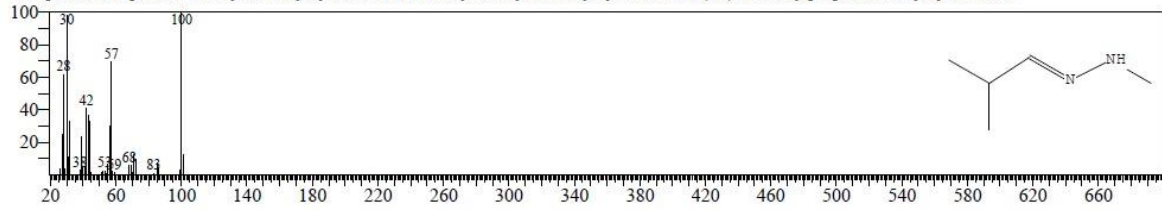
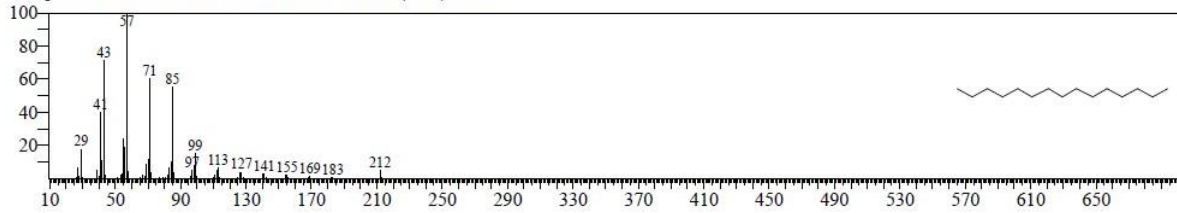


SUPPLEMENTARY MATERIAL

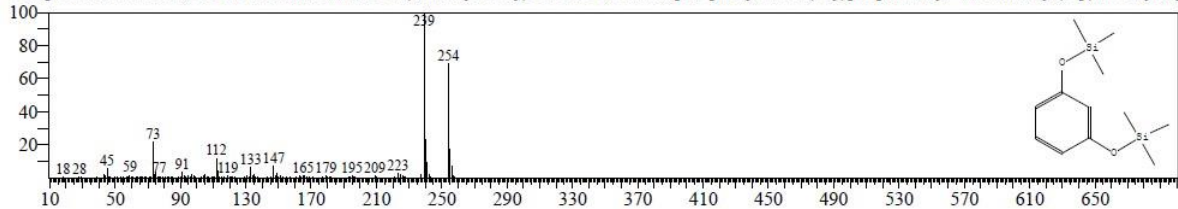
Hit#:1 Entry:2132 Library:NIST17R.lib
 SI:81 Formula:C5H12N2 CAS:16713-37-4 MolWeight:100 RetIndex:868
 CompName:Propanal, 2-methyl-, methylhydrazone \$\$ Isobutyraldehyde methylhydrazone \$\$ (1E)-2-Methylpropanal methylhydrazone #



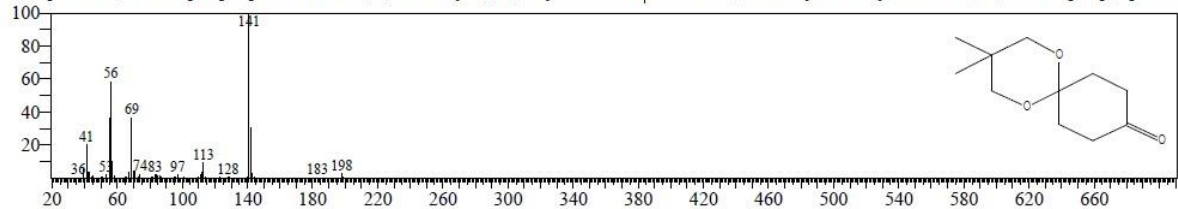
Hit#:1 Entry:23844 Library:NIST17R.lib
 SI:76 Formula:C15H32 CAS:629-62-9 MolWeight:212 RetIndex:1512
 CompName:Pentadecane \$\$ n-Pentadecane \$\$ CH3(CH2)13CH3



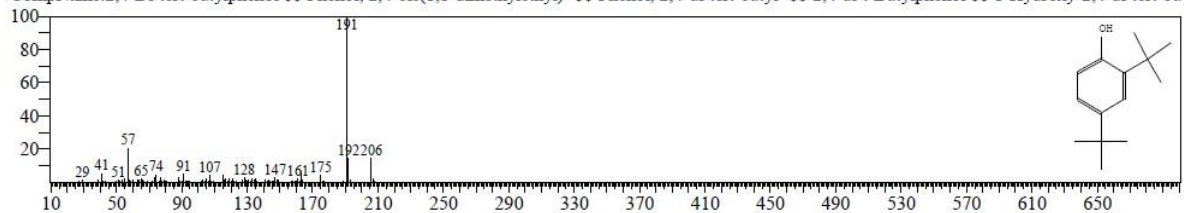
Hit#:1 Entry:29052 Library:NIST17R.lib
 SI:55 Formula:C12H22O2Si2 CAS:4520-29-0 MolWeight:254 RetIndex:1276
 CompName:Resorcinol, 2TMS derivative \$\$ 1,3-Bis(trimethylsiloxy)benzene \$\$ Silane, [1,3-phenylenebis(oxy)]bis(trimethyl-



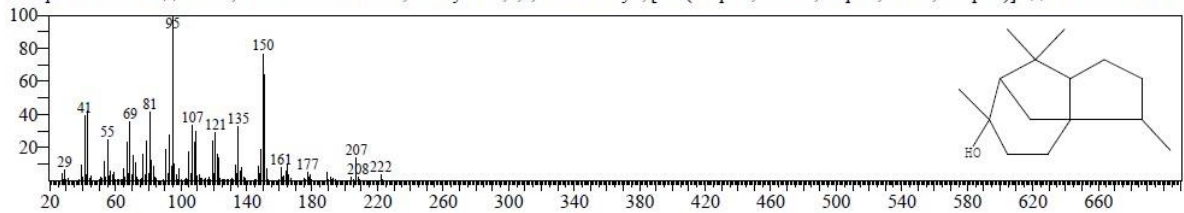
Hit#:1 Entry:21165 Library:NIST17R.lib
 SI:72 Formula:C11H18O3 CAS:69225-59-8 MolWeight:198 RetIndex:1517
 CompName:1,5-Dioxaspiro[5.5]undecan-9-one, 3,3-dimethyl- \$\$ 1,4-Cyclohexanedione mono-2,2-dimethyl-trimethylene ketal \$\$ 1,5-Dioxaspiro[5.5]undec-



Hit#:1 Entry:22785 Library:NIST17R.lib
 SI:97 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
 CompName:2,4-Di-tert-butylphenol \$\$ Phenol, 2,4-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,4-di-tert-butyl- \$\$ 2,4-di-tert-butylphenol \$\$ 1-Hydroxy-2,4-di-tert-butyl-

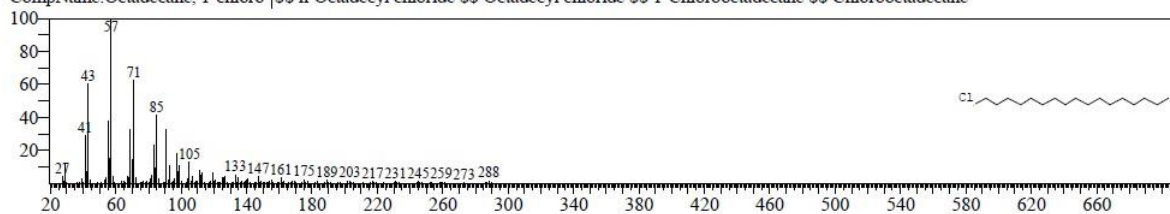


Hit#:1 Entry:25364 Library:NIST17R.lib
 SI:58 Formula:C15H26O CAS:77-53-2 MolWeight:222 RetIndex:1543
 CompName:Cedrol \$\$ 1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,6.alpha.,7.beta.,8a.alpha.)]- \$\$ 8.beta.H-Cedran-

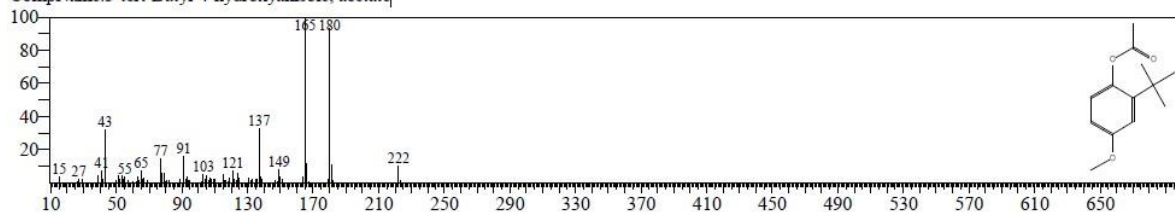


SUPPLEMENTARY MATERIAL

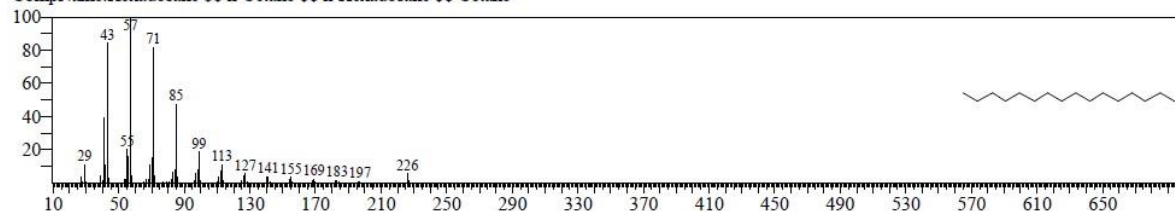
Hit#:1 Entry:32089 Library:NIST17R.lib
 SI:70 Formula:C18H37Cl CAS:3386-33-2 MolWeight:288 RetIndex:2036
 CompName:Octadecane, 1-chloro-|\$\$ n-Octadecyl chloride \$\$ Octadecyl chloride \$\$ 1-Chlorooctadecane \$\$ Chlorooctadecane



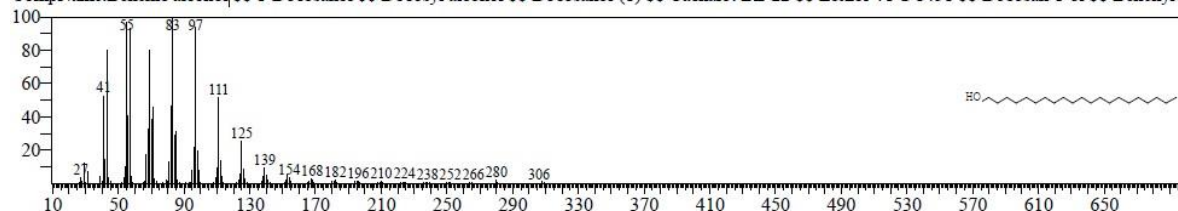
Hit#:1 Entry:25256 Library:NIST17R.lib
 SI:67 Formula:C13H18O3 CAS:91401-26-2 MolWeight:222 RetIndex:1576
 CompName:3-tert-Butyl-4-hydroxyanisole, acetate|



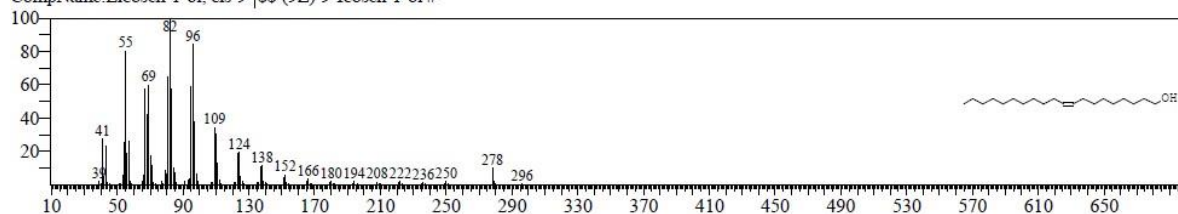
Hit#:1 Entry:25988 Library:NIST17R.lib
 SI:82 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1612
 CompName:Hexadecane \$\$ n-Cetane \$\$ n-Hexadecane \$\$ Cetane



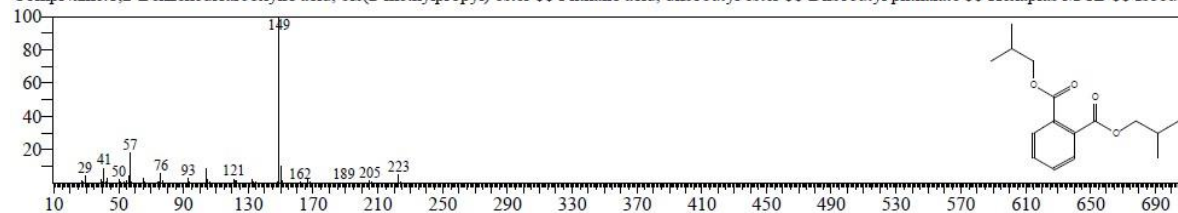
Hit#:1 Entry:34738 Library:NIST17R.lib
 SI:92 Formula:C22H46O CAS:661-19-8 MolWeight:326 RetIndex:2451
 CompName:Behenic alcohol|\$\$ 1-Docosanol \$\$ Docosyl alcohol \$\$ Docosanol-(1) \$\$ Cachalot BE-22 \$\$ Loxiol VPG 1451 \$\$ Docosan-1-ol \$\$ Behenyl a



Hit#:1 Entry:32767 Library:NIST17R.lib
 SI:86 Formula:C20H40O CAS:112248-30-3 MolWeight:296 RetIndex:2260
 CompName:Eicosen-1-ol, cis-9-|\$\$ (9Z)-9-Icosen-1-ol #



Hit#:1 Entry:31274 Library:NIST17R.lib
 SI:92 Formula:C16H22O4 CAS:84-69-5 MolWeight:278 RetIndex:1908
 CompName:1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester \$\$ Phthalic acid, diisobutyl ester \$\$ Diisobutyl phthalate \$\$ Hexaplas M/1B \$\$ Isobuty

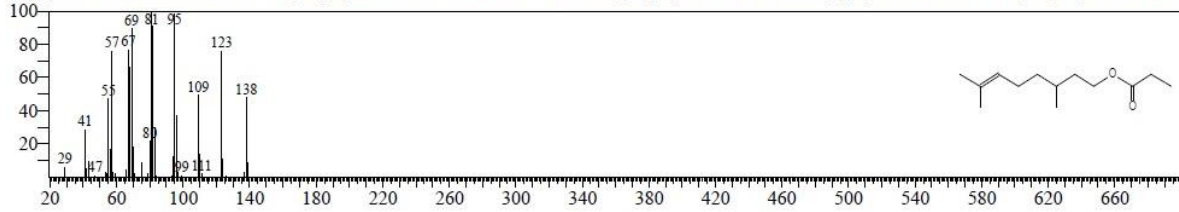


SUPPLEMENTARY MATERIAL

Hit#:1 Entry:23758 Library:NIST17R.lib

SI:79 Formula:C13H24O2 CAS:141-14-0 MolWeight:212 RetIndex:1402

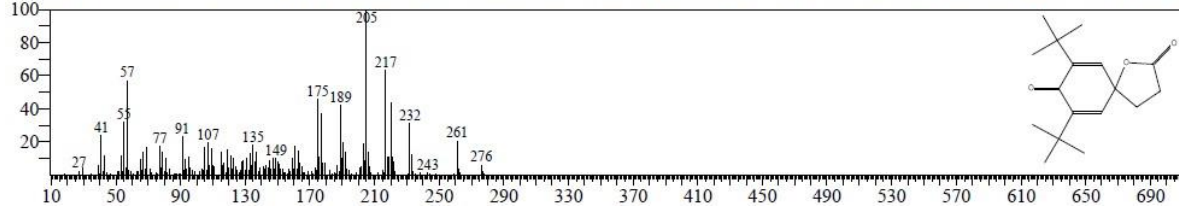
CompName:6-Octen-1-ol, 3,7-dimethyl-, propanoate \$\$ 6-Octen-1-ol, 3,7-dimethyl-, propionate \$\$ Citronellyl propanoate \$\$ Citronellyl n-propionate \$\$ 3,



Hit#:1 Entry:31118 Library:NIST17R.lib

SI:87 Formula:C17H24O3 CAS:82304-66-3 MolWeight:276 RetIndex:2081

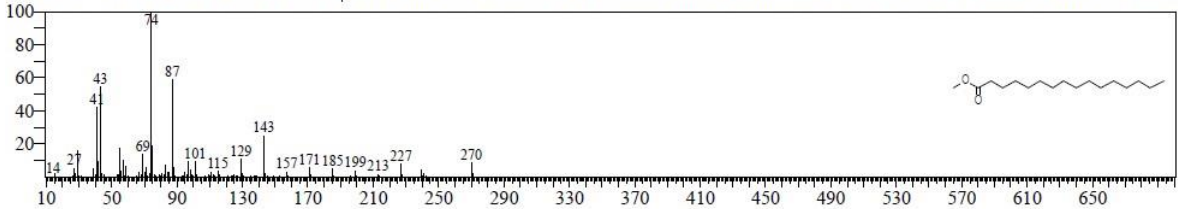
CompName:7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione \$\$ 1-Oxa-spiro[4.5]deca-6,9-diene-2,8-dione, 7,9-di-tert-butyl- \$\$ 7,9-Di-tert-butyl-1



Hit#:1 Entry:30645 Library:NIST17R.lib

SI:90 Formula:C17H34O2 CAS:112-39-0 MolWeight:270 RetIndex:1878

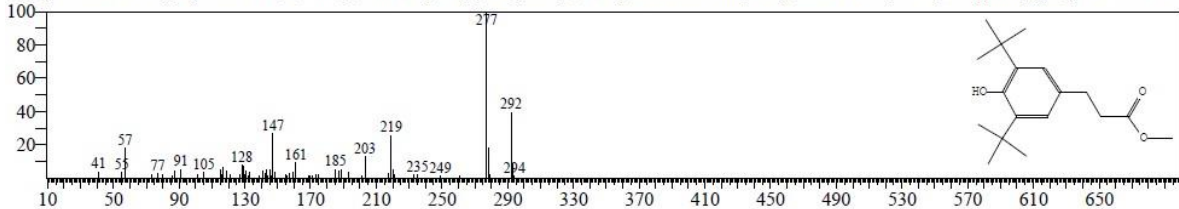
CompName:Hexadecanoic acid, methyl ester \$\$ Palmitic acid, methyl ester \$\$ n-Hexadecanoic acid methyl ester \$\$ Metholene 2216 \$\$ Methyl hexadecanoic



Hit#:1 Entry:32424 Library:NIST17R.lib

SI:92 Formula:C18H28O3 CAS:6386-38-5 MolWeight:292 RetIndex:2134

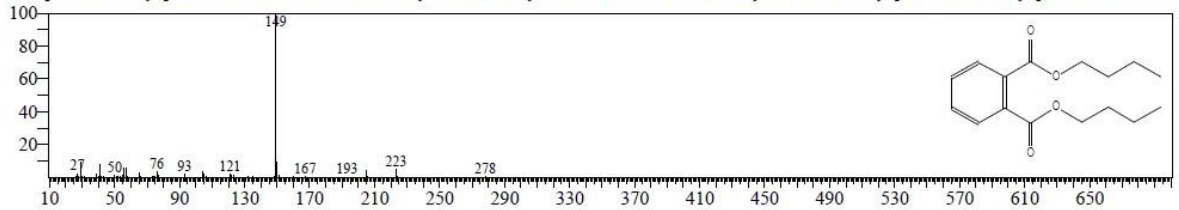
CompName:Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester \$\$ Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoate \$\$ Meti



Hit#:1 Entry:31277 Library:NIST17R.lib

SI:95 Formula:C16H22O4 CAS:84-74-2 MolWeight:278 RetIndex:2037

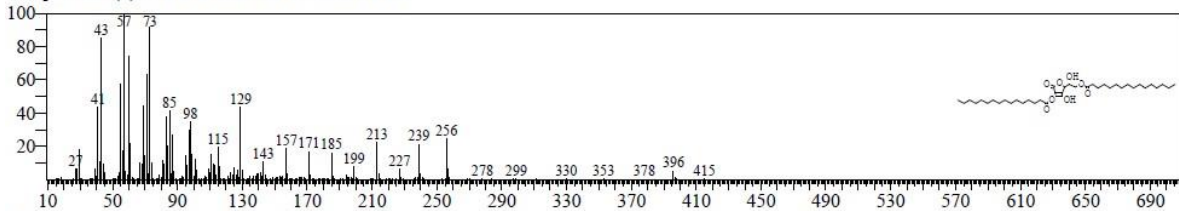
CompName:Dibutyl phthalate \$\$ 1,2-Benzenedicarboxylic acid, dibutyl ester \$\$ Phthalic acid, dibutyl ester \$\$ n-Butyl phthalate \$\$ Butyl phthalate \$\$ Cellu



Hit#:1 Entry:3516 Library:NIST17M2.lib

SI:78 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765

CompName:1-(+)-Ascorbic acid 2,6-dihexadecanoate

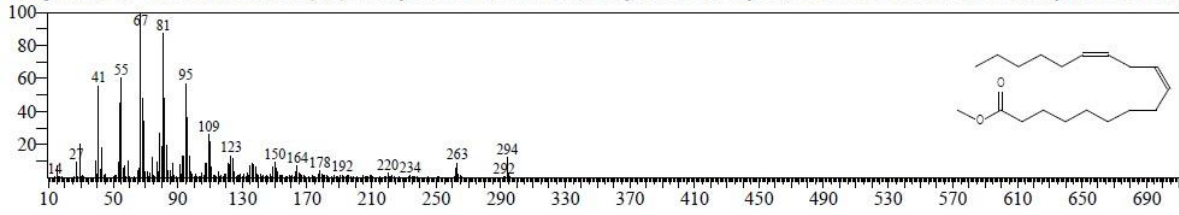


SUPPLEMENTARY MATERIAL

Hit#:1 Entry:32589 Library:NIST17R.lib

SI:85 Formula:C19H34O2 CAS:112-63-0 MolWeight:294 RetIndex:2093

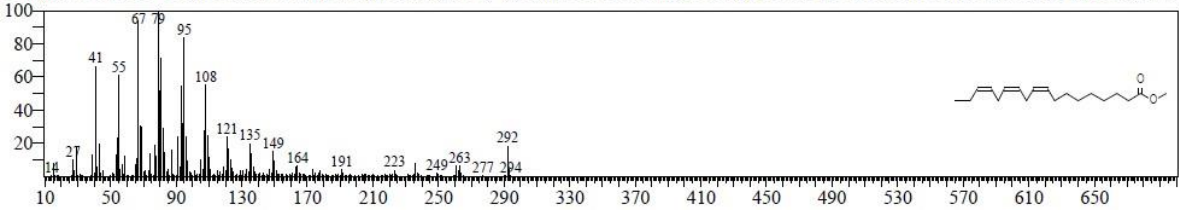
CompName:9,12-Octadecadienoic acid (Z,Z)-, methyl ester \$\$ Linoleic acid, methyl ester \$\$ Methyl cis,cis-9,12-octadecadienoate \$\$ Methyl linoleate \$\$ M



Hit#:1 Entry:32440 Library:NIST17R.lib

SI:83 Formula:C19H32O2 CAS:301-00-8 MolWeight:292 RetIndex:2101

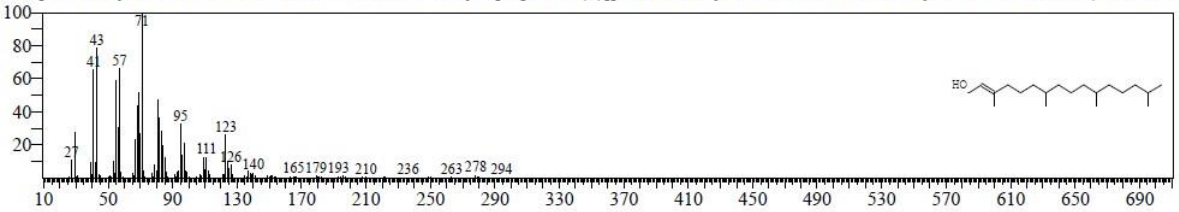
CompName:9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- \$\$ Linolenic acid, methyl ester \$\$ Methyl all-cis-9,12,15-octadecatrienoate \$\$ Methyl lino



Hit#:1 Entry:32763 Library:NIST17R.lib

SI:89 Formula:C20H40O CAS:150-86-7 MolWeight:296 RetIndex:2045

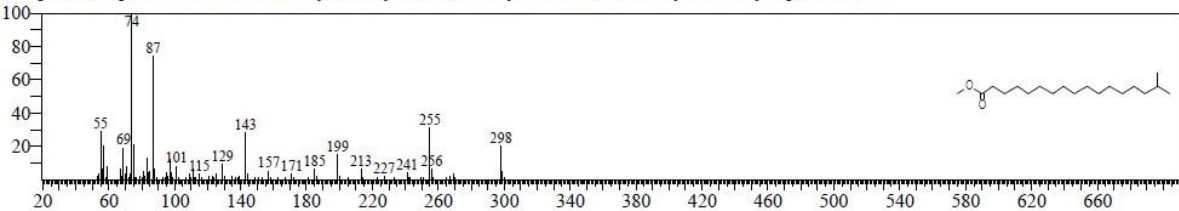
CompName:Phytol \$\$ 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*(E)]]- \$\$ trans-Phytol \$\$ 3,7,11,15-Tetramethyl-2-hexadecen-1-ol-, (2E,7R,11R



Hit#:1 Entry:32877 Library:NIST17R.lib

SI:82 Formula:C19H38O2 CAS:5129-61-3 MolWeight:298 RetIndex:2013

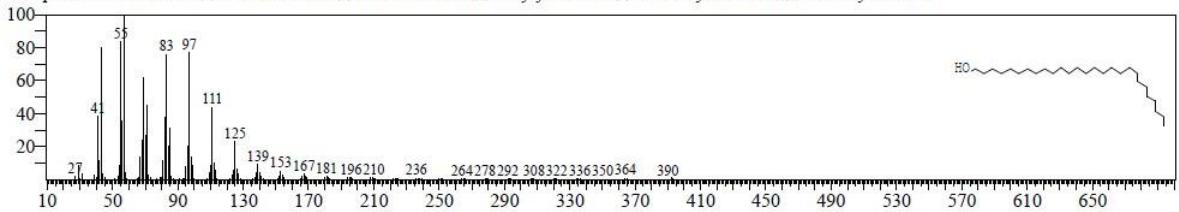
CompName:Heptadecanoic acid, 16-methyl-, methyl ester \$\$ Methyl isostearate \$\$ Methyl 16-methylheptadecanoate



Hit#:1 Entry:37818 Library:NIST17R.lib

SI:82 Formula:C28H58O CAS:557-61-9 MolWeight:410 RetIndex:3047

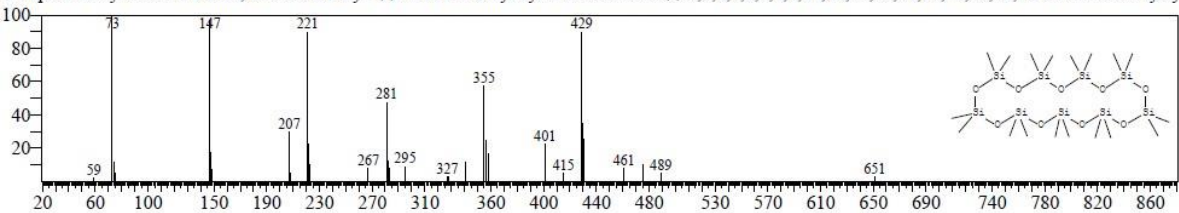
CompName:Octacosanol \$\$ 1-Octacosanol \$\$ n-Octacosanol \$\$ Cluytyl alcohol \$\$ Montanyl alcohol \$\$ Octacosyl alcohol



Hit#:1 Entry:39158 Library:NIST17R.lib

SI:61 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860

CompName:Cyclononasiloxane, octadecamethyl- \$\$ Octadecamethyl-cyclononasiloxane \$\$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

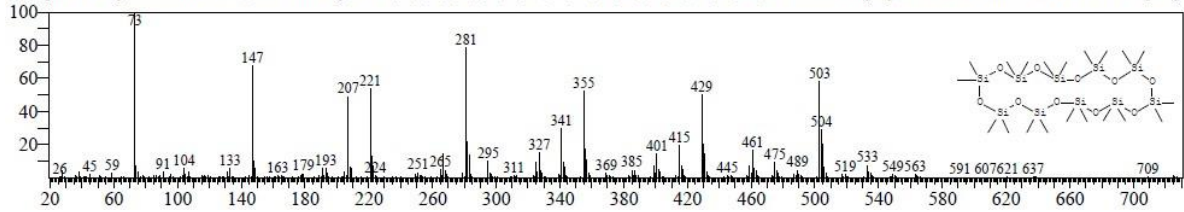


SUPPLEMENTARY MATERIAL

Hit#:1 Entry:4634 Library:NIST17M2.lib

SI:47 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067

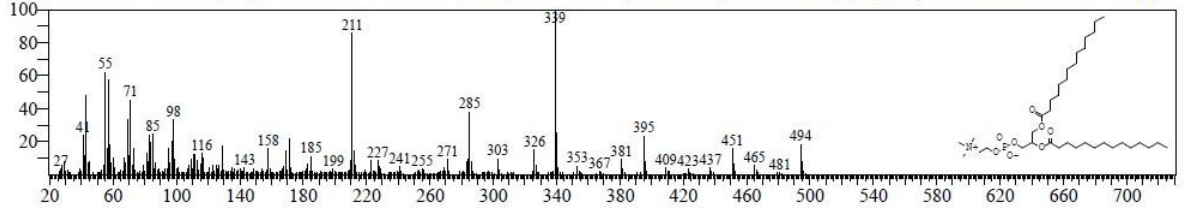
CompName:Cyclodecasiloxane, eicosamethyl- \$\$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # \$\$ Eicosamethyl-cy



Hit#:1 Entry:3933 Library:NIST17M2.lib

SI:51 Formula:C36H72NO8P CAS:18194-24-6 MolWeight:677 RetIndex:0

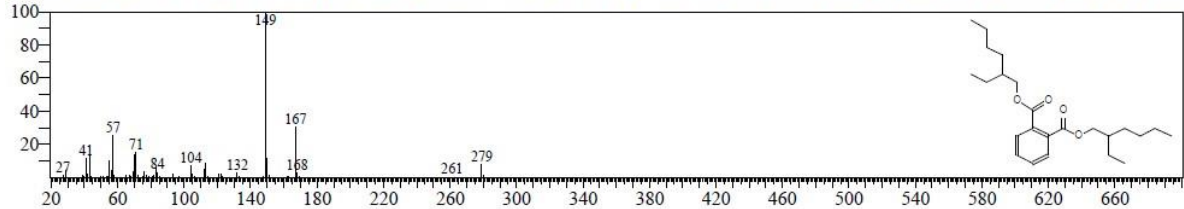
CompName:3,5,9-Trioxa-4-phosphatricosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-7-[(1-oxotetradecyl)oxy]-, hydroxide, inner salt, 4-oxide, (R)- \$



Hit#:1 Entry:37380 Library:NIST17R.lib

SI:73 Formula:C24H38O4 CAS:117-81-7 MolWeight:390 RetIndex:2704

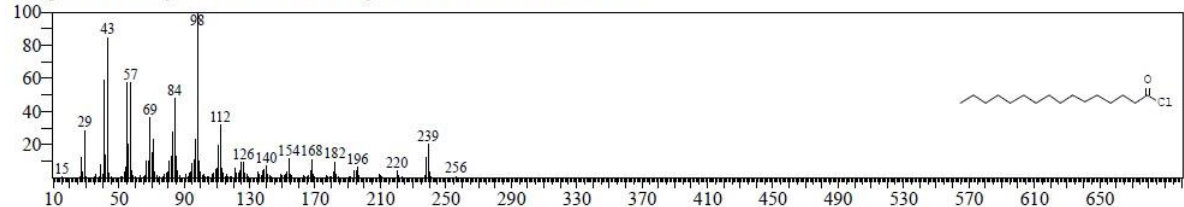
CompName:Bis(2-ethylhexyl) phthalate \$\$ Phthalic acid, bis(2-ethylhexyl) ester \$\$ Bis(2-ethylhexyl) 1,2-benzenedicarboxylate \$\$ Bisoflex 81 \$\$ Compou



Hit#:1 Entry:30936 Library:NIST17R.lib

SI:62 Formula:C16H31ClO CAS:112-67-4 MolWeight:274 RetIndex:1924

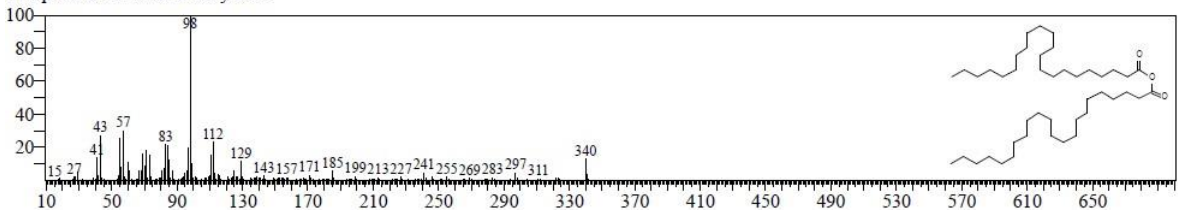
CompName:Palmitoyl chloride \$\$ Hexadecanoyl-chloride- \$\$ Palmitic acid chloride



Hit#:1 Entry:3711 Library:NIST17M2.lib

SI:64 Formula:C44H86O3 CAS:55726-23-3 MolWeight:662 RetIndex:4698

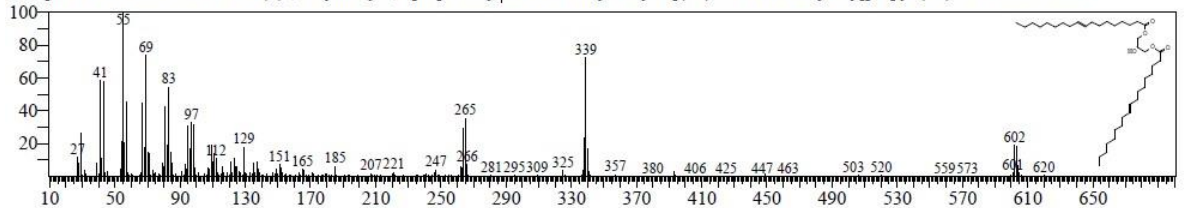
CompName:Docosanoic anhydride



Hit#:5 Entry:2775 Library:NIST17M2.lib

SI:54 Formula:C39H72O5 CAS:2465-32-9 MolWeight:620 RetIndex:4411

CompName:9-Octadecenoic acid (Z)-, 2-hydroxy-1,3-propanediyl]ester \$\$ 2-Hydroxy-3-[(9E)-9-octadecenoyloxy]propyl (9E)-9-octadecenoate #

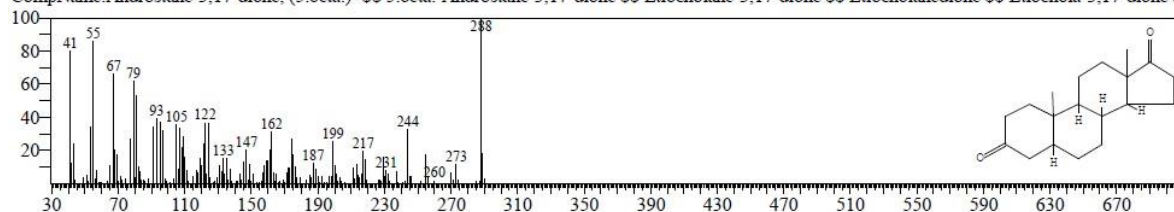


SUPPLEMENTARY MATERIAL

Hit#:1 Entry:32107 Library:NIST17R.lib

SI:34 Formula:C19H28O2 CAS:1229-12-5 MolWeight:288 RetIndex:2112

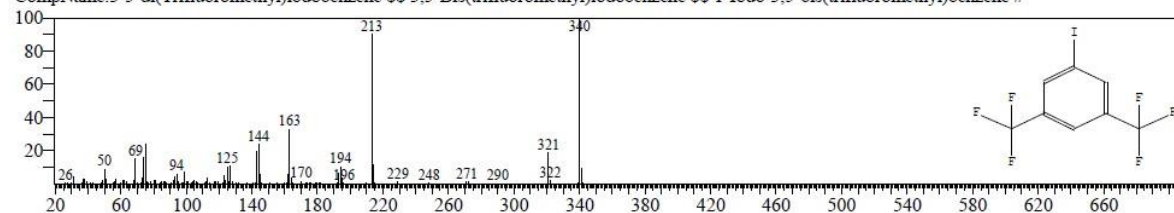
CompName:Androstane-3,17-dione, (5.beta.)- \$\$ 5.beta.-Androstane-3,17-dione \$\$ Etiocholane-3,17-dione \$\$ Etiocholanedione \$\$ Etiochola-3,17-dione \$



Hit#:1 Entry:35459 Library:NIST17R.lib

SI:31 Formula:C8H3F6I CAS:328-73-4 MolWeight:340 RetIndex:979

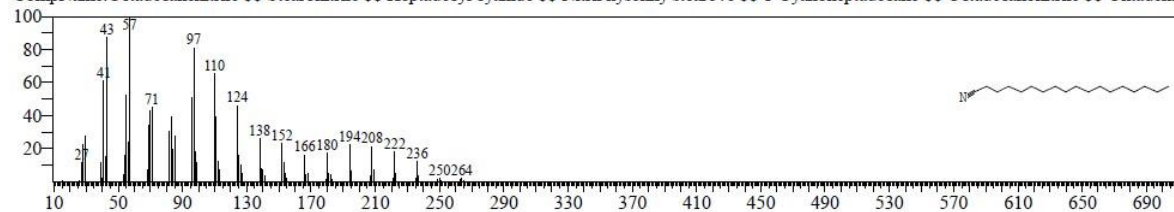
CompName:3,5-di(Trifluoromethyl)iodobenzene \$\$ 3,5-Bis(trifluoromethyl)iodobenzene \$\$ 1-Iodo-3,5-bis(trifluoromethyl)benzene #



Hit#:1 Entry:30132 Library:NIST17R.lib

SI:37 Formula:C18H35N CAS:638-65-3 MolWeight:265 RetIndex:2056

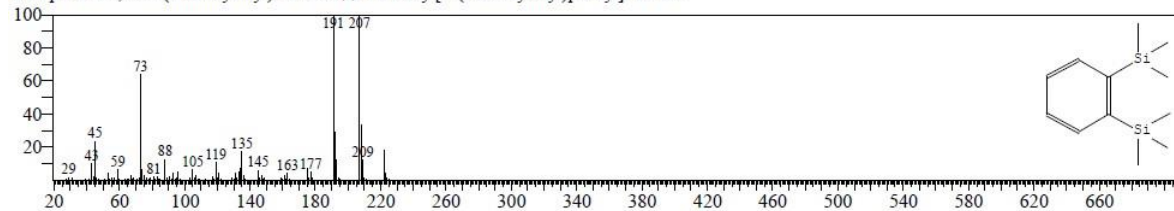
CompName:Octadecanenitrile \$\$ Stearonitrile \$\$ Heptadecyl cyanide \$\$ Nitril kyseliny stearove \$\$ 1-Cyanoheptadecane \$\$ Octadecanonitrile \$\$ Oktadeka



Hit#:1 Entry:25239 Library:NIST17R.lib

SI:40 Formula:C12H22Si2 CAS:17151-09-6 MolWeight:222 RetIndex:1124

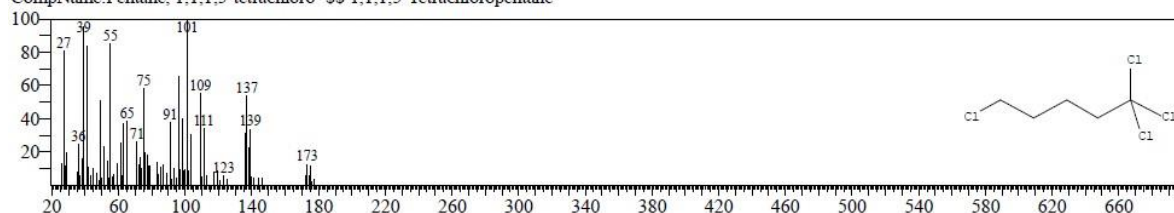
CompName:1,2-Bis(trimethylsilyl)benzene \$\$ Trimethyl[2-(trimethylsilyl)phenyl]silane #



Hit#:1 Entry:22949 Library:NIST17R.lib

SI:31 Formula:C5H8Cl4 CAS:2467-10-9 MolWeight:208 RetIndex:1131

CompName:Pentane, 1,1,1,5-tetrachloro- \$\$ 1,1,1,5-Tetrachloropentane



Hit#:1 Entry:3710 Library:NIST17M2.lib

SI:76 Formula:C42H63O4P CAS:95906-11-9 MolWeight:662 RetIndex:0

CompName:Tris(2,4-di-tert-butylphenyl) phosphate \$\$ Phenol, 2,4-bis(1,1-dimethylethyl)-, 1,1',1''-phosphate \$\$ Phenol, 2,4-bis(1,1-dimethylethyl)-, phosph

