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Chromatogram C87-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-008.qgd

Peak Report TIC

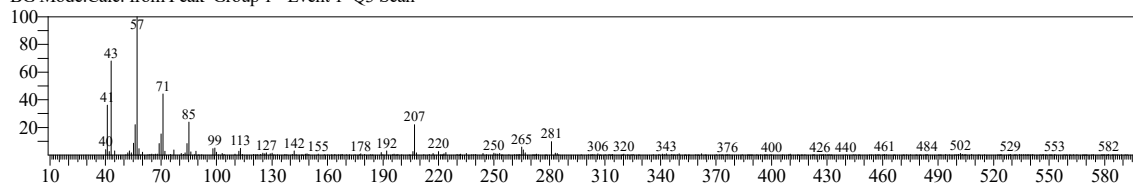| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.944	46154	23.13	25534	23.77	1.81	85	Dodecane
2	9.687	37976	19.03	27127	25.25	1.40	88	Undecane
3	15.471	50339	25.22	23467	21.84	2.15	84	2,4-Di-tert-butylphenol
4	31.914	50875	25.49	21393	19.91	2.38	33	Epinephrine-3TMS
5	31.955	14234	7.13	9910	9.22	1.44	23	2-Hydroxyhippuric acid-3TMS
		199578	100.00	107431	100.00			

Library

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<< Target >>
Line#:1   R.Time:7.945(Scan#:690) MassPeaks:277
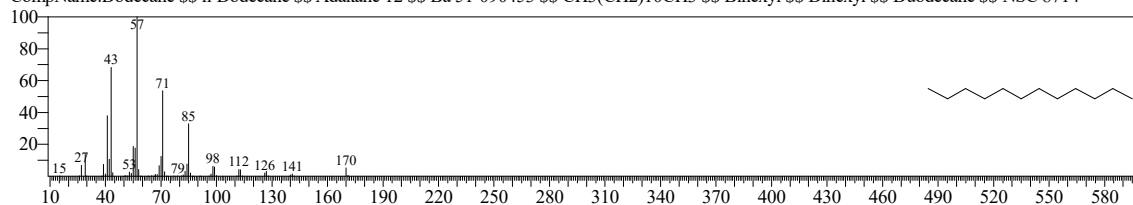RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(5990)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:30057 Library:NIST20M1.lib
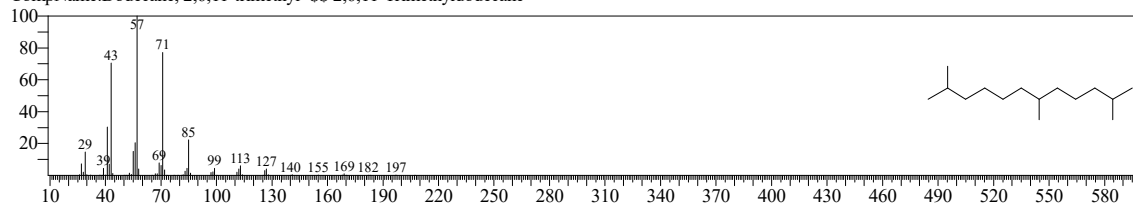SI:85 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:2 Entry:25291 Library:NIST20R.lib
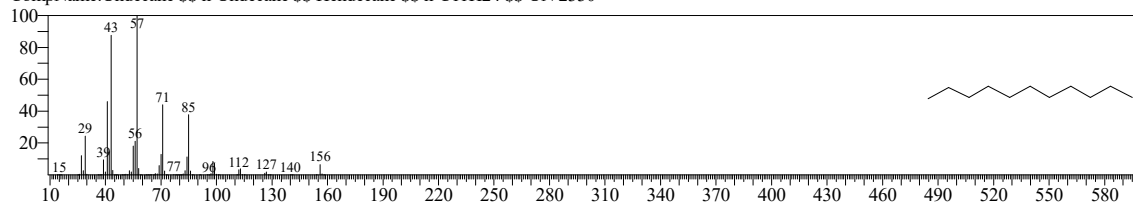SI:85 Formula:C15H32 CAS:31295-56-4 MolWeight:212 RetIndex:1320
CompName:Dodecane, 2,6,11-trimethyl- $$ 2,6,11-Trimethyldodecane

Hit#:3 Entry:12897 Library:NIST20R.lib
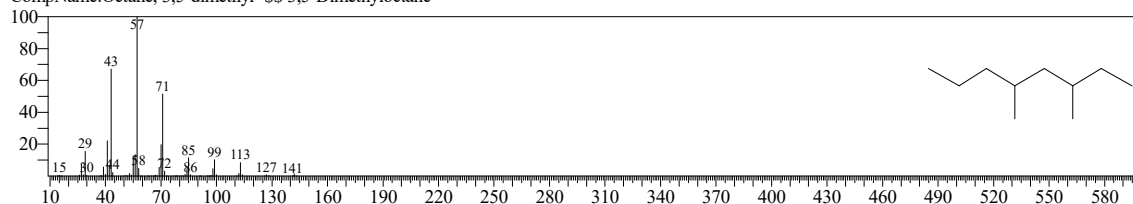SI:85 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:4 Entry:13631 Library:NIST20M1.lib
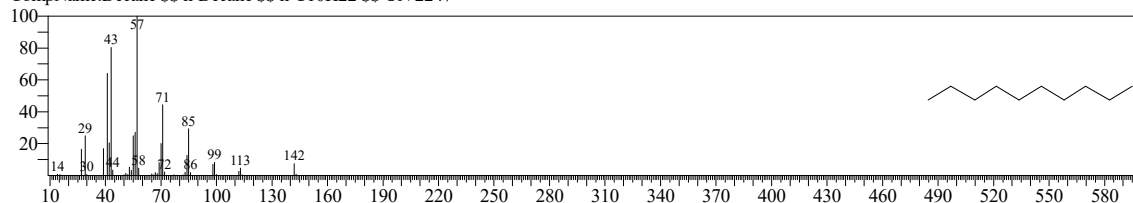SI:85 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887
CompName:Octane, 3,5-dimethyl- $$ 3,5-Dimethyloctane

Hit#:5 Entry:13604 Library:NIST20M1.lib
SI:84 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
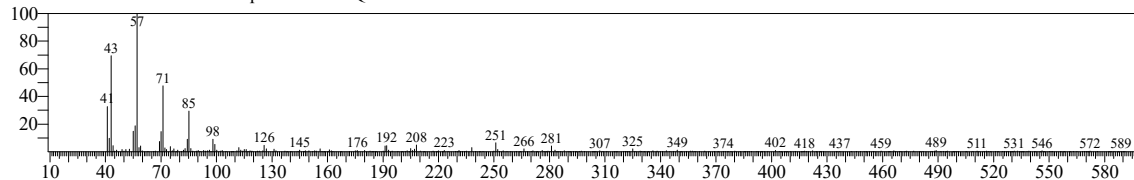CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

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<< Target >>
Line#:2 R.Time:9.685(Scan#:1038) MassPeaks:315
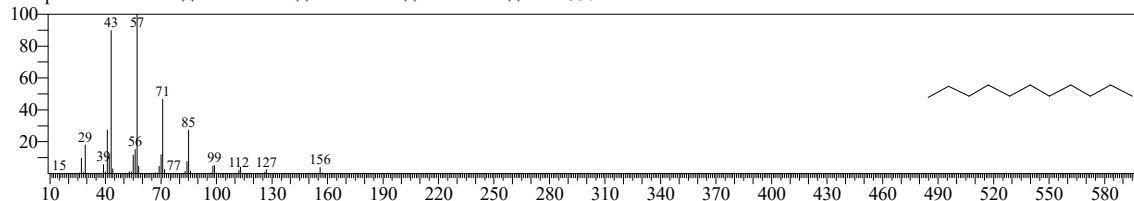RawMode:Averaged 9.680-9.690(1037-1039) BasePeak:57.05(5512)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:21042 Library:NIST20M1.lib
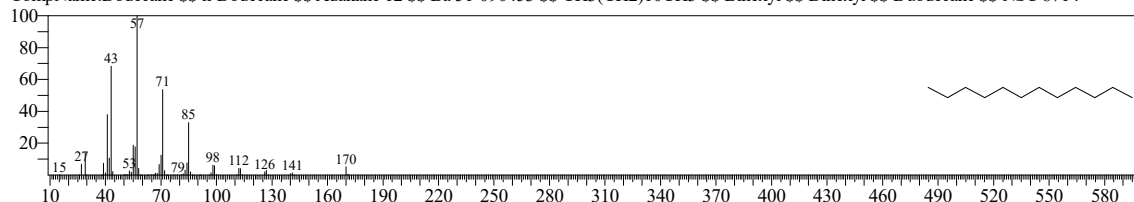SI:88 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:30057 Library:NIST20M1.lib
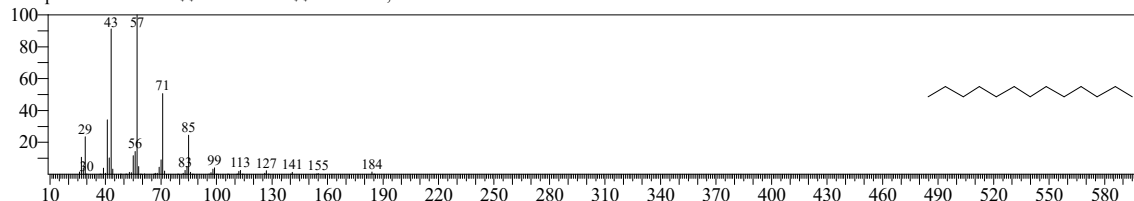SI:88 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:3 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
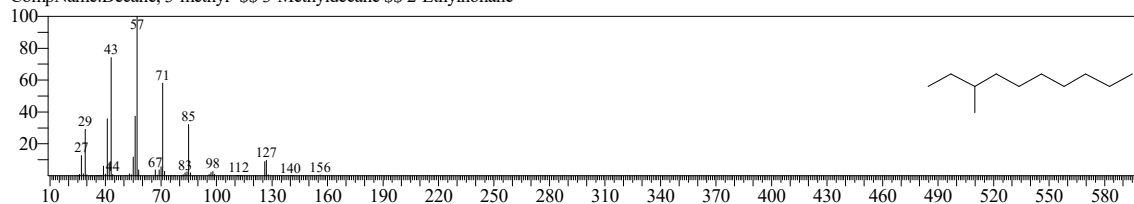CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:4 Entry:12893 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:13151-34-3 MolWeight:156 RetIndex:1051
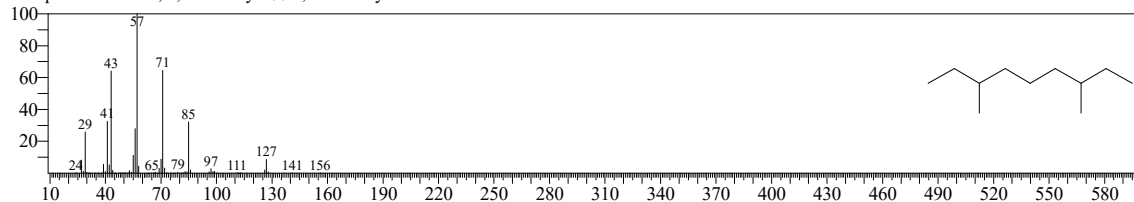CompName:Decane, 3-methyl- $$ 3-Methyldecane $$ 2-Ethylnonane

Hit#:5 Entry:21047 Library:NIST20M1.lib
SI:86 Formula:C11H24 CAS:17302-32-8 MolWeight:156 RetIndex:986
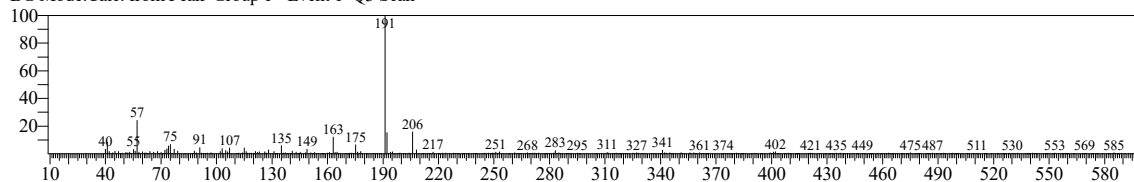CompName:Nonane, 3,7-dimethyl- $$ 3,7-Dimethylnonane

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<< Target >>
Line#:3   R.Time:15.470(Scan#:2195) MassPeaks:333
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.15(7298)
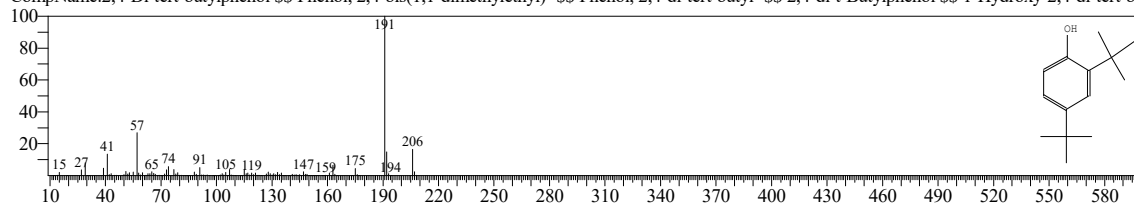BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:24086 Library:NIST20R.lib
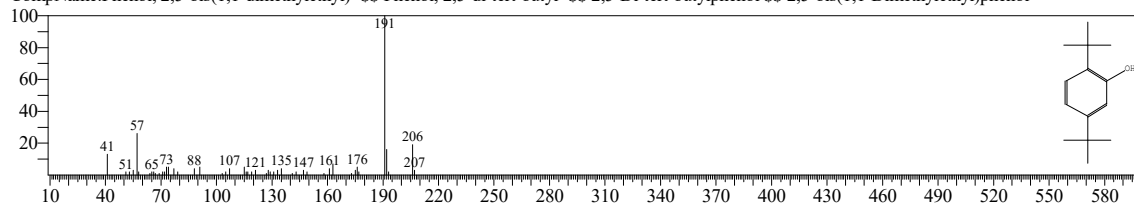SI:84 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu

Hit#:2 Entry:24098 Library:NIST20R.lib
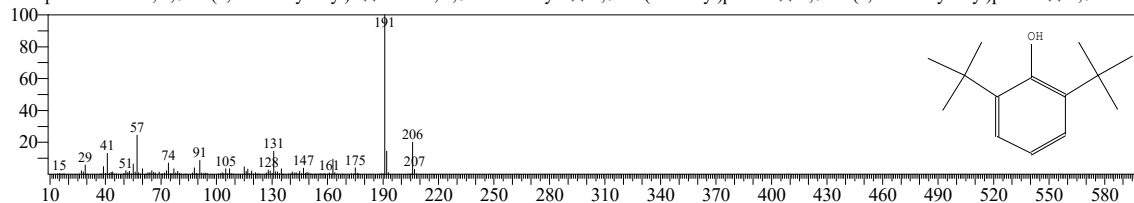SI:83 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol

Hit#:3 Entry:59031 Library:NIST20M1.lib
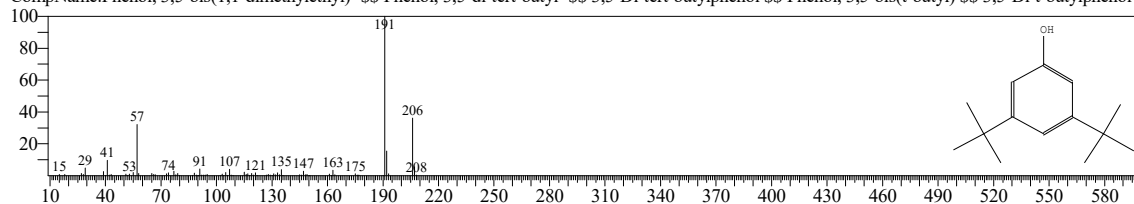SI:83 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

Hit#:4 Entry:24110 Library:NIST20R.lib
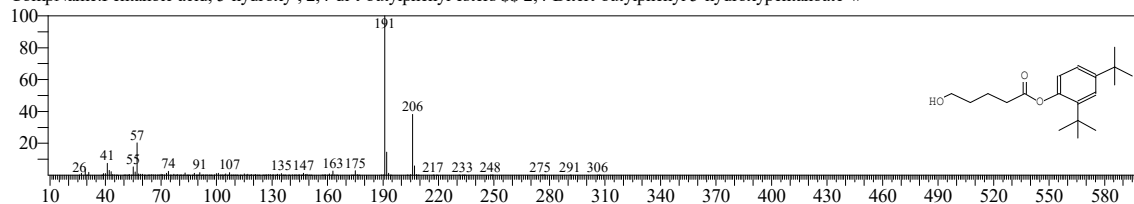SI:81 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $

Hit#:5 Entry:170993 Library:NIST20M1.lib
SI:79 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255
CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters $$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #
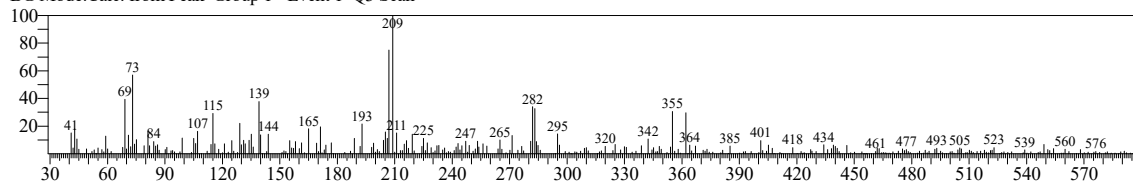
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<< Target >>
Line#:4   R.Time:31.915(Scan#:5484) MassPeaks:328
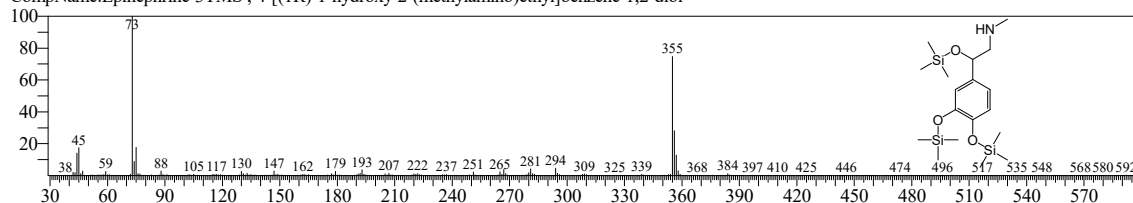RawMode:Averaged 31.910-31.920(5483-5485) BasePeak:209.00(1646)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
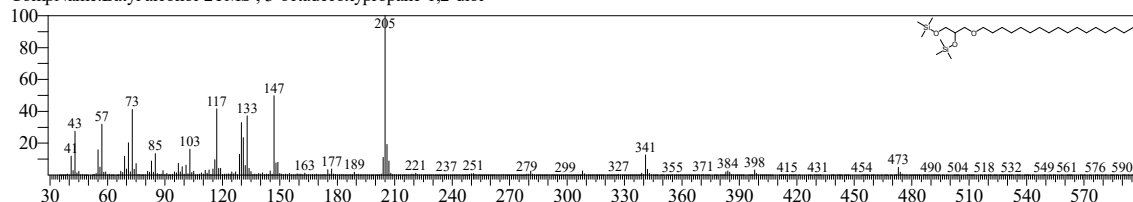SI:33 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:2 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
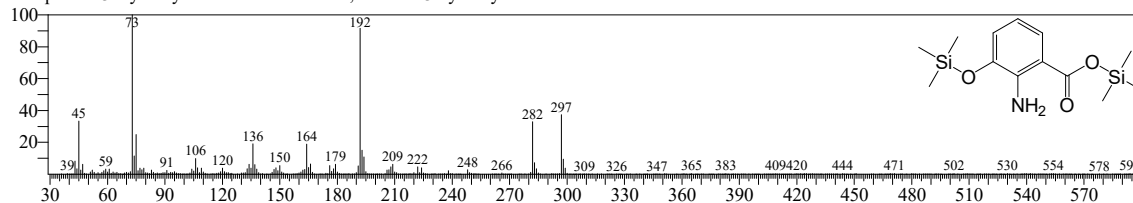SI:32 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

Hit#:3 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
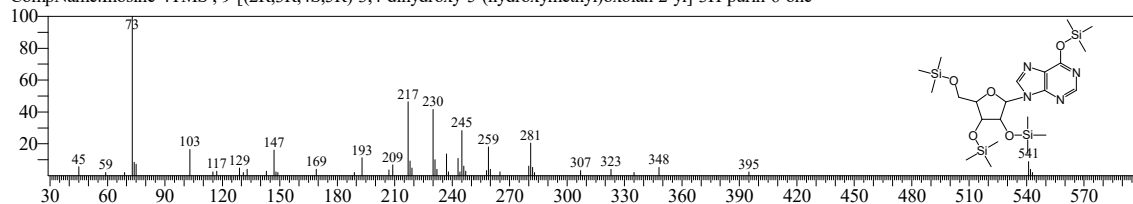SI:32 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:4 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
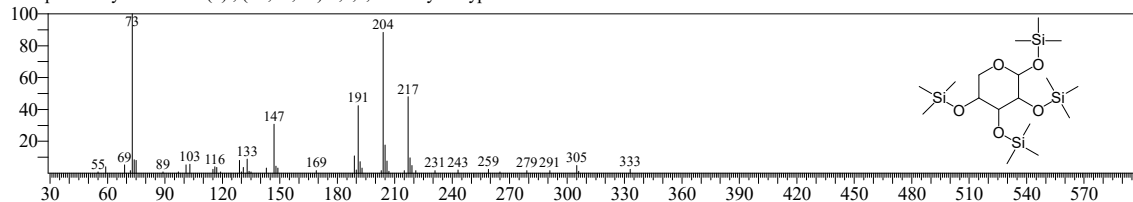SI:32 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

Hit#:5 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
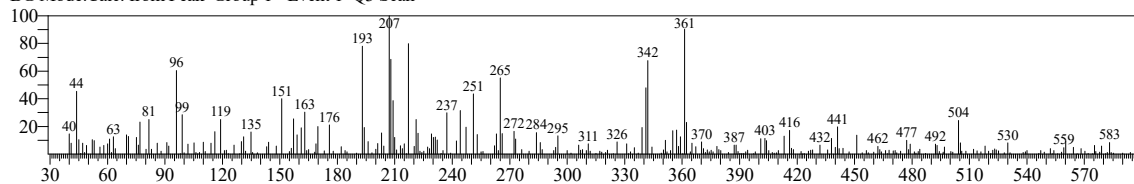CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

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<< Target >>
Line#:5　R.Time:31.955(Scan#:5492)　MassPeaks:298
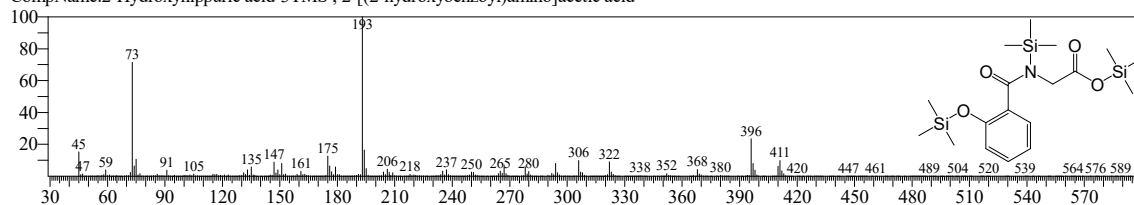RawMode:Averaged 31.950-31.960(5491-5493) BasePeak:207.05(819)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1　Entry:420　Library:OA_TMS_DB5_67min_V3.lib
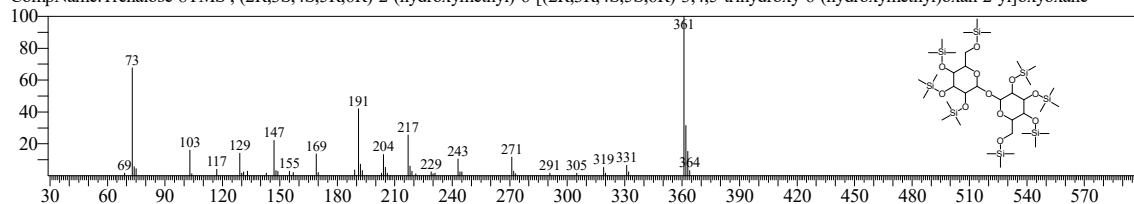SI:23　Formula:C18H33NO4Si3　CAS:487-54-7　MolWeight:411　RetIndex:1973
CompName:2-Hydroxyhippuric acid-3TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid

Hit#:2　Entry:552　Library:OA_TMS_DB5_67min_V3.lib
SI:23　Formula:C36H86O11Si8　CAS:99-20-7　MolWeight:918　RetIndex:2812
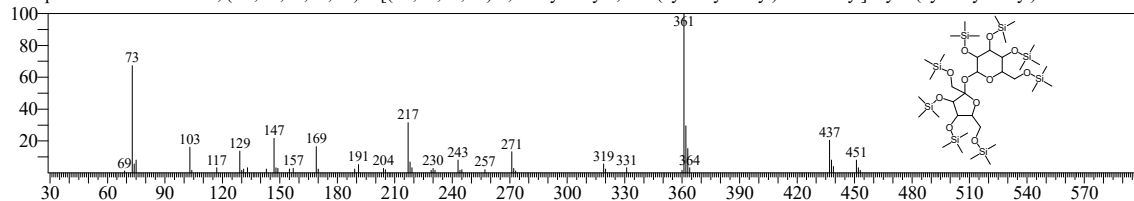CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

Hit#:3　Entry:541　Library:OA_TMS_DB5_67min_V3.lib
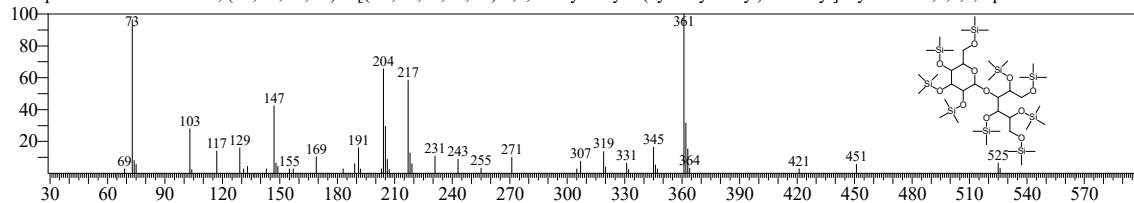SI:21　Formula:C36H86O11Si8　CAS:57-50-1　MolWeight:918　RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3

Hit#:4　Entry:559　Library:OA_TMS_DB5_67min_V3.lib
SI:20　Formula:C39H96O11Si9　CAS:585-88-6　MolWeight:992　RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:5　Entry:315　Library:OA_TMS_DB5_67min_V3.lib
SI:20　Formula:C16H30O4Si3　CAS:99-50-3　MolWeight:370　RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid