TNAU

Analyzed by	: Admin		
Analyzed	: 04-Aug-22 6:12:21 PM		
Sample Type	: Unknown		
Level #	: 1		
Sample Name	: C42-2		
Sample ID	: C42-2		
IS Amount	: [1]=1		
Sample Amount	: 1		
Dilution Factor	: 1		
Vial #	: 3		
Injection Volume	: 1.00		
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-003.qgd		
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-003.qgd		
Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm		
Org Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm		
Report File	:		
Tuning File	: D:\GCMS-8040NX\Aug 2022\Tuning Data\TUNING 04082022.qgt		
[Comment]			
Jerry samples			
Modified by	: Admin		
Modified	: 05-Aug-22 4:11:12 PM		

Chromatogram C42-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-003.qgd

Peak Report TIC

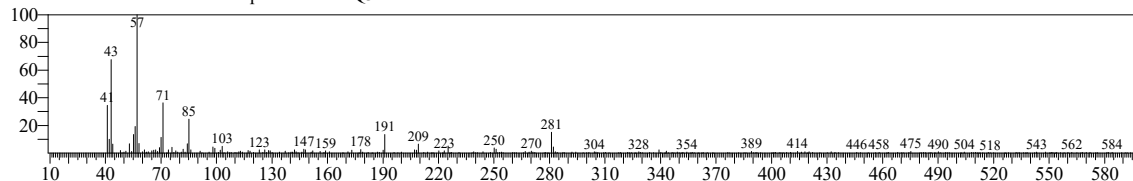| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.953	36448	6.01	19595	8.30	1.86	82	Tridecane
2	9.693	51131	8.43	27060	11.46	1.89	86	Undecane
3	16.472	23172	3.82	15390	6.52	1.51	86	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
4	19.927	360645	59.49	120866	51.19	2.98	98	Dimethyl palmitamine
5	28.713	25325	4.18	10609	4.49	2.39	29	Glutaric acid-2TMS
6	29.308	34739	5.73	11011	4.66	3.15	35	3-Hydroxybenzoic acid-2TMS
7	30.299	55908	9.22	13482	5.71	4.15	27	Trehalose-8TMS
8	30.727	8179	1.35	8366	3.54	0.98	35	Inosine-4TMS
9	30.937	10662	1.76	9729	4.12	1.10	35	Galactose-5TMS(1)
		606209	100.00	236108	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:7.955(Scan#:692) MassPeaks:283
RawMode:Averaged 7.950-7.960(691-693) BasePeak:57.10(4299)
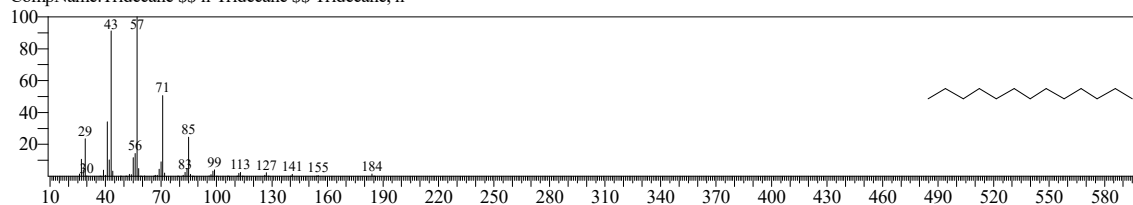BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:40226 Library:NIST20M1.lib
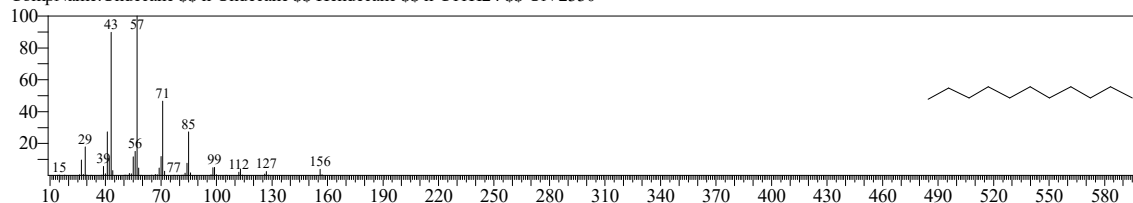SI:82 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:2 Entry:21042 Library:NIST20M1.lib
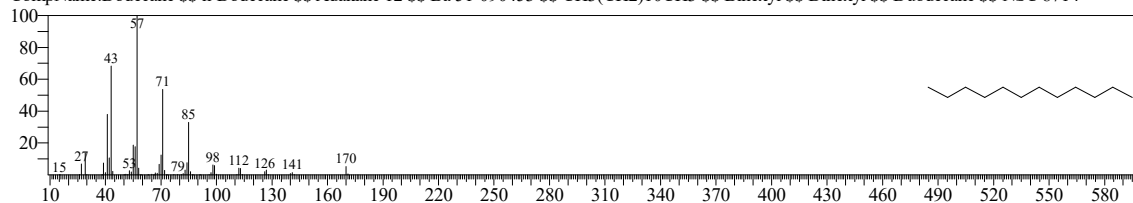SI:82 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:82 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#:4 Entry:40255 Library:NIST20M1.lib
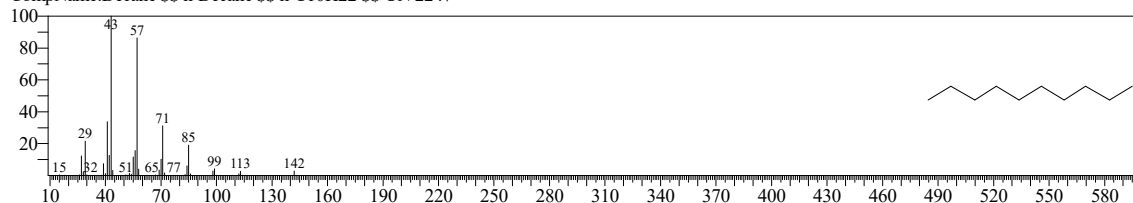SI:81 Formula:C13H28 CAS:62108-21-8 MolWeight:184 RetIndex:1185
CompName:Decane, 6-ethyl-2-methyl- $$ 6-Ethyl-2-methyldecane #

Hit#:5 Entry:9444 Library:NIST20R.lib
SI:81 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
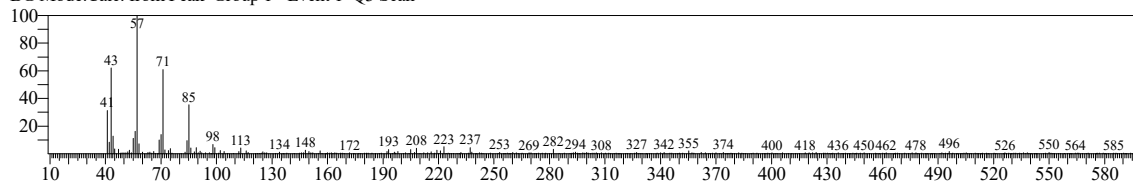CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

TNAU

<< Target >>
Line#:2 R.Time:9.695(Scan#:1040) MassPeaks:359
RawMode:Averaged 9.690-9.700(1039-1041) BasePeak:57.10(5156)
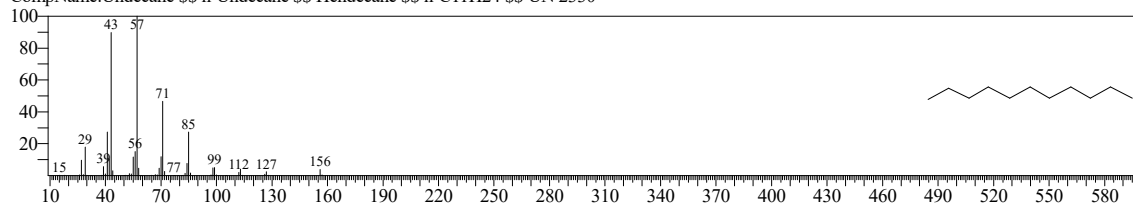BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:21042 Library:NIST20M1.lib
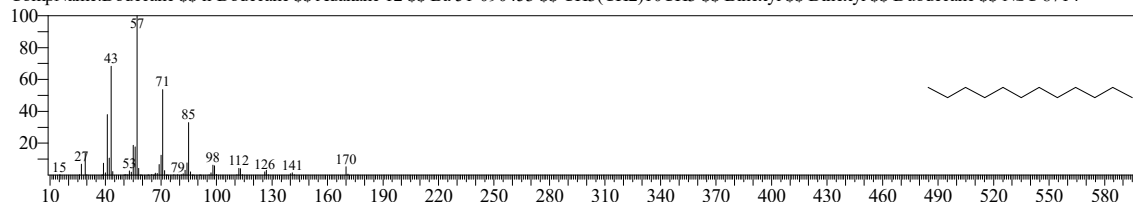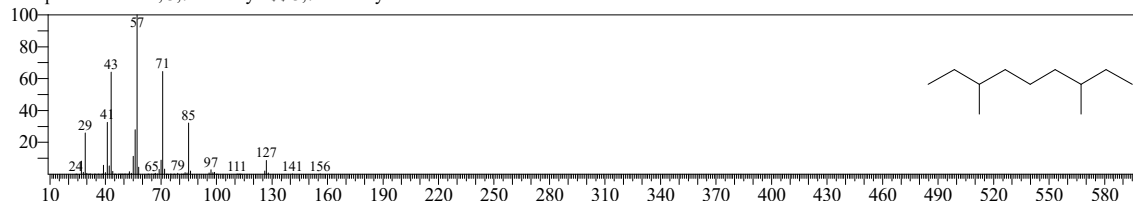SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:30057 Library:NIST20M1.lib
SI:86 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:21047 Library:NIST20M1.lib
SI:85 Formula:C11H24 CAS:17302-32-8 MolWeight:156 RetIndex:986
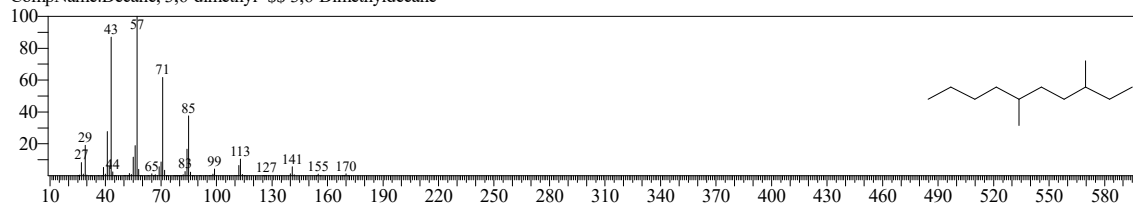CompName:Nonane, 3,7-dimethyl- $$ 3,7-Dimethylnonane

Hit#:4 Entry:30051 Library:NIST20M1.lib
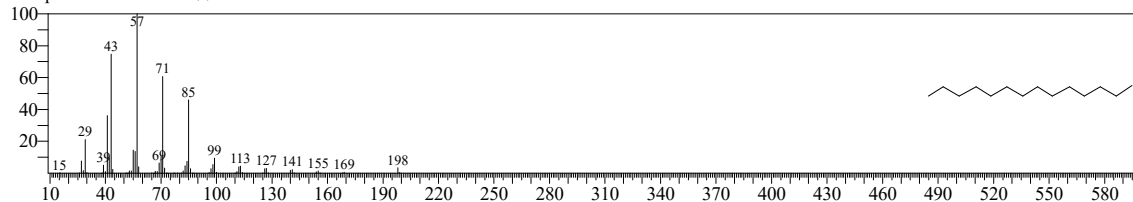SI:85 Formula:C12H26 CAS:17312-53-7 MolWeight:170 RetIndex:1086
CompName:Decane, 3,6-dimethyl- $$ 3,6-Dimethyldecane

Hit#:5 Entry:22497 Library:NIST20R.lib
SI:85 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
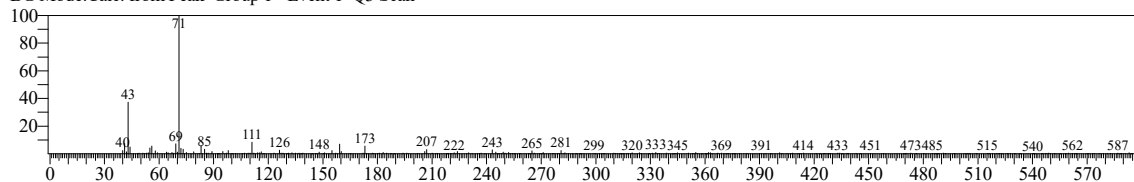CompName:Tetradecane $$ n-Tetradecane

TNAU

<< Target >>
Line#:3 R.Time:16.470(Scan#:2395) MassPeaks:268
RawMode:Averaged 16.465-16.475(2394-2396) BasePeak:71.00(6976)
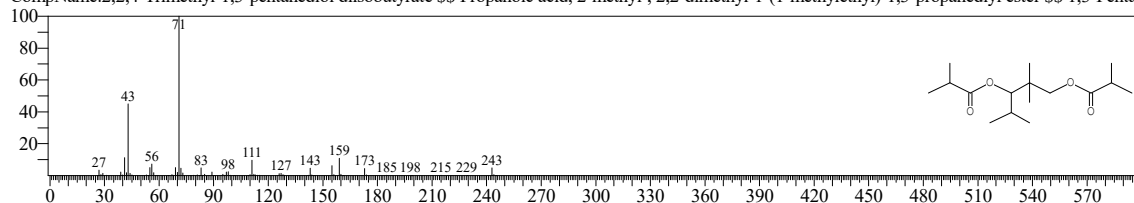BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34622 Library:NIST20R.lib
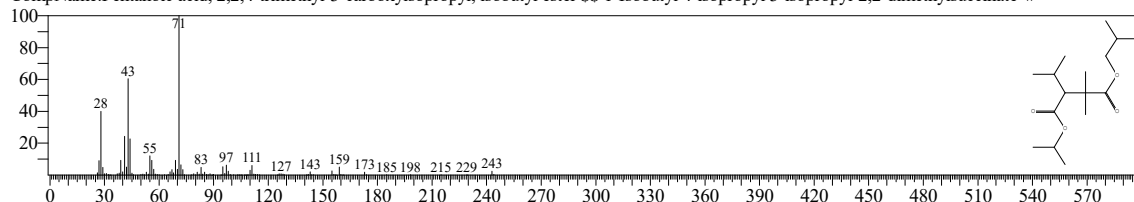SI:86 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan

Hit#:2 Entry:146809 Library:NIST20M1.lib
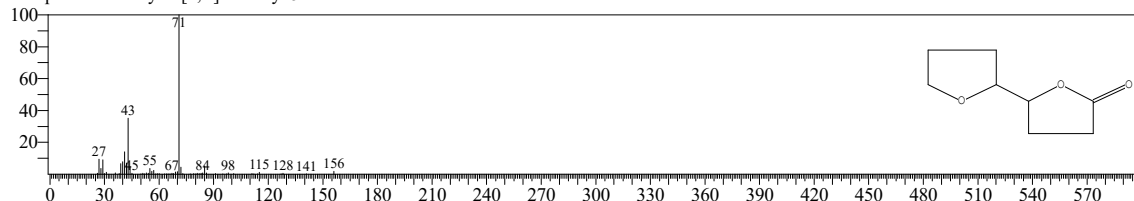SI:81 Formula:C16H30O4 CAS:0-00-0 MolWeight:286 RetIndex:1605
CompName:Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester $$ 1-Isobutyl 4-isopropyl 3-isopropyl-2,2-dimethylsuccinate #

Hit#:3 Entry:20598 Library:NIST20M1.lib
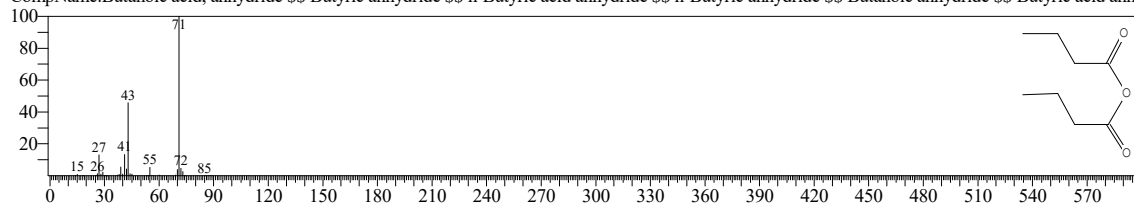SI:80 Formula:C8H12O3 CAS:19680-00-3 MolWeight:156 RetIndex:1316
CompName:Tetrahydro[2,2']bifuranyl-5-one

Hit#:4 Entry:21815 Library:NIST20M1.lib
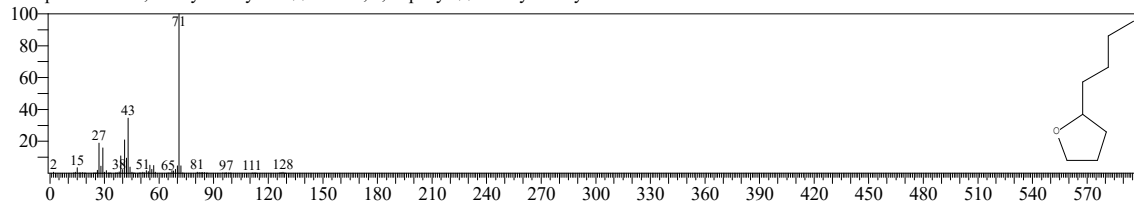SI:78 Formula:C8H14O3 CAS:106-31-0 MolWeight:158 RetIndex:1120
CompName:Butanoic acid, anhydride $$ Butyric anhydride $$ n-Butyric acid anhydride $$ n-Butyric anhydride $$ Butanoic anhydride $$ Butyric acid anhy

Hit#:5 Entry:7968 Library:NIST20M1.lib
SI:78 Formula:C8H16O CAS:1004-29-1 MolWeight:128 RetIndex:948
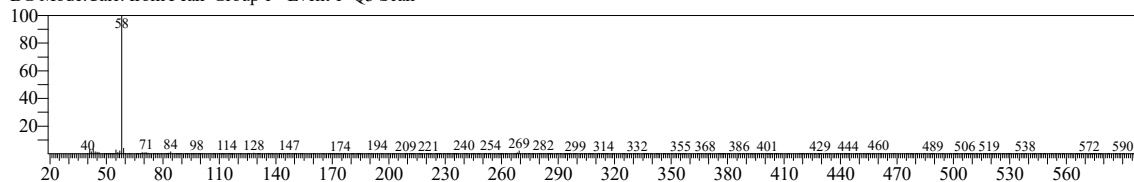CompName:Furan, 2-butyltetrahydro- $$ Octane, 1,4-epoxy- $$ 2-Butyltetrahydrofuran

<< Target >>
Line#:4   R.Time:19.925(Scan#:3086) MassPeaks:284
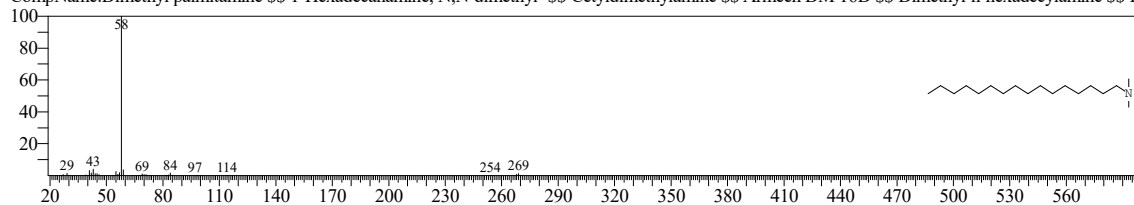RawMode:Averaged 19.920-19.930(3085-3087) BasePeak:58.10(89028)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:32974 Library:NIST20R.lib
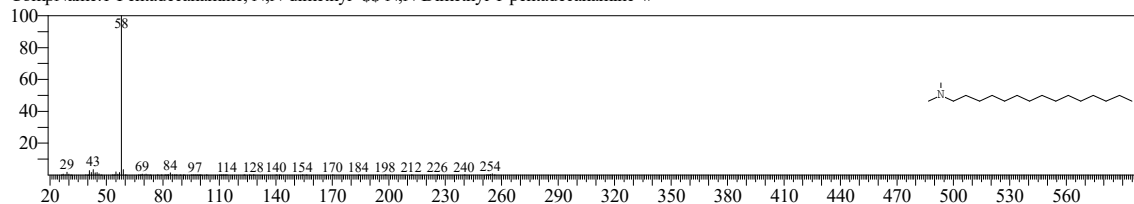SI:98 Formula:C18H39N CAS:112-69-6 MolWeight:269 RetIndex:1860
CompName:Dimethyl palmitamine $$ 1-Hexadecanamine, N,N-dimethyl- $$ Cetyldimethylamine $$ Armeen DM 16D $$ Dimethyl-n-hexadecylamine $$ D

Hit#:2 Entry:110833 Library:NIST20M1.lib
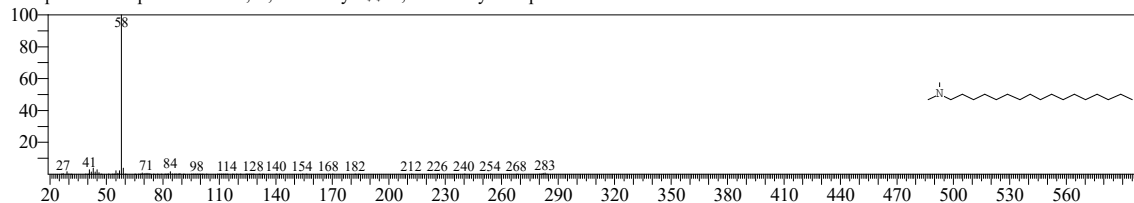SI:97 Formula:C17H37N CAS:17678-60-3 MolWeight:255 RetIndex:1760
CompName:1-Pentadecanamine, N,N-dimethyl- $$ N,N-Dimethyl-1-pentadecanamine #

Hit#:3 Entry:143326 Library:NIST20M1.lib
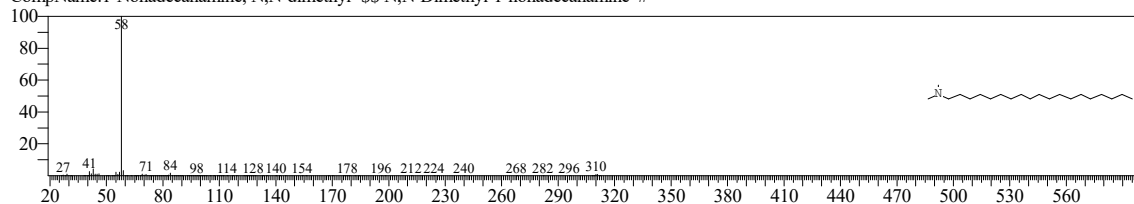SI:96 Formula:C19H41N CAS:3002-57-1 MolWeight:283 RetIndex:1959
CompName:1-Heptadecanamine, N,N-dimethyl- $$ N,N-Dimethyl-1-heptadecanamine #

Hit#:4 Entry:176597 Library:NIST20M1.lib
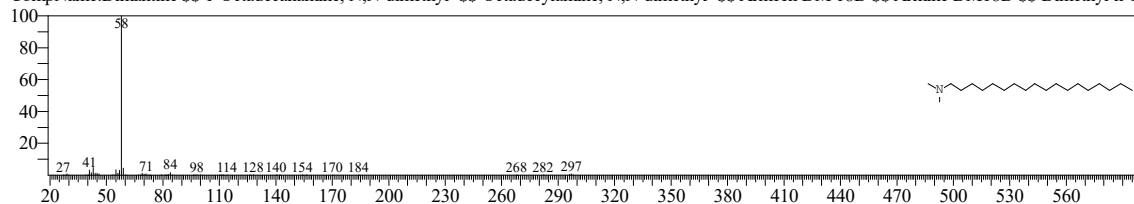SI:96 Formula:C21H45N CAS:49859-87-2 MolWeight:311 RetIndex:2158
CompName:1-Nonadecanamine, N,N-dimethyl- $$ N,N-Dimethyl-1-nonadecanamine #

Hit#:5 Entry:160142 Library:NIST20M1.lib
SI:96 Formula:C20H43N CAS:124-28-7 MolWeight:297 RetIndex:2058
CompName:Dimantine $$ 1-Octadecanamine, N,N-dimethyl- $$ Octadecylamine, N,N-dimethyl- $$ Armeen DM 18D $$ Armine DM18D $$ Dimethyl-n-oc
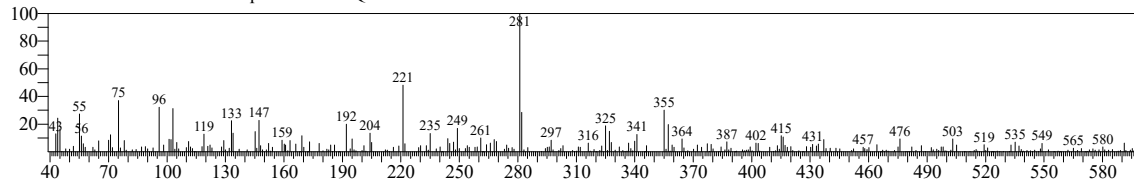
TNAU

<< Target >>
Line#:5 R.Time:28.715(Scan#:4844) MassPeaks:315
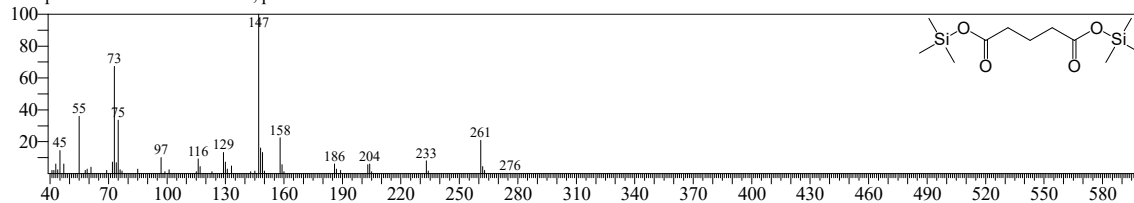RawMode:Averaged 28.710-28.720(4843-4845) BasePeak:281.05(1817)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:115 Library:OA_TMS_DB5_67min_V3.lib
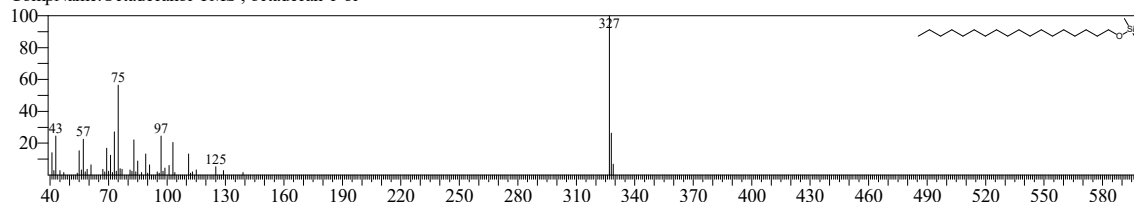SI:29 Formula:C11H24O4Si2 CAS:110-94-1 MolWeight:276 RetIndex:1403
CompName:Glutaric acid-2TMS ; pentanedioic acid

Hit#:2 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
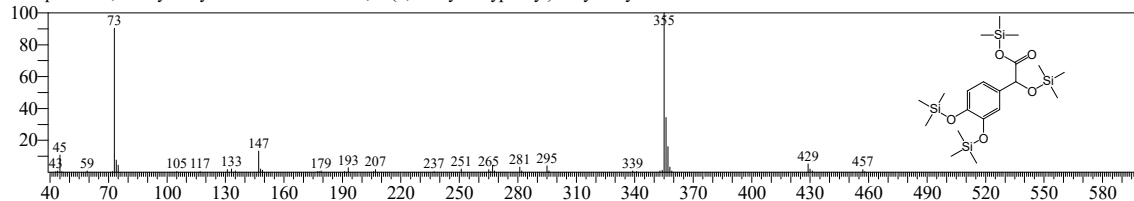SI:29 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol

Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
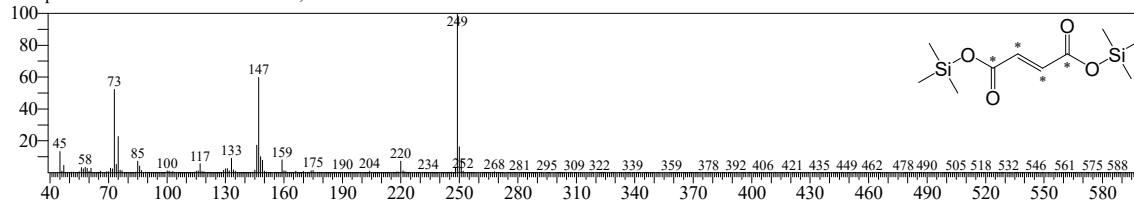SI:28 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:4 Entry:100 Library:OA_TMS_DB5_67min_V3.lib
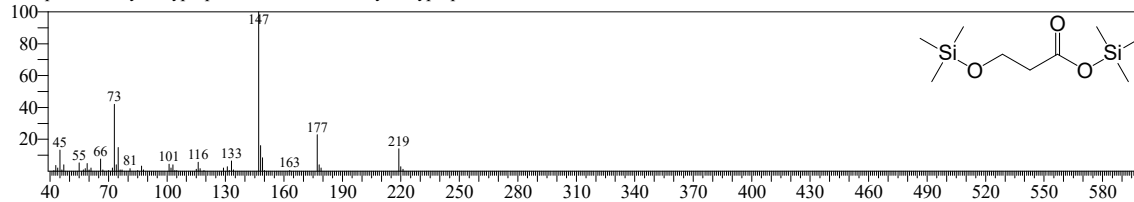SI:28 Formula: CAS:0-00-0 MolWeight:264 RetIndex:1346
CompName:Fumaric acid-13C4-2TMS ;

Hit#:5 Entry:30 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C9H22O3Si2 CAS:503-66-2 MolWeight:234 RetIndex:1145
CompName:3-Hydroxypropionic acid-2TMS ; 3-hydroxypropanoic acid
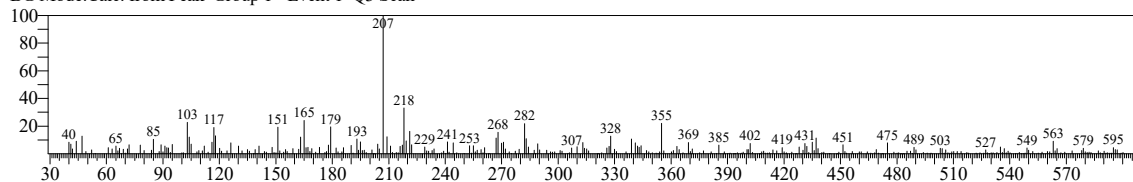
<< Target >>
Line#:6 R.Time:29.310(Scan#:4963) MassPeaks:324
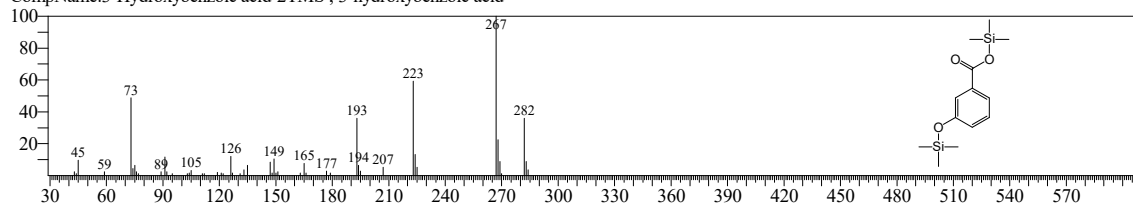RawMode:Averaged 29.305-29.315(4962-4964) BasePeak:207.05(2184)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
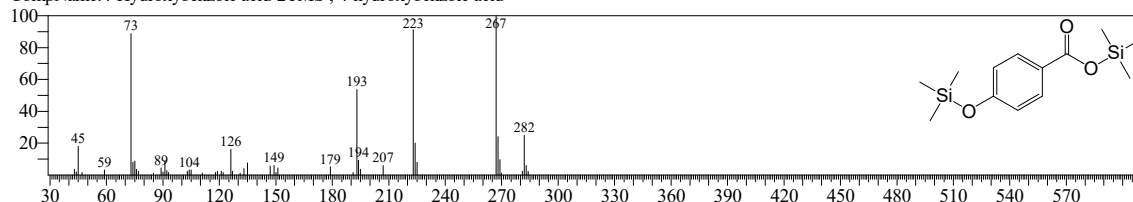SI:35 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
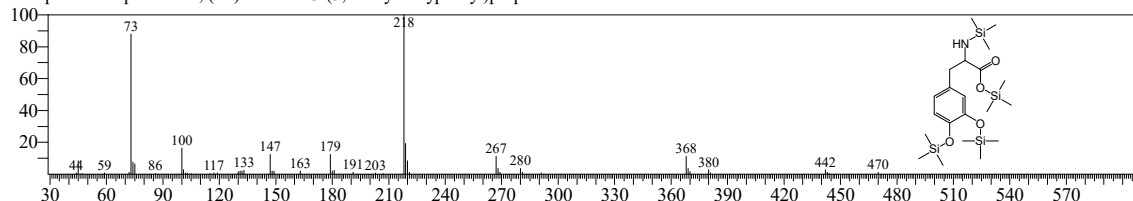SI:33 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:3 Entry:463 Library:OA_TMS_DB5_67min_V3.lib
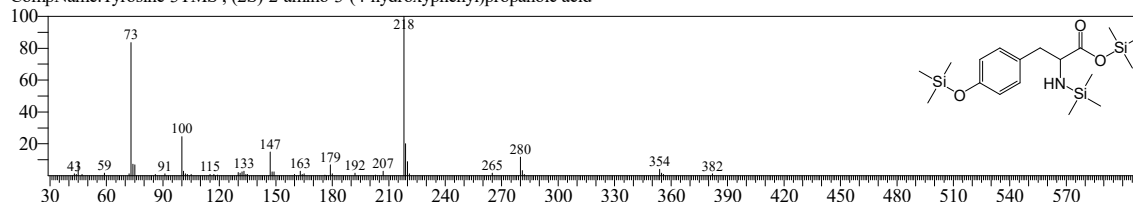SI:31 Formula:C21H43NO4Si4 CAS:59-92-7 MolWeight:485 RetIndex:2123
CompName:Dopa-4TMS ; (2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoic acid

Hit#:4 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
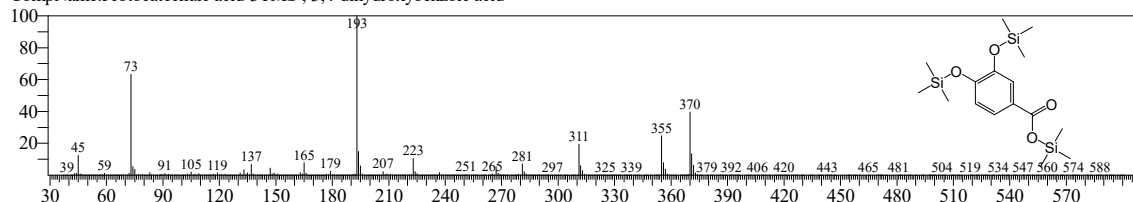SI:30 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid
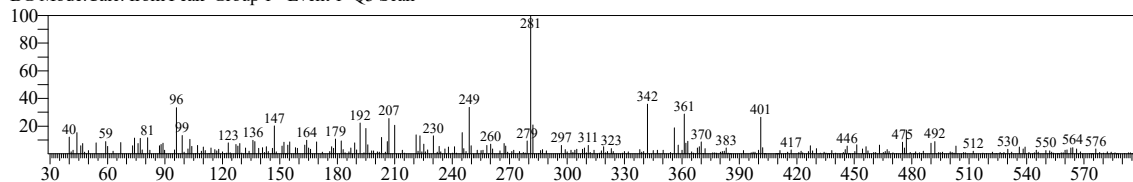
TNAU

<< Target >>
Line#:7   R.Time:30.300(Scan#:5161) MassPeaks:314
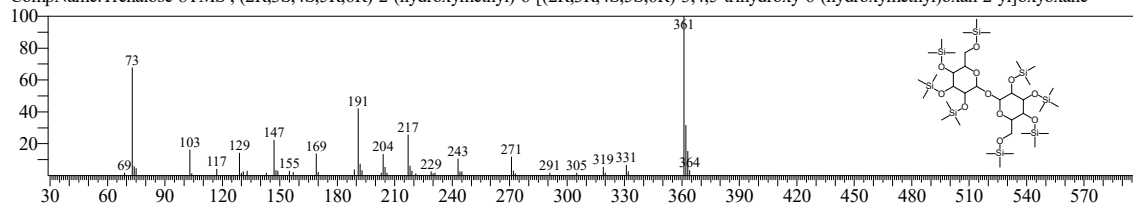RawMode:Averaged 30.295-30.305(5160-5162) BasePeak:281.05(1892)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
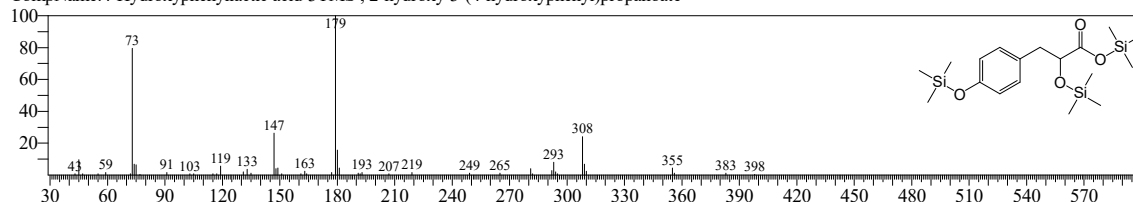SI:27 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

Hit#:2 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
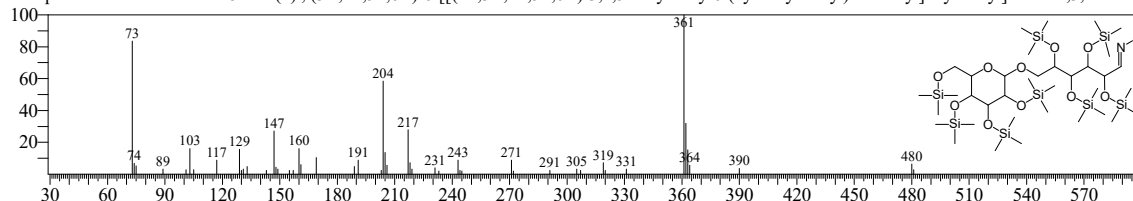SI:25 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

Hit#:3 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
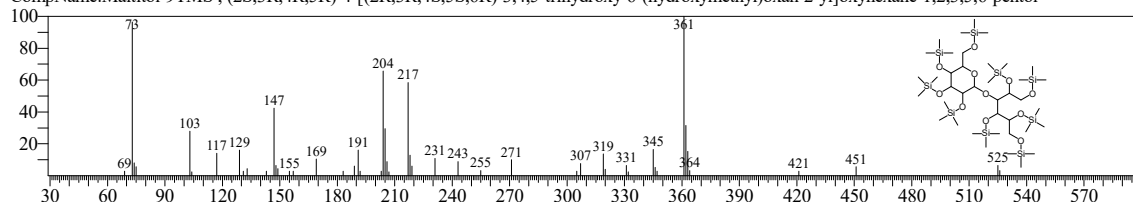SI:24 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

Hit#:4 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
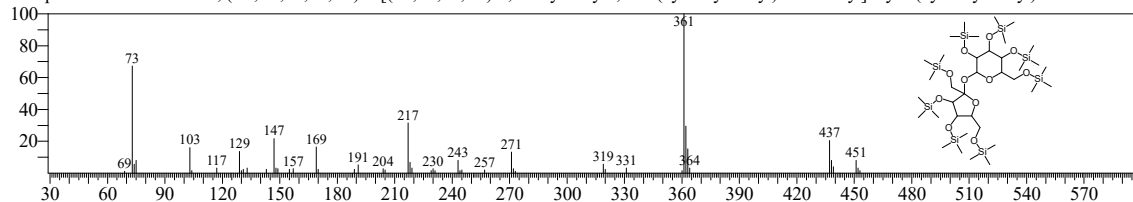CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:5 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:24 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
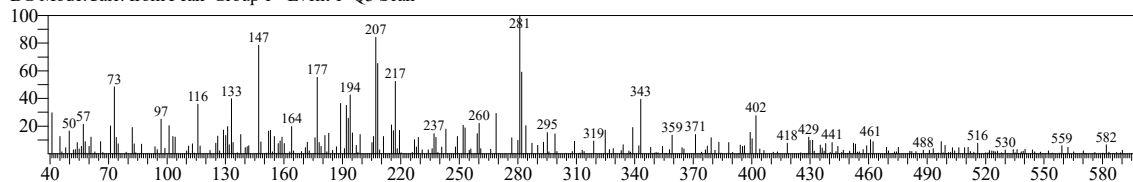
TNAU

<< Target >>
Line#:8 R.Time:30.725(Scan#:5246) MassPeaks:277
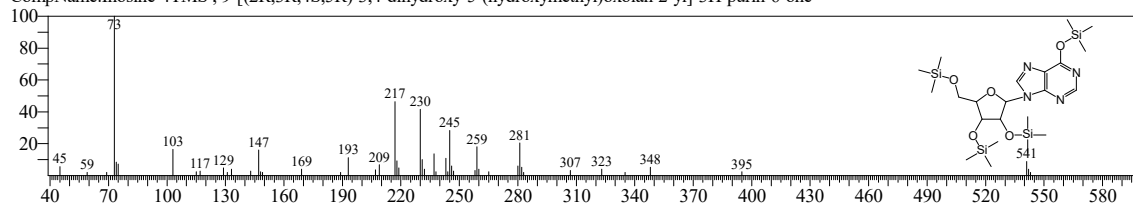RawMode:Averaged 30.720-30.730(5245-5247) BasePeak:281.05(834)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
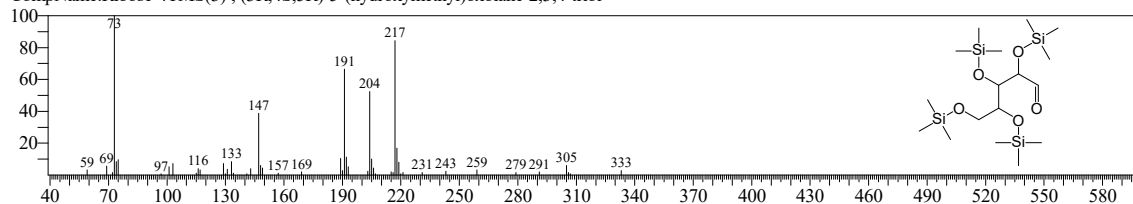SI:35 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

Hit#:2 Entry:236 Library:OA_TMS_DB5_67min_V3.lib
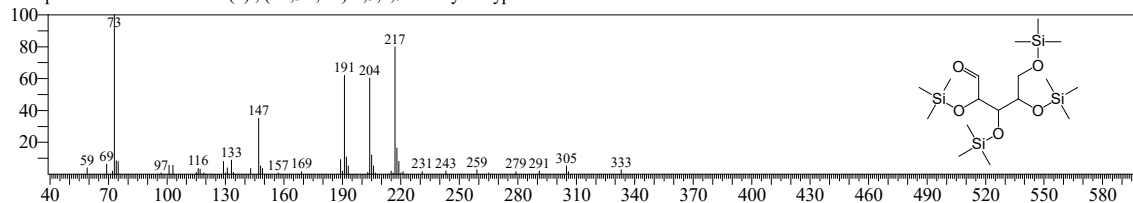SI:34 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1673
CompName:Ribose-4TMS(3) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

Hit#:3 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
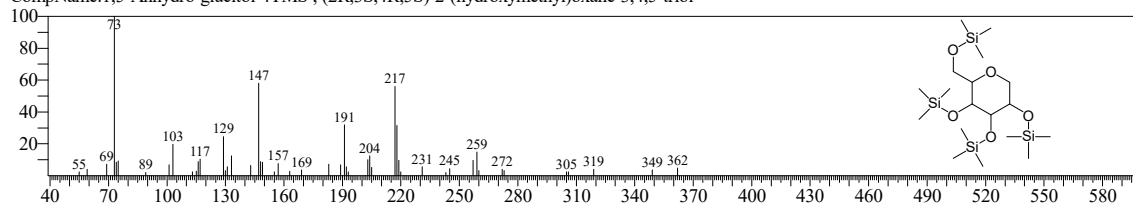SI:33 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:4 Entry:351 Library:OA_TMS_DB5_67min_V3.lib
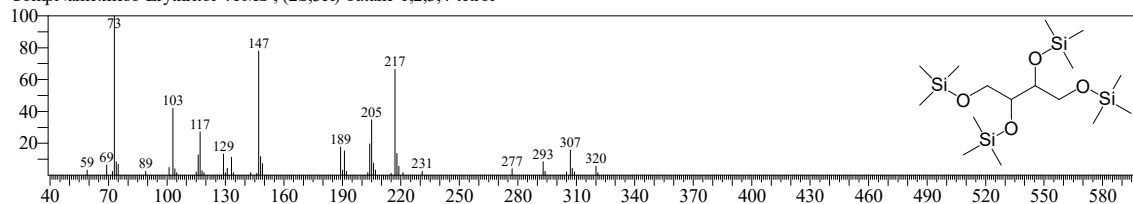SI:33 Formula:C18H44O5Si4 CAS:154-58-5 MolWeight:452 RetIndex:1876
CompName:1,5-Anhydro-glucitol-4TMS ; (2R,3S,4R,5S)-2-(hydroxymethyl)oxane-3,4,5-triol

Hit#:5 Entry:155 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C16H42O4Si4 CAS:149-32-6 MolWeight:410 RetIndex:1521
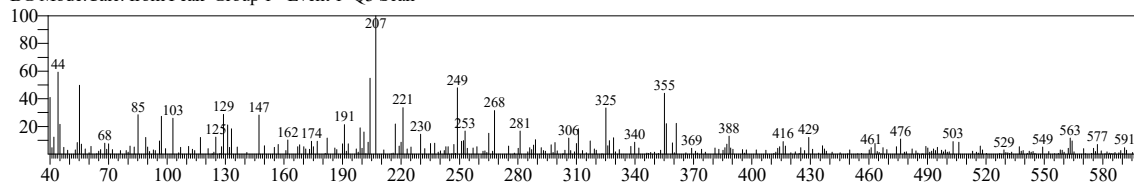CompName:meso-Erythritol-4TMS ; (2S,3R)-butane-1,2,3,4-tetrol

TNAU

<< Target >>
Line#:9 R.Time:30.935(Scan#:5288) MassPeaks:292
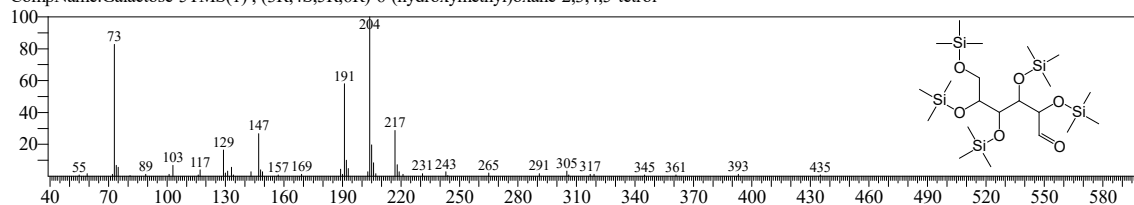RawMode:Averaged 30.930-30.940(5287-5289) BasePeak:207.05(1274)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
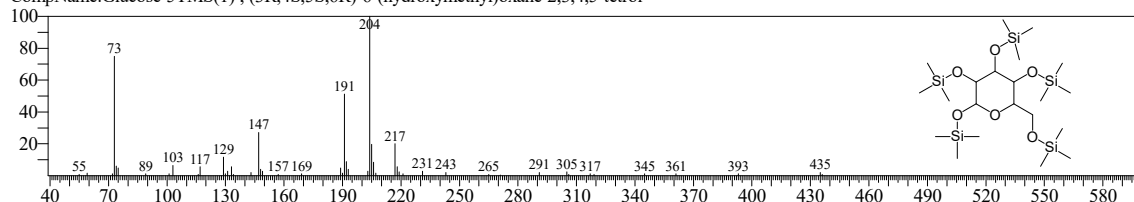SI:35 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1824
CompName:Galactose-5TMS(1) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:2 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
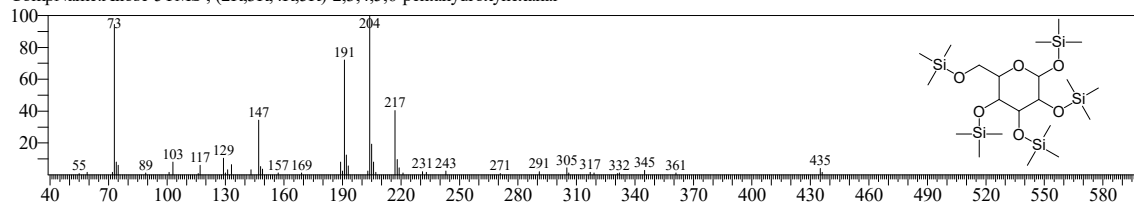SI:34 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:3 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
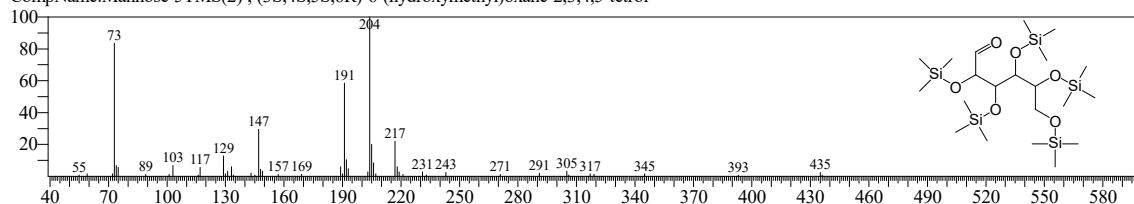SI:34 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

Hit#:4 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:5 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol