



Figure S1. Representative two-dimensional chromatograms for Fuji, Gala, Ambrosia, Golden and Envy apples.

Table S1. Identified molecules on apple surface.

Molecules
(2,5-Dimethoxyphenyl)acetone
(2-Aziridinylethyl)amine
(2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trien-1-yl stearate
(3a?,4?,7?,7a?)-3a,4,7,7a-Tetrahydro-4,7-methano-1H-indene
(4,4-Dimethyl-5-methylene-4,5-dihydro-3H-pyrrol-2-yl)-(4,4-dimethyl-5-methylene-pyrrolidin-2-ylidene)-acetonitrile
2,5-Dimethoxy-4-Iodoamphetamine, N-trimethylsilyl-
3,4,5-Trimethoxyamphetamine, N-(trimethylsilyl)-
4-Methylephedrine, N-trimethylsilyl-, trimethylsilyl ether
4-Methyl-N-ethyl-norephedrine, N-trimethylsilyl-, trimethylsilyl ether
MBDB, N-trimethylsilyl-
N-Ethylcathinone ephedrine, N-trimethylsilyl-, trimethylsilyl ether
Phenylpropanolamine, N-trimethylsilyl-, trimethylsilyl ether
p-Methoxyamphetamine, N-trimethylsilyl-
(R)-(-)-Phenylephrine, N-trimethylsilyl-, bis(trimethylsilyl) ether
(R)-9-[(S)-2-(Hydroxymethyl)pyrrolidin-1-yl]-3-methyl-3,4-dihydro-2H-benzo[b][1,4,5]oxathiazepine 1,1-dioxide
(S,E)-8,12,15,15-Tetramethyl-4-methylenebicyclo[9.3.1]pentadeca-7,11-diene
(Z)-2-(Heptadec-10-en-1-yl)-4,5-dihydro-1H-imidazole
(Z)-Docos-13-enamide, N-TMS
(Z)-Docos-9-enenitrile
[1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-tetramethyl-
1-(1-Butoxy-2-propoxy)-2-propanol, TMS derivative
1-(2,4-Dimethoxyphenyl)-propan-2-one
1-(2,5-Dimethoxyphenyl)-1-[(trimethylsilyl)oxy]propan-2-amine
1-(2-Methoxy-1-methylethoxy)-2-propanol, TMS derivative
1-(Ethoxycarbonylmethyl)pyridinium bromide
1,1,3,3,5,5,7,7-Octamethyl-7-(2-methylpropoxy)tetrasiloxan-1-ol
1,11-Dodecadiene
1,15-Hexadecadiene
1,19-Eicosadiene
1,2,3-Butanetriol, 3TMS derivative
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
1,2-Benzenedicarboxylic acid, dinonyl ester
1,2-Benzenediol, O-(4-methoxybenzoyl)-O'-(2-furoyl)-
1,2-Benzisothiazole
1,2-Cyclohexanedicarboxylic acid, 2-ethylhexyl nonyl ester
1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl nonyl ester
1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl nonyl ester
1,2-Cyclohexanedicarboxylic acid, dinonyl ester
1,2-Cyclohexanedicarboxylic acid, heptadecyl 2-methylcyclohexyl ester
1,2-Ethenediol, 2TMS derivative
1,3,5-Trioxepane
1,3-Bis(trimethylsilyloxy)pentane
1,3-di-iso-propylnaphthalene
1,3-Dioxolane, 2-butyl-
1,3-Dioxolane, 2-heptyl-
1,3-Dipentyl-heptabarbital
1,3-Diphenyl-2-azafluorene
1,3-Propanediol, 2TMS derivative
1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
1,4-Butanediol, 2TMS derivative
1,5-Anhydroglucitol, 4TMS derivative
1,5-Heptadiene, 3,4-dimethyl-
1,6-Dioxacyclododecane-7,12-dione
1,8,11-Heptadecatriene, (Z,Z)-
10,18-Bisnorabieta-8,11,13-triene

10H-Phenoxaphosphine, 2-chloro-8-ethyl-10-hydroxy-, 10-oxide
10-Undecen-1-ol, TMS derivative
10-Undecen-1-yl acetate
11,14-Eicosadienoic acid
11,14-Eicosadienoic acid, methyl ester
11-Eicosenoic acid, (E)-,TMS derivative
11-Hexacosyne
11-Hydroxy-.DELTA.-9-tetrahydrocannabinol, bis(trimethylsilyl) ether
11-Octadecynenitrile
13-Bromotetradecanoic acid
13-Docosen-1-ol, (Z)-
13-Docosenamide, (Z)-
16-Octadecenoic acid, methyl ester
18-Methyl-eicosane-1,2-diol, isopropylidene derivative
19-Norepietiocholanolone acetate
1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, tridecyl ester
1-Butoxy-2-propanol, TMS derivative
1-Chloroundecane
1-Cyclohexylethanol, TMS derivative
1-Decanol, 2-methyl-
1-Decene
1-Deoxypentitol, 4TMS derivative
1-Diphenyl(tert-butyl)silyloxy-4-methoxybenzene
1-Dodecanol
1-Dodecanol, 2-hexyl-
1-Dodecanol, TMS derivative
1-Ethyl-2-dimethyl(octyl)silyloxycyclohexane
1-Heneicosanol
1-Hexacosene
1-Hexadecanol, 3,7,11,15-tetramethyl-
1-Hexadecanol, TBDMS derivative
1-Hexadecanol, TMS derivative
1-Hexanone, 5-methyl-1-phenyl-
1-Hexene, 2,5,5-trimethyl-
1H-Imidazole, 2-heptadecyl-4,5-dihydro-
1H-Imidazole, 4,5-dihydro-2-hexadec-9Z-enyl-
1H-Indene, 1-ethylidene-
1H-Indene, 1-hexadecyl-2,3-dihydro-
1H-Indene, 1-methylene-
1H-Quinolin-2-one, 5,8-dimethoxy-1,4-dimethyl-
1-Methyl-5-mercaptotetrazole
1-Mono-isobutyrim, 2TMS derivative
1-Monolinolein, 2TMS derivative
1-Monomyristin, 2TMS derivative
1-Monopalmitin, 2TMS derivative
1-Naphthalenecarboxamide, N-(3-chlorophenyl)-
1-Naphthamide, N-(4-chlorophenyl)-
1-Octacosanol, 2,4,6,8-tetramethyl-, (all-R)-
1-Octadecanol, TBDMS derivative
1-Octadecanol, TMS derivative
1-Octanol, 2,2-dimethyl-
1-Octanol, 2-butyl-
1-Octanol, 3,7-dimethyl-
1-Octene, 6-methyl-
1-Pentanol, 2-ethyl-4-methyl-
1-Pentene, 2,4,4-trimethyl-
1-Phenyl-1,2-ethanediol, 2TMS derivative
1-Propanol, TMS derivative

1-Propene-1-thiol
 1-Tetracosene
 1-Tetradecene
 1-Tricosene
 1-Undecanol, TMS derivative
 2-(2,5-Dimethoxy-phenyl)-propionaldehyde
 2(3H)-Furanone, 5-hexyldihydro-
 2-(4'-Methoxyphenyl)-2-(3'-methyl-4'methoxyphenyl)propane
 2,2,7,7-Tetramethyltricyclo[6.2.1.0(1,6)]undec-4-en-3-one
 2,2-Dimethyl-3-heptene trans
 2,2'-Dithiobisethanol, 2TMS derivative
 2,2'-Heptamethylene-di-2-imidazoline
 2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (, (R*,R*)-)
 2,3-Butanediol, 2TMS derivative
 2,3-Dihydro-1H-2-isopropylcyclopenta[b]quinoxaline
 2,3-Dihydroxypropyl icosanoate, 2TMS derivative
 2,3-Dimethoxyphenol, TMS
 2,4,6,8-Tetramethyl-1-undecene
 2,4,6-Tris(1,1-dimethylethyl)-4-methylcyclohexa-2,5-dien-1-one
 2,4,7,9-Tetramethyl-5-decyne-4,7-diol, 2TMS derivative
 2,4-Dichlorobenzoic acid, TMS derivative
 2,4-Dihydroxybenzoic acid, 3TMS derivative
 2,4-Di-tert-butylphenol
 2,4-Thiazolidinedione
 2,5-cyclohexadiene-1,4-dione, 2-(1,1-dimethylethyl)-5-(2-methyl-2-propen-1-yl)-
 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-
 2,5-Dihydroxy-4-methoxyacetophenone
 2,5-Dimethoxy-4-methylamphetamine, N-(trimethylsilyl)-
 2,5-Dimethoxybenzoic acid, TMS derivative
 2,5-Dimethoxymandelic acid, di-TMS
 2,5-Dimethoxyphenol, TMS
 2',5'-Dimethoxypropiophenone
 2,5-Hexanediol, 2TMS derivative
 2,6,8-Trimethyl-4-nonyl acetate
 2,6-Bis(tert-butyl)phenol, TMS derivative
 2,6-Dimethyldecane
 2,6-di-tert-Butyl-4-(dimethylaminomethyl)phenol
 2-[2-[2-Methoxyethoxy]ethoxy-1,3-dioxalane
 2-Acetoxyindane
 2-Acetylmethylamino-4,5,6,7-tetrahydrobenzothiazol-7-one
 2-Allyl-1,4-dimethoxybenzene
 2-Amino-2-deoxyhexose, 5TMS derivative
 2-Amino-4-(1-ethylpropyl)-4H-benzo[h]chromene-3-carbonitrile
 2-Aminobenzoxazole, 2TBDMS derivative
 2-Aminomalonic acid, N,O,O,-TMS
 2-Aminosuccinonitrile
 2-Benzothiazolamine, N-ethyl-
 2-Butene-1,4-diol, (E)-, 2TMS derivative
 2-Butylamine, N-tetradecyl-
 2-Decanol, TMS derivative
 2-Decene, 7-methyl-, (Z)-
 2-Dodecene, (Z)-
 2-Ethoxyethanol, TMS derivative
 2-Ethyl-acridone
 2-Ethylhexanal ethylene glycol acetal
 2-Ethylhexanoic acid, TMS derivative
 2H-Cyclopropa[a]naphthalen-2-one, 1,1a,4,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, (1a?,7?,7a?,7b?)-
 2-Heptanol, TBDMS derivative

2-Hexene, 3,5,5-trimethyl-
2-Hexene, 3,5-dimethyl-
2-Hexyl-1-octanol
2-Hydroxy-2-methylbutyric acid, 2TMS derivative
2-Hydroxy-4-methoxybenzaldehyde, TMS derivative
2-Hydroxy-5-methoxybenzaldehyde, TMS derivative
2-Hydroxymandelic acid, ethyl ester, di-TMS
2-Imidazolidinone
2-Isopropyl-5-methyl-1-heptanol
2-Methoxybenzoic acid, 2,3-dichlorophenyl ester
2-Methyl-1,2-bis(trimethylsilyloxy)butane
2-Methyl-1,3-butanediol, 2TMS derivative
2-Methyl-1,3-butanediol, TBDMS derivative
2-Methyl-3-buten-2-ol, TMS derivative
2-Methylbicyclo[3.2.1]octane
2-Methyl-E-7-hexadecene
2-Monomyristin, 2TMS derivative
2-Monostearin, 2TMS derivative
2-Naphthalenol, 8-amino-
2-Nonenal
2-Oxopentanoic acid, TMS derivative
2-Palmitoylglycerol, 2TMS derivative
2-Pentanethiol, 2-methyl-
2-Phenylisopropanol, TMS derivative
2-Propanol, 1-[2-(2-methoxy-1-methylethoxy)-1-methylethoxy]-
2-Propanol, 2-methyl-
2-Propanone, 1,1,3,3-tetrabutoxy-
2-tert-Butoxytetrahydrofuran
2-Undecanethiol, 2-methyl-
3,3,13,13-Tetraethylpentadecane
3,3-Dichloropropyne
3,4-Dimethoxymandelic acid, di-TMS
3,4-Dimethyl-2-(3-methyl-butyl)-benzoic acid, methyl ester
3,5-Diacetyl-4-methyl-1-phenyl-1,4-dihydropyridine
3,5-Dimethoxymandelic acid, di-TMS
3,5-Dimethoxymandelic amide, di-TMS
3,7-Dimethyloctyl acetate
3-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propanenitrile
3-[3-(4-Hydroxyphenyl)-3-oxoprop-1-en-1-yl]-6-methylchromen-4-one
3-Allyl-5-(1H-indol-3-ylmethyl)-2-thioxo-imidazolidin-4-one
3-Chlorobenzoic acid, TMS derivative
3-Dodecanol, 3,7,11-trimethyl-
3-Ethyl-2-methyl-2-heptanol
3-Ethyl-3-methylheptane
3-Ethyl-3-methylnonadecane
3-Ethylpentan-3-ol, trimethylsilyl ether
3H-1,2,4-Triazole-3-thione, 5-amino-1,2-dihydro-
3-Hydroxy-3-phenylbutan-2-one
3-Hydroxybutyric acid, 2TMS derivative
3-Methoxyamphetamine, 4-trimethylsilyloxy, N-trimethylsilyl-
3-Methoxy-benzoic acid 3,4-dimethyl-phenyl ester
3-Methyl-1,3-bis(trimethylsilyloxy)butane
3-Methyl-2-butanol, TMS derivative
3-Methylvaleric acid, TMS
3-pentulosonic acid, 2,4,5-tris-O-(trimethylsilyl)-, trimethylsilyl ester
3-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-2,4b,8,8-tetramethyl-, (4bS,8aS)-
3-Phenyl-2-butanol, TMS derivative
3-Phenyllactic acid, 2TMS derivative

3-Pyridinol, TMS derivative
4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-
4-Benzyl-4,5-dihydroisoxazole
4-Chlorobenzoic acid, TMS derivative
4-Cyano-4-methylthio-tetracyclo(6,2,1,1(3,6).0(2,7)dodec-9-ene
4-Decene, 7-methyl-, (E)-
4-Dodecene, (E)-
4-Hydroxy-3,4,6-trimethylhept-5-enoic acid lactone
4-Methoxybenzoic acid, 4-isopropylphenyl ester
4-Methoxyphenol, TMS derivative
4-Methylethcathinone, N-trimethylsilyl-
4-Methylpentan-2-ol, tert-butyldimethylsilyl ether
4-Methylvaleric acid, TMS derivative
4-Pentene-2-ol, 2-methyl
4-Pyridinol, TMS derivative
4-Trimethylsilylphenol
5,2,1,6,3,4-[2,3]Butanediyl[1,4]diylidenedipentaleno[2,1,6-cde:2',1',6'-gha]pentalene, hexadecahydro-
5,5-Dimethyl-1,3-dioxane-2-ethanol, TMS derivative
5,6,7,8,9,10-Hexahydrobenzocyclooctene
5,6-Dimethyl-4-phenyl-3-cyanopyridine-2(1H)-thione
5?-Androstan-3?-ol, O-acetyl-
5?-Androstan-3?-ol, O-ethyl-
5-Cyano-2-methyl-4-methylthio-6-phenylpyrimidine
5-Dodecene, (E)-
5-Eicosene, (E)-
5-Ethyldecane
5-Hydroxytryptophan, 4TMS derivative
5-Methyl-2-(2-methyl-2-tetrahydrofuryl)tetrahydrofuran
5-Methyluridine, 3TMS derivative
5-Nitro-3-phenyl-1H-indazole
5-Nonanol, TMS derivative
5-Oxoproline, 2TMS derivative
6-(4-Fluorophenyl)-4-phenyl-3-cyanopyridine-2(1H)-thione
6,9-Heptadecadiene
6-Dodecyne
6-Methoxy-3-methylbenzofuran
6-Nonenal, (E)-
6-Tetradecene, (E)-
6-Tridecene
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin
7-Isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene
7-Methyl-Z-tetradecen-1-ol acetate
7-Tetradecene, (E)-
8-Hexadecyne
8-Methyl-6-nonenamide
8-Methylnonanoic acid, trimethylsilyl ester
9(E),11(E)-Conjugated linoleic acid, trimethylsilyl ester
9,10-Anthracenedione, 1,4-diamino-2,3-dihydro-
9,11-Octadecadienoic acid, methyl ester, (E,E)-
9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-
9,12-Octadecadienoic acid (Z,Z)-
9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester
9,12-Octadecadienoic acid (Z,Z)-, methyl ester
9,12-Octadecadienoic acid, ethyl ester
9,12-Octadecadienoic acid, methyl ester
9-Octadecen-1-ol, (Z)-
9-Octadecen-1-ol, acetate, (Z)-

9-Octadecenamide, (Z)-
 9-Octadecenitrile, (Z)-
 9-Octadecenoic acid, (E)-, TMS derivative
 9-Octadecynitrile
 9-Tricosene, (Z)-
 Acetic acid, 7,7,10a,12a-tetramethyl-2,5-dioxo-1,2,3,4,4a,4b,5,7,8,9,10,10a,10b,11,12,12a-hexadecahydro-1-azachrysen-8-yl
 ester
 Acetic acid, bis[(trimethylsilyl)oxyl]-, trimethylsilyl ester
 Acetic acid, dimethoxy-, methyl ester
 Acetic acid, TMS derivative
 Acrylic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester
 Adonitol, 5TMS derivative
 Ala-?-Ala, N-trimethylsilyl-, trimethylsilyl ester
 Alanine, N-methyl-n-butoxycarbonyl-, undecyl ester
 Alanine, N-methyl-N-ethoxycarbonyl-, dodecyl ester
 Alanine, N-methyl-N-ethoxycarbonyl-, pentadecyl ester
 Alanine, N-methyl-N-isobutoxycarbonyl-, isohexyl ester
 Alanine, N-methyl-N-methoxycarbonyl-, undecyl ester
 Alanylalanine, N,N'-dimethyl-N'-methoxycarbonyl-, hexyl ester
 Alanylalanine, N,N'-dimethyl-N'-methoxycarbonyl-, pentyl ester
 Alanylglycine, 2TMS derivative
 Allonic acid, ?-lactone, 4TMS derivavative
 alpha-(4-DIMETHYLAMINOPHENYL)-?(9-PHENANTHRYL)DECANE
 alpha-D-(-)-Lyxopyranose, 4TMS derivative
 alpha-D-(+)-Talopyranose, 5TMS derivative
 alpha-D-Allopyranose, 5TMS derivative
 alpha-D-Arabinopyranose, 4TMS derivative
 alpha-D-Glucopyranose, 5TMS derivative
 alpha-D-Mannopyranose, 5TMS derivative
 alpha-D-Xylopyranose, 4TMS derivative
 alpha-Farnesene
 alpha-Hydroxyisobutyric acid, 2TMS derivative
 alpha-L-6-Deoxymannopyranose, 4TMS derivative
 alpha-Methyl-L-tyrosine, 3TMS derivative
 Androstane, (5?)-
 Anthra[1,9-cd]pyrazol-6(2H)-one
 Anthranilic acid, TMS derivative
 Arabinitol, 5TMS derivative
 Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)-
 Arabinose, 4TMS derivative
 Arachidic acid, TMS derivative
 Aspartic acid, 3TMS derivative
 Behenic acid, TMS derivative
 Benzaldehyde, 2,5-dimethoxy-
 Benzamide, N-(1,1-dimethylethyl)-
 Benzamide, N-propyl-
 Benzenamine, 4-(6-methyl-2-benzothiazolyl)-
 Benzenamine, N,N-diethyl-3-methyl-
 Benzenamine, N,N-diethyl-4-methyl-
 Benzene, (1-butylheptyl)-
 Benzene, (1-methyldodecyl)-
 Benzene, (1-methylethyl)-
 Benzene, (1-methyltridecyl)-
 Benzene, (1-methylundecyl)-
 Benzene, (1-pentylheptyl)-
 Benzene, [1-[[1-(1-methylethyl)-3-butenyl]oxy]ethyl]-, [S-(R*,R*)]-
 Benzene, 1,1'-(1-ethenyl-1,3-propanediyl)bis-
 Benzene, 1,1'-(oxydiethylidene)bis-

Benzene, 1,2,3-trimethyl-
Benzene, 1,2,4-trimethyl-
Benzene, 1,4-dimethoxy-
Benzene, 1-ethyl-2-methyl-
Benzene, 1-ethyl-3-methyl-
Benzene, 1-ethyl-4-methyl-
Benzene, 1-methyl-4-propyl-
Benzene, 4-butyl-1,2-dimethoxy-
Benzene, propyl-
Benzeneacetic acid, TBDMS derivative
Benzeneethanol, γ -ethenyl-
Benzenemethanol, γ -(1-aminobutyl)-, N-trimethylsilyl-, trimethylsilyl ether
Benzenemethanol, γ,γ -dimethyl-
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester
Benzoic acid, 2-hydroxy-3-[(2-hydroxy-4-methoxy-6-propylbenzoyl)oxy]-4-methoxy-6-propyl-, methyl ester
Benzoic acid, methyl ester
Benzoic Acid, TBDMS derivative
Benzoic Acid, TMS derivative
Benzophenone
Benzothiazole
Benzothiazole, 2-(4-amino-3-methylphenyl)-
Benzothiazole, 2-(o-aminophenyl)-4-methyl-
Benzyl alcohol, TMS derivative
beta-D-(+)-Mannopyranose, 5TMS derivative
beta-D-(+)-Talopyranose, 5TMS derivative
beta-D-Allopyranose, 5TMS derivative
beta-D-Glucopyranose, 5TMS derivative
beta-Hydroxypyruvic acid, trimethylsilyl ether, trimethylsilyl ester
beta-L-Arabinopyranose, 4TMS derivative
Biphenyl-4,4'-dicarboxylic acid, bis-(4-pentyl-phenyl) ester
Bisphenol A monomethyl ether, TMS derivative
Bisphenol A, 2TMS derivative
Bisphenol A, TMS derivative
Boric acid, 3TMS derivative
Butanal, oxime
Butane, 2,3-dimethoxy-2-methyl-
Butane-1,3-diol, 1-methylene-3-methyl-, bis(trimethylsilyl)ether
Butanedioic acid, 2TMS derivative
Butyl 9,12,15-octadecatrienoate
Butyl 9,12-octadecadienoate
Butylated Hydroxytoluene
Butylone, N-trimethylsilyl-
Butyric Acid, TMS derivative
Cadaverine, 4TMS derivative
Carbitol, TMS derivative
Chavicol TMS
Cholesterol, TMS derivative
Chrysophanol, 2TMS derivative
Citric acid, 4TMS derivative
Cyanuric acid, 3TMS derivative
Cyclobutanecarboxylic acid, 2-propenyl ester
Cyclododecane
Cyclohexane, (1-hexadecylheptadecyl)-
Cyclohexane, 1-methyl-4-(1-methylethenyl)-, trans-
Cyclohexanemethanol, 4-methyl-, trans-
Cyclohexanol, TMS derivative
Cyclohexanone, 3,3,5-trimethyl-
Cyclohexene, 1-butyl-

Cyclohexene,3-propyl-
 Cyclooctane, 1,4-dimethyl-, cis-
 Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-
 Cyclopentane, 1,1,3,3-tetramethyl-
 Cyclopentane, 1,1'-hexadecylidenebis-
 Cyclopentane, nonyl-
 Cyclopentane, undecyl-
 Cyclopentanone, 2,2,4-trimethyl-
 Cyclopropane, 1-(1-hydroxy-1-heptyl)-2-methylene-3-pentyl-
 Cyclopropane, 1-hexyl-2-methyl-
 Cyclopropane, 1-methyl-2-(3-methylpentyl)-
 D-(-)-Erythrofuranose, tris(trimethylsilyl) ether (isomer 1)
 D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1)
 D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 2)
 D-(-)-Fructopyranose, 5TMS derivative (isomer 1)
 D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1)
 D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 2)
 D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 1)
 D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2)
 D-(+)-Arabitol, 5TMS derivative
 D-(+)-Galactopyranose, 5TMS derivative (isomer 2)
 D-(+)-Talofuranose, pentakis(trimethylsilyl) ether (isomer 2)
 D-(+)-Xylose, 4TMS derivative
 D-Alanine, N-ethoxycarbonyl-, undecyl ester
 D-Allofuranose, pentakis(trimethylsilyl) ether
 D-Arabinopyranose, 4TMS derivative (isomer 2)
 Decane
 Decane, 2,3,5-trimethyl-
 Decane, 2,6,7-trimethyl-
 Decane, 4-methyl-
 Decane, 5,6-dimethyl-
 Decanoic acid, TMS derivative
 Decyl oleate
 D-Erythro-Pentitol, 2-deoxy-1,3,4,5-tetrakis-O-(trimethylsilyl)-
 D-Fructose, 5TMS derivative
 D-Fucitol, 5TMS derivative
 D-Glucopyranose, 5TMS derivative
 D-Glucose, 5TMS derivative
 Dicyclopentadiene
 Diethyl aminomalonate, TMS derivative
 Diethylene glyco, TMS derivative
 Diethylene glycol, 2TMS derivative
 Diethylene glycol, n-butyl ether, trimethylsilyl ether
 Diglycerol, 4TMS derivative
 Dihydroxyacetone, 2TMS derivative
 Dimethyl hexopyranosiduronate, ?-D-, 3TMS derivative
 Dinaphtho(1,2-b:2',1'-d)thiophene
 Disulfide, di-tert-dodecyl
 dl-2-Phenyl-1,2-propanediol
 dl-7-Azatryptophan
 dl-Alanine ethyl ester
 DL-Arabinopyranose, 4TMS derivative
 D-Lyxose, 4TMS derivative
 D-Mannopyranose, 5TMS derivative
 D-Mannose, 5TMS derivative
 D-Norleucine, N-ethoxycarbonyl-, dodecyl ester
 Docosane
 Docosanol, TBDMS derivative

Docosyl octyl ether
Dodecane
Dodecane, 2,6,11-trimethyl-
Dodecane, 2,7,10-trimethyl-
Dodecane, 4,6-dimethyl-
Dodecanoic acid, ethenyl ester
Dodecanoic acid, methyl ester
Dodecanoic acid, TMS derivative
Dopamine, 4TMS derivative
D-Psicofuranose, pentakis(trimethylsilyl) ether (isomer 1)
D-Psicofuranose, pentakis(trimethylsilyl) ether (isomer 2)
D-Psicopyranose, 5TMS derivative (isomer 2)
D-Ribofuranose, 5-deoxy-5-(methylsulfinyl)-1,2,3-tris-O-(trimethylsilyl)-
D-Ribose, 4TMS derivative
D-Xylopyranose, 4TMS derivative
D-Xylose, 4TMS derivative
E-11(12-Cyclopropyl)dodecen-1-ol acetate
E-11-Hexadecen-1-ol
E-8-Methyl-9-tetradecen-1-ol acetate
E-9-Tetradecenoic acid
Eicosane
Eicosane, 2-methyl-
Eicosanenitrile
Eicosanoic acid, methyl ester
Eicosyl nonyl ether
Ephedrine, 2TMS derivative
Erythritol, 4TMS derivative
Ethanimidic acid, N-(trimethylsilyl)-, trimethylsilyl ester
Ethanone, 1,1'-(1,4-phenylene)bis-
Ethyl 3-hydroxybutyrate, TMS derivative
Ethyl 9,12-hexadecadienoate
Ethylene glycol - Adipate - Diethylene glycol
Ethylene glycol butyl ether, trimethylsilyl ether
Ethylene glycol, 2TMS derivative
Ethylene glycol, TMS derivative
Ethylene sebacate
Formamide, N-methyl-
Fructofuranoside, methyl 1,3,4,6-tetrakis-O-(trimethylsilyl)-, ?-D-
Fumaric acid, pent-4-en-2-yl tetradecyl ester
Furfuryl alcohol, TMS derivative
Galactopyranose, 5TMS derivative
Gluconolactone (3R,4S,5R,6R)-, 4TMS derivative
Gluconolactone, 4TMS derivative
Glucopyranose, 5TMS derivative
Glucose, 5TMS derivative
Glucuronolactone, trisO-(trimethylsilyl)-
Glyceric acid, 3TMS derivative
Glycerol monostearate, 2TMS derivative
Glycerol, 3TMS derivative
Glycine, 3TMS derivative
Glycine, di-TMS
Glycine, N-methyl-N-ethoxycarbonyl-, decyl ester
Glycine, N-methyl-N-ethoxycarbonyl-, nonyl ester
Glycine, N-methyl-N-ethoxycarbonyl-, octyl ester
Glycolic acid, 2TMS derivative
Glyoxime, 2TMS derivative
Heneicosane
Heneicosane, 11-decyl-

Heneicosane, 3-methyl-
Heneicosanoic acid, TMS derivative
Henicos-1-ene
Hentriacontane
Heptacosane
Heptadecane
Heptadecane, 2,6,10,15-tetramethyl-
Heptadecane, 2-methyl-
Heptadecanenitrile
Heptadecanoic acid, glycerine-(1)-monoester, bis-O-trimethylsilyl-
Heptadecanoic acid, TMS derivative
Heptamethyl-3-phenyl-1,4-cyclohexadiene
Heptanamide, 4-ethyl-5-methyl-
Heptane, 2,2,4,6,6-pentamethyl-
Heptane, 2,5,5-trimethyl-
Heptane, 3,3,5-trimethyl-
Heptanoic acid, TMS derivative
Hexacosane
Hexacosanoic acid, TMS derivative
Hexadecanamide
Hexadecane
Hexadecane, 2,6,10,14-tetramethyl-
Hexadecane, 2,6,11,15-tetramethyl-
Hexadecane, 2-methyl-
Hexadecane, 7-methyl-
Hexadecane-1,2-diol
Hexadecanenitrile
Hexadecanoic acid, butyl ester
Hexadecanoic acid, methyl ester
Hexan-3-ol, trimethylsilyl ether
Hexane, 4-ethyl-2-methyl-
Hexanedioic acid, 2TMS derivative
Hexanedioic acid, bis(2-ethylhexyl) ester
Hexanedioic acid, dioctyl ester
Hexanoic acid, TMS derivative
Hexatriacontane
Hexopyranose, 5TMS derivative
Hexyl octyl ether
Hydroquinone, TMS derivative
Hydroxylamine, methyl-(1-phenylethyl)-
Hydroxylamine, O-(3-methylbutyl)-
Hydroxylamine, O-pentyl-
Indane
Indeno[2',1':4,5]thieno[3,2-b]thiopyran
Inosose-2, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, myo-
Isobutanol, TMS derivative
Isobutyl triacontyl ether
Isopropyl alcohol, TMS derivative
Isopropyl palmitate
Isopropylamine, N-tert-butyldimethylsilyl-
Isoquinoline, 1,2,3,4-tetrahydro-6,7-dimethoxy-
Isoquinoline, 3,4-dihydro-6,7-dimethoxy-1-[3-methoxyphenyl]-
L-(-)-Arabitol, 5TMS derivative
L-(-)-Sorbofuranose, pentakis(trimethylsilyl) ether
L-(+)-Rhamnopyranose, 4TMS derivative
L-5-Oxoproline, , 2TMS derivative
Labda-8(20),14-dien-13-ol, (13S)-, O-TMS
Lactic acid dimer, bis(trimethylsilyl)-

Lactic Acid, 2TMS derivative
L-Alanine ethylamide, (S)-
L-Alanine, 2TMS derivative
L-Aspartic acid, diethyl ester
Levoglucosan, 3TMS derivative
Levulinic acid, TMS derivative
L-Homophenylalanine, N-(n-pentyl)-, pentyl ester
Lignoceric acid, TMS derivative
Linoleyl acetate
Linolool oxide, (Z)-, TMS derivative
L-Norleucine, N-ethoxycarbonyl-, decyl ester
L-Norleucine, N-methoxycarbonyl-, isohexyl ester
L-Norleucine, N-methoxycarbonyl-, octyl ester
L-Norleucine, N-methoxycarbonyl-, pentyl ester
L-Norvaline, N-ethoxycarbonyl-, isohexyl ester
L-Norvaline, N-ethoxycarbonyl-, nonyl ester
L-Norvaline, N-methoxycarbonyl-, heptyl ester
L-Norvaline, N-methoxycarbonyl-, nonyl ester
L-Norvaline, N-methoxycarbonyl-, octyl ester
L-Norvaline, N-methoxycarbonyl-, pentyl ester
L-Norvaline, N-methoxycarbonyl-, tetradecyl ester
L-Norvaline, n-propargyloxycarbonyl-, heptyl ester
L-Norvaline, n-propargyloxycarbonyl-, propargyl ester
L-Norvaline, n-propoxycarbonyl-, undecyl ester
L-Norvaline, trimethylsilyl ester
L-Phenylalanine, 2TMS derivative
L-Rhamnose, 4TMS derivative
L-Sorbopyranose, (1S,2R,3S)-, 5TMS derivative
L-Threitol, 4TMS derivative
L-Threonine, 3TMS derivative
L-Val-L-Leu, N-trimethylsilyl-, trimethylsilyl ester
Malic acid, 3TMS derivative
Malonic acid, bis(2-trimethylsilylethyl) ester
m-Aminophenylacetylene
Mercaptoethanol, 2TMS derivative
Mesitylene
meso-Erythritol, 4TMS derivative
Metanephine, 3TMS derivative
Methamphetamine, N-TMS
Methiopropamine, N-trimethylsilyl-
Methyl (2R,3R,4S)-2,4-dimethyl-3-hydroxyhexanoate
Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative
Methyl 4-methoxysalicylate, TMS derivative
Methyl 9-cis,11-trans-octadecadienoate
Methyl galactoside, 4TMS derivative
Methyl pentopyranoside, 3TMS derivative
Methyl stearate
Methyl vinyl ketone
Methyl Z-11-tetradecenoate
Monolaurin, 2TMS derivative
m-Toluic acid, TMS derivative
Myristic acid, TMS derivative
Naphthalene
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-
Naphthalene, 1-methyl-
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-
n-Hexadecanoic acid

n-Nonadecanol-1
Nonacosan-10-ol, O-TMS
Nonadecanenitrile
Nonadecanoic acid, TMS derivative
Nonane, 2,6-dimethyl-
Nonane, 5-methyl-5-propyl-
Nonanoic acid, TMS derivative
n-Propyl 9,12-octadecadienoate
N-Trimethylsilylstearamide
Octacosane
Octadecanamide
Octadecanamide, N-(2-methylpropyl)-N-nitroso-
Octadecane
Octadecane, 2-methyl-
Octadecanenitrile
Octadecanoic acid, 2-methylpropyl ester
Octadecanoic acid, 2-oxo-, methyl ester
Octadecanoic acid, ethenyl ester
Octadecanoic acid, phenylmethyl ester
Octaethylene glycol, 2TMS derivative
Octan-2-yl palmitate
Octane, 2,3,6,7-tetramethyl-
Octane, 2,3,7-trimethyl-
Octane, 3,3-dimethyl-
Octane, 3,5-dimethyl-
Octane, 6-ethyl-2-methyl-
Octanoic acid, TMS derivative
Octopamine, 4TMS derivative
Oleamide, TMS derivative
Oleic Acid
Oleic Acid, (Z)-, TMS derivative
Oleic acid, butyl ester
Orthoformic acid, triisobutyl ester
Oxalic acid, 2TMS derivative
Oxalic acid, heptyl propyl ester
Oxime-, methoxy-phenyl-
Palmitelaidic acid, TMS derivative
Palmitic Acid, TMS derivative
Palmitoleamide
Palmitoleonitrile
p-Anisic acid, tridec-2-ynyl ester
Pentacosane
Pentacosanoic acid, trimethylsilyl ester
Pentadecane
Pentadecane, 2,6,10,14-tetramethyl-
Pentadecane, 2,6,10-trimethyl-
Pentadecanoic acid, 14-methyl-, methyl ester
Pentadecanoic acid, glycerine-(1)-monoester, bis-O-trimethylsilyl-
Pentadecanoic acid, TMS derivative
Pentanamide
Pentanoic acid, 2,4-dimethyl-3-oxo-, methyl ester
Pentanoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester
Pentanoic acid, 3-methyl-2-oxo-, methyl ester
Pentanoic acid, 4-oxo-, pentyl ester
Pentyl linoleate
Phenanthrene, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, (4aS-trans)-
Phenethylamine, ?-methyl-N-propyl-
Phenol, 2,4-bis(1-methylethyl)-, acetate

Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate
Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-
Phenol, TMS derivative
phenoxyethanol, TMS derivative
p-Hydroxydiisopropylbenzene, TMS derivative
Pipelic acid, 2TMS derivative
Pipelic acid, N-ethoxycarbonyl-, dodecyl ester
Pipelic acid, N-octyloxycarbonyl-, undecyl ester
Propanal, 2-methyl-
Propanamide, N-(1-naphthyl)-2-methyl-
Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-
Propanetriol, 2-methyl-, tris-O-(trimethylsilyl)-
Propanoic acid, 2-methyl-, hexyl ester
Propylene glycol, 2TMS derivative
Propylparaben, TMS derivative
Pyrogallol, 3TMS derivative
Pyroglutamic acid, TMS derivative
Pyrrole-2-carboxylic acid, 2TMS derivative
Pyruvic acid, butyl ester
Pyruvic acid, TMS derivative
Quinoline, 1,2-dihydro-2,2,4-trimethyl-
Resorcinol, TMS derivative
Ribitol, 5TMS derivative
Ribonic acid, 2,3,4,5-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester
Salsoline
Serine, 3TMS derivative
s-Indacen-1(2H)-one, 3,5,6,7-tetrahydro-3,3,4,5,8-hexamethyl-
Squalene
Stearic acid, TMS derivative
Sulfurous acid, isobutyl pentyl ester
Supraene
Synephrine, N,O,O'-tris-trimethylsilyl
Talose, 5TMS derivative
Tetracosanol, O-TMS
Tetracyano-p-quinodimethane
Tetradecane
Tetradecanenitrile
Tetradecanoic acid, 10,13-dimethyl-, methyl ester
Tetradecanoic acid, 2-oxo-, ethyl ester
Tetradecanoic acid, dimethyl(isopropyl)silyl ester
Tetrahydrogeranyl formate
Thiourea, tetramethyl-
Tolycaine
trans,trans-9,12-Octadecadienoic acid, propyl ester
trans-13-Octadecenoic acid
trans-9-Octadecenoic acid, pentyl ester
Tri(1,2-propyleneglycol), monomethyl ether
Tributyl acetylcitrate
Tridecane
Tridecane, 3-methylene-
Tridecane, 4-methyl-
Tridecanoic acid, TMS derivative
Triethanolamine, 3TMS derivative
Triethylene glycol, 2TMS derivative
Trimethylolpropane, 3TMS derivative
Trimethylsilyl tricosanoate
Trimethylsilylserine
Triphenylphosphine oxide

Tris(trimethylsilyl)carbamate
Trisaminol, 3-OTMS
Tromethamine, 4TMS derivative
Undecane, 2,5-dimethyl-
Undecane, 2,6-dimethyl-
Undecane, 3,9-dimethyl-
Undecane, 3-methyl-
Undecane, 4-methyl-
Undecane, 5-methyl-
Undecanoic acid, 11-amino-
Uracil, 2TMS derivative
Urazole
Urea, 2TMS derivative
Valine, N-methyl-N-ethoxycarbonyl-, isohexyl ester
Xylitol, 5TMS derivative
Xylose, 4TMS derivative
Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate

Table S2: Molecules with different abundances between apple groups

	FC	raw.pval
1,2,3-Butanetriol, 3TMS derivative	43.391	0.001848
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	3.1702	0.016918
1,2-Benzenediol, O-4-methoxybenzoyl -O'-2-furoyl-	2.7326	0.003042
1,2-Cyclohexanedicarboxylic acid, heptadecyl 2-methylcyclohexyl ester	2.2178	0.019562
1-Butoxy-2-propanol, TMS derivative	2.5963	0.008612
1-Chloroundecane	3.1714	0.00242
1-Ethoxycarbonylmethylpyridinium bromide	1.7768	0.000777
1H-Pyrazolo[3,4-d]pyrimidin-4-amine	0.57424	0.013792
1H-Quinolin-2-one, 5,8-dimethoxy-1,4-dimethyl-	0.55028	0.033273
1-Methyl-5-mercaptotetrazole	0.50372	0.047957
1-Octacosanol, 2,4,6,8-tetramethyl-, all-R-	0.53936	0.002067
1-Tetradecene	2.3593	0.018466
1-Undecanol, TMS derivative	1.6669	0.029171
2,4,6-Tris(1,1-dimethylethyl-4-methylcyclohexa-2,5-dien-1-one	2.582	0.035173
2,4-Dichlorobenzoic acid, TMS derivative	9.7553	4.44E-06
2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	0.65213	0.005792
2,5-Dimethoxyphenylacetone	2.9865	0.027463
2,6,8-Trimethyl-4-nonyl acetate	1.6622	0.004345
2,6-Dimethyldecane	2.1435	0.026926
2,6-di-tert-Butyl-4-dimethylaminomethylphenol	1.7458	0.009767
2-Acetoxyindane	0.47058	0.014991
2-Amino-2-deoxyhexose, 5TMS derivative	0.32526	0.006777
2-Benzothiazolamine, N-ethyl-	0.63035	0.01005
2-Butylamine, N-tetradecyl-	2.6107	1.76E-06
2-Ethoxyethanol, TMS derivative	3.2334	0.046455
2-Propanol, 1-2-2-methoxy-1-methylethoxy-1-methylethoxy-	7.2175	0.013011
2-Propanol, 2-methyl-	2.1136	0.02089
3,4-Dimethoxymandelic acid, di-TMS	0.41598	0.000826
3,5-Diacetyl-4-methyl-1-phenyl-1,4-dihydropyridine	0.61988	0.004208
3,5-Dimethoxymandelic acid, di-TMS	0.55152	0.04622
3,5-Dimethoxymandelic amide, di-TMS	3.0032	0.008269
3-Chlorobenzoic acid, TMS derivative	7.528	4.79E-05
3-Ethyl-2-methyl-2-heptanol	2.4836	0.025418
3-Ethyl-3-methylheptane	1.8323	0.002771

3H-1,2,4-Triazole-3-thione, 5-amino-1,2-dihydro-	0.47736	0.016553
3-Methoxy-benzoic acid 3,4-dimethyl-phenyl ester	2.2539	0.017459
3-Methyl-2-butanol, TMS derivative	1.6862	0.024834
4,4-Dimethyl-5-methylene-4,5-dihydro-3H-pyrrol-2-yl-4,4-dimethyl-5-methylene-pyrrolidin-2-ylidene-acetonitrile	0.61988	0.004208
4-Chlorobenzoic acid, TMS derivative	7.5359	4.77E-05
4-Decene, 7-methyl-, E-	1.7794	0.008838
4-Methoxybenzoic acid, 4-isopropylphenyl ester	1.8093	0.012482
5,2,1,6,3,4-2,3Butanediyl1,4diylidenedipentaleno2,1,6-cde2',1',6'-ghapentalene, hexadecahydro-	0.44444	0.002067
5-Phenylvaleric acid, tert-butyldimethylsilyl ester	3.347	0.00341
6-Methoxy-3-methylbenzofuran	14.175	0.000413
9,12-Octadecadienoic acid Z,Z-, methyl ester	3.0499	0.000197
9E,11E-Conjugated linoleic acid, trimethylsilyl ester	1.669	0.001769
9-Octadecenoic acid, E-, TMS derivative	1.6862	0.024834
Alanylalanine, N,N'-dimethyl-N'-methoxycarbonyl-, hexyl ester	0.48236	0.017379
alpha-Farnesene	4.6891	0.000584
Anthra1,9-cdpyrazol-62H-one	6.8279	0.020787
Anthranilic acid, TMS derivative	5.0707	0.000411
Benzaldehyde, 2,5-dimethoxy-	0.4192	0.000115
Benzaldehyde, 2-hydroxy-5-nitro-, 2-iodophenylhydrazone	1.8687	0.003163
Benzenamine, 4-6-methyl-2-benzothiazolyl-	3.8256	1.34E-08
Benzene, 1,1'-1-ethenyl-1,3-propanediylbis-	0.54504	0.01181
Benzene, 1-pentylheptyl-	2.1272	0.005165
Benzeneacetic acid, TMS derivative	5.3755	0.007656
Benzothiazole, 2-o-aminophenyl-4-methyl-	2.2101	6.35E-05
Boric acid, 3TMS derivative	0.29856	0.00099
Butanal, oxime	2.3494	0.007812
Chrysophanol, 2TMS derivative	1.7043	0.006695
Cyclopentane, 1,1'-hexadecylidenebis-	0.4522	0.005536
Cyclopropane, 1-1-hydroxy-1-heptyl-2-methylene-3-pentyl-	0.23274	7.72E-05
Dinaphtho1,2-b2',1'-dthiophene	2.3156	0.018455
Docosanol, TBDMS derivative	1.9921	0.024672
Dodecane, 4,6-dimethyl-	1.5406	0.007414
D-Xylopyranose, 4TMS derivative	1.9769	0.044205
Eicosane	2.3172	0.037552
Ethanimidic acid, N-trimethylsilyl-, trimethylsilyl ester	0.38458	0.047868
Formamide, N-methyl-	2.4858	0.024985
Glycerol monostearate, 2TMS derivative	5.0057	0.010721
Glycine, N-methyl-N-ethoxycarbonyl-, nonyl ester	0.48215	0.021337
Heneicosane, 3-methyl-	7.2758	0.000941
Heptane, 2,2,4,6,6-pentamethyl-	2.1414	0.014204
Hexadecanamide	3.1738	0.002398
Indeno2',1'4,5thieno3,2-bthiopyran	3.6723	1.51E-05
Inosose-2, 1,3,4,5,6-pentakis-O-trimethylsilyl-, myo-	0.51892	0.039516
Isopropylamine, N-tert-butyldimethylsilyl-	0.47798	0.01671
Labda-820,14-dien-13-ol, 13S-, O-TMS	1.8424	0.006407
l-Norleucine, N-ethoxycarbonyl-, decyl ester	0.60649	0.042664
Methyl 3,4-dimethoxyphenylhydroxyacetate, TMS derivative	1.9183	0.044643
Methyl 9-cis,11-trans-octadecadienoate	2.2668	0.002531
Naphthalene, 1-methyl-	3.718	0.011475
n-Nonadecanol-1	1.5084	0.011911
Nonane, 2,6-dimethyl-	1.8323	0.002771
Octadecanamide, N-2-methylpropyl-N-nitroso-	0.32678	0.005701
Octane, 2,3,7-trimethyl-	1.9888	0.000603
Oleic Acid, Z-, TMS derivative	1.5842	0.020916
Oxalic acid, heptyl propyl ester	0.66044	0.016778
Phenol, 2,4-bis1-methylethyl-, acetate	2.663	0.000517
pm-4-Fluoroephedrine, N-trimethylsilyl-, trimethylsilyl ether	0.53528	0.034911

pm-p-Methoxyamphetamine, N-trimethylsilyl-	0.61052	0.02702
Propylene glycol, 2TMS derivative	3.0575	0.026156
Propylparaben, TMS derivative	3.3474	0.010665
Pyrrole-2-carboxylic acid, 2TMS derivative	0.65725	0.04564
R-9-S-2-Hydroxymethylpyrrolidin-1-yl-3-methyl-3,4-dihydro-2H-benzob1,4,5oxathiazepine 1,1-dioxide	4.7391	0.005459
R---Phenylephrine, N-trimethylsilyl-, bistrimethylsilyl ether	0.45322	0.011866
Serine, 3TMS derivative	0.43595	0.041998
Stearic acid hydrazide	3.1148	0.02159
Sulfurous acid, isobutyl pentyl ester	0.56612	0.008681
trans-13-Octadecenoic acid	0.34168	0.043301
Tridecane, 4-methyl-	1.6391	0.00429
Trimethylsilylserine	0.43595	0.041998