\_93 |
| Decane | Alkane | 13 | A\_152 |
| 3-Heptanone | Ketones | 13 | A\_25 |
| Undecane | Alkane | 12 | A\_154 |
| Trichloroethene | Halo-Hydrocarbons | 11 | A\_100 |
| Phenol | Alcohol | 11 | A\_62 |
| Octadecane | Alkane | 10 | A\_177 |
| n-Nonane | Alkane | 9 | A\_147 |
| Sevoflurane | Other | 9 | A\_299 |
| Nonadecane | Alkane | 8 | A\_178 |
| Dihydro-2(3H)-furanone | Ketones | 6 | A\_27 |
| 2-Ethyl-1-Hexanol | Alcohol | 6 | A\_67 |
| 2-Methyl heptane | Alkane | 5 | A\_141 |
| 2-Pentanone | Ketones | 5 | A\_28 |
| Benzaldehyde | Aldehyde | 5 | A\_279 |
| Octanal | Aldehyde | 5 | A\_281 |
| Sulfur dioxide | VSC | 5 | A\_4 |
| 3-Methyl nonane | Alkane | 5 | A\_121 |
| Isoprene | Terpens | 4 | A\_187 |
| Dimethyl selenide | Other | 4 | A\_285 |
| 2-Pinene | Terpens | 4 | A\_198 |
| Octane | Alkane | 3 | A\_142 |
| Myrcene | Terpens | 3 | A\_196 |
| (-)-beta-Pinene | Terpens | 3 | A\_203 |
| Toluene | Aromatics | 3 | A\_213 |
| o-Xylene | Aromatics | 3 | A\_221 |
| 2,6-Dimethyloctane | Alkane | 2 | A\_150 |
| 2,6-Dimethyloctane | Alkane | 2 | A\_150 |
| Allyl methyl disulfide | VSC | 2 | A\_17 |
| p-Xylene | Aromatics | 2 | A\_219 |
| Azulene | Aromatics | 2 | A\_228 |
| 3-Sulfo-L-alanine | VSC | 2 | A\_20 |
| 1,3,5-Trimethylbenzene | Aromatics | 1 | A\_209 |
| Propylcyclopentane | Alkane | 1 | A\_138 |
| Ethylcyclohexane | Alkane | 1 | A\_139 |
| Pentadecane | Alkane | 1 | A\_169 |
| (2E)-2-butenyl methyl sulfide | VSC | 1 | A\_16 |
| Acetone | Ketones | 1 | A\_21 |
| 3-Carene | Terpens | 1 | A\_197 |
| 2-Butanone | Ketones | 1 | A\_23 |
| Phthalic anhydride | Aromatics | 1 | A\_233 |
| Acetic acid | Acid | 1 | A\_260 |
| Acetaldehyde | Aldehyde | 1 | A\_273 |
| Menthone | Ketones | 1 | A\_40 |
| Ethanol | Alcohol | 1 | A\_46 |