SUPPLEMENTARY INFORMATION

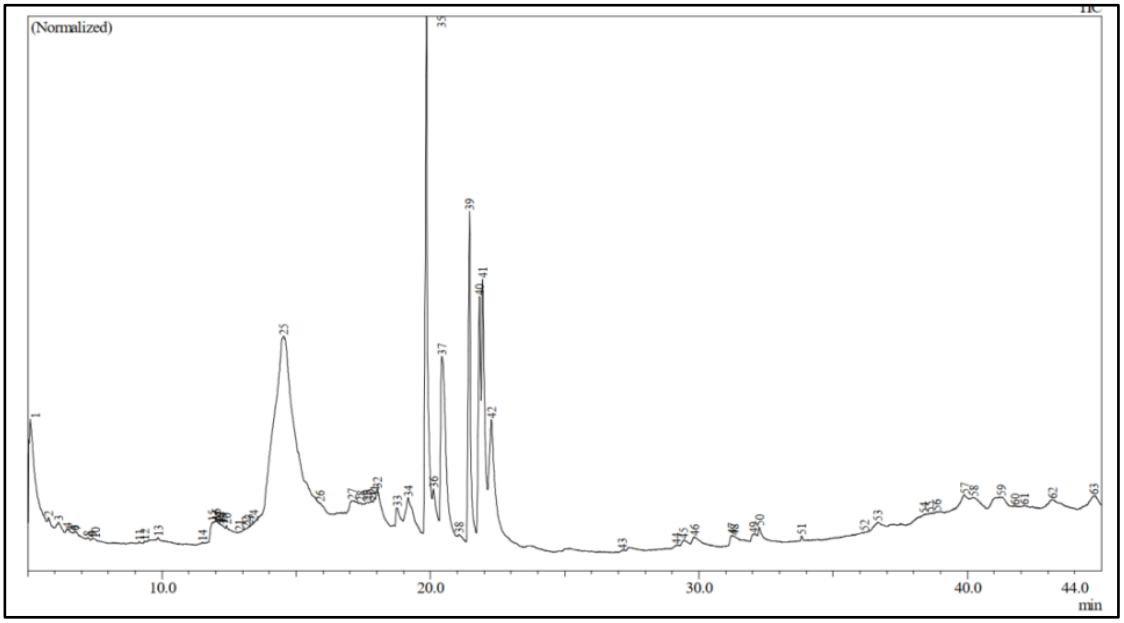


Figure 1. GC-MS chromatogram results of ethyl acetate extract from LU_3 isolate

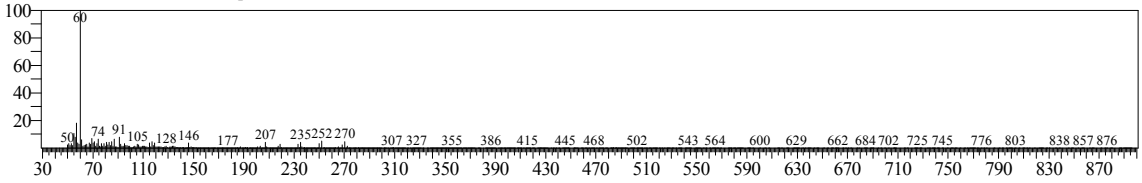
Library

<< Target >>

Line#:1 R.Time:5.092(Scan#:12) MassPeaks:582

RawMode:Averaged 5.083-5.100(11-13) BasePeak:60.05(462429)

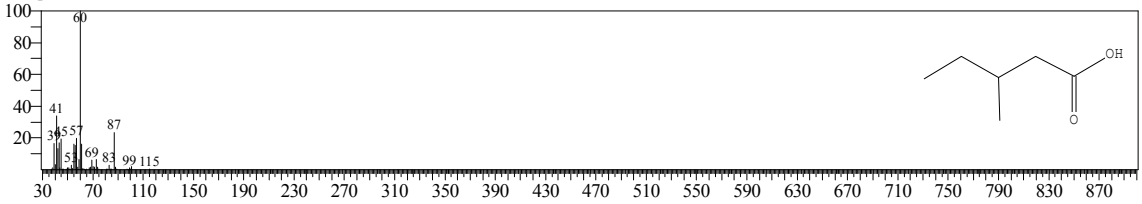
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Hit#:1 Entry:16944 Library:Wiley9.lib

SI:77 Formula:C6H12O2 CAS:105-43-1 MolWeight:116 RetIndex:0

CompName:3 METHYL PENTANOIC ACID $$ 3 METHYL VALERIC ACID $$ PENTANOIC ACID, 3-METHYL- $$ 3-METHYLPENTANOIC ACID $$ .BE

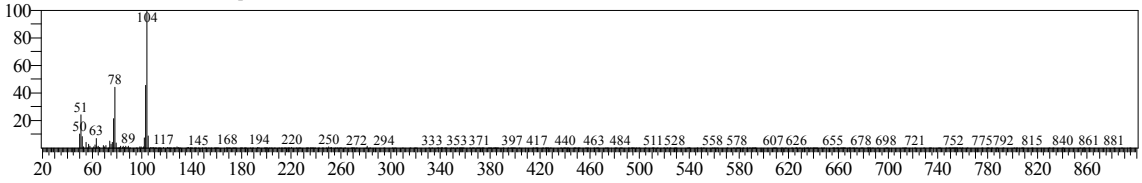


<< Target >>

Line#:2 R.Time:5.775(Scan#:94) MassPeaks:322

RawMode:Averaged 5.767-5.783(93-95) BasePeak:104.15(32364)

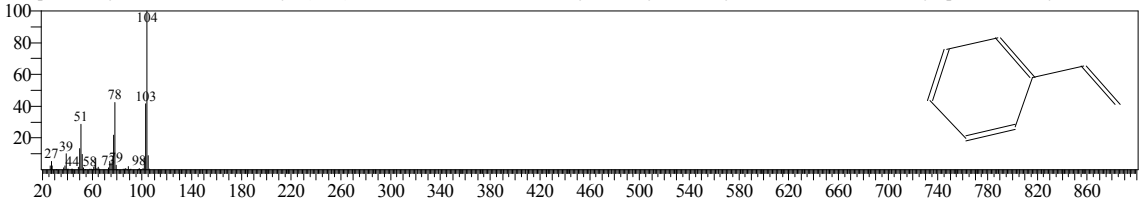
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Hit#:1 Entry:10301 Library:Wiley9.lib

SI:95 Formula:C8H8 CAS:100-42-5 MolWeight:104 RetIndex:0

CompName:Styrene $$ Benzene, ethenyl- (CAS) $$ ETHENYLBENZENE $$ Styrol $$ Styrole $$ Styrolene $$ Cinnamene $$ Styropol SO $$ Vinylbenzol $$ I

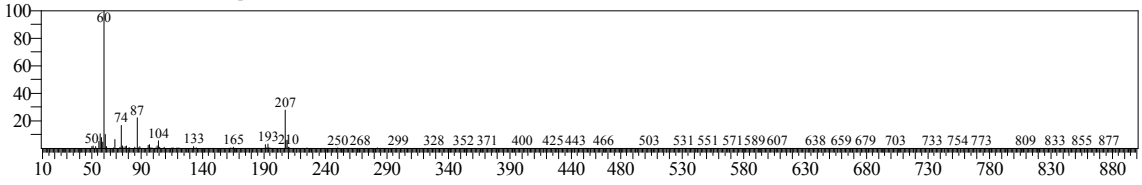


<< Target >>

Line#:3 R.Time:6.142(Scan#:138) MassPeaks:431

RawMode:Averaged 6.133-6.150(137-139) BasePeak:60.05(46660)

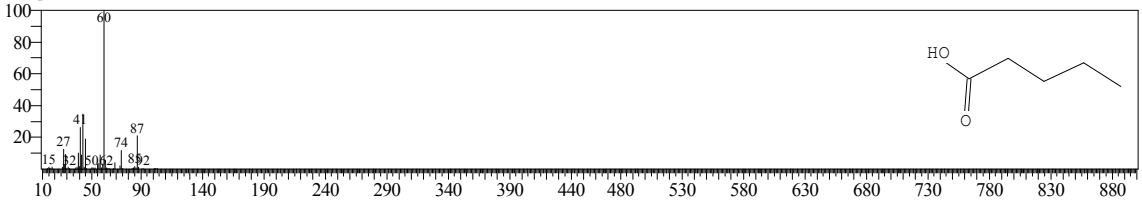
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



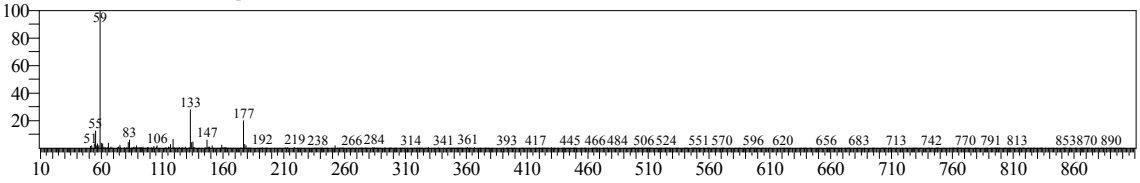
Hit#:1 Entry:8168 Library:WILEY8.LIB

SI:78 Formula:C5H10O2 CAS:109-52-4 MolWeight:102 RetIndex:0

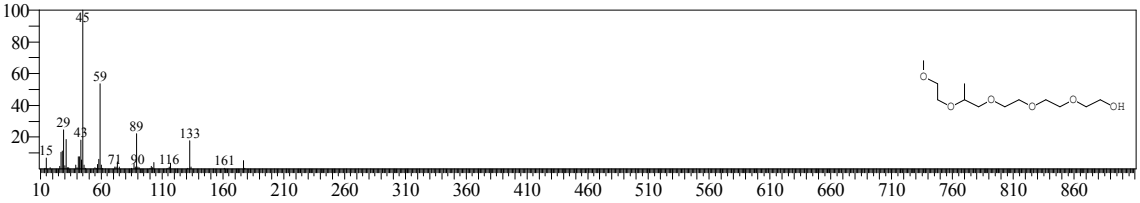
CompName:PENTANOIC ACID $$ AMMONIUM VALERATE $$ PENTANOATE $$ POTASSIUM VALERATE $$ SODIUM PENTANOATE $$ SODIUM VA



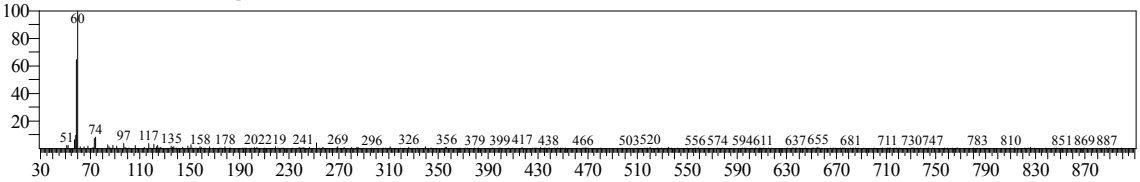
<< Target >>
Line#:4 R.Time:6.458(Scan#:176) MassPeaks:426
RawMode:Averaged 6.450-6.467(175-177) BasePeak:59.10(20358)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



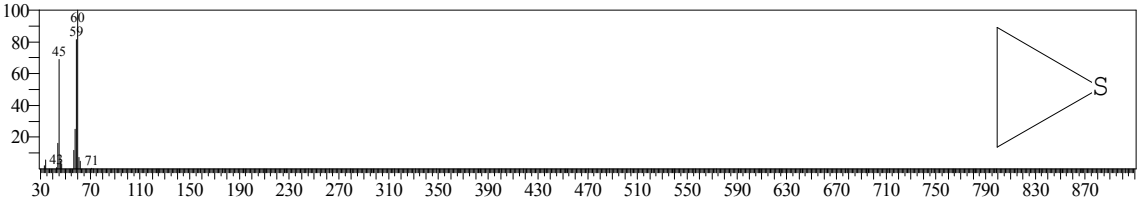
Hit#:1 Entry:295940 Library:Wiley9.lib
SI:74 Formula:C12H26O6 CAS:0-00-0 MolWeight:266 RetIndex:0
CompName:2-Methoxyethoxy-2-methylethyl 2-[(2'-hydroxyethoxy)ethoxy]ethyl ether $$ MeOEPE3 $$ 2-METHOXYETHOXY-2-METHYLETHYL 2-[(2'-HYI



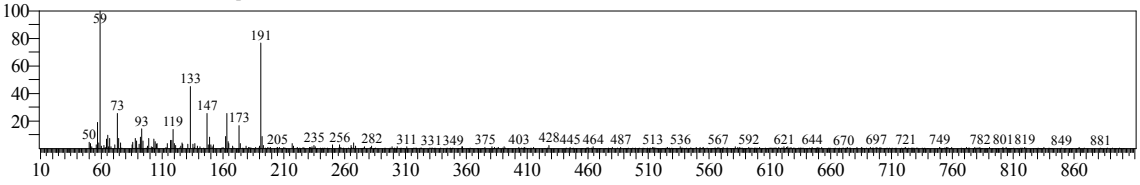
<< Target >>
Line#:5 R.Time:6.617(Scan#:195) MassPeaks:395
RawMode:Averaged 6.608-6.625(194-196) BasePeak:60.05(5245)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



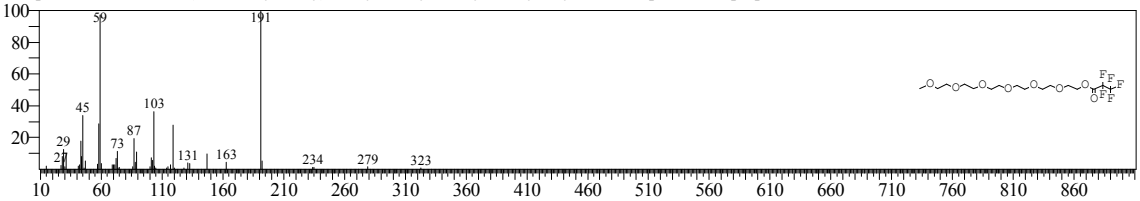
Hit#:1 Entry:686 Library:WILEY8.LIB
SI:78 Formula:C2H4S CAS:420-12-2 MolWeight:60 RetIndex:0
CompName:THIIRANE $$ 2,3-DIHYDROTHIIRENE $$ AETHYLENSULFID $$ AETHYLENSULFID [GERMAN] $$ AI3-52351 $$ CCRIS 782 $$ EINECS



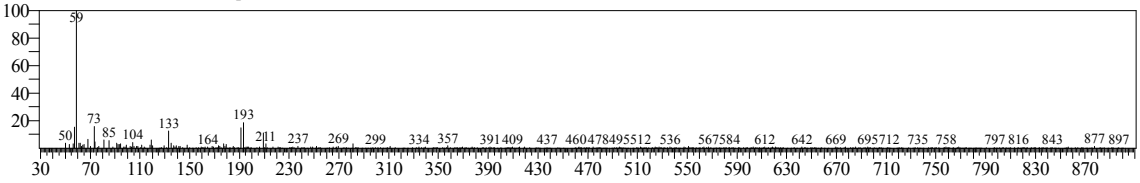
<< Target >>
Line#:6 R.Time:6.742(Scan#:210) MassPeaks:443
RawMode:Averaged 6.733-6.750(209-211) BasePeak:59.10(3265)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



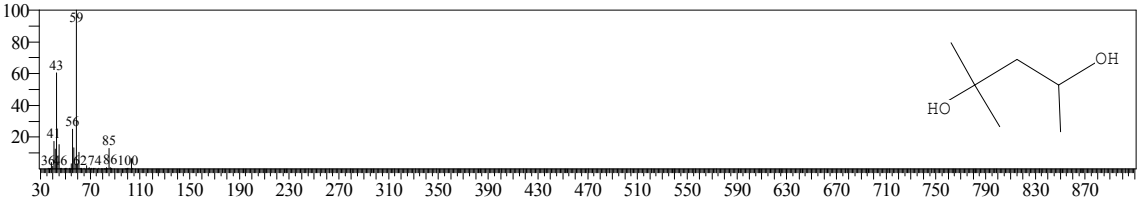
Hit#:1 Entry:282859 Library:NIST17.lib
SI:65 Formula:C16H27F5O8 CAS:0-00-0 MolWeight:442 RetIndex:1930
CompName:2-[2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate



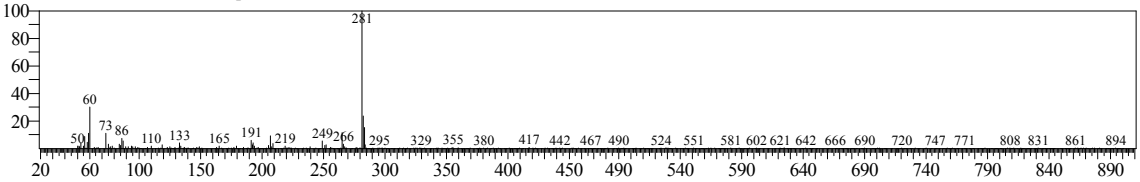
<< Target >>
Line#:7 R.Time:6.792(Scan#:216) MassPeaks:507
RawMode:Averaged 6.783-6.800(215-217) BasePeak:59.10(4744)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



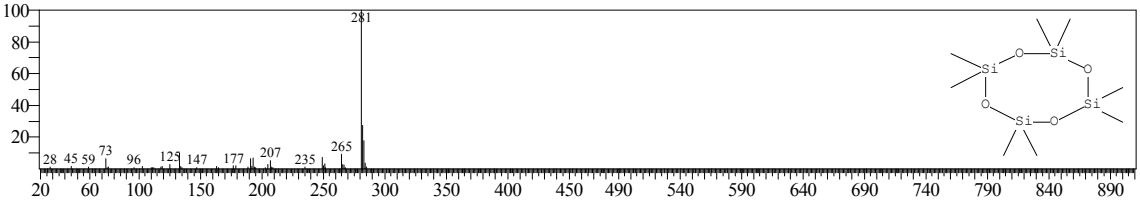
Hit#:1 Entry:15700 Library:WILEY8.LIB
SI:61 Formula:C6H14O2 CAS:107-41-5 MolWeight:118 RetIndex:0
CompName:1,2-HEXANEDIOL $$ 2,4-PENTANEDIOL, 2-METHYL- $$ 2-METHYLPENTANE-2,4-DIOL $$ (+-)-2-METHYL-2,4-PENTANEDIOL $$ .ALP



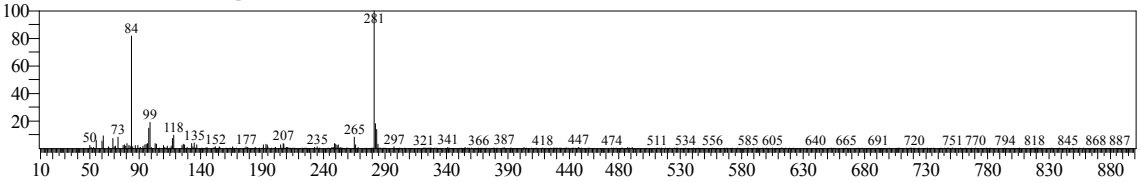
<< Target >>
Line#:8 R.Time:7.233(Scan#:269) MassPeaks:443
RawMode:Averaged 7.225-7.242(268-270) BasePeak:281.25(8150)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



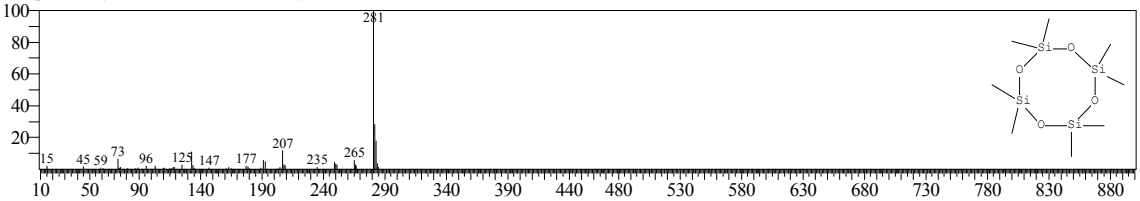
Hit#:1 Entry:234038 Library:WILEY8.LIB
SI:77 Formula:C8H24O4Si4 CAS:556-67-2 MolWeight:296 RetIndex:0
CompName:2,2,4,4,6,6,8,8-OCTAMETHYL-1,3,5,7,2,4,6,8-TETRAOXATETRASILOCANE $$ 2,2,4,4,6,6,8,8-OCTAMETHYL-[1,3,5,7,2,4,6,8]TETRAOXA



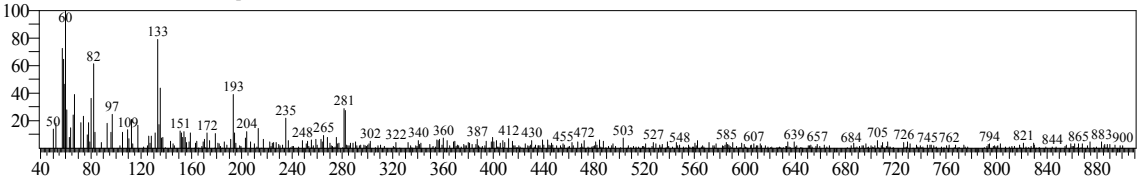
<< Target >>
Line#:9 R.Time:7.417(Scan#:291) MassPeaks:460
RawMode:Averaged 7.408-7.425(290-292) BasePeak:281.25(6429)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



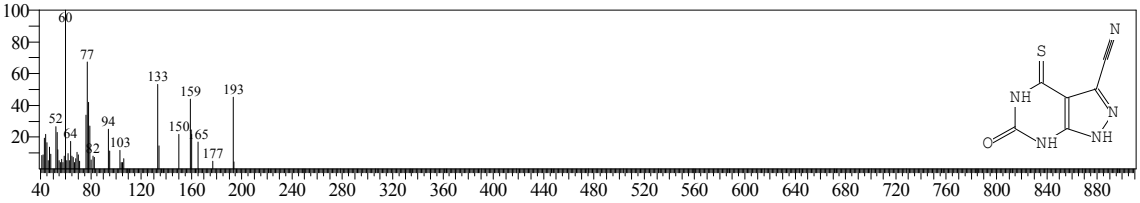
Hit#:1 Entry:171254 Library:NIST17.lib
SI:64 Formula:C8H24O4Si4 CAS:556-67-2 MolWeight:296 RetIndex:827
CompName:Cyclotetrasiloxane, octamethyl-



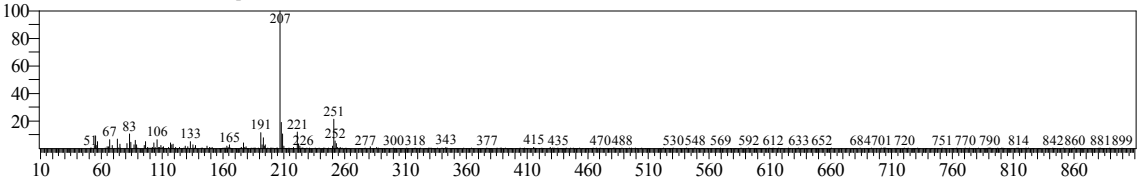
<< Target >>
Line#:10 R.Time:7.525(Scan#:304) MassPeaks:460
RawMode:Averaged 7.517-7.533(303-305) BasePeak:60.05(723)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



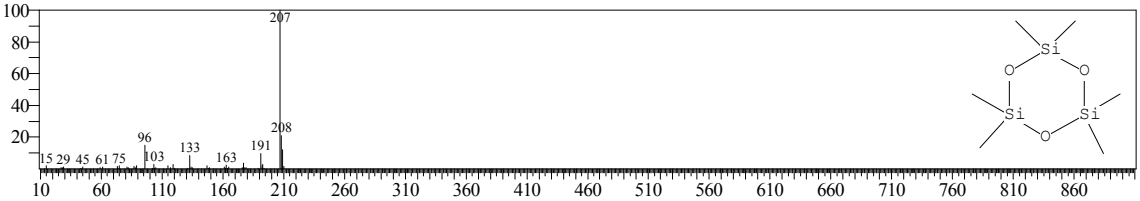
Hit#:1 Entry:35807 Library:NIST147.LIB
SI:49 Formula:C6H3N5OS CAS:0-00-0 MolWeight:193 RetIndex:0
CompName:3-Cyano-6-oxopyrazolo[3,4-d]pyrimidin-4-thione $$ 6-Oxo-4-thioxo-4,5,6,7-tetrahydro-1H-pyrazolo[3,4-d]pyrimidine-3-carbonitrile # $$



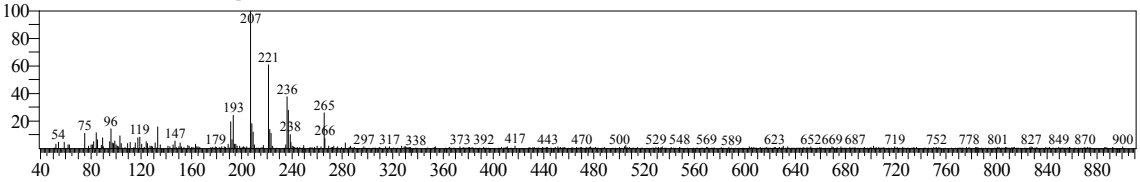
<< Target >>
Line#:11 R.Time:9.158(Scan#:500) MassPeaks:447
RawMode:Averaged 9.150-9.167(499-501) BasePeak:207.20(8024)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



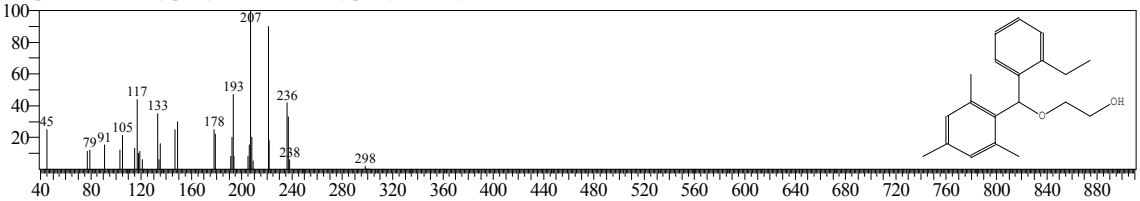
Hit#:1 Entry:92668 Library:NIST17.lib
SI:71 Formula:C6H18O3Si3 CAS:541-05-9 MolWeight:222 RetIndex:620
CompName:Cyclotrisiloxane, hexamethyl-



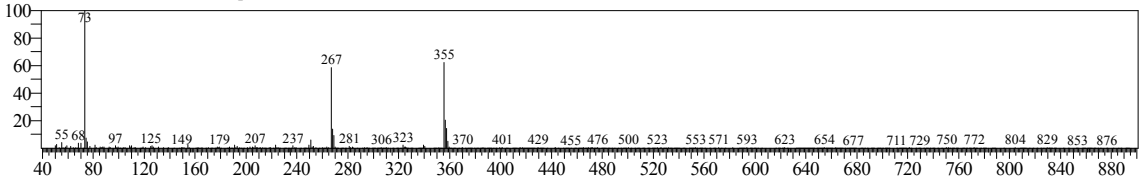
<< Target >>
Line#:12 R.Time:9.350(Scan#:523) MassPeaks:582
RawMode:Averaged 9.342-9.358(522-524) BasePeak:207.20(3232)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



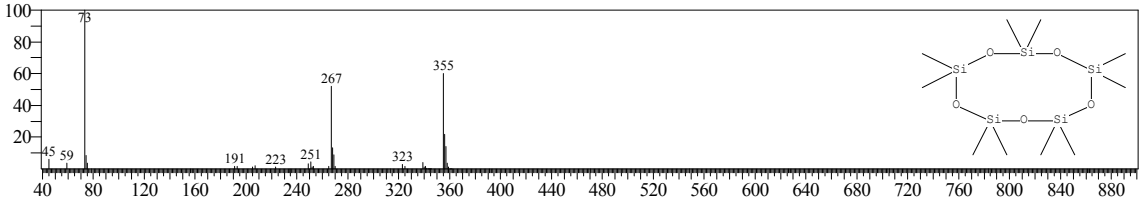
Hit#:1 Entry:371029 Library:Wiley9.lib
SI:63 Formula:C20H26O2 CAS:0-00-0 MolWeight:298 RetIndex:0
CompName:2-[(2'-Ethylphenyl)(2",4",6'-trimethylphenyl)methoxy]ethanol



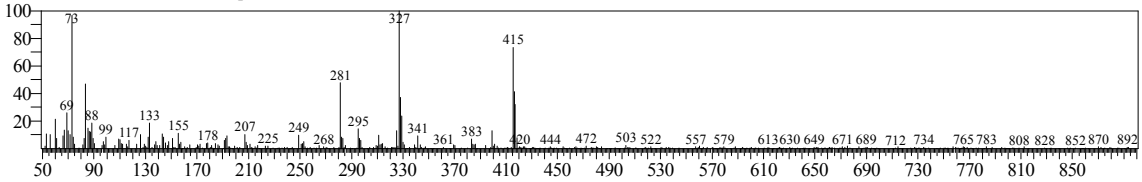
<< Target >>
Line#:13 R.Time:9.850(Scan#:583) MassPeaks:487
RawMode:Averaged 9.842-9.858(582-584) BasePeak:73.10(12072)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



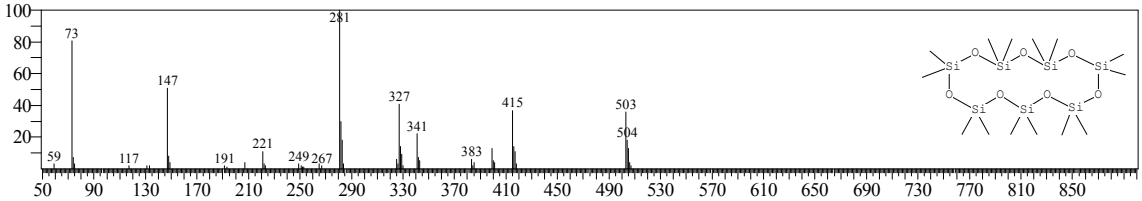
Hit#:1 Entry:502115 Library:Wiley9.lib
SI:91 Formula:C10H30O5Si5 CAS:541-02-6 MolWeight:370 RetIndex:0
CompName:Cyclopentasiloxane, decamethyl- (CAS) $$ Dimethylsiloxane pentamer $$ DECAMETHYL-CYCLOPENTASILOXANE $$ Decamethylcyclopenta



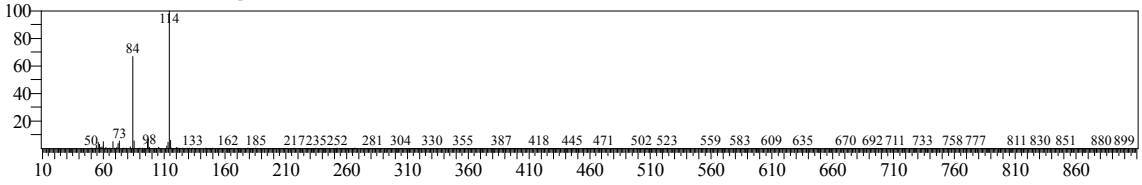
<< Target >>
Line#:14 R.Time:11.500(Scan#:781) MassPeaks:422
RawMode:Averaged 11.492-11.508(780-782) BasePeak:327.20(2011)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



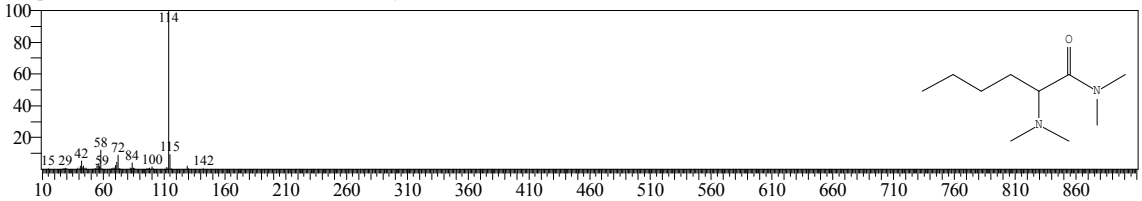
Hit#:1 Entry:298256 Library:NIST17.lib
SI:53 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl-



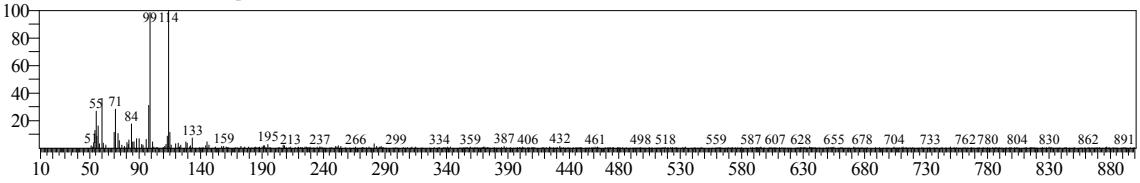
<< Target >>
Line#:15 R.Time:11.883(Scan#:827) MassPeaks:477
RawMode:Averaged 11.875-11.892(826-828) BasePeak:114.15(31482)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



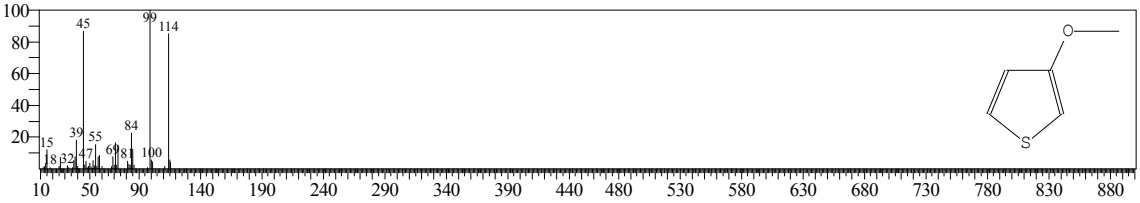
Hit#:1 Entry:57660 Library:NIST17.lib
SI:79 Formula:C10H22N2O CAS:0-00-0 MolWeight:186 RetIndex:1201
CompName:DL-Norleucine amide, N,N,N'N'-tetramethyl-



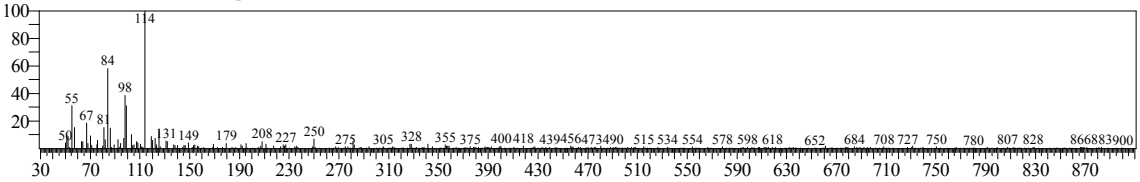
<< Target >>
Line#:16 R.Time:12.025(Scan#:844) MassPeaks:521
RawMode:Averaged 12.017-12.033(843-845) BasePeak:114.15(4818)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



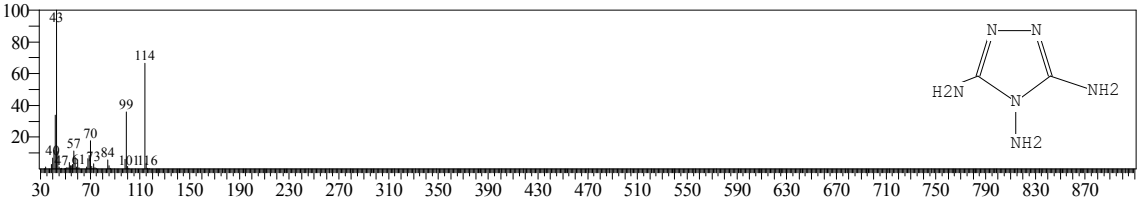
Hit#:1 Entry:7891 Library:NIST17.lib
SI:74 Formula:C5H6OS CAS:17573-92-1 MolWeight:114 RetIndex:870
CompName:Thiophene, 3-methoxy-



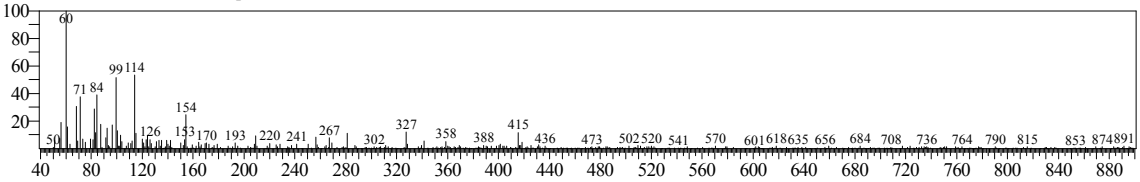
<< Target >>
Line#:17 R.Time:12.125(Scan#:856) MassPeaks:424
RawMode:Averaged 12.117-12.133(855-857) BasePeak:114.20(2128)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



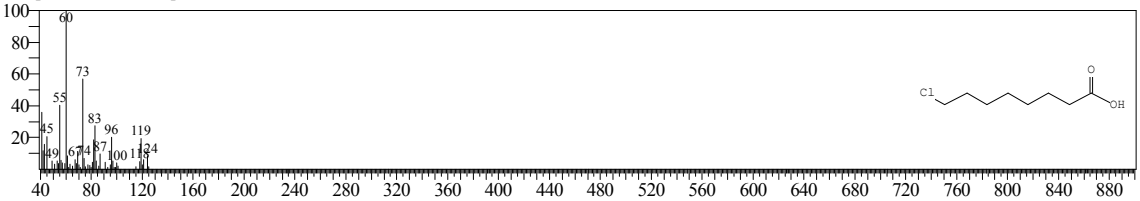
Hit#:1 Entry:7813 Library:NIST17.lib
SI:57 Formula:C2H6N6 CAS:473-96-1 MolWeight:114 RetIndex:1363
CompName:Guanazine



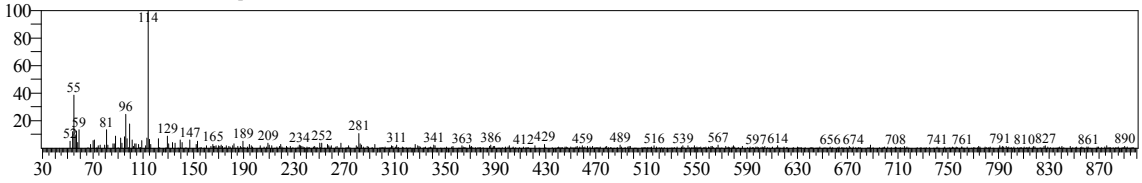
<< Target >>
Line#:18 R.Time:12.175(Scan#:862) MassPeaks:412
RawMode:Averaged 12.167-12.183(861-863) BasePeak:60.05(1587)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



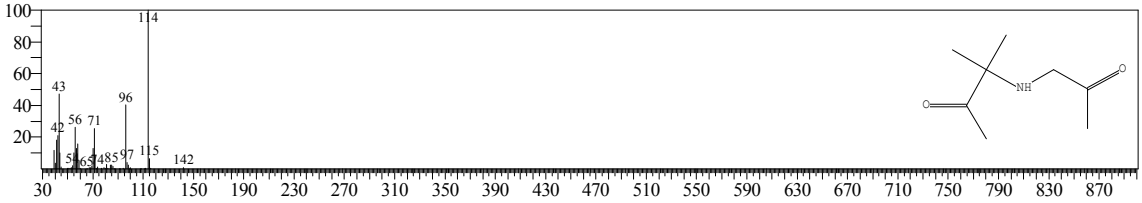
Hit#:1 Entry:49881 Library:NIST17.lib
SI:56 Formula:C8H15ClO2 CAS:1795-62-6 MolWeight:178 RetIndex:1398
CompName:8-Chlorocapric acid



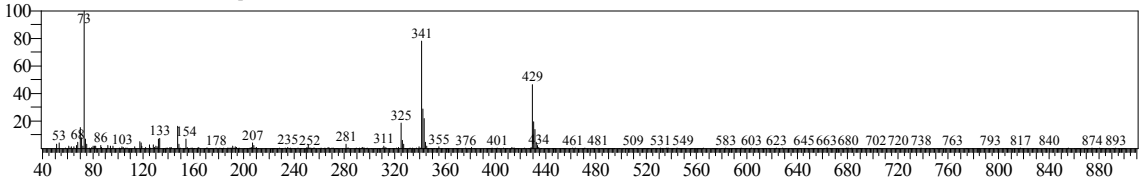
<< Target >>
Line#:19 R.Time:12.258(Scan#:872) MassPeaks:515
RawMode:Averaged 12.250-12.267(871-873) BasePeak:114.15(2623)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



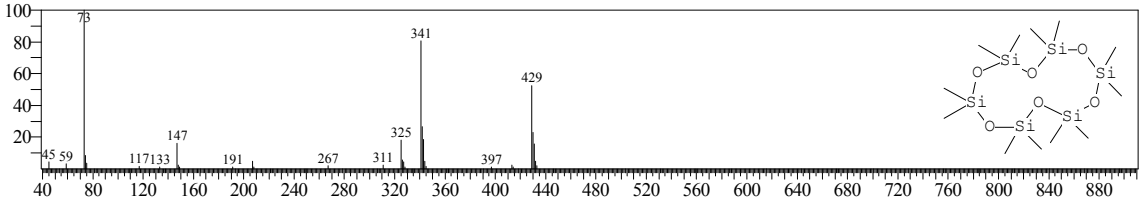
Hit#:1 Entry:32928 Library:NIST17.lib
SI:64 Formula:C8H15NO2 CAS:103634-54-4 MolWeight:157 RetIndex:1202
CompName:Butane-2-one, 3-methyl-3-(2-oxopropylamino)-



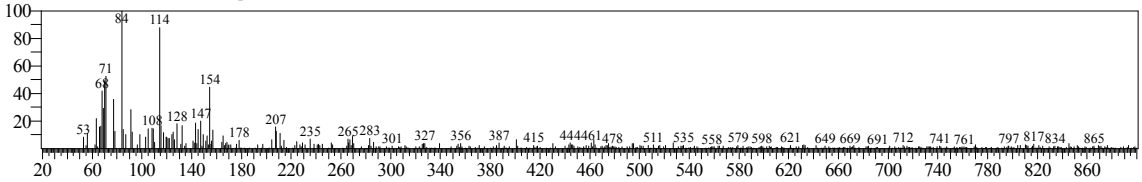
<< Target >>
Line#:20 R.Time:12.400(Scan#:889) MassPeaks:423
RawMode:Averaged 12.392-12.408(888-890) BasePeak:73.10(10426)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



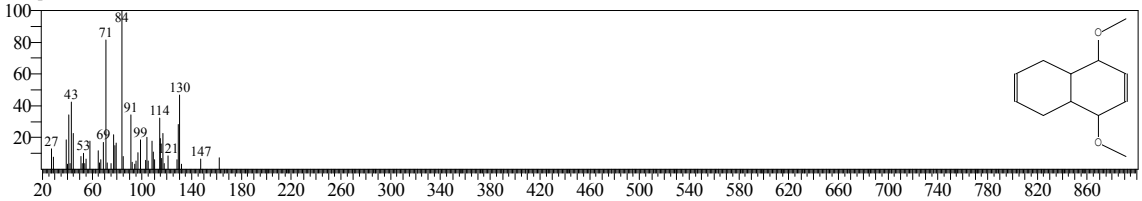
Hit#:1 Entry:27091 Library:NIST27.LIB
SI:86 Formula:C12H36O6Si6 CAS:540-97-6 MolWeight:444 RetIndex:0
CompName:Cyclohexasiloxane, dodecamethyl-



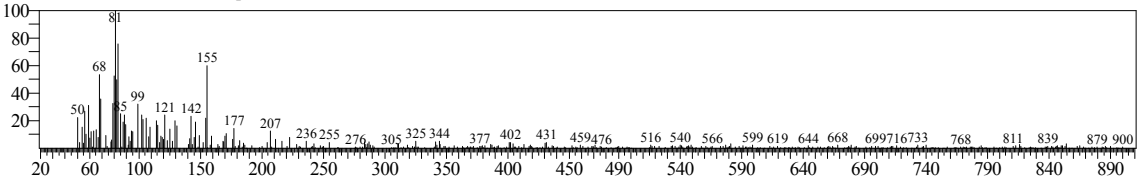
<< Target >>
Line#:21 R.Time:12.883(Scan#:947) MassPeaks:468
RawMode:Averaged 12.875-12.892(946-948) BasePeak:84.10(1190)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



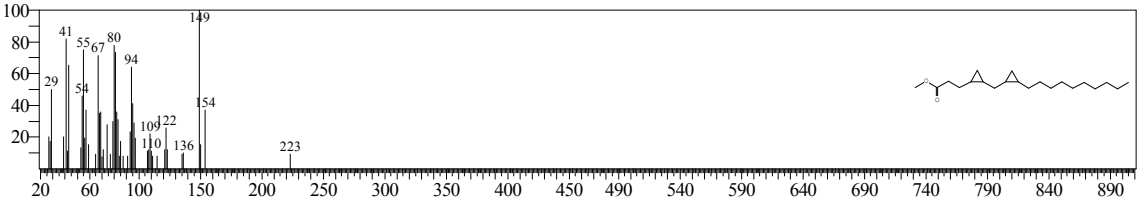
Hit#:1 Entry:95757 Library:WILEY8.LIB
SI:55 Formula:C12H18O2 CAS:0-00-0 MolWeight:194 RetIndex:0
CompName:1,4-DIMETHOXY-1,4,4A,5,8,8A-HEXAHYDRONAPHTHALENE $$ 1,4-DIMETHOXY-1,4,4A,5,8,8A-HEXAHYDRO-NAPHTHALENE



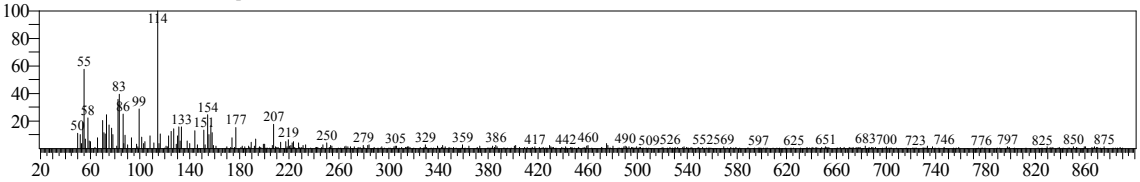
<< Target >>
Line#:22 R.Time:13.125(Scan#:976) MassPeaks:407
RawMode:Averaged 13.117-13.133(975-977) BasePeak:81.15(1415)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



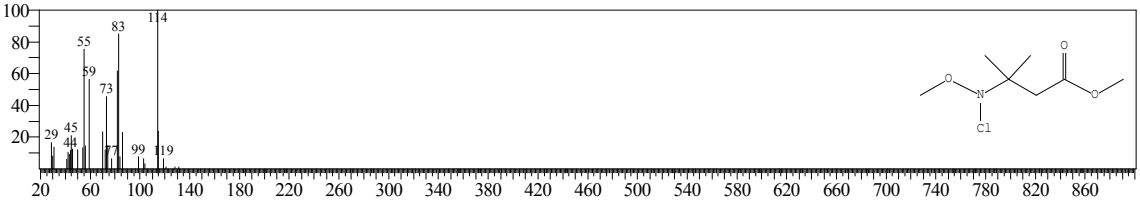
Hit#:1 Entry:104375 Library:NIST147.LIB
SI:54 Formula:C21H38O2 CAS:10152-67-7 MolWeight:322 RetIndex:0
CompName:Cyclopropanepropionic acid, 2-[(2-decylcyclopropyl)methyl]-, methyl ester $$ Methyl 3-(2-[(2-decylcyclopropyl)methyl]cyclopropyl)propanoate #



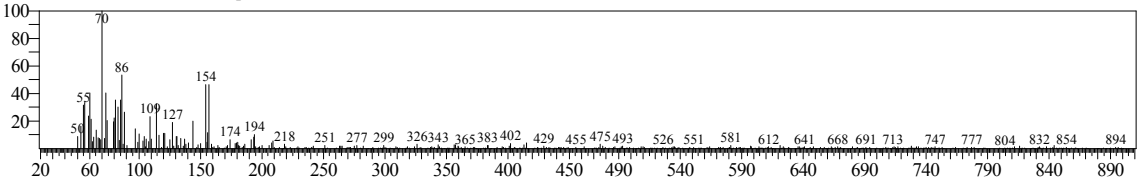
<< Target >>
Line#:23 R.Time:13.233(Scan#:989) MassPeaks:448
RawMode:Averaged 13.225-13.242(988-990) BasePeak:114.15(2220)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



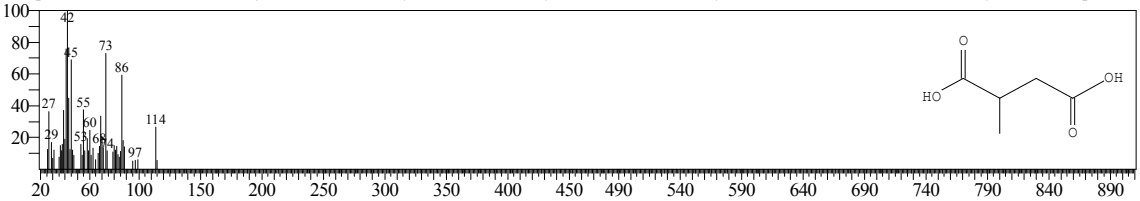
Hit#:1 Entry:65740 Library:NIST17.lib
SI:61 Formula:C7H14ClNO3 CAS:70569-70-9 MolWeight:195 RetIndex:1101
CompName:Methyl 3-methyl-3-(methoxy-chloro)amino-butanoate



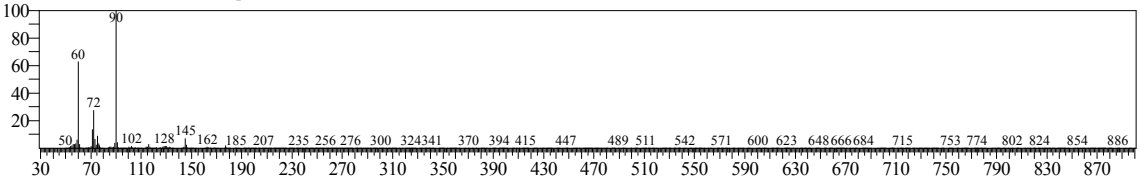
<< Target >>
Line#:24 R.Time:13.417(Scan#:1011) MassPeaks:428
RawMode:Averaged 13.408-13.425(1010-1012) BasePeak:70.10(2213)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



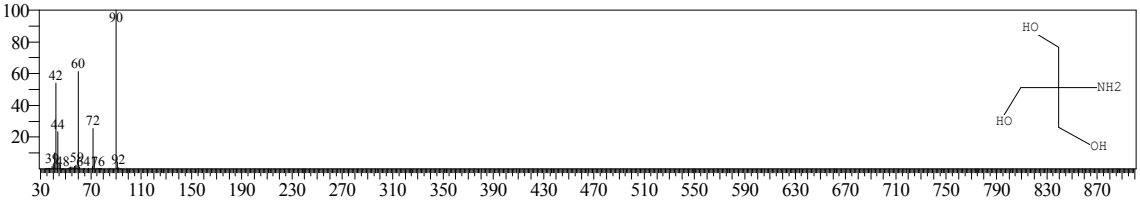
Hit#:1 Entry:28942 Library:Wiley9.lib
SI:63 Formula:C5H8O4 CAS:498-21-5 MolWeight:132 RetIndex:0
CompName:Butanedioic acid, methyl- (CAS) $$ 2-Methylsuccinic acid $$ Pyrotartaric acid $$ Methylsuccinic acid $$ Succinic acid, methyl- $$ 1,2-Propanedic



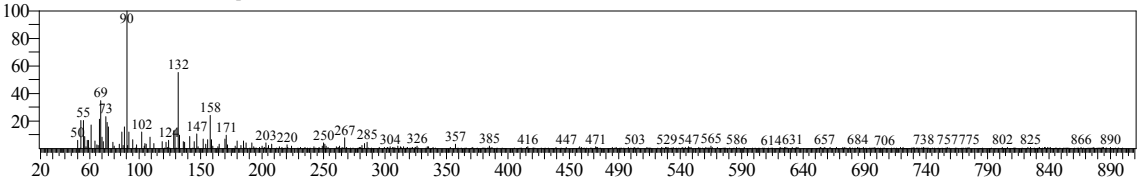
<< Target >>
Line#:25 R.Time:14.525(Scan#:1144) MassPeaks:520
RawMode:Averaged 14.517-14.533(1143-1145) BasePeak:90.15(1019586)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



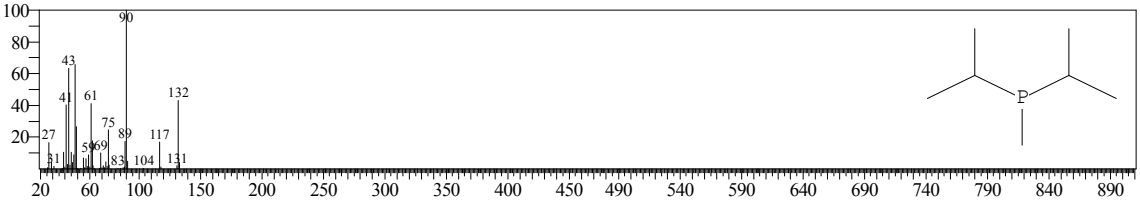
Hit#:1 Entry:19526 Library:Wiley9.lib
SI:88 Formula:C4H11NO3 CAS:77-86-1 MolWeight:121 RetIndex:0
CompName:1,3-Propanediol, 2-amino-2-(hydroxymethyl)- (CAS) $$ THAM $$ Tris $$ Tham-E $$ Trizma $$ Talatrol $$ Pehanorm $$ Trisamin $$ Trisamine $$ A



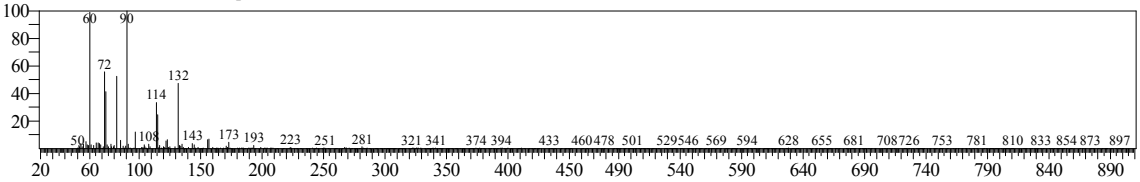
<< Target >>
Line#:26 R.Time:15.892(Scan#:1308) MassPeaks:479
RawMode:Averaged 15.883-15.900(1307-1309) BasePeak:90.10(3681)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



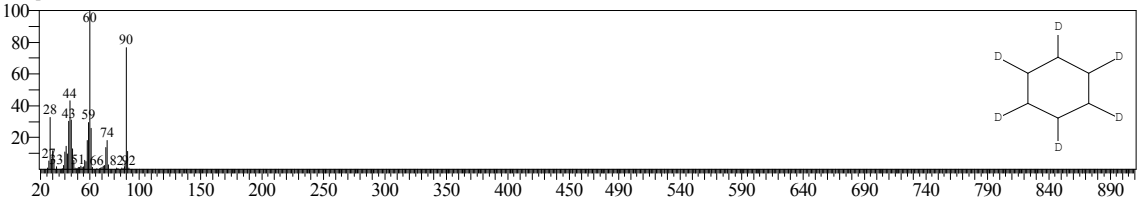
Hit#:1 Entry:24815 Library:WILEY8.LIB
SI:56 Formula:C7H17P CAS:60054-88-8 MolWeight:132 RetIndex:0
CompName:DIISOPROPYL(METHYL)PHOSPHINE # $$ DIISOPROPYL(METHYL)PHOSPHINE $$ PHOSPHINE, METHYLBIS(1-METHYLETHYL)-



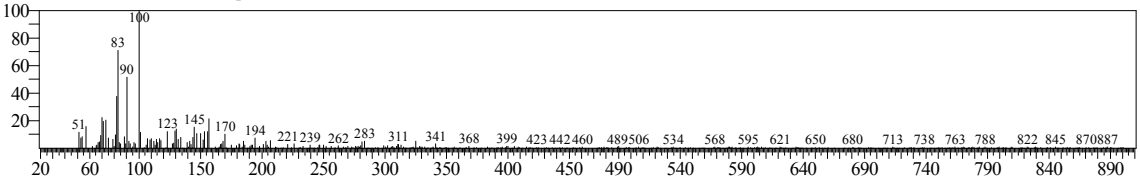
<< Target >>
Line#:27 R.Time:17.083(Scan#:1451) MassPeaks:460
RawMode:Averaged 17.075-17.092(1450-1452) BasePeak:90.15(22339)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



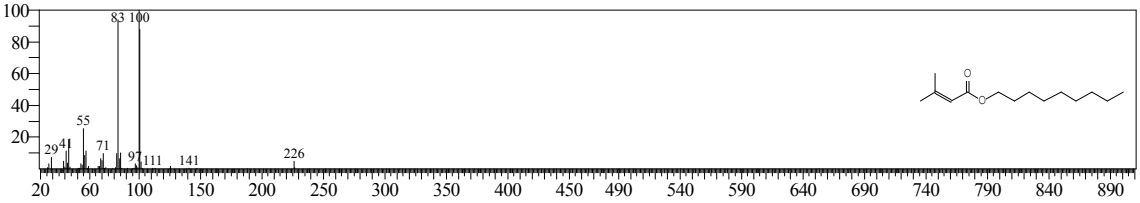
Hit#:1 Entry:3348 Library:Wiley9.lib
SI:63 Formula:C6H6D6 CAS:0-00-0 MolWeight:84 RetIndex:0
CompName:CYCLOHEXAN, 1,2,3,4,5,6-HEXADEUTERO- $$ CYCLOHEXANE



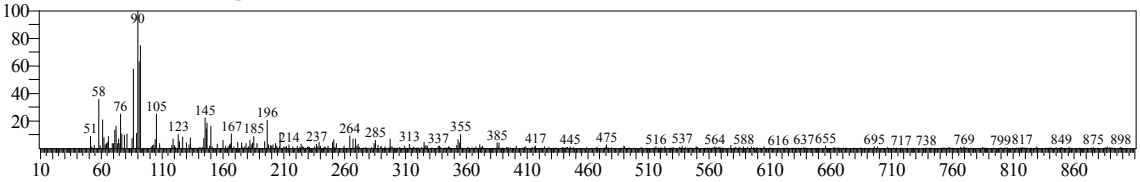
<< Target >>
Line#:28 R.Time:17.408(Scan#:1490) MassPeaks:423
RawMode:Averaged 17.400-17.417(1489-1491) BasePeak:100.15(3623)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



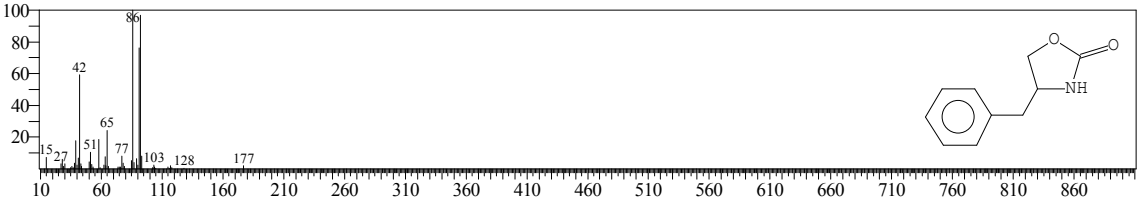
Hit#:1 Entry:98252 Library:NIST17.lib
SI:55 Formula:C14H26O2 CAS:0-00-0 MolWeight:226 RetIndex:1565
CompName:3-Methyl-2-butenoic acid, nonyl ester



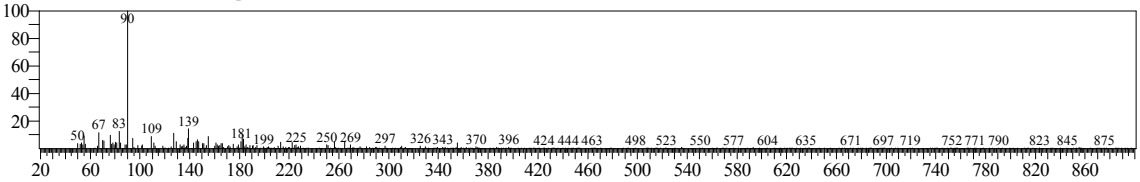
<< Target >>
Line#:29 R.Time:17.633(Scan#:1517) MassPeaks:474
RawMode:Averaged 17.625-17.642(1516-1518) BasePeak:90.15(3181)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



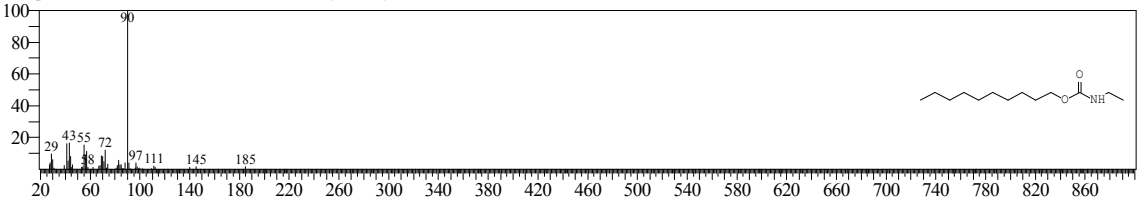
Hit#:1 Entry:27694 Library:NIST147.LIB
SI:57 Formula:C10H11NO2 CAS:90719-32-7 MolWeight:177 RetIndex:0
CompName:(S)-4-Benzyl-2-oxazolidinone $$ 4-Benzyl-1,3-oxazolidin-2-one # $$



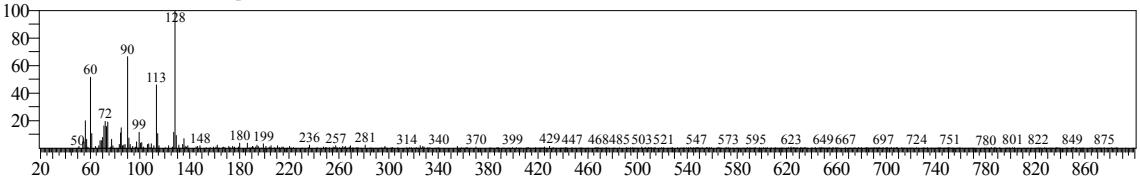
<< Target >>
Line#:30 R.Time:17.758(Scan#:1532) MassPeaks:512
RawMode:Averaged 17.750-17.767(1531-1533) BasePeak:90.15(6017)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



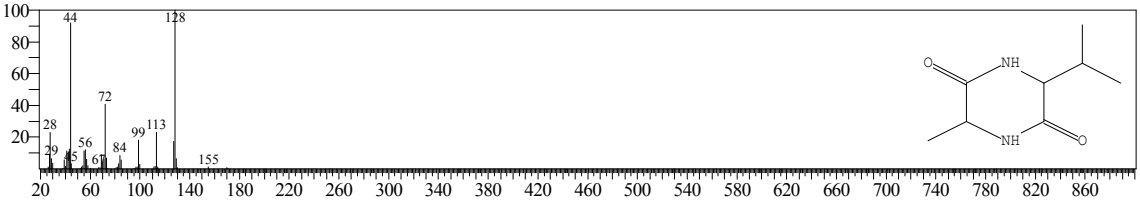
Hit#:1 Entry:101106 Library:NIST17.lib
SI:54 Formula:C13H27NO2 CAS:0-00-0 MolWeight:229 RetIndex:1679
CompName:Carbonic acid, monoamide, N-ethyl-, decyl ester



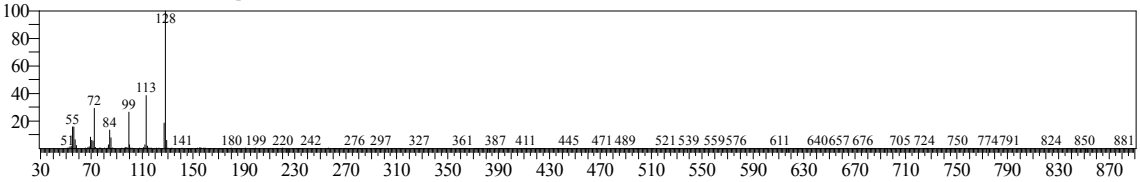
<< Target >>
Line#:31 R.Time:17.925(Scan#:1552) MassPeaks:477
RawMode:Averaged 17.917-17.933(1551-1553) BasePeak:128.20(7415)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



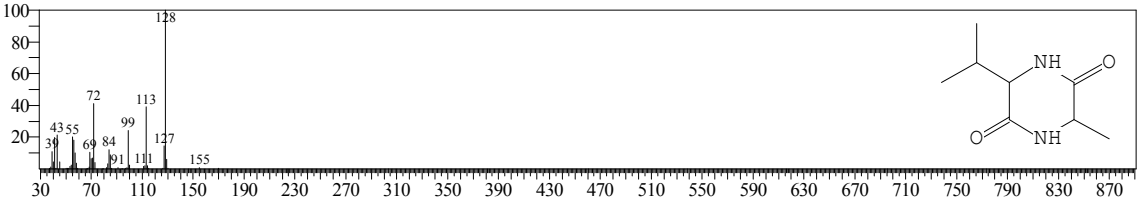
Hit#:1 Entry:64822 Library:WILEY8.LIB
SI:69 Formula:C8H14N2O2 CAS:22160-42-5 MolWeight:170 RetIndex:0
CompName:3-ISOPROPYL-6-METHYL-PIPERAZINE-2,5-DIONE $$ 3-ISOPROPYL-6-METHYL-2,5-PIPERAZINEDIONE



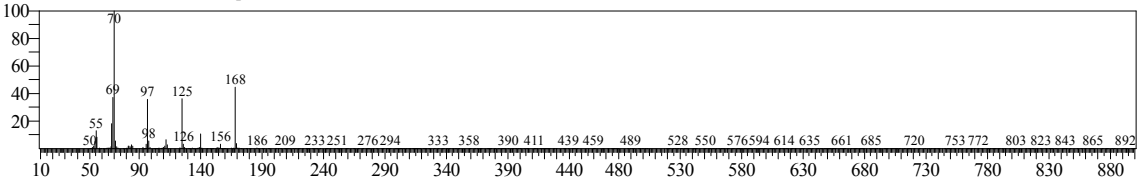
<< Target >>
Line#:32 R.Time:18.017(Scan#:1563) MassPeaks:403
RawMode:Averaged 18.008-18.025(1562-1564) BasePeak:128.20(72725)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



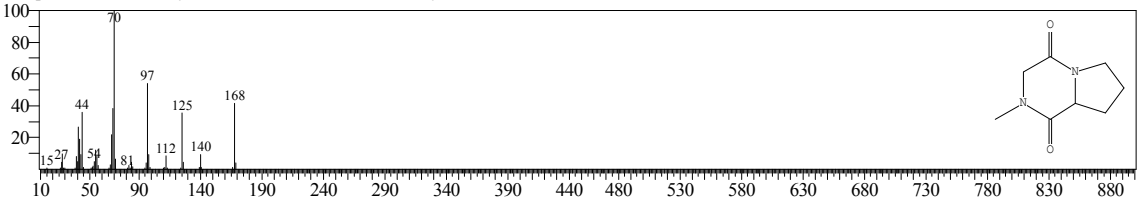
Hit#:1 Entry:24153 Library:NIST147.LIB
SI:96 Formula:C8H14N2O2 CAS:22160-42-5 MolWeight:170 RetIndex:0
CompName:2,5-Piperazinedione, 3-methyl-6-(1-methylethyl)- $$ 3-Isopropyl-6-methyl-2,5-piperazinedione # $$



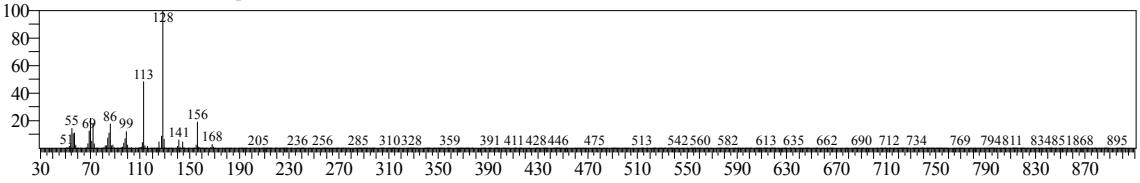
<< Target >>
Line#:33 R.Time:18.750(Scan#:1651) MassPeaks:419
RawMode:Averaged 18.742-18.758(1650-1652) BasePeak:70.15(81774)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



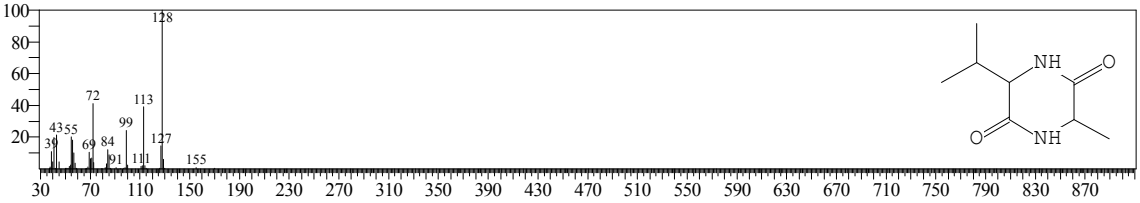
Hit#:1 Entry:41300 Library:NIST17.lib
SI:94 Formula:C8H12N2O2 CAS:0-00-0 MolWeight:168 RetIndex:1562
CompName:1,4-diazabicyclo[4.3.0]nonan-2,5-dione, 3-methyl



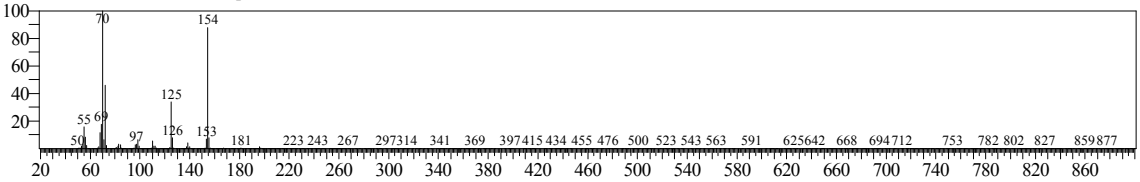
<< Target >>
Line#:34 R.Time:19.167(Scan#:1701) MassPeaks:438
RawMode:Averaged 19.158-19.175(1700-1702) BasePeak:128.20(114204)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



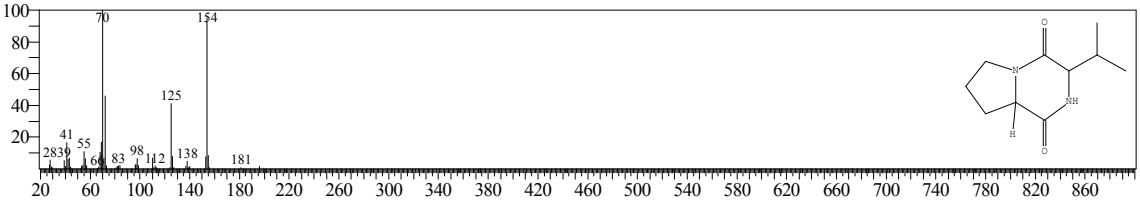
Hit#:1 Entry:24153 Library:NIST147.LIB
SI:85 Formula:C8H14N2O2 CAS:22160-42-5 MolWeight:170 RetIndex:0
CompName:2,5-Piperazinedione, 3-methyl-6-(1-methylethyl)- $$ 3-Isopropyl-6-methyl-2,5-piperazinedione # $$



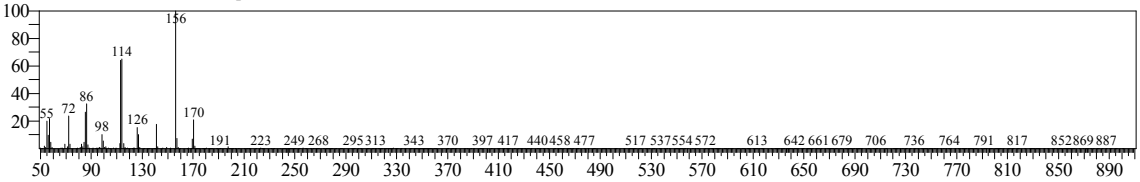
<< Target >>
Line#:35 R.Time:19.850(Scan#:1783) MassPeaks:498
RawMode:Averaged 19.842-19.858(1782-1784) BasePeak:70.15(2078204)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



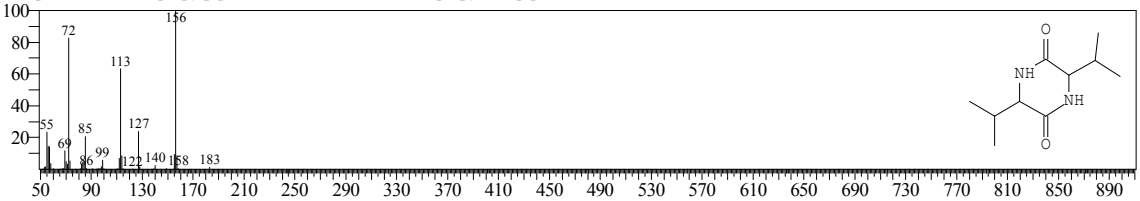
Hit#:1 Entry:67023 Library:NIST17.lib
SI:98 Formula:C10H16N2O2 CAS:2854-40-2 MolWeight:196 RetIndex:1600
CompName:Cyclo(L-prolyl-L-valine)



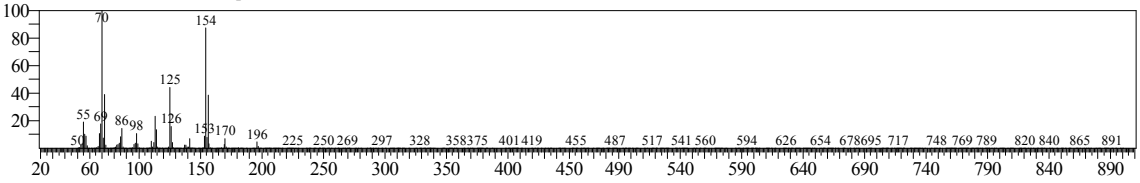
<< Target >>
Line#:36 R.Time:20.117(Scan#:1815) MassPeaks:449
RawMode:Averaged 20.108-20.125(1814-1816) BasePeak:156.25(58675)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



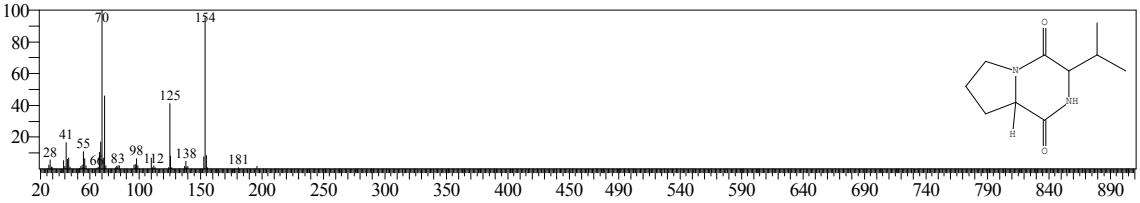
Hit#:1 Entry:38860 Library:NIST147.LIB
SI:79 Formula:C10H18N2O2 CAS:5625-44-5 MolWeight:198 RetIndex:0
CompName:3,6-Diisopropylpiperazin-2,5-dione $$ 3,6-Diisopropyl-2,5-piperazinedione # $$



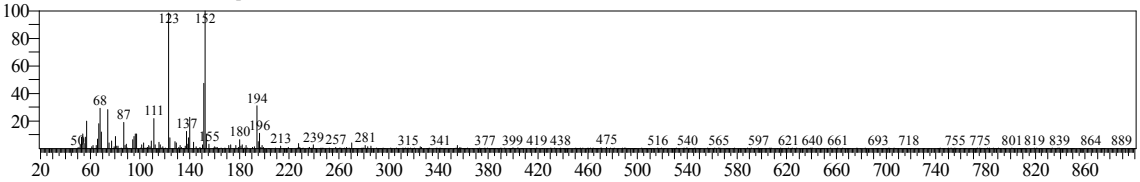
<< Target >>
Line#:37 R.Time:20.417(Scan#:1851) MassPeaks:457
RawMode:Averaged 20.408-20.425(1850-1852) BasePeak:70.15(490502)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



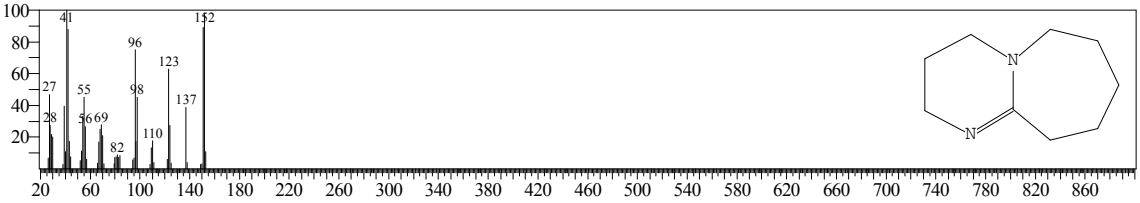
Hit#:1 Entry:67023 Library:NIST17.lib
SI:87 Formula:C10H16N2O2 CAS:2854-40-2 MolWeight:196 RetIndex:1600
CompName:Cyclo(L-prolyl-L-valine)



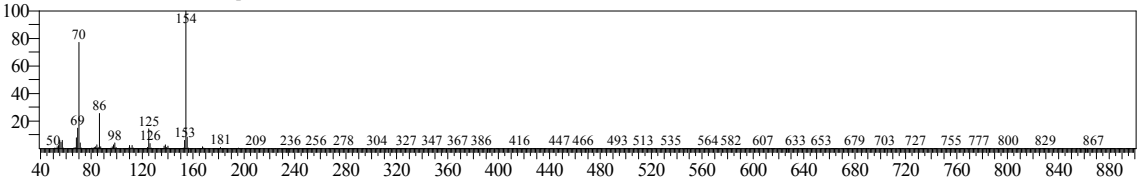
<< Target >>
Line#:38 R.Time:21.067(Scan#:1929) MassPeaks:457
RawMode:Averaged 21.058-21.075(1928-1930) BasePeak:152.20(8301)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



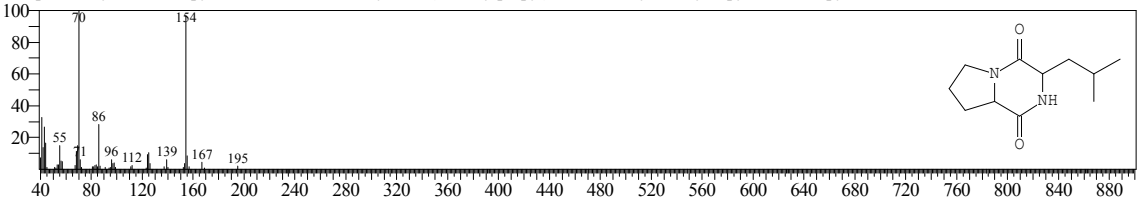
Hit#:1 Entry:53910 Library:Wiley9.lib
SI:65 Formula:C9H16N2 CAS:6674-22-2 MolWeight:152 RetIndex:0
CompName:Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro- $$ 1,5-Diazabicyclo[5.4.0]undec-5-ene $$ DBU $$ 2,3,4,6,7,8,9,10-Octahydropyrimido[1,2-a]a



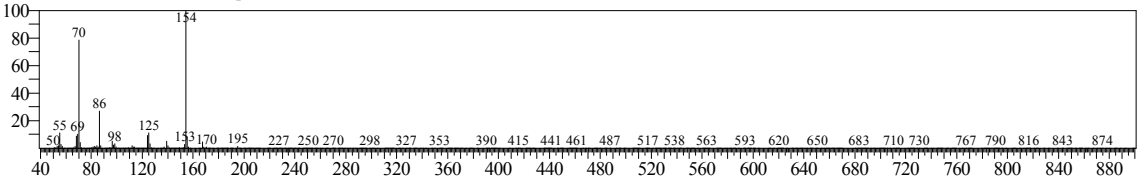
<< Target >>
Line#:39 R.Time:21.458(Scan#:1976) MassPeaks:524
RawMode:Averaged 21.450-21.467(1975-1977) BasePeak:154.20(1652979)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



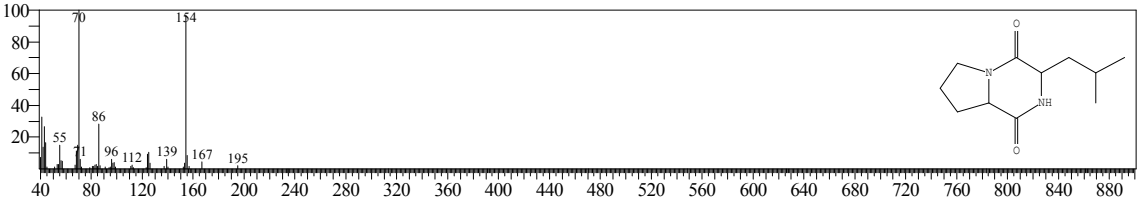
Hit#:1 Entry:45514 Library:NIST147.LIB
SI:92 Formula:C11H18N2O2 CAS:5654-86-4 MolWeight:210 RetIndex:0
CompName:Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)- $$ 3-Isobutylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione # $$



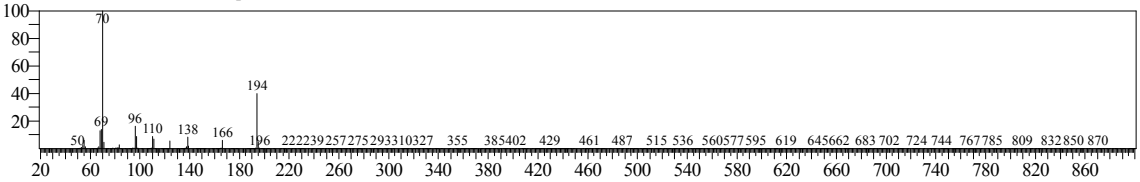
<< Target >>
Line#:40 R.Time:21.825(Scan#:2020) MassPeaks:486
RawMode:Averaged 21.817-21.833(2019-2021) BasePeak:154.20(745004)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



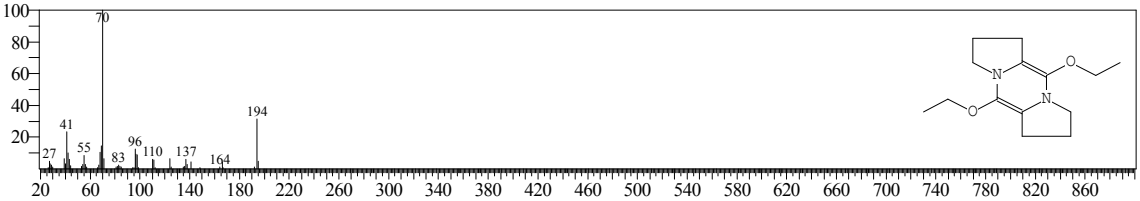
Hit#:1 Entry:81070 Library:NIST17.lib
SI:94 Formula:C11H18N2O2 CAS:5654-86-4 MolWeight:210 RetIndex:1699
CompName:Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-



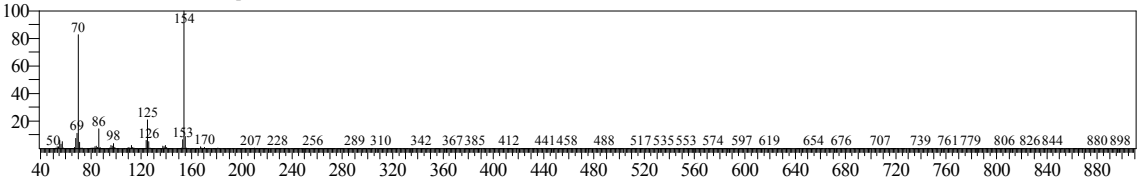
<< Target >>
Line#:41 R.Time:21.942(Scan#:2034) MassPeaks:477
RawMode:Averaged 21.933-21.950(2033-2035) BasePeak:70.15(978492)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



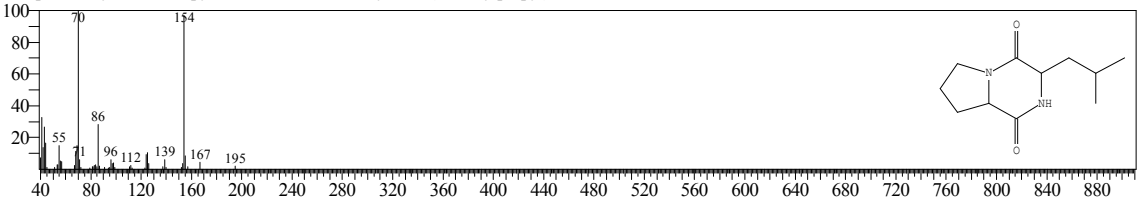
Hit#:1 Entry:67533 Library:NIST147.LIB
SI:91 Formula:C14H22N2O2 CAS:0-00-0 MolWeight:250 RetIndex:0
CompName:5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a;1',2'-d]pyrazine $$ 5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a:1,2-d]pyrazin



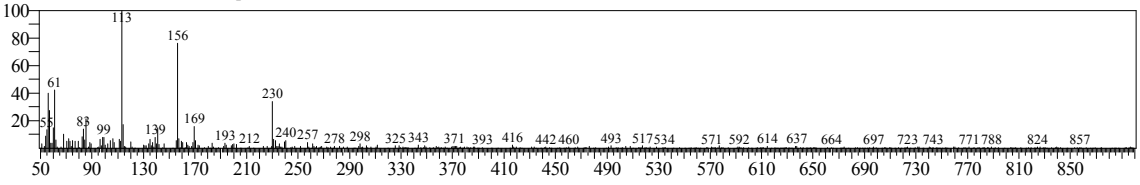
<< Target >>
Line#:42 R.Time:22.267(Scan#:2073) MassPeaks:527
RawMode:Averaged 22.258-22.275(2072-2074) BasePeak:154.20(406275)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



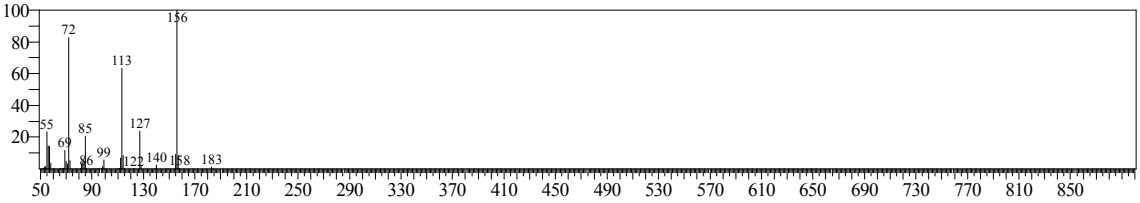
Hit#:1 Entry:81070 Library:NIST17.lib
SI:91 Formula:C11H18N2O2 CAS:5654-86-4 MolWeight:210 RetIndex:1699
CompName:Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-



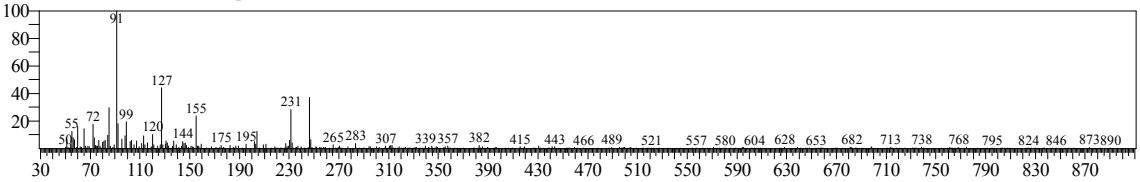
<< Target >>
Line#:43 R.Time:27.133(Scan#:2657) MassPeaks:413
RawMode:Averaged 27.125-27.142(2656-2658) BasePeak:113.15(3232)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



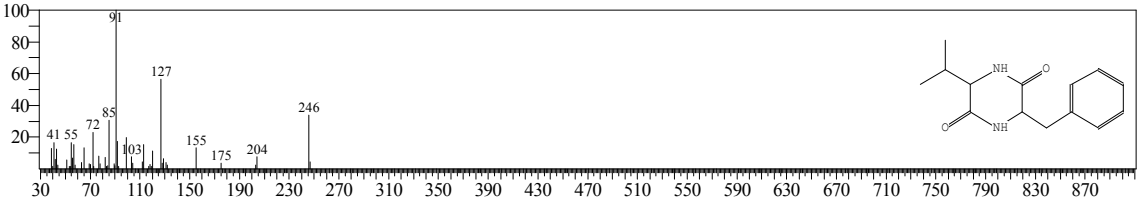
Hit#:1 Entry:137882 Library:Wiley9.lib
SI:63 Formula:C10H18N2O2 CAS:5625-44-5 MolWeight:198 RetIndex:0
CompName:3,6-Diisopropylpiperazin-2,5-dione $$ 3,6-Diisopropyl-2,5-piperazinedione $$ 3,6-Diisopropyl-2,5-piperazinedione (computer-generated name) $$



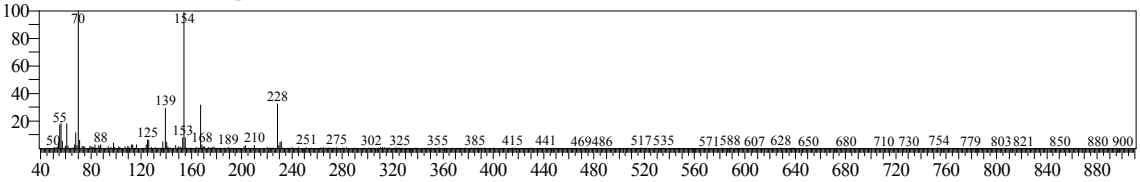
<< Target >>
Line#:44 R.Time:29.150(Scan#:2899) MassPeaks:484
RawMode:Averaged 29.142-29.158(2898-2900) BasePeak:91.15(5256)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



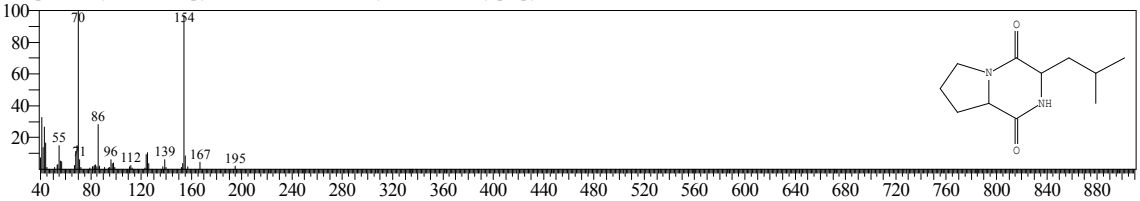
Hit#:1 Entry:118467 Library:NIST17.lib
SI:77 Formula:C14H18N2O2 CAS:14474-71-6 MolWeight:246 RetIndex:1976
CompName:2,5-Piperazinedione, 3-benzyl-6-isopropyl-



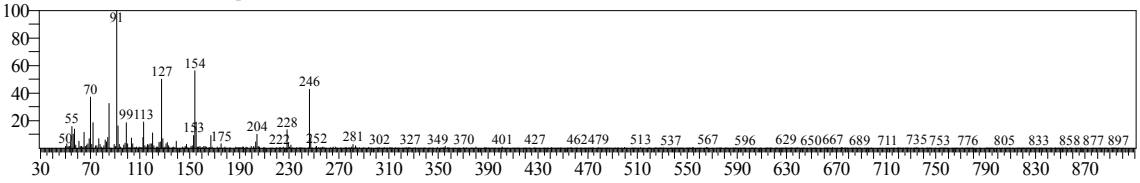
<< Target >>
Line#:45 R.Time:29.425(Scan#:2932) MassPeaks:499
RawMode:Averaged 29.417-29.433(2931-2933) BasePeak:70.15(15874)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



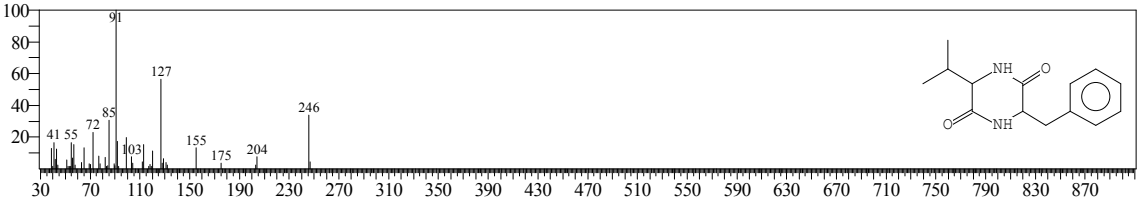
Hit#:1 Entry:81070 Library:NIST17.lib
SI:77 Formula:C11H18N2O2 CAS:5654-86-4 MolWeight:210 RetIndex:1699
CompName:Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-



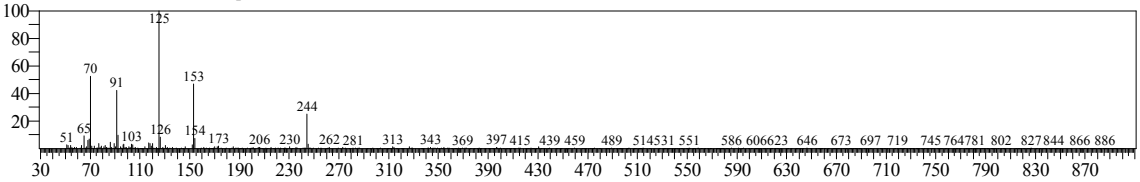
<< Target >>
Line#:46 R.Time:29.833(Scan#:2981) MassPeaks:569
RawMode:Averaged 29.825-29.842(2980-2982) BasePeak:91.15(15193)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



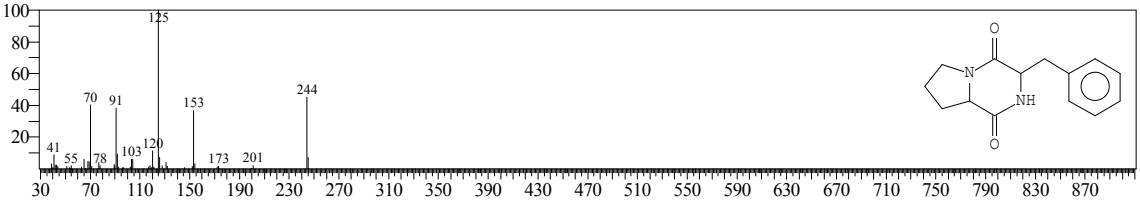
Hit#:1 Entry:65433 Library:NIST147.LIB
SI:81 Formula:C14H18N2O2 CAS:14474-71-6 MolWeight:246 RetIndex:0
CompName:2,5-Piperazinedione, 3-benzyl-6-isopropyl- $$ 3-Benzyl-6-isopropyl-2,5-piperazinedione # $$



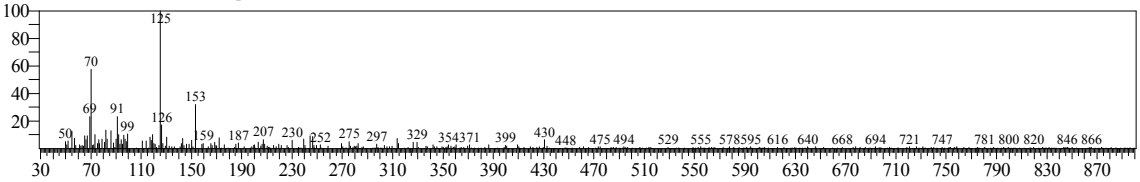
<< Target >>
Line#:47 R.Time:31.242(Scan#:3150) MassPeaks:462
RawMode:Averaged 31.233-31.250(3149-3151) BasePeak:125.20(15078)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



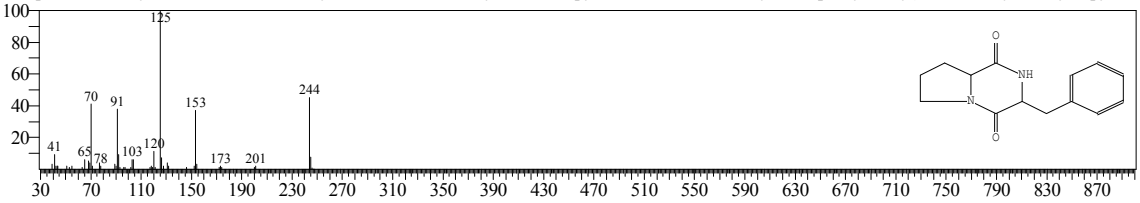
Hit#:1 Entry:64408 Library:NIST147.LIB
SI:87 Formula:C14H16N2O2 CAS:14705-60-3 MolWeight:244 RetIndex:0
CompName:Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(phenylmethyl)- $$ 3-Benzylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione # $$



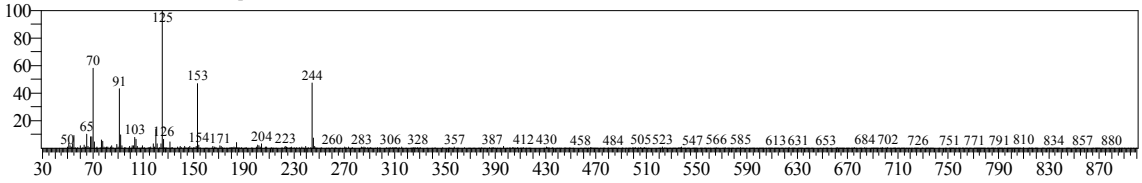
<< Target >>
Line#:48 R.Time:31.317(Scan#:3159) MassPeaks:438
RawMode:Averaged 31.308-31.325(3158-3160) BasePeak:125.20(2860)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



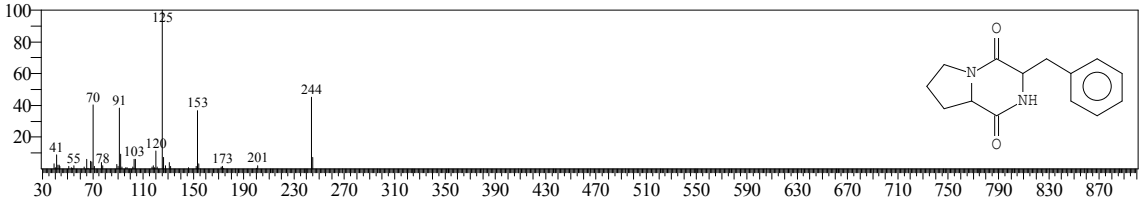
Hit#:1 Entry:245346 Library:Wiley9.lib
SI:60 Formula:C14H16N2O2 CAS:14705-60-3 MolWeight:244 RetIndex:0
CompName:3-benzyl-1,4-diaza-2,5-dioxobicyclo[4.3.0]nonane $$ Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(phenylmethyl)- $$ 3-Benzylhexahydropyrrol



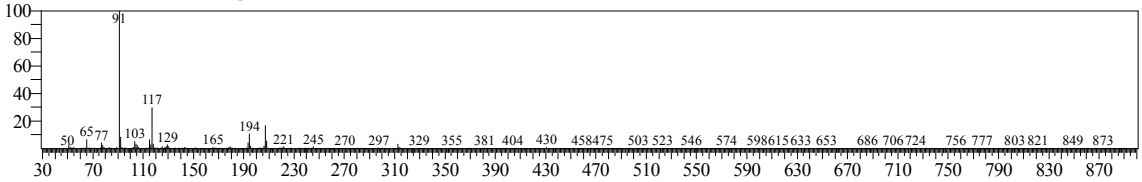
<< Target >>
Line#:49 R.Time:32.033(Scan#:3245) MassPeaks:509
RawMode:Averaged 32.025-32.042(3244-3246) BasePeak:125.20(15856)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



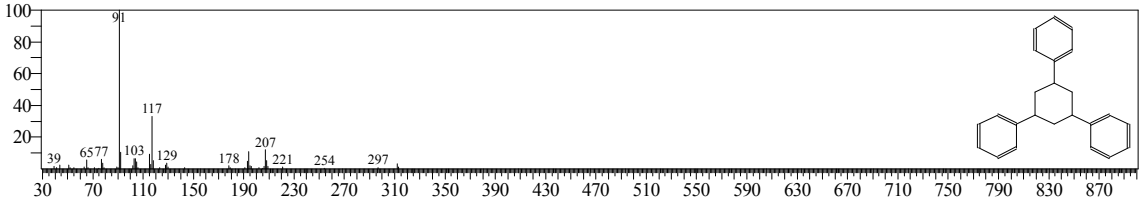
Hit#:1 Entry:64408 Library:NIST147.LIB
SI:89 Formula:C14H16N2O2 CAS:14705-60-3 MolWeight:244 RetIndex:0
CompName:Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(phenylmethyl)- $$ 3-Benzylhexahydropyrrolo[1,2-a]pyrazine-1,4-dione # $$



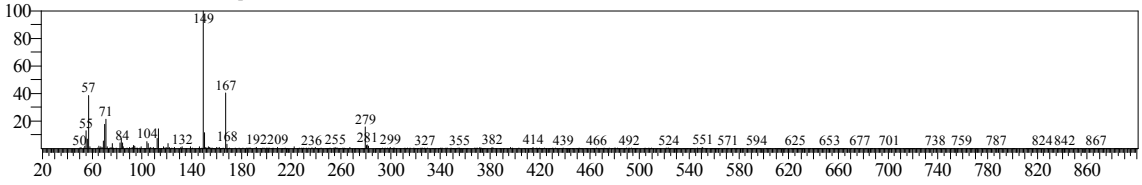
<< Target >>
Line#:50 R.Time:32.250(Scan#:3271) MassPeaks:459
RawMode:Averaged 32.242-32.258(3270-3272) BasePeak:91.15(59187)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



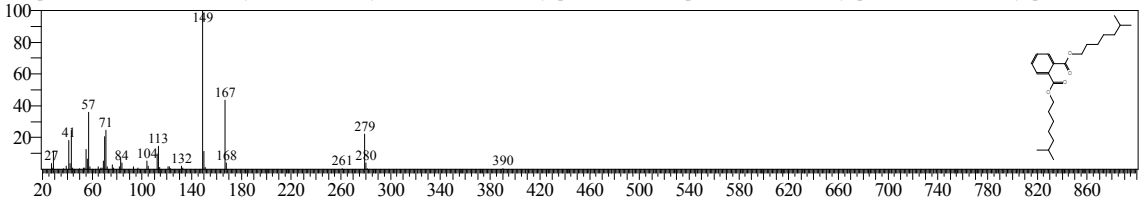
Hit#:1 Entry:190281 Library:NIST17.lib
SI:93 Formula:C24H24 CAS:28336-57-4 MolWeight:312 RetIndex:2624
CompName:Cyclohexane, 1,3,5-triphenyl-



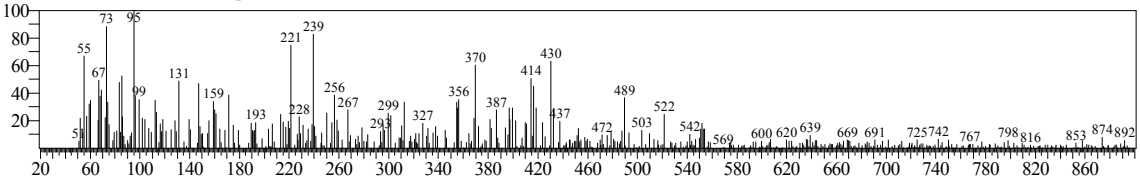
<< Target >>
Line#:51 R.Time:33.825(Scan#:3460) MassPeaks:496
RawMode:Averaged 33.817-33.833(3459-3461) BasePeak:149.15(21316)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



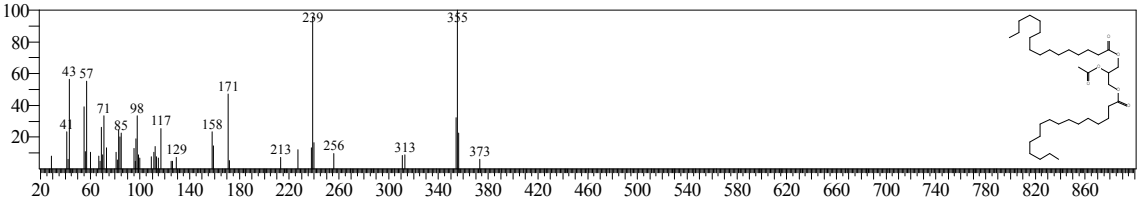
Hit#:1 Entry:530942 Library:Wiley9.lib
SI:93 Formula:C24H38O4 CAS:27554-26-3 MolWeight:390 RetIndex:0
CompName:1,2-Benzenedicarboxylic acid, diisooctyl ester (CAS) $$ Isooctyl phthalate $$ Hexaplas M/O $$ Diisooctyl phthalate $$ Di-isooctyl phthalate $$ IS



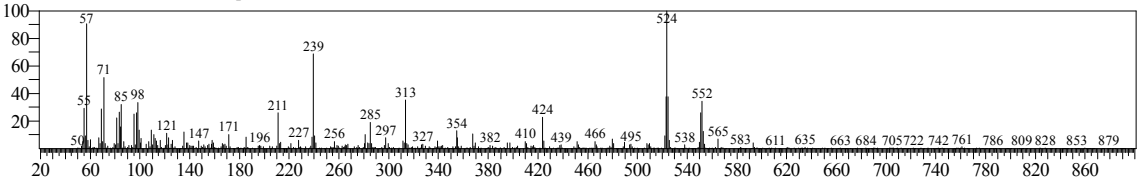
<< Target >>
Line#:52 R.Time:36.167(Scan#:3741) MassPeaks:482
RawMode:Averaged 36.158-36.175(3740-3742) BasePeak:95.15(772)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



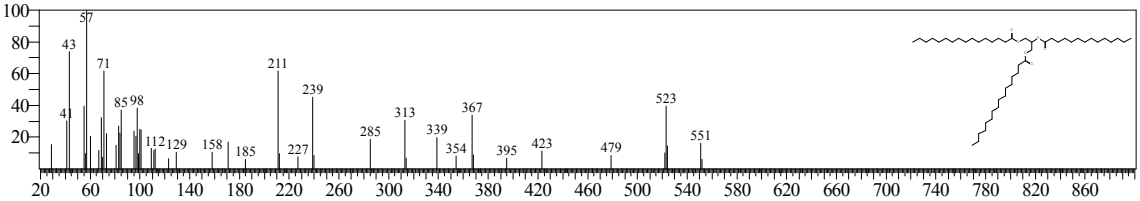
Hit#:1 Entry:303604 Library:NIST17.lib
SI:44 Formula:C37H70O6 CAS:58546-06-8 MolWeight:610 RetIndex:4137
CompName:Glycerol 2-acetate 1,3-dipalmitate



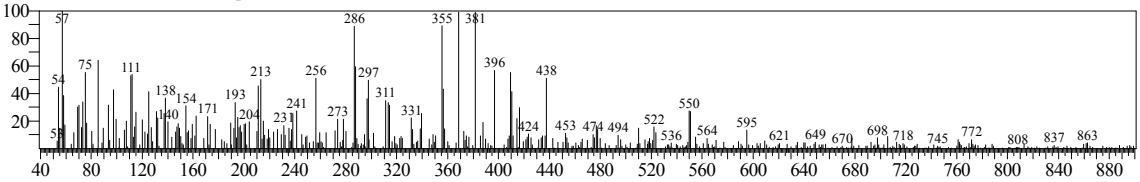
<< Target >>
Line#:53 R.Time:36.667(Scan#:3801) MassPeaks:508
RawMode:Averaged 36.658-36.675(3800-3802) BasePeak:523.80(7999)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



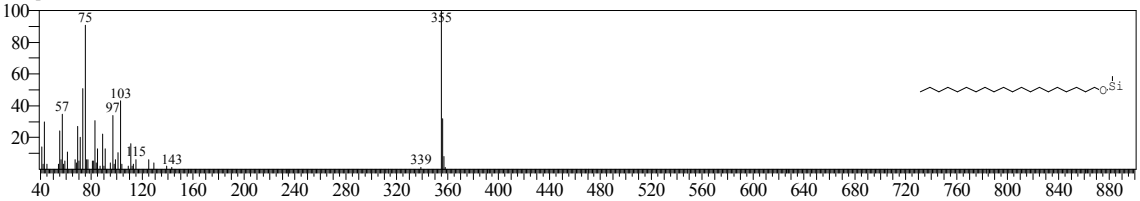
Hit#:1 Entry:146822 Library:NIST147.LIB
SI:77 Formula:C49H94O6 CAS:56599-89-4 MolWeight:778 RetIndex:0
CompName:Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester $$ 3-(Palmitoyloxy)-2-(tetradecanoyloxy)propyl palmitate # $$



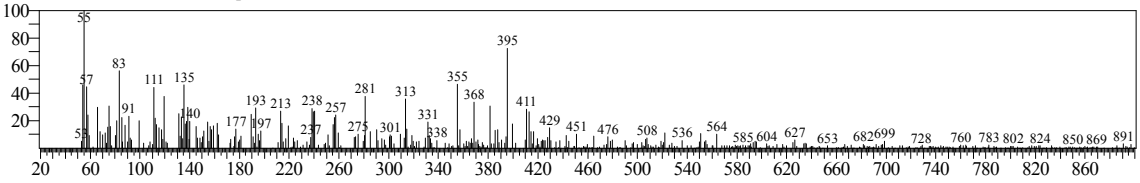
<< Target >>
Line#:54 R.Time:38.383(Scan#:4007) MassPeaks:439
RawMode:Averaged 38.375-38.392(4006-4008) BasePeak:57.10(1040)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



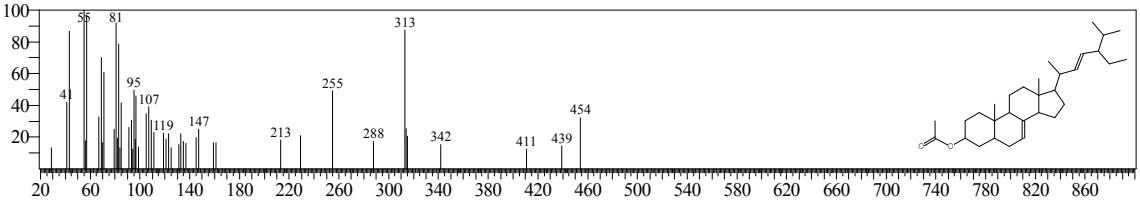
Hit#:1 Entry:503883 Library:Wiley9.lib
SI:34 Formula:C23H50OSi CAS:0-00-0 MolWeight:370 RetIndex:0
CompName:1HO-20:0 TMS



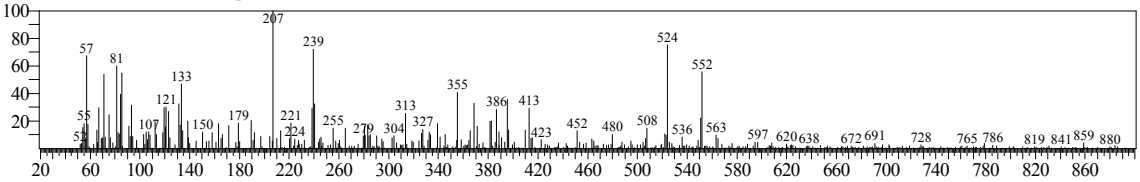
<< Target >>
Line#:55 R.Time:38.600(Scan#:4033) MassPeaks:456
RawMode:Averaged 38.592-38.608(4032-4034) BasePeak:55.10(1317)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



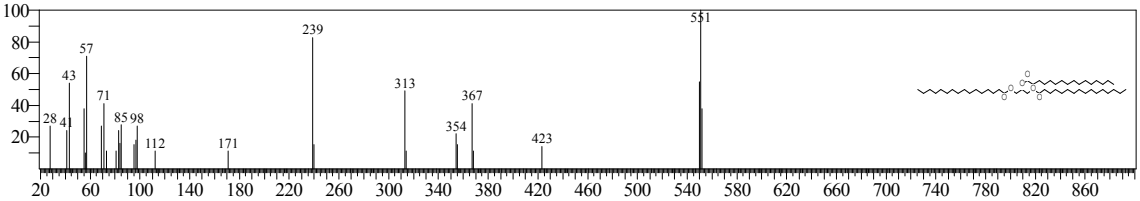
Hit#:1 Entry:137678 Library:NIST147.LIB
SI:41 Formula:C31H50O2 CAS:4651-46-1 MolWeight:454 RetIndex:0
CompName:Stigmasta-7,22-dien-3-ol, acetate, (3.beta.,5.alpha.,22E)- $$ 5.alpha.-Stigmasta-7,22-dien-3.beta.-ol, acetate $$ .alpha.-Spinasterol acetate $$ .alpha



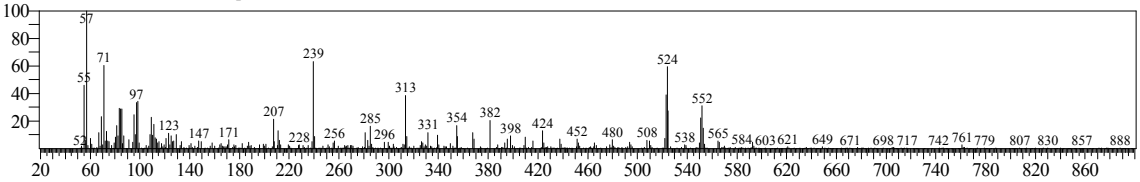
<< Target >>
Line#:56 R.Time:38.867(Scan#:4065) MassPeaks:456
RawMode:Averaged 38.858-38.875(4064-4066) BasePeak:207.15(1558)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



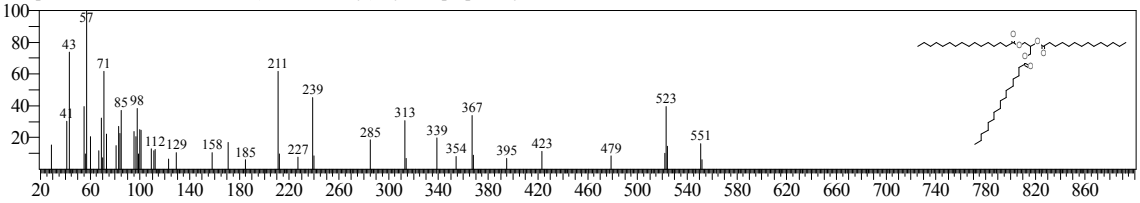
Hit#:1 Entry:658901 Library:Wiley9.lib
SI:42 Formula:C51H98O6 CAS:555-44-2 MolWeight:806 RetIndex:0
CompName:Hexadecanoic acid, 1,2,3-propanetriyl ester (CAS) $$ Tripalmitin $$ GLYCERYL TRIHEXADECANOATE $$ Palmitin, tri- $$ Spezialfett 116 $$ .a



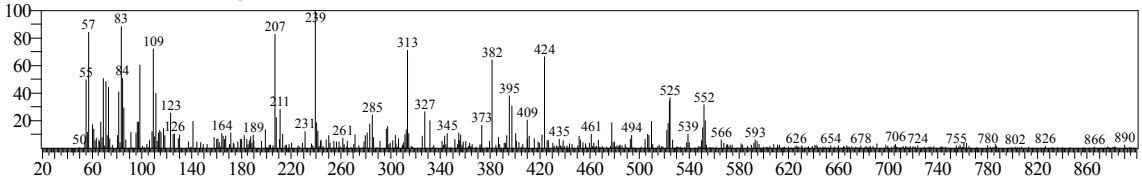
<< Target >>
Line#:57 R.Time:39.900(Scan#:4189) MassPeaks:503
RawMode:Averaged 39.892-39.908(4188-4190) BasePeak:57.10(7914)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



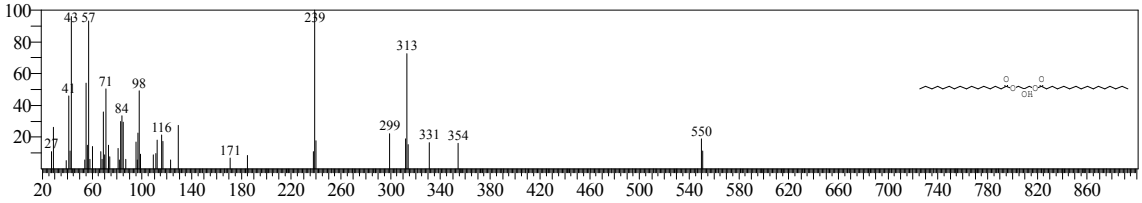
Hit#:1 Entry:306120 Library:NIST17.lib
SI:74 Formula:C49H94O6 CAS:56599-89-4 MolWeight:778 RetIndex:5330
CompName:Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester



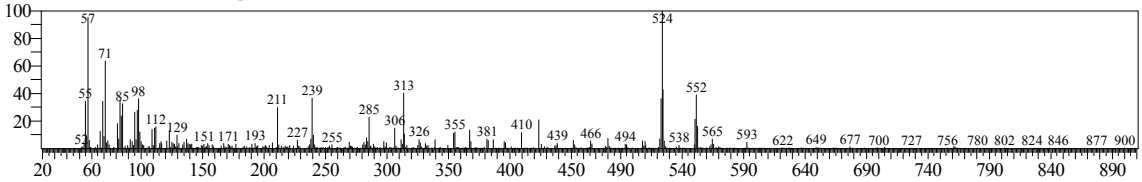
<< Target >>
Line#:58 R.Time:40.233(Scan#:4229) MassPeaks:449
RawMode:Averaged 40.225-40.242(4228-4230) BasePeak:239.40(2196)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



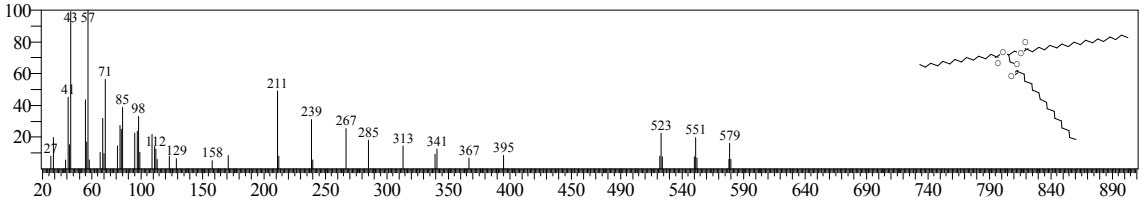
Hit#:1 Entry:386723 Library:WILEY8.LIB
SI:58 Formula:C35H68O5 CAS:502-52-3 MolWeight:568 RetIndex:0
CompName:HEXADECANOIC ACID, 2-HYDROXY-1,3-PROPANEDIYL ESTER $$ 2-HYDROXY-3-(PALMITOYLOXY)PROPYL PALMITATE # $$ .ALP



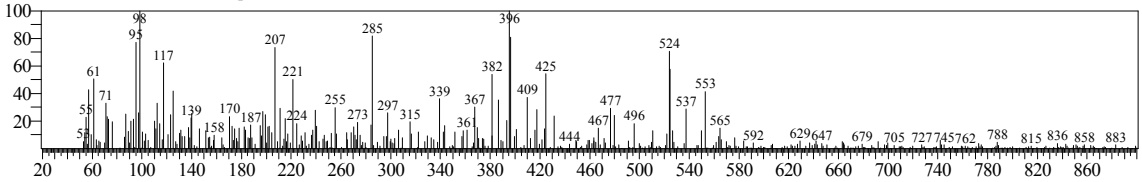
<< Target >>
Line#:59 R.Time:41.267(Scan#:4353) MassPeaks:523
RawMode:Averaged 41.258-41.275(4352-4354) BasePeak:523.85(11170)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



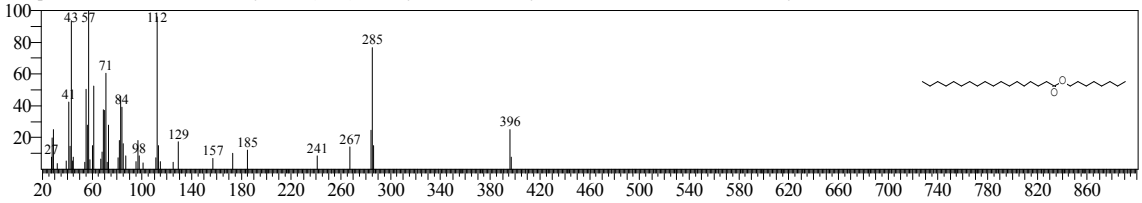
Hit#:1 Entry:397617 Library:WILEY8.LIB
SI:75 Formula:C51H98O6 CAS:56554-26-8 MolWeight:806 RetIndex:0
CompName:OCTADECANOIC ACID, 3-[(1-OXOHEXADECYL)OXY]-2-[(1-OXOTETRADECYL)OXY]PROPYL ESTER $$ 3-(PALMITOYLOXY)-2-(TET



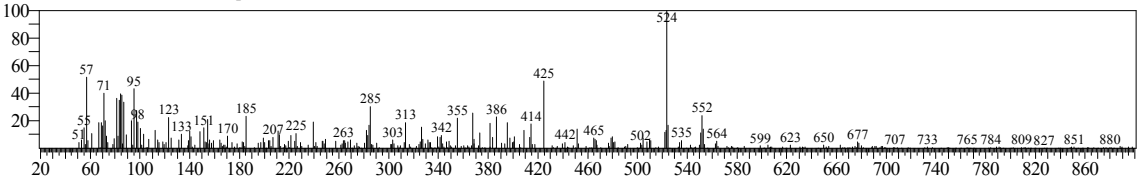
<< Target >>
Line#:60 R.Time:41.767(Scan#:4413) MassPeaks:419
RawMode:Averaged 41.758-41.775(4412-4414) BasePeak:395.60(1083)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



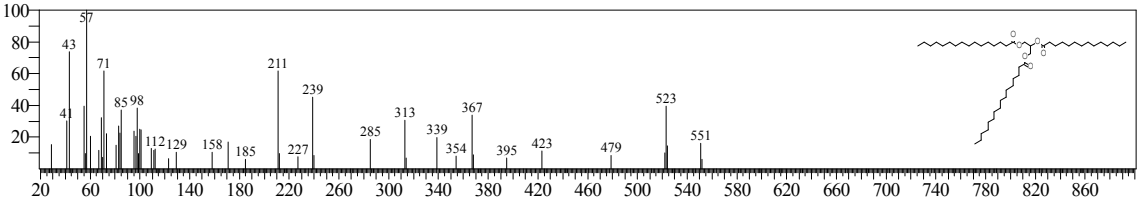
Hit#:1 Entry:538086 Library:Wiley9.lib
SI:35 Formula:C26H52O2 CAS:109-36-4 MolWeight:396 RetIndex:0
CompName:Octadecanoic acid, octyl ester (CAS) $$ Octyl stearate $$ Octyl octadecanoate $$ Stearic acid, octyl ester $$ OCTADECANSAEURE, OCTYLEST



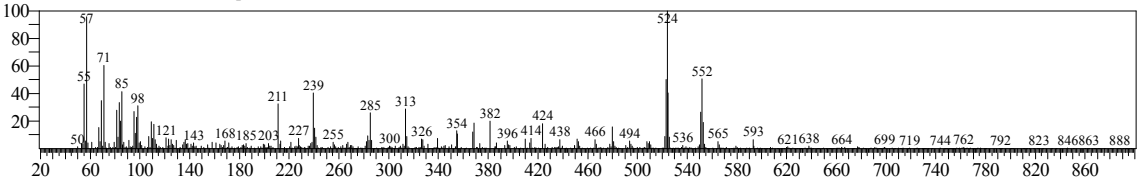
<< Target >>
Line#:61 R.Time:42.133(Scan#:4457) MassPeaks:368
RawMode:Averaged 42.125-42.142(4456-4458) BasePeak:523.80(2583)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



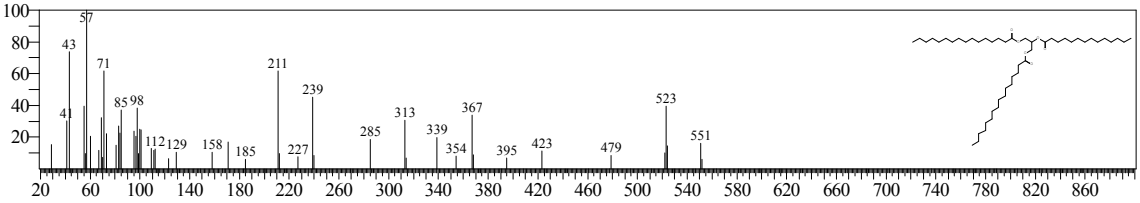
Hit#:1 Entry:306120 Library:NIST17.lib
SI:58 Formula:C49H94O6 CAS:56599-89-4 MolWeight:778 RetIndex:5330
CompName:Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester



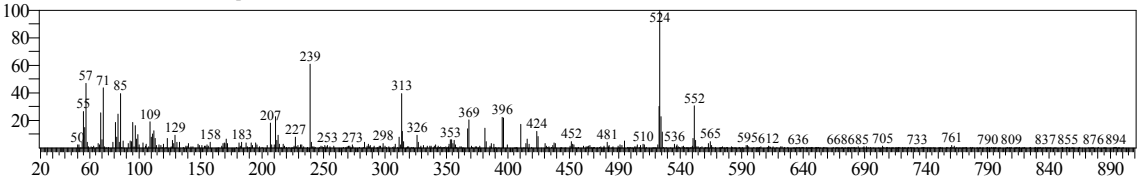
<< Target >>
Line#:62 R.Time:43.175(Scan#:4582) MassPeaks:522
RawMode:Averaged 43.167-43.183(4581-4583) BasePeak:523.85(9048)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Hit#:1 Entry:146822 Library:NIST147.LIB
SI:73 Formula:C49H94O6 CAS:56599-89-4 MolWeight:778 RetIndex:0
CompName:Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester $$ 3-(Palmitoyloxy)-2-(tetradecanoyloxy)propyl palmitate # $$



<< Target >>
Line#:63 R.Time:44.758(Scan#:4772) MassPeaks:521
RawMode:Averaged 44.750-44.767(4771-4773) BasePeak:523.80(7120)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Hit#:1 Entry:146822 Library:NIST147.LIB
SI:65 Formula:C49H94O6 CAS:56599-89-4 MolWeight:778 RetIndex:0
CompName:Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester $$ 3-(Palmitoyloxy)-2-(tetradecanoyloxy)propyl palmitate # $$

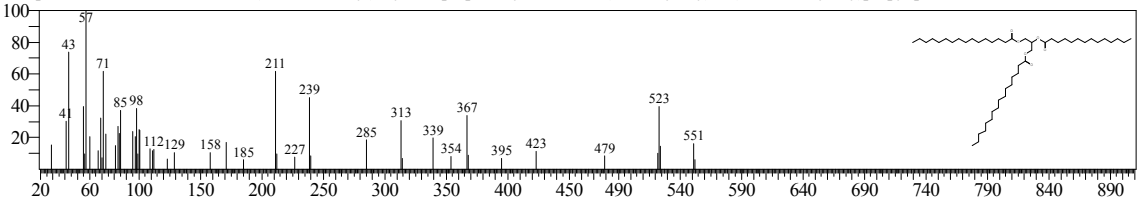


Figure 2. Representative GC–MS mass spectra of major compounds identified from the ethyl acetate extract of isolate LU_3. Spectral matching was performed using the NIST 17 and Wiley 9 libraries. Only compounds with a library match score ≥90% were considered for biological interpretation.

Table 1. GC-MS results of ethyl acetate extract compounds from LU_3 bacterial isolate

Peak	Retention Time	Identified Compound	Library Match (%)	Area (%)
1	5.090	3 methyl pentanoic acid	77	4.95
2	5.772	Styrene	95	0.08
3	6.144	Pentanoic acid	78	0.21
4	6.460	2-Methoxyethoxy-2-methylethyl 2-[(2' hydroxyethoxy) ethoxy]ethyl ether	74	0.07
5	6.617	Thiirane	78	0.01
6	6.746	2-[2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy] ethoxy]ethyl 2,2,3,3,3-pentafluor	65	0.02
7	6.792	1,2-Hexanediol	61	0.04
8	7.236	2,2,4,4,6,6,8,8-octamethyl-1,3,5,7,2,4,6,8-tetraoxatetrasiloca	77	0.02
9	7.416	Cyclotetrasiloxane, octamethyl	64	0.04
10	7.525	3-Cyano-6-oxopyrazolo[3,4-d]pyrimidin-4-thione	49	0.01
11	9.156	Cyclotrisiloxane, hexamethyl-	71	0.01
12	9.350	2-[(2'-Ethylphenyl)(2",4",6'-trimethylphenyl)methoxy]ethan	63	0.00
13	9.853	Cyclopentasiloxane, decamethyl- (CAS)	91	0.03
14	11.503	Cycloheptasiloxane, tetradecamethyl-	53	0.01
15	11.883	Dl-Norleucine amide, N,N,N'N'-tetramethy	79	0.42
16	12.025	Thiophene, 3-methoxy-	74	0.51
17	12.125	Guanazine	57	0.11
18	12.175	8-Chlorocapric acid	56	0.12
19	12.258	Butane-2-one, 3-methyl-3-(2-oxopropylamino)-	64	0.15
20	12.402	Cyclohexasiloxane, dodecamethyl	86	0.07
21	12.883	1,4-Dimethoxy-1,4,4a,5,8,8a-	55	0.01

		hexahydronaphthale		
22	13.125	Cyclopropanepropionic acid, 2-[(2-decylcyclopropyl)methyl]-, methyl ester	54	0.07
23	13.233	Methyl 3-methyl-3-(methoxy-chloro)amino-butanoate	61	0.05
24	13.417	Butanedioic acid, methyl- (CAS)	63	0.20
25	14.526	1,3-Propanediol, 2-amino-2-(hydroxymethyl)- (CAS)	88	31.08
26	15.892	Diisopropyl(methyl)phosphine	56	0.41
27	17.083	Cyclohexan, 1,2,3,4,5,6-hexadeutero	63	0.85
28	17.408	3-Methyl-2-butenoic acid, nonyl ester	55	0.42
29	17.633	(S)-4-Benzyl-2-oxazolidinone	57	0.68
30	17.758	Carbonic acid, monoamide, N-ethyl-, decyl ester	54	0.56
31	17.925	3-Isopropyl-6-methyl-piperazine-2,5-dione	69	0.36
32	18.014	2,5-Piperazinedione, 3-methyl-6-(1-methylethyl)	96	1.29
33	18.752	1,4-diazabicyclo[4.3.0]nonan-2,5-dione, 3-methyl	94	0.64
34	19.170	2,5-Piperazinedione, 3-methyl-6-(1-methylethyl)-	85	1.80
35	19.853	Cyclo(L-prolyl-L-valine)	98	10.95
36	20.113	3,6-Diisopropylpiperazin-2,5-dione	79	0.21
37	20.420	Cyclo(L-prolyl-L-valine)	87	7.05
38	21.065	Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-	65	0.09
39	21.454	Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(2-methylpropy)	92	6.12
40	21.828	Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(2-methylpropyl)	94	4.50
41	21.944	5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2-a]	91	6.14
42	22.268	Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(2-methylpropyl)	91	5.99
43	27.133	3,6-Diisopropylpiperazin-2,5-dione	63	0.02

44	29.150	2,5-Piperazinedione, 3-benzyl-6-isopropyl	77	0.10
45	29.429	Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(2-Methylpropyl)	77	0.28
46	29.832	2,5-Piperazinedione, 3-benzyl-6-isopropyl-	81	0.36
47	31.242	Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(phenylmethyl)-	87	0.21
48	31.317	3-benzyl-1,4-diaza-2,5-dioxobicyclo[4.3.0]nonane	60	0.13
49	32.033	Pyrrolo[1,2-a]pyrazine-1,4-dione,hexahydro-3-(phenylmethyl)	89	0.27
50	32.251	Cyclohexane, 1,3,5-triphenyl-	93	0.34
51	33.823	1,2-Benzenedicarboxylic acid, diisooctyl ester (CAS)	83	0.06
52	36.167	Glycerol 2-acetate 1,3-dipalmitate	44	0.02
53	36.668	Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester	77	0.39
54	38.383	1HO-20:0 TMS (trimethylsilyl)	34	0.54
55	38.600	Stigmasta-7,22-dien-3-ol, acetate, (3.beta.,5.alpha.,22E)	41	0.53
56	38.867	Hexadecanoic acid, 1,2,3-propanetriyl ester (CAS)	42	0.68
57	39.899	Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester	74	2.68
58	40.233	Hexadecanoic acid, 2-hydroxy-1, 3-propanediyl ester	58	1.64
59	41.264	Octadecanoic acid, 3-[(1-oxohexadecyl)oxy]-2-[(1-oxotetradecy	75	2.54
60	41.767	Octadecanoic acid, octyl ester (CAS)	35	0.40
61	42.133	Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester	58	0.57
62	43.177	Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester	73	1.73
63	44.760	Hexadecanoic acid, 2-[(1-oxotetradecyl)oxy]-1,3-propanediyl ester	65	0.17