TNAU

Chromatogram T87-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-028.qgd

Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.941	54302	1.37	31725	1.41	1.71	91	Undecane
2	9.685	52566	1.32	29634	1.32	1.77	90	Dodecane
3	12.650	32639	0.82	7405	0.33	4.41	39	Epinephrine-3TMS
4	12.727	161875	4.08	101983	4.55	1.59	89	Cyclohexasiloxane, dodecamethyl-
5	14.825	14459	0.36	5741	0.26	2.52	41	3,4-Dihydroxymandelic acid-4TMS
6	14.944	507282	12.78	343875	15.33	1.48	94	Cycloheptasiloxane, tetradecamethyl-
7	15.467	67286	1.70	43560	1.94	1.54	91	2,4-Di-tert-butylphenol
8	16.910	460584	11.60	305976	13.64	1.51	92	Cyclooctasiloxane, hexadecamethyl-
9	18.602	357324	9.00	236931	10.56	1.51	91	Cyclononasiloxane, octadecamethyl-
10	20.106	265991	6.70	171518	7.65	1.55	87	Cyclodecasiloxane, eicosamethyl-
11	21.482	208988	5.27	127192	5.67	1.64	85	Cyclooctasiloxane, hexadecamethyl-
12	22.725	201777	5.08	120893	5.39	1.67	87	Cyclononasiloxane, octadecamethyl-
13	23.874	177576	4.47	105486	4.70	1.68	87	Cyclodecasiloxane, eicosamethyl-
14	24.958	168659	4.25	97123	4.33	1.74	86	Cyclodecasiloxane, eicosamethyl-
15	25.976	146458	3.69	92905	4.14	1.58	85	Tetracosamethyl-cyclododecasiloxane
16	26.931	140237	3.53	75419	3.36	1.86	84	Tetracosamethyl-cyclododecasiloxane
17	27.821	121813	3.07	60155	2.68	2.02	82	Tetracosamethyl-cyclododecasiloxane
18	28.360	21517	0.54	13181	0.59	1.63	27	3,4-Dihydroxymandelic acid-4TMS
19	28.402	9529	0.24	7904	0.35	1.21	28	3,4-Dihydroxymandelic acid-4TMS
20	28.525	16457	0.41	6418	0.29	2.56	27	4-Aminobenzoic acid-2TMS
21	28.705	125254	3.16	62859	2.80	1.99	82	Tetracosamethyl-cyclododecasiloxane
22	29.205	33579	0.85	8821	0.39	3.81	38	4-Hydroxybenzoic acid-2TMS

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
23	29.488	64379	1.62	9294	0.41	6.93	39	3-Hydroxybenzoic acid-2TMS
24	29.722	115629	2.91	41434	1.85	2.79	80	Tetracosamethyl-cyclododecasiloxane
25	30.272	11140	0.28	10207	0.46	1.09	36	Hypoxanthine-2TMS
26	30.305	8683	0.22	10813	0.48	0.80	32	Phosphoric acid-3TMS
27	30.955	67206	1.69	24991	1.11	2.69	51	3,4-Dihydroxymandelic acid-4TMS
28	30.990	12615	0.32	12518	0.56	1.01	32	3-Hydroxybenzoic acid-2TMS
29	31.297	15399	0.39	7663	0.34	2.01	32	Vanilmandelic acid-3TMS
30	31.431	54611	1.38	12597	0.56	4.34	37	4-Aminobenzoic acid-2TMS
31	31.900	54229	1.37	13259	0.59	4.09	35	4-Hydroxybenzoic acid-2TMS
32	32.005	47319	1.19	8298	0.37	5.70	37	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid
33	32.485	71302	1.80	14161	0.63	5.04	44	3,4-Dihydroxymandelic acid-4TMS
34	32.813	75015	1.89	10938	0.49	6.86	41	4-Aminobenzoic acid-2TMS
35	32.928	25402	0.64	9907	0.44	2.56	39	Chloramphenicol-2TMS
		3969081	100.00	2242784	100.00			

Library

<< Target >>
Line#:1   R.Time:7.940(Scan#:689) MassPeaks:300
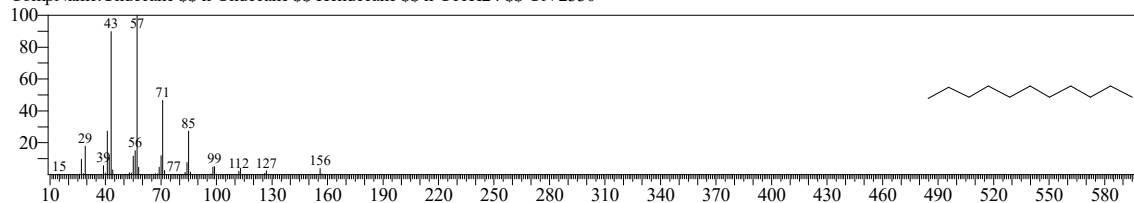RawMode:Averaged 7.935-7.945(688-690) BasePeak:57.10(7302)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:21042 Library:NIST20M1.lib
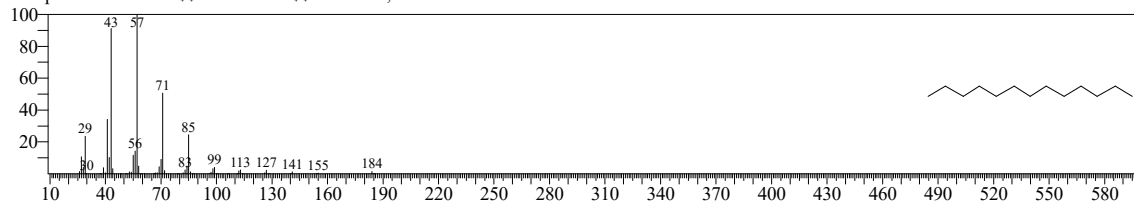SI:91 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:40226 Library:NIST20M1.lib
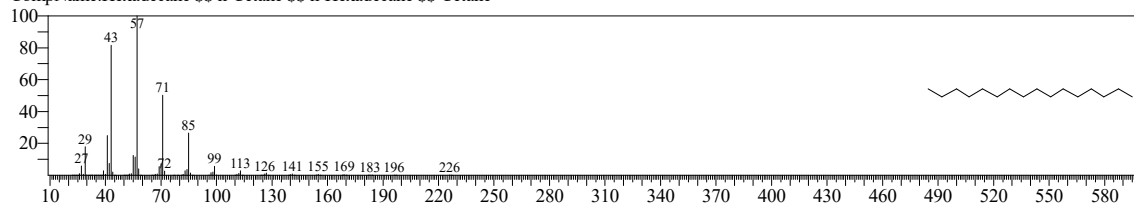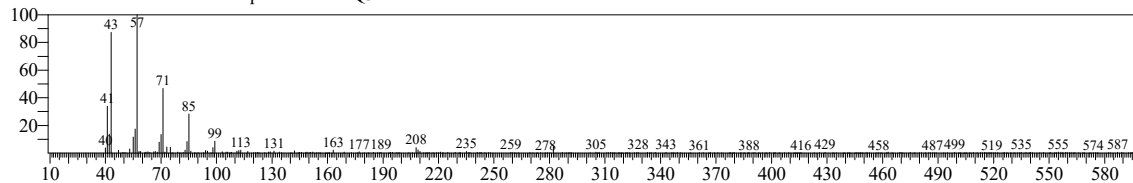SI:91 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:3 Entry:27737 Library:NIST20R.lib
SI:89 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

TNAU

<< Target >>
Line#:1 R.Time:7.940(Scan#:689) MassPeaks:300
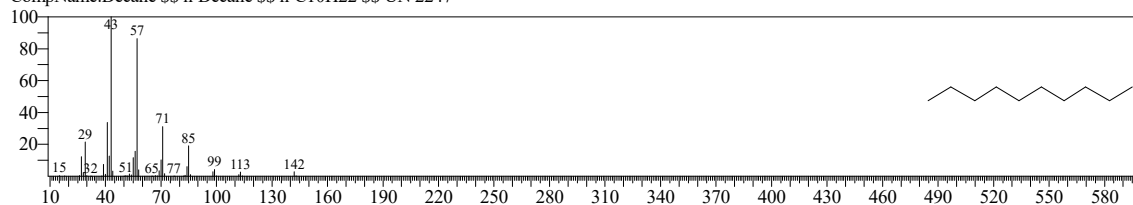RawMode:Averaged 7.935-7.945(688-690) BasePeak:57.10(7302)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:4 Entry:9444 Library:NIST20R.lib
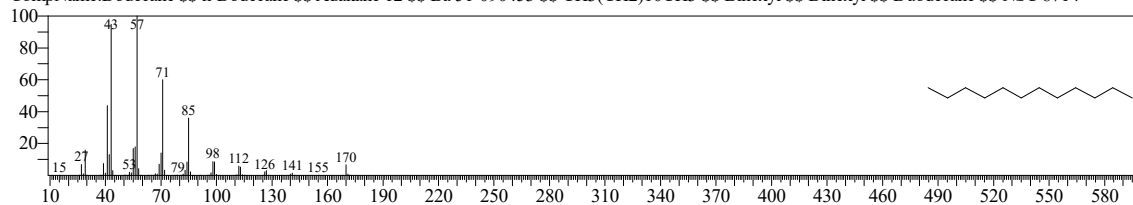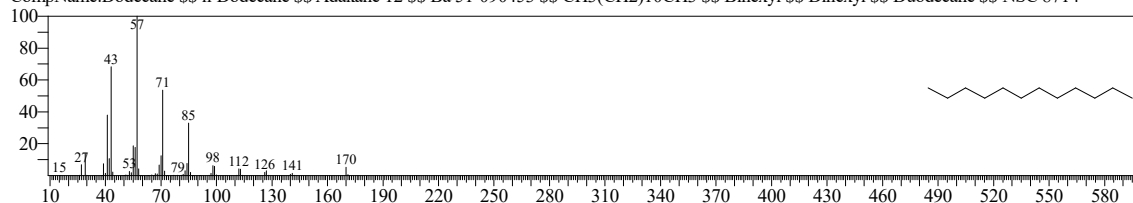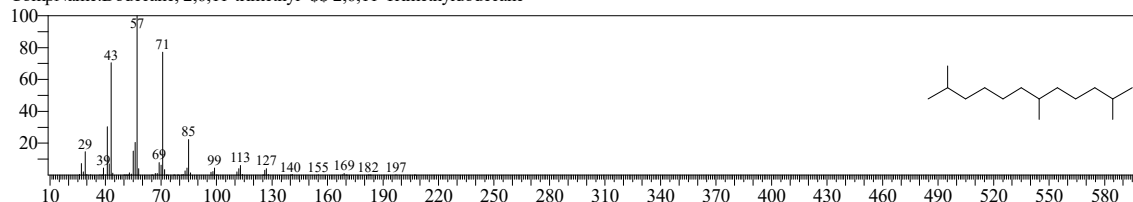SI:89 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

Hit#:5 Entry:16191 Library:NIST20R.lib
SI:89 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

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<< Target >>
Line#:2   R.Time:9.685(Scan#:1038) MassPeaks:309
RawMode:Averaged 9.680-9.690(1037-1039) BasePeak:57.10(6188)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:30057 Library:NIST20M1.lib
SI:90 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:90 Formula:C15H32 CAS:31295-56-4 MolWeight:212 RetIndex:1320
CompName:Dodecane, 2,6,11-trimethyl- $$ 2,6,11-Trimethyldodecane

Hit#:3 Entry:22497 Library:NIST20R.lib
SI:90 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

Hit#:4 Entry:12898 Library:NIST20R.lib
SI:90 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:5 Entry:27736 Library:NIST20R.lib
SI:90 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane
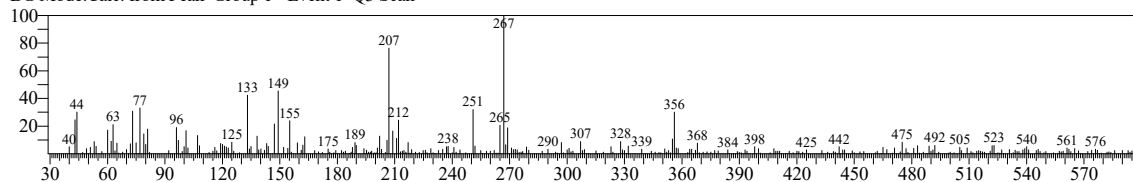
TNAU

<< Target >>
Line#:3 R.Time:12.650(Scan#:1631) MassPeaks:310
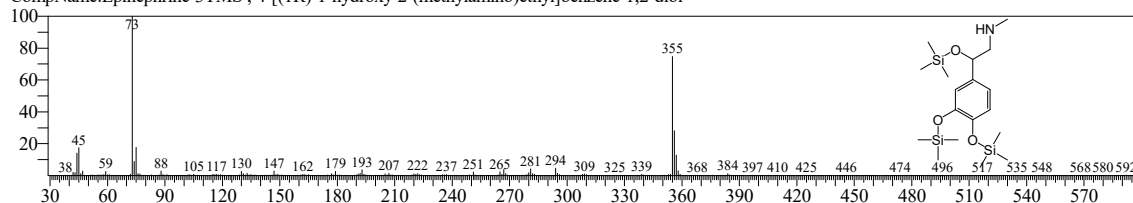RawMode:Averaged 12.645-12.655(1630-1632) BasePeak:266.90(663)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
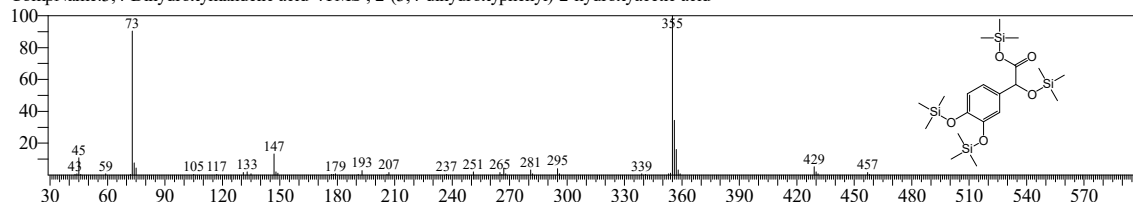SI:39 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
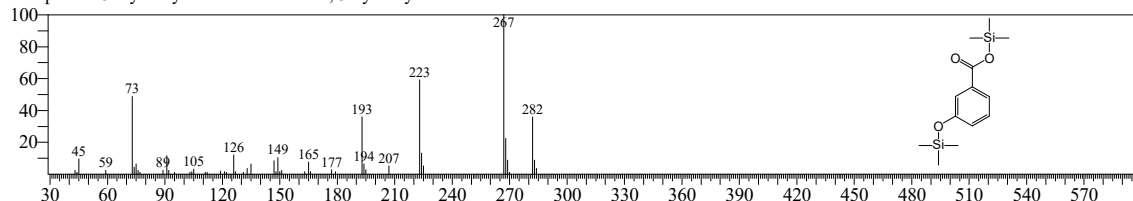SI:39 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:4 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
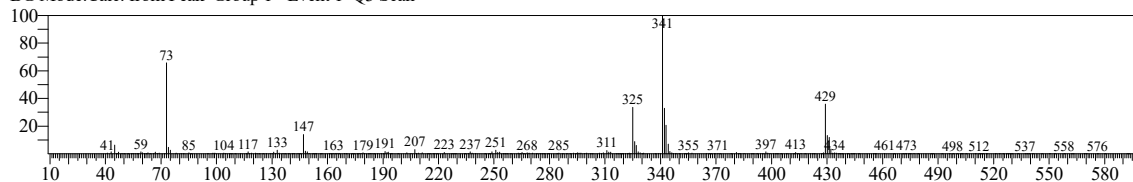CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

TNAU

<< Target >>
Line#:4 R.Time:12.725(Scan#:1646) MassPeaks:298
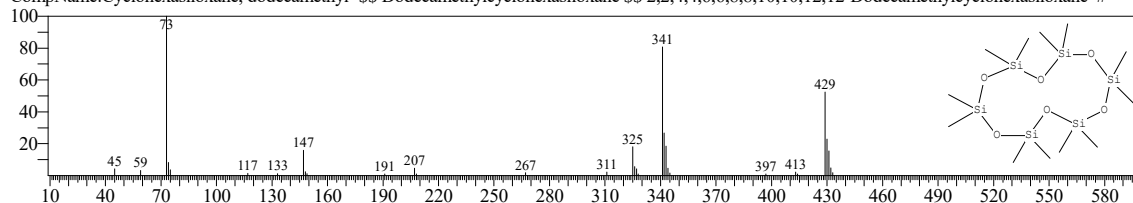RawMode:Averaged 12.720-12.730(1645-1647) BasePeak:341.00(21033)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:42510 Library:NIST20R.lib
SI:89 Formula:C12H36O6Si6 CAS:540-97-6 MolWeight:444 RetIndex:1240
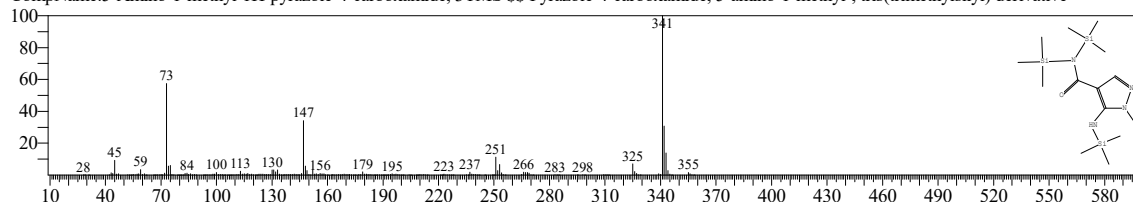CompName:Cyclohexasiloxane, dodecamethyl- $$ Dodecamethylcyclohexasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12-Dodecamethylcyclohexasiloxane #

Hit#:2 Entry:225481 Library:NIST20M1.lib
SI:76 Formula:C14H32N4OSi3 CAS:0-00-0 MolWeight:356 RetIndex:1819
CompName:5-Amino-1-methyl-1H-pyrazole-4-carboxamide, 3TMS $$ Pyrazole-4-carboxamide, 5-amino-1-methyl-, tris(trimethylsilyl) derivative

Hit#:3 Entry:210499 Library:NIST20M1.lib
SI:70 Formula:C15H31NO2Si3 CAS:0-00-0 MolWeight:341 RetIndex:1697
CompName:4-Amino-1,2-benzenediol, O,O',N-tris(trimethylsilyl)- $$ 4-Aminopyrocatechol, O,O',N-tris(trimethylsilyl)- $$ 4-Amino-1,2-benzenediol, 3TMS

Hit#:4 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
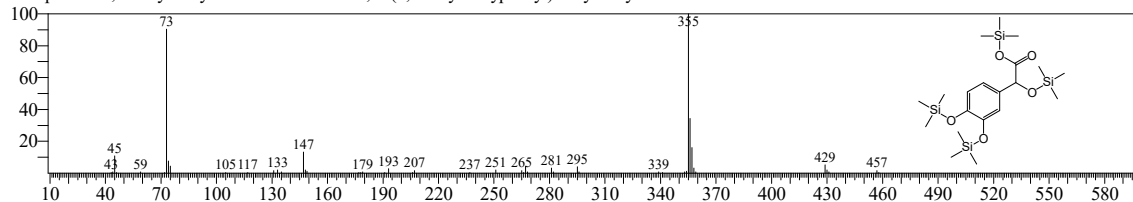SI:56 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid

Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:52 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid
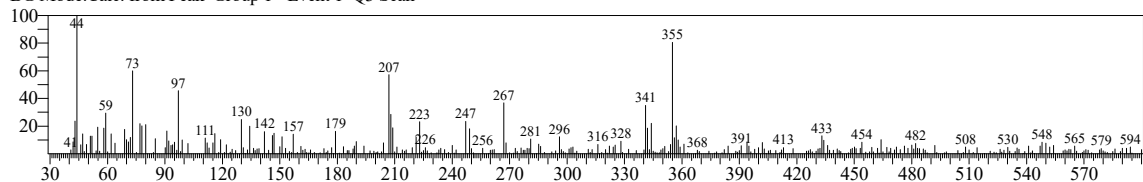
TNAU

<< Target >>
Line#:5 R.Time:14.825(Scan#:2066) MassPeaks:329
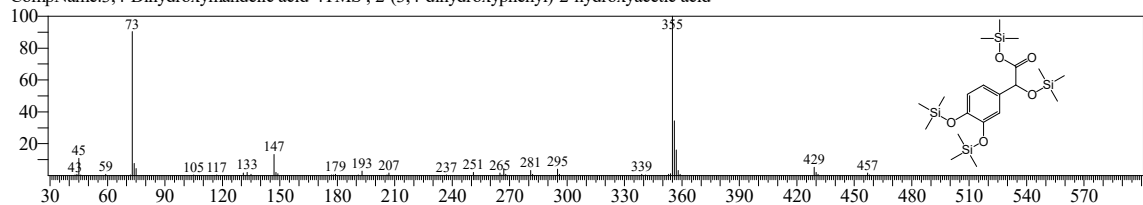RawMode:Averaged 14.820-14.830(2065-2067) BasePeak:44.05(445)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
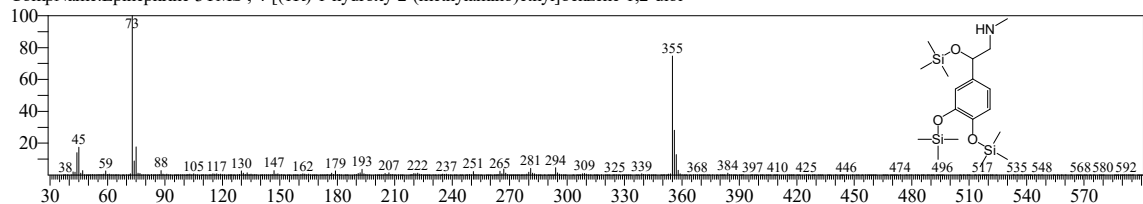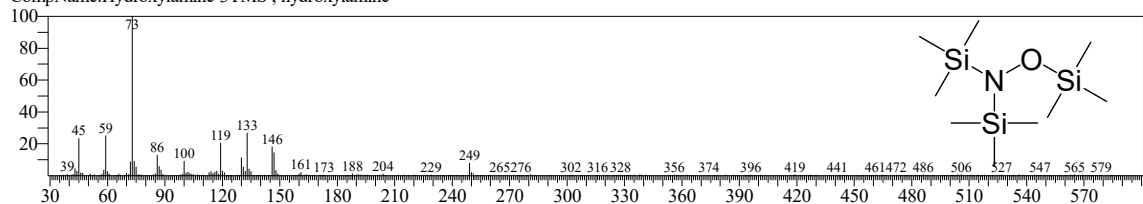SI:41 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 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#:3 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#:4 Entry:20 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H27NOSi3 CAS:7803-49-8 MolWeight:249 RetIndex:1127
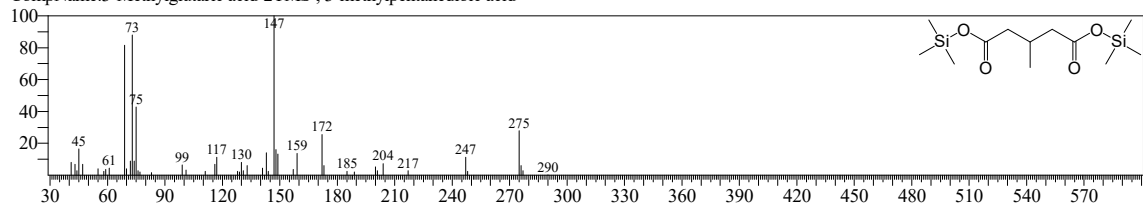CompName:Hydroxylamine-3TMS ; hydroxylamine

Hit#:5 Entry:119 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C12H26O4Si2 CAS:626-51-7 MolWeight:290 RetIndex:1426
CompName:3-Methylglutaric acid-2TMS ; 3-methylpentanedioic acid
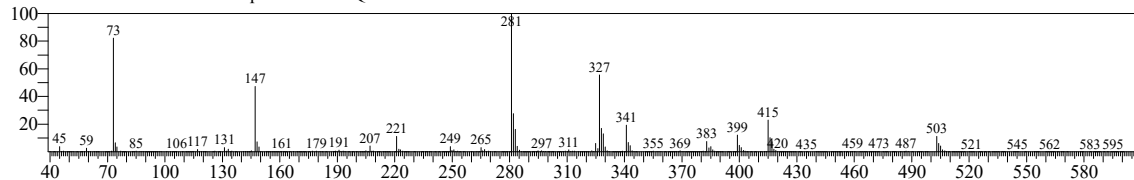
TNAU

<< Target >>
Line#:6   R.Time:14.945(Scan#:2090) MassPeaks:402
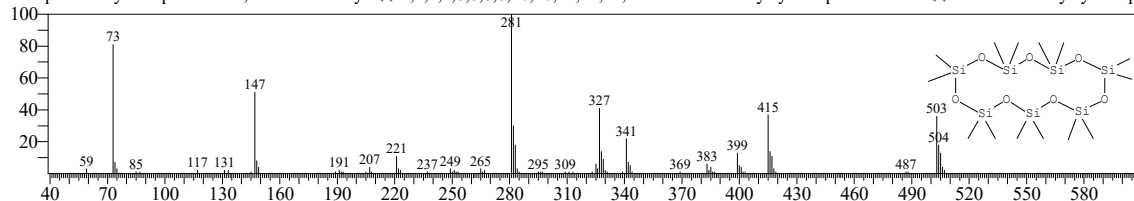RawMode:Averaged 14.940-14.950(2089-2091) BasePeak:281.05(51843)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:43264 Library:NIST20R.lib
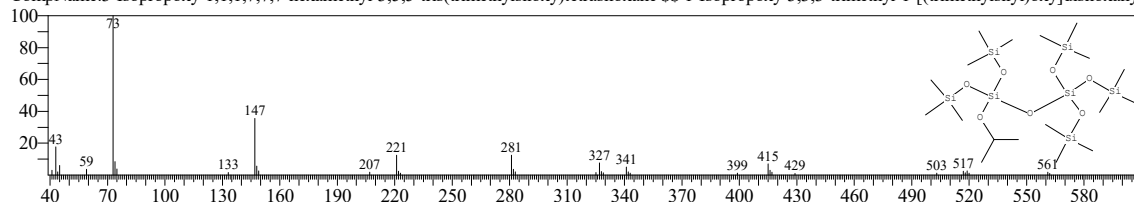SI:94 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohept

Hit#:2 Entry:41637 Library:NIST20M2.lib
SI:72 Formula:C18H52O7Si7 CAS:71579-69-6 MolWeight:576 RetIndex:1648
CompName:3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane $$ 1-Isopropoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl

Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:48 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

Hit#:4 Entry:247 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula: CAS:0-00-0 MolWeight:343 RetIndex:1688
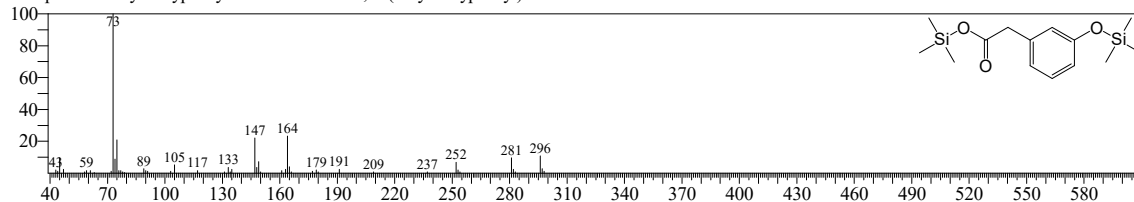CompName:Taurine-13C2-3TMS ;

Hit#:5 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
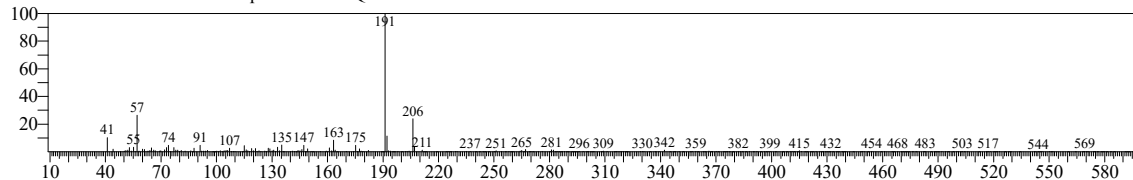CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

TNAU

<< Target >>
Line#:7 R.Time:15.465(Scan#:2194) MassPeaks:326
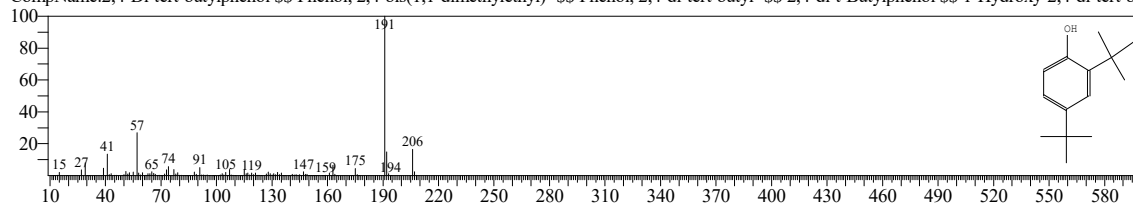RawMode:Averaged 15.460-15.470(2193-2195) BasePeak:191.15(13323)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:24086 Library:NIST20R.lib
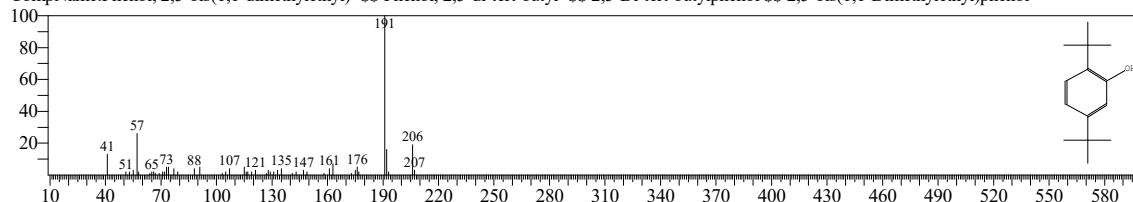SI:91 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu

Hit#:2 Entry:24098 Library:NIST20R.lib
SI:89 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
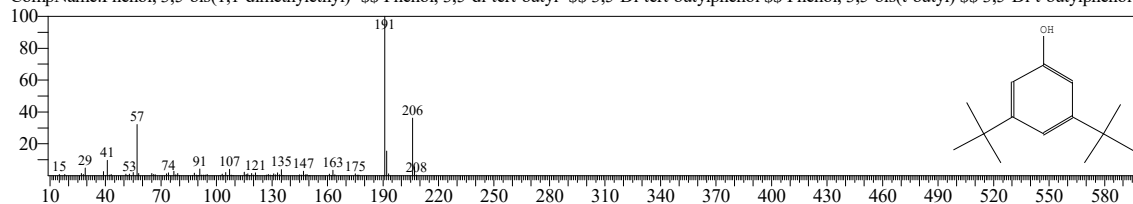SI:89 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

Hit#:4 Entry:24110 Library:NIST20R.lib
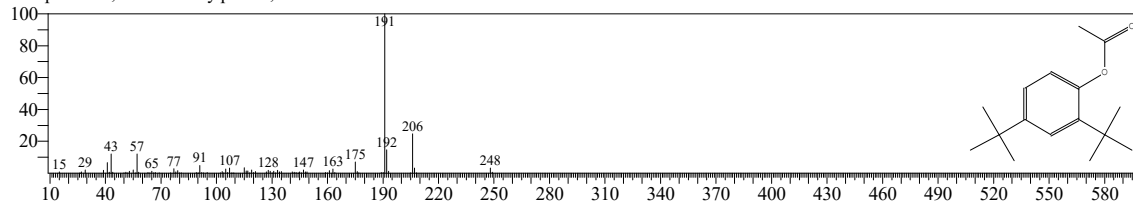SI:88 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $

Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:83 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
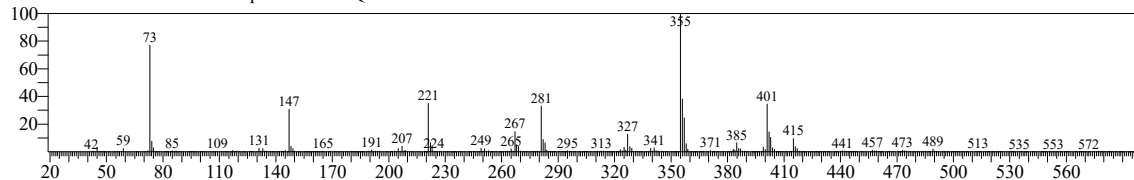CompName:2,4-Di-tert-butylphenol, acetate

TNAU

<< Target >>
Line#:8 R.Time:16.910(Scan#:2483) MassPeaks:386
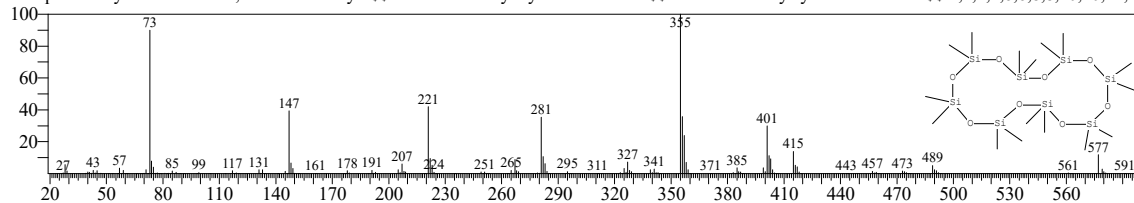RawMode:Averaged 16.905-16.915(2482-2484) BasePeak:355.05(46317)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:42384 Library:NIST20M2.lib
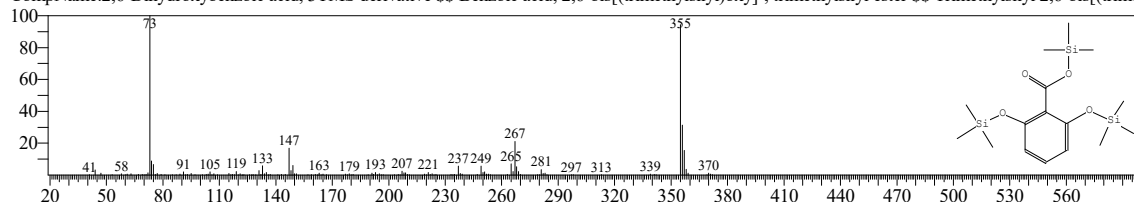SI:92 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12

Hit#:2 Entry:238200 Library:NIST20M1.lib
SI:72 Formula:C16H30O4Si3 CAS:3782-85-2 MolWeight:370 RetIndex:1765
CompName:2,6-Dihydroxybenzoic acid, 3TMS derivative $$ Benzoic acid, 2,6-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester $$ Trimethylsilyl 2,6-bis[(trimet

Hit#:3 Entry:42693 Library:NIST20R.lib
SI:71 Formula:C14H42O5Si6 CAS:107-52-8 MolWeight:458 RetIndex:1252
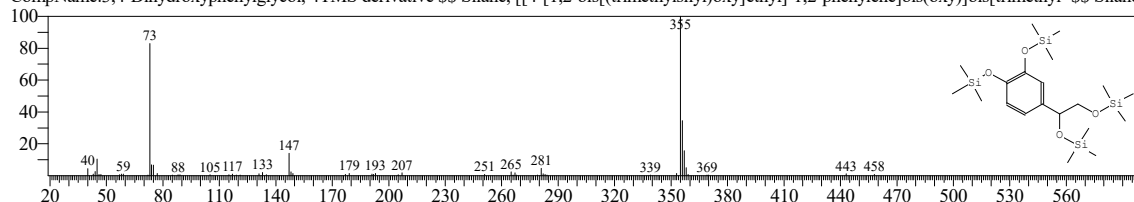CompName:Hexasiloxane, tetradecamethyl- $$ Tetradecamethylhexasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,11-Tetradecamethylhexasiloxane #

Hit#:4 Entry:42703 Library:NIST20R.lib
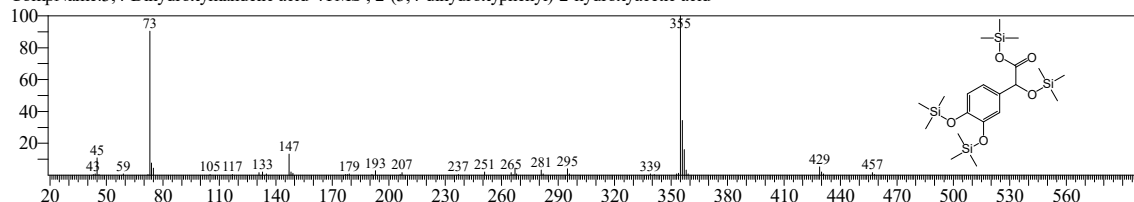SI:71 Formula:C20H42O4Si4 CAS:56114-62-6 MolWeight:458 RetIndex:1993
CompName:3,4-Dihydroxyphenylglycol, 4TMS derivative $$ Silane, [[4-[1,2-bis[(trimethylsilyl)oxy]ethyl]-1,2-phenylene]bis(oxy)]bis[trimethyl- $$ Silane,

Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:70 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
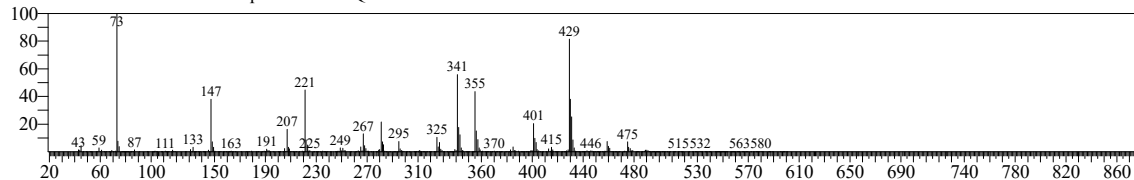CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

TNAU

<< Target >>
Line#:9　R.Time:18.600(Scan#:2821)　MassPeaks:377
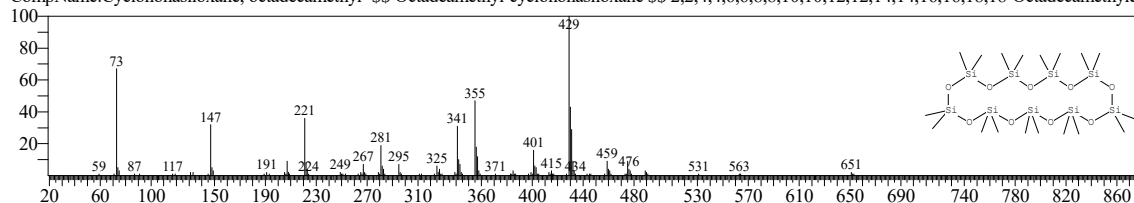RawMode:Averaged 18.595-18.605(2820-2822) BasePeak:73.05(27233)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1　Entry:43659　Library:NIST20R.lib
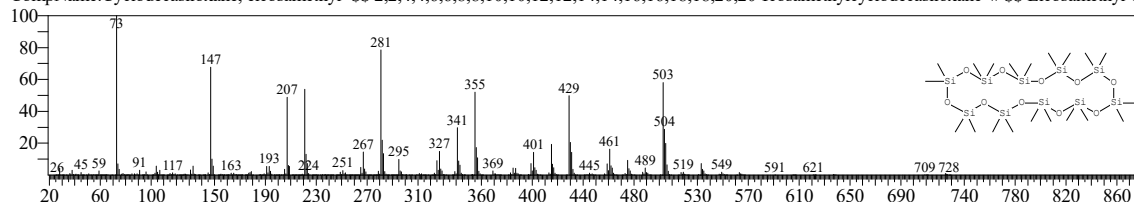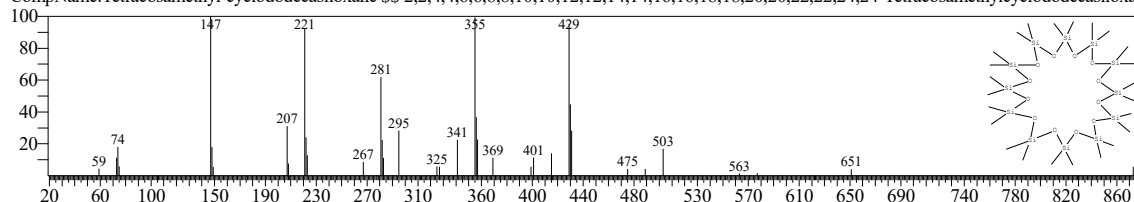SI:91　Formula:C18H54O9Si9　CAS:556-71-8　MolWeight:666　RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:2　Entry:45685　Library:NIST20M2.lib
SI:76　Formula:C20H60O10Si10　CAS:18772-36-6　MolWeight:740　RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3　Entry:38404　Library:NIST20M2.lib
SI:74　Formula:C16H48O6Si7　CAS:541-01-5　MolWeight:532　RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #

Hit#:4　Entry:46368　Library:NIST20M2.lib
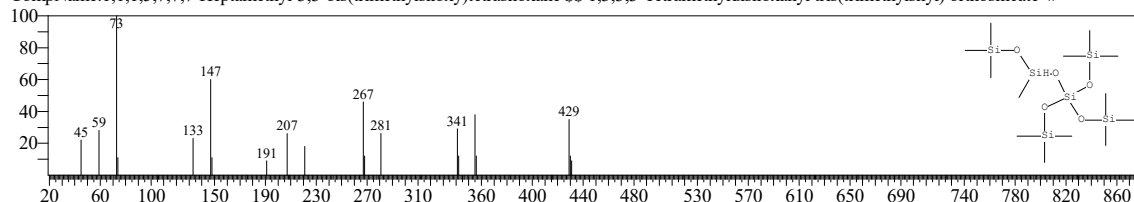SI:74　Formula:C24H72O12Si12　CAS:18919-94-3　MolWeight:888　RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:5　Entry:20636　Library:NIST20M2.lib
SI:73　Formula:C13H40O5Si6　CAS:38147-00-1　MolWeight:444　RetIndex:1297
CompName:1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane $$ 1,3,3,3-Tetramethyldisiloxanyl tris(trimethylsilyl) orthosilicate #
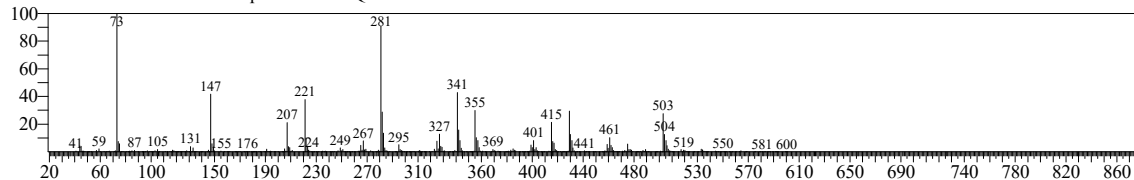
TNAU

<< Target >>
Line#:10 R.Time:20.105(Scan#:3122) MassPeaks:359
RawMode:Averaged 20.100-20.110(3121-3123) BasePeak:73.05(18784)
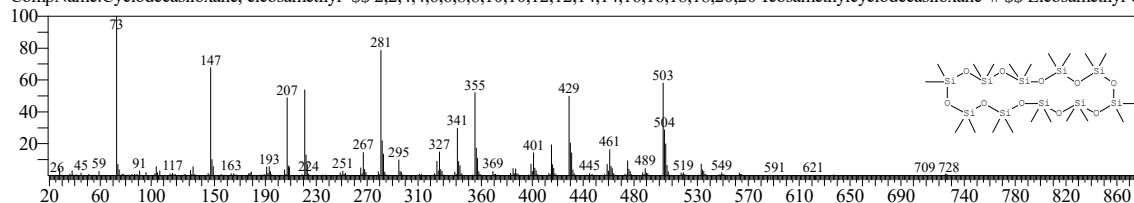BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:45685 Library:NIST20M2.lib
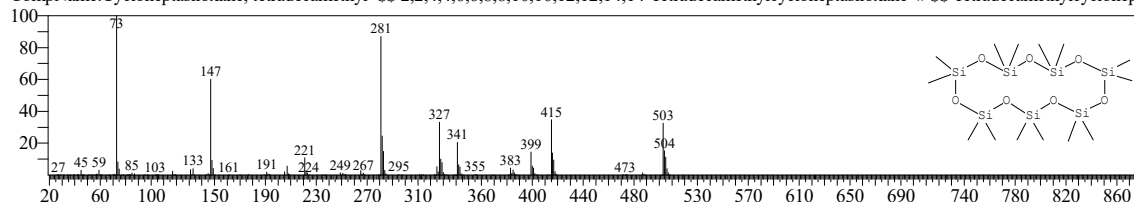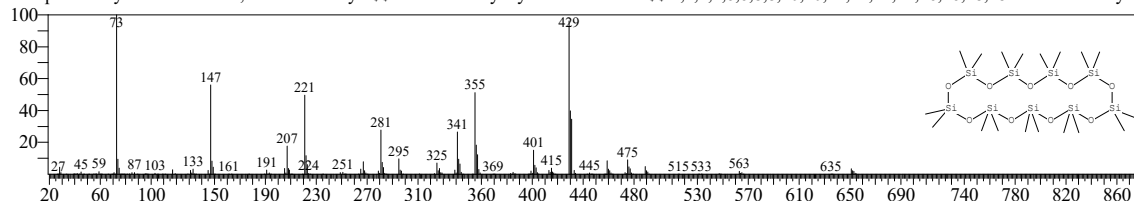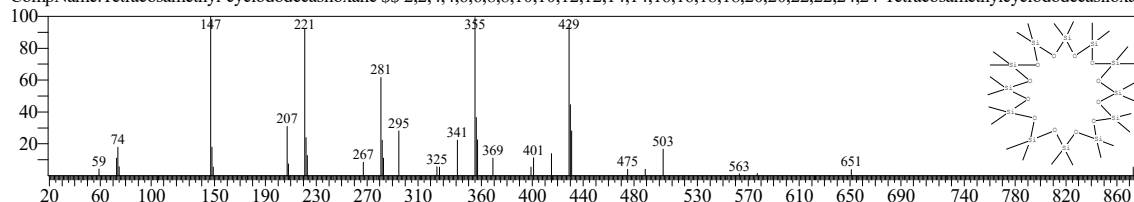SI:87 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:2 Entry:36969 Library:NIST20M2.lib
SI:79 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohept

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:77 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:46368 Library:NIST20M2.lib
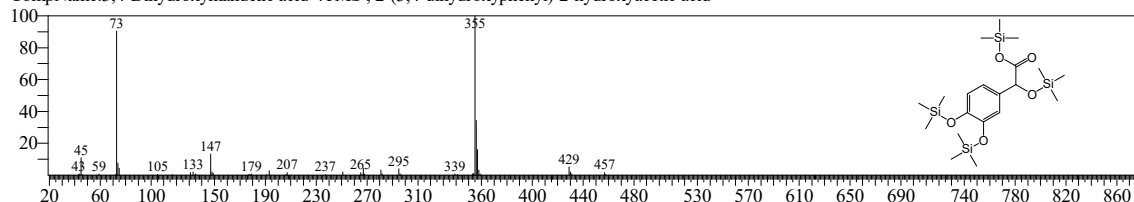SI:72 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:56 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid
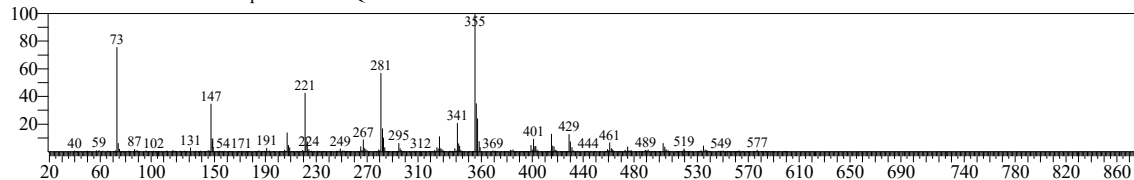
TNAU

<< Target >>
Line#:11 R.Time:21.480(Scan#:3397) MassPeaks:373
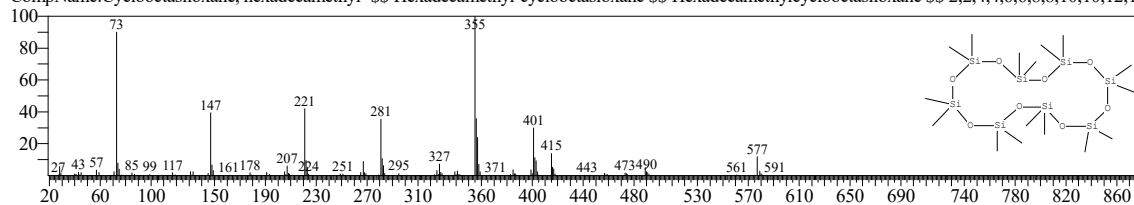RawMode:Averaged 21.475-21.485(3396-3398) BasePeak:355.05(16585)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:42384 Library:NIST20M2.lib
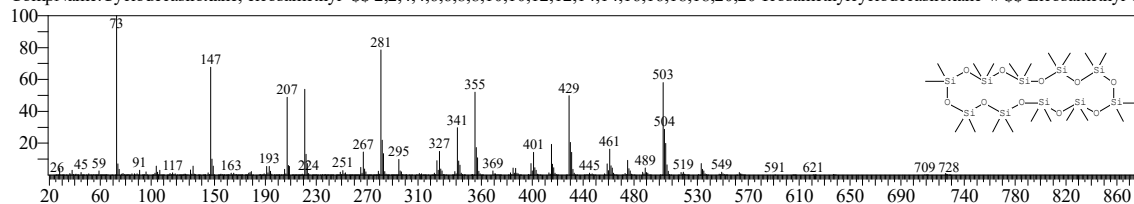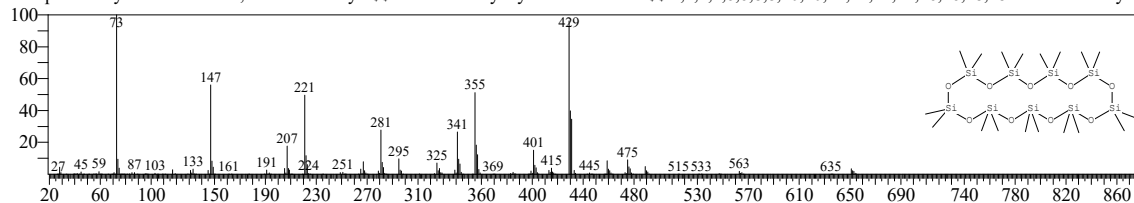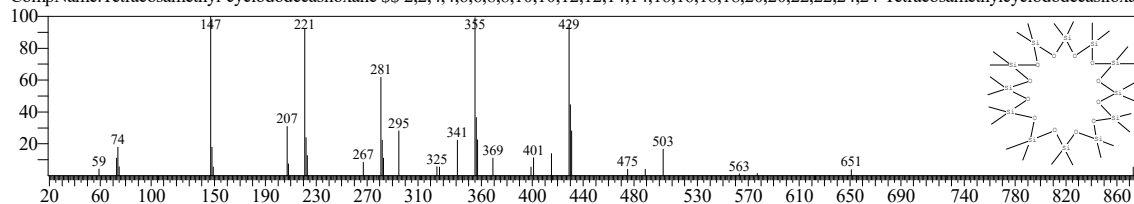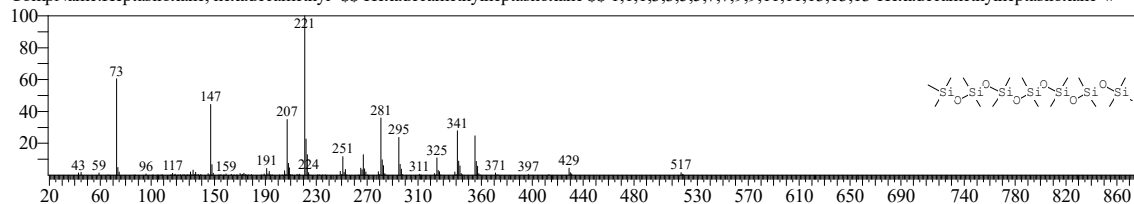SI:85 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12

Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:80 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:79 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:46368 Library:NIST20M2.lib
SI:78 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:73 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
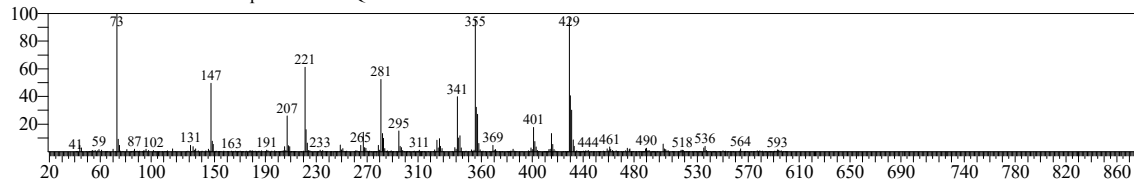
TNAU

<< Target >>
Line#:12 R.Time:22.725(Scan#:3646) MassPeaks:388
RawMode:Averaged 22.720-22.730(3645-3647) BasePeak:73.05(10692)
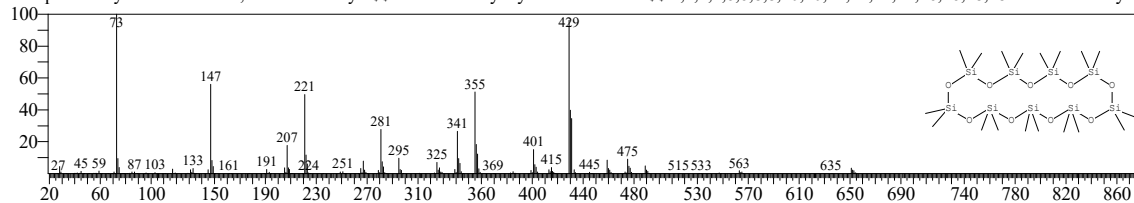BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:44570 Library:NIST20M2.lib
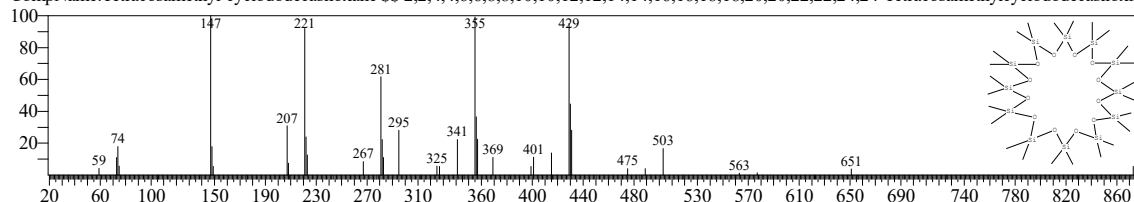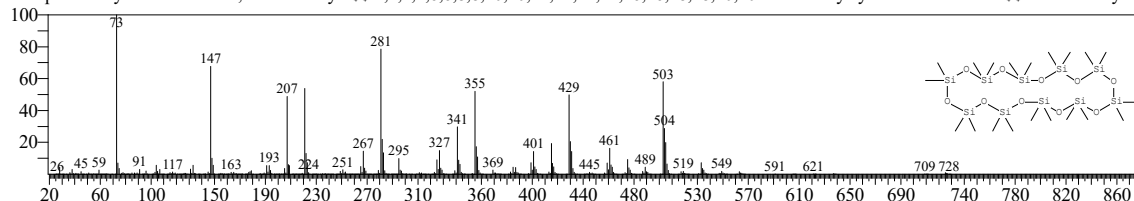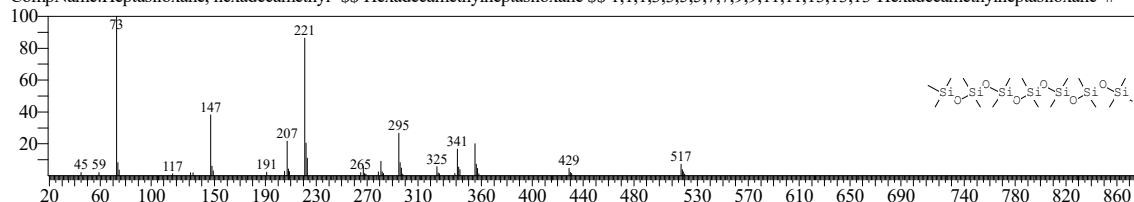SI:87 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:2 Entry:46368 Library:NIST20M2.lib
SI:83 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:3 Entry:45685 Library:NIST20M2.lib
SI:80 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:4 Entry:38404 Library:NIST20M2.lib
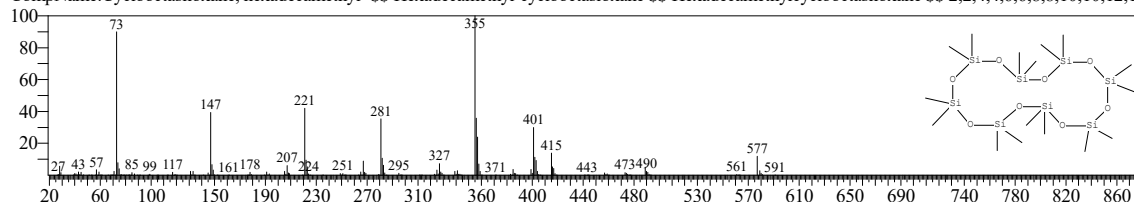SI:74 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #

Hit#:5 Entry:42384 Library:NIST20M2.lib
SI:73 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12
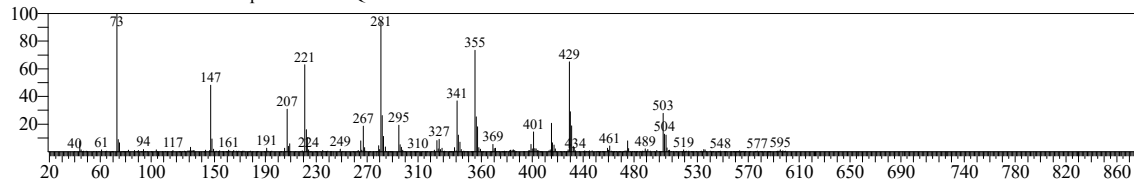
TNAU

<< Target >>
Line#:13 R.Time:23.875(Scan#:3876) MassPeaks:342
RawMode:Averaged 23.870-23.880(3875-3877) BasePeak:73.05(9606)
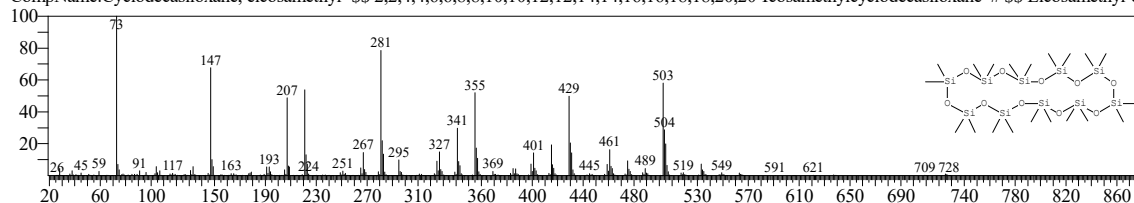BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:45685 Library:NIST20M2.lib
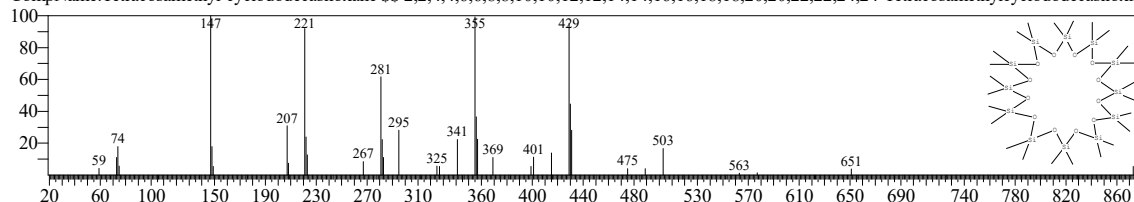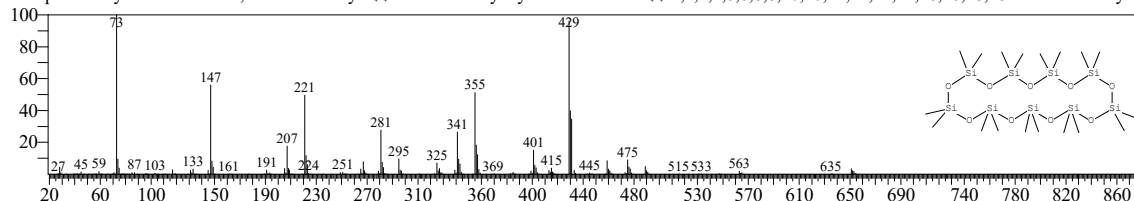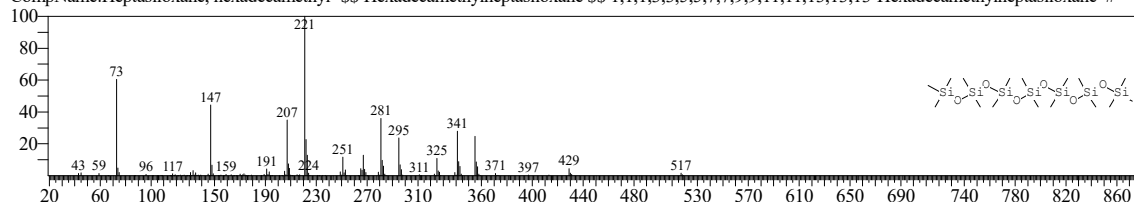SI:87 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:2 Entry:46368 Library:NIST20M2.lib
SI:81 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:81 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:43312 Library:NIST20R.lib
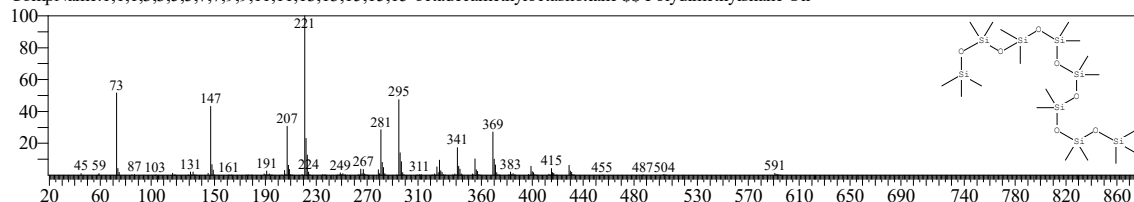SI:73 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #

Hit#:5 Entry:42942 Library:NIST20M2.lib
SI:72 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil
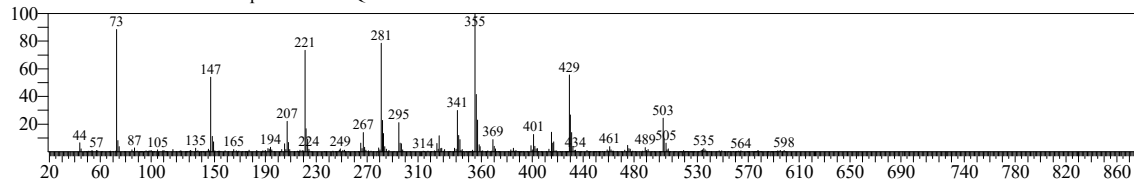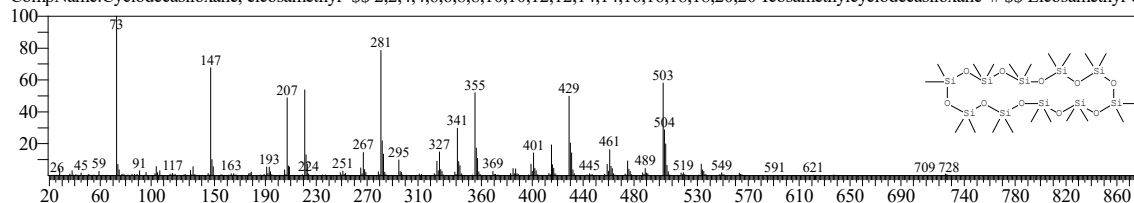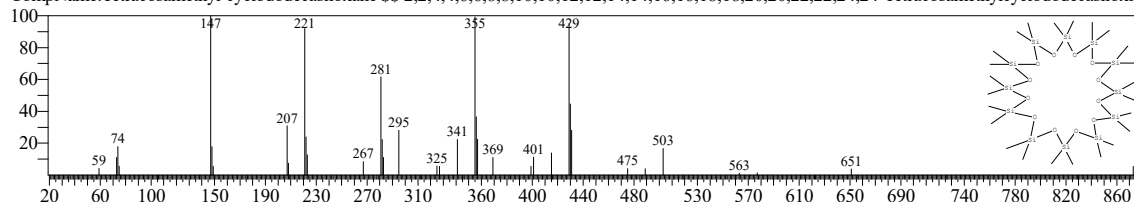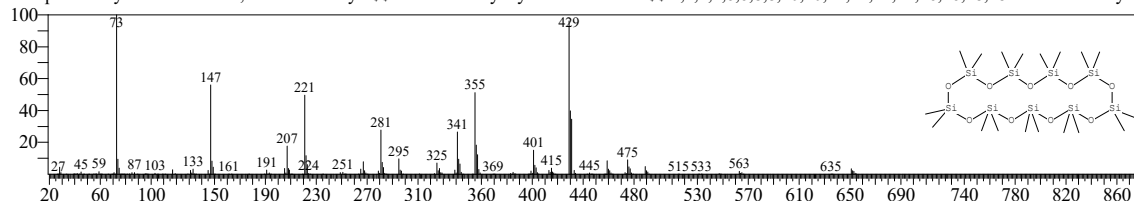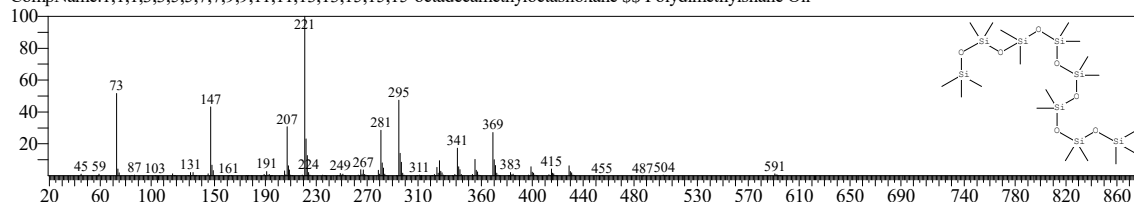
TNAU

<< Target >>
Line#:14 R.Time:24.955(Scan#:4092) MassPeaks:335
RawMode:Averaged 24.950-24.960(4091-4093) BasePeak:355.05(8728)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:45685 Library:NIST20M2.lib
SI:86 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:2 Entry:46368 Library:NIST20M2.lib
SI:84 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:80 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
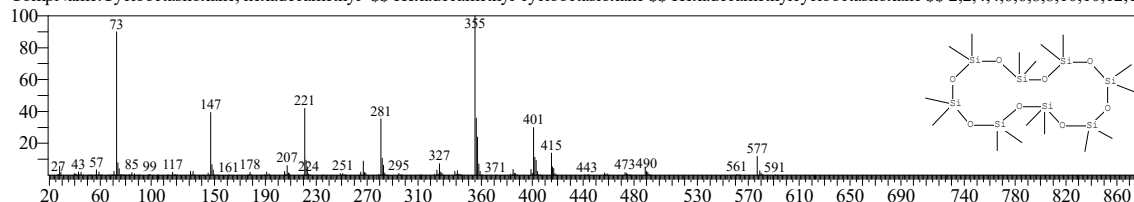SI:74 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:42384 Library:NIST20M2.lib
SI:73 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12
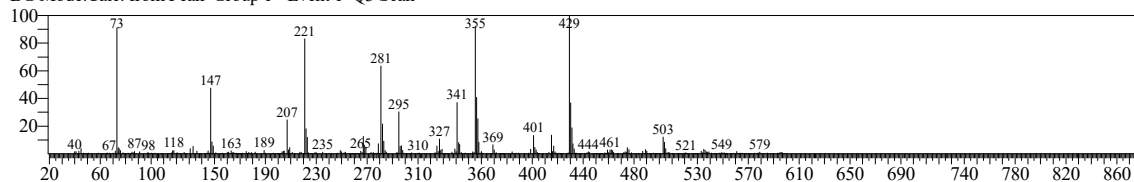
TNAU

<< Target >>
Line#:15   R.Time:25.975(Scan#:4296) MassPeaks:325
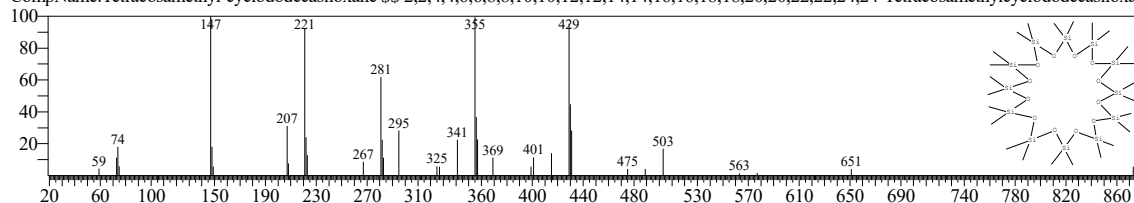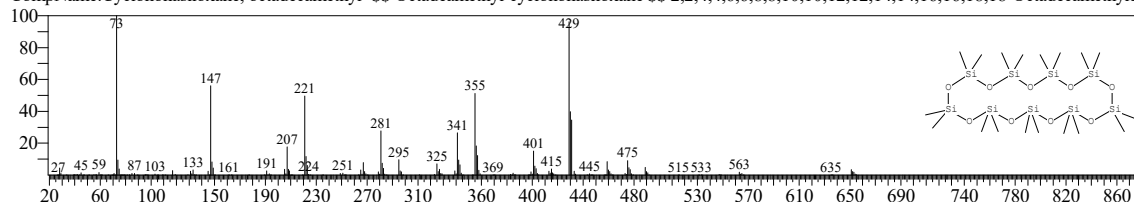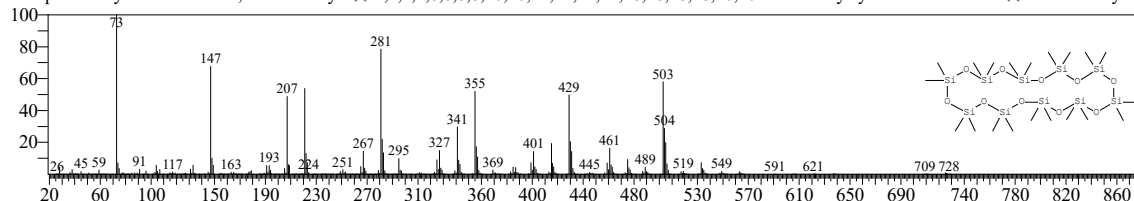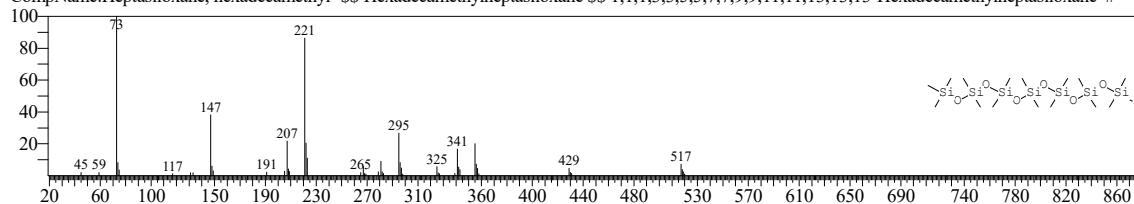RawMode:Averaged 25.970-25.980(4295-4297) BasePeak:429.10(8038)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:85 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:44570 Library:NIST20M2.lib
SI:83 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:3 Entry:45685 Library:NIST20M2.lib
SI:81 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:4 Entry:38404 Library:NIST20M2.lib
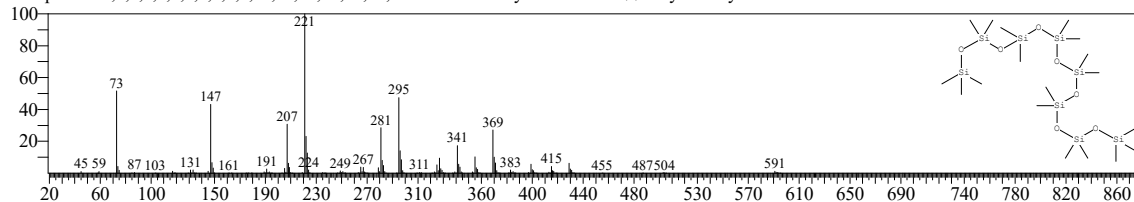SI:75 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #

Hit#:5 Entry:42942 Library:NIST20M2.lib
SI:74 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil
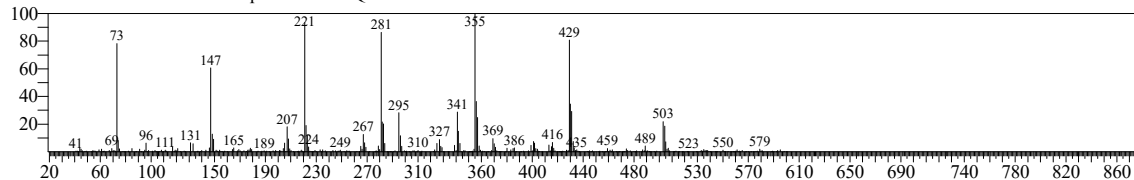
TNAU

<< Target >>
Line#:16   R.Time:26.930(Scan#:4487) MassPeaks:331
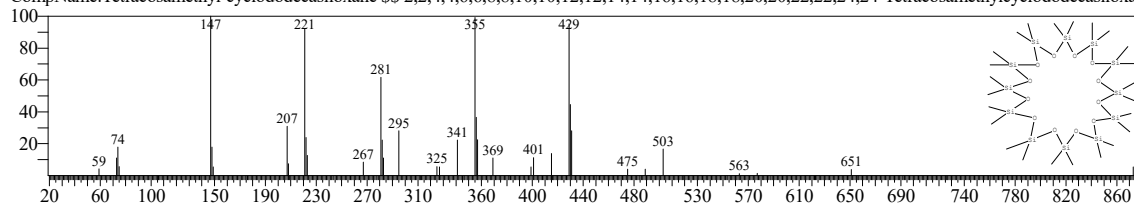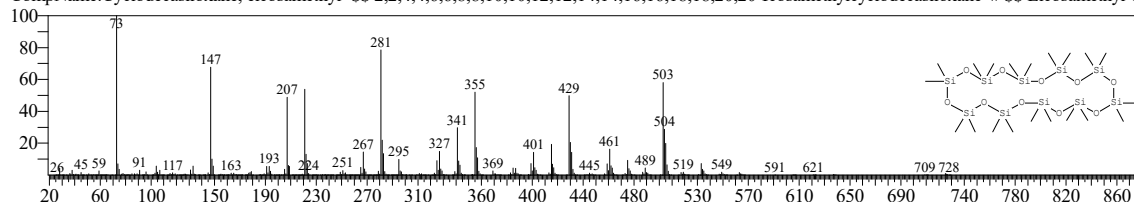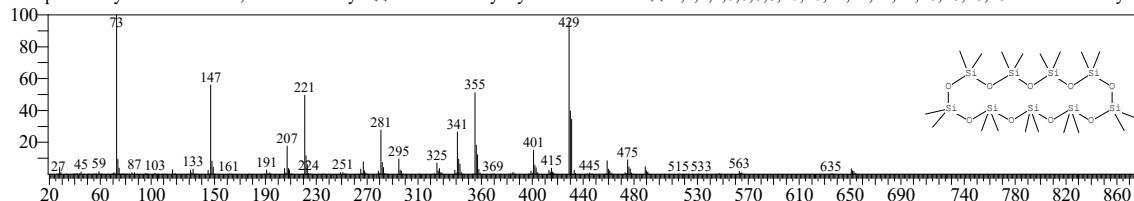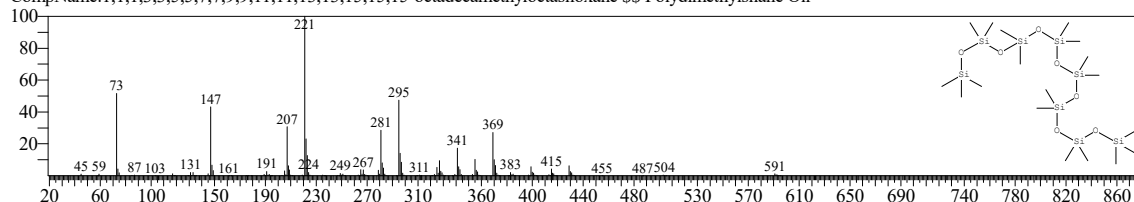RawMode:Averaged 26.925-26.935(4486-4488) BasePeak:355.05(6270)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:84 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:81 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:80 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
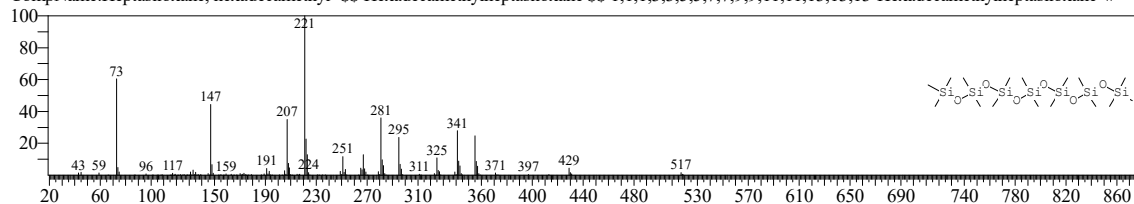SI:74 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:73 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
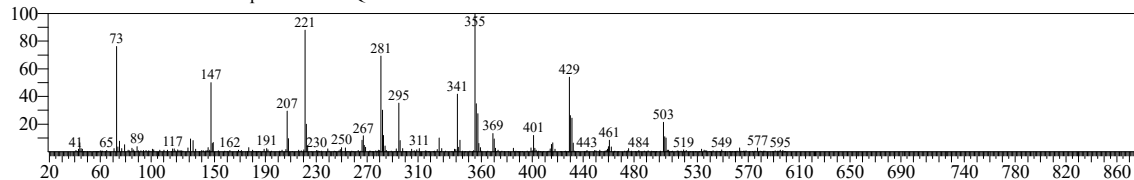
TNAU

<< Target >>
Line#:17 R.Time:27.820(Scan#:4665) MassPeaks:314
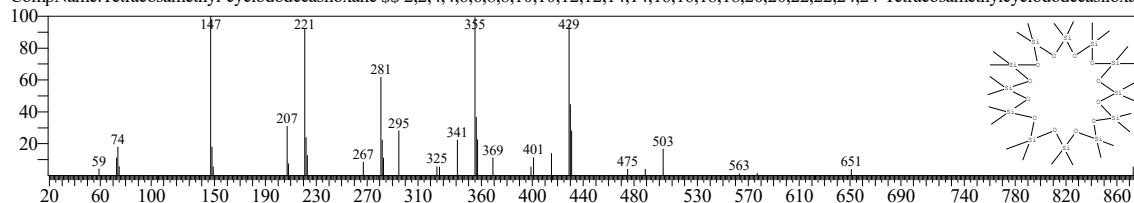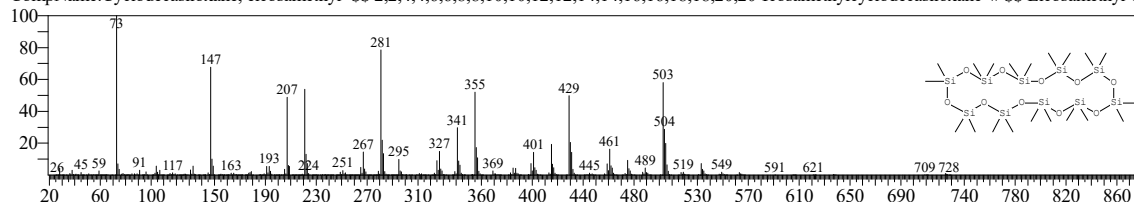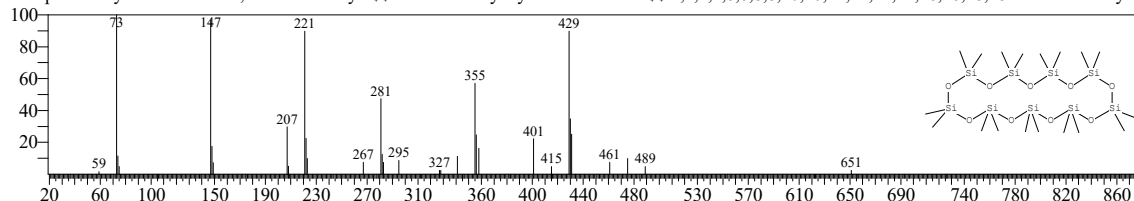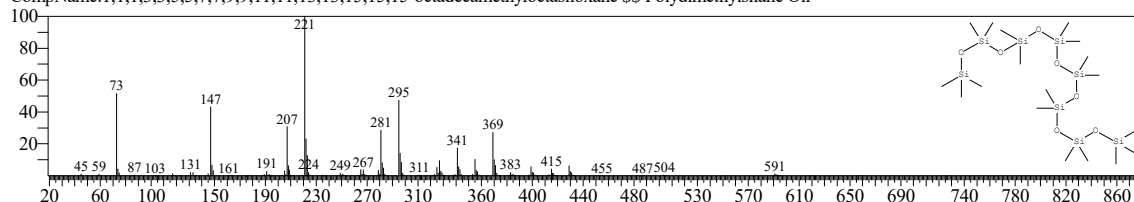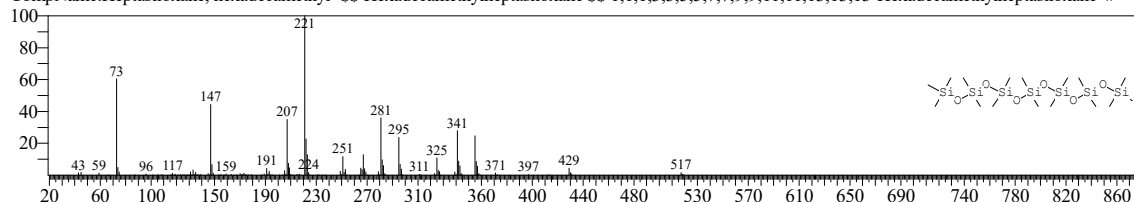RawMode:Averaged 27.815-27.825(4664-4666) BasePeak:355.05(5625)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:82 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:80 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:43658 Library:NIST20R.lib
SI:79 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
SI:74 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:72 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
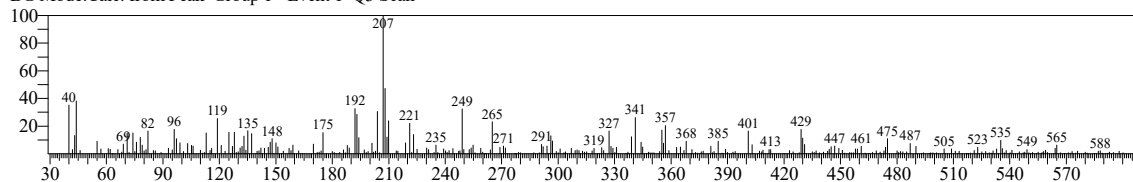
TNAU

<< Target >>
Line#:18 R.Time:28.360(Scan#:4773) MassPeaks:309
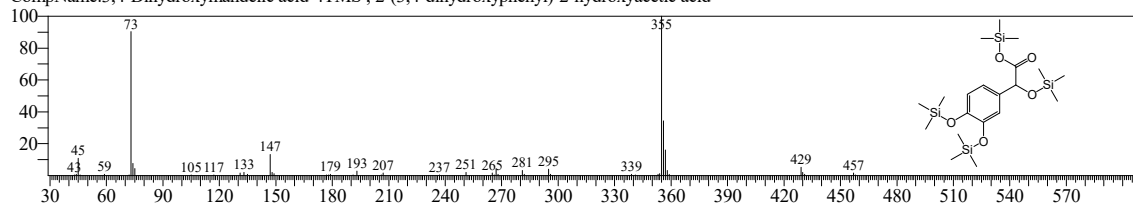RawMode:Averaged 28.355-28.365(4772-4774) BasePeak:207.05(1360)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
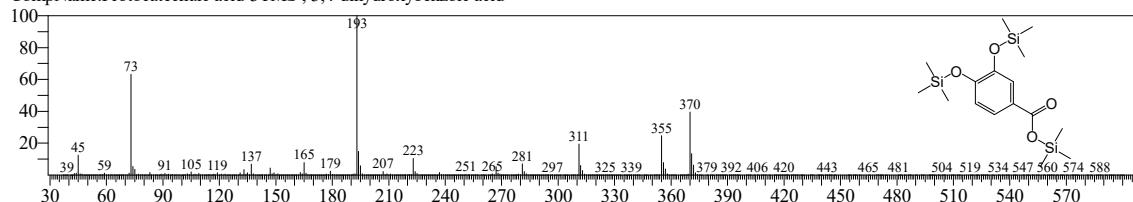SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

Hit#:3 Entry:359 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:4 Entry:329 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C11H27NO4SSi2 CAS:820-10-0 MolWeight:325 RetIndex:1848
CompName:Methionine sulfone-2TMS ; 2-amino-4-methylsulfonylbutanoic acid

Hit#:5 Entry:420 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H33NO4Si3 CAS:487-54-7 MolWeight:411 RetIndex:1973
CompName:2-Hydroxyhippuric acid-3TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid
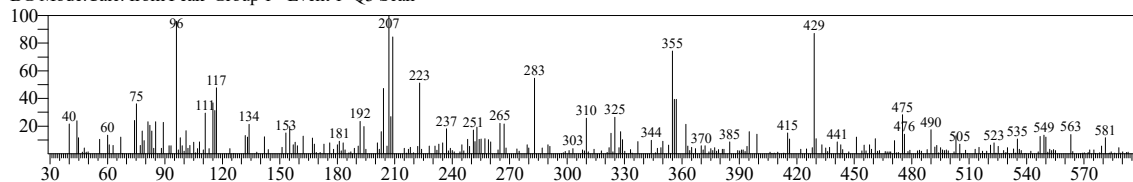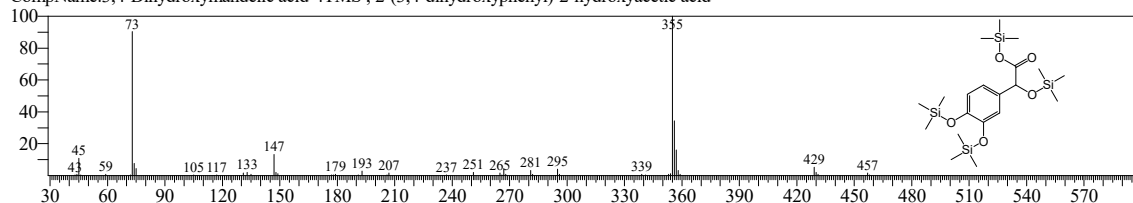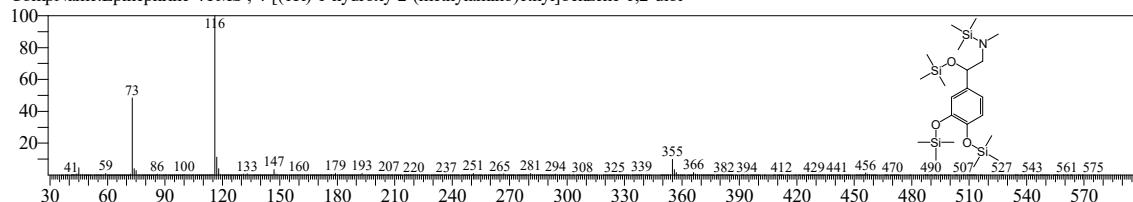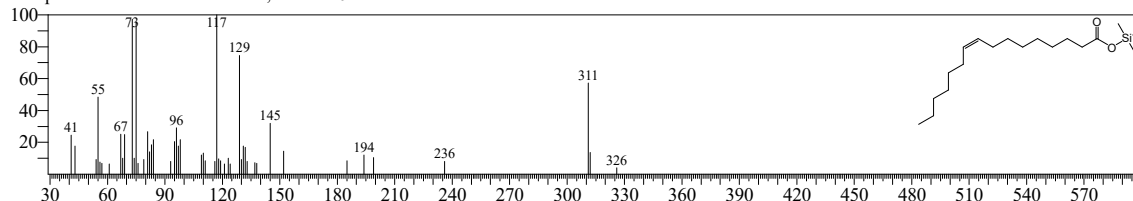
TNAU

<< Target >>
Line#:19 R.Time:28.400(Scan#:4781) MassPeaks:298
RawMode:Averaged 28.395-28.405(4780-4782) BasePeak:207.00(628)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 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#:2 Entry:431 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C21H45NO3Si4 CAS:51-43-4 MolWeight:471 RetIndex:1989
CompName:Epinephrine-4TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:3 Entry:442 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C19H38O2Si CAS:373-49-9 MolWeight:326 RetIndex:2028
CompName:Palmitoleic acid-TMS ; hexadec-9-enoic acid

Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:5 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
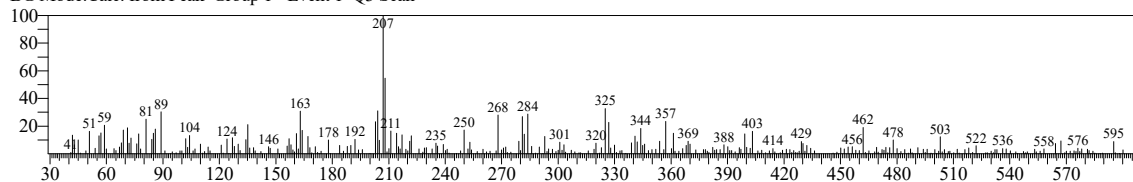CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

TNAU

<< Target >>
Line#:20 R.Time:28.525(Scan#:4806) MassPeaks:318
RawMode:Averaged 28.520-28.530(4805-4807) BasePeak:207.05(829)
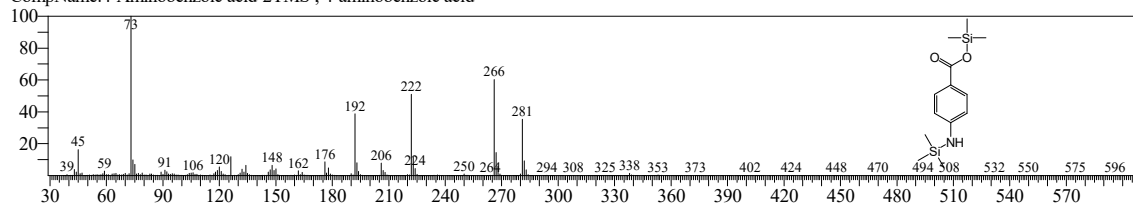BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
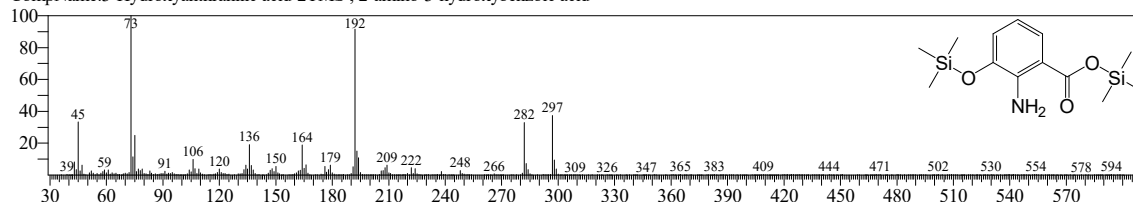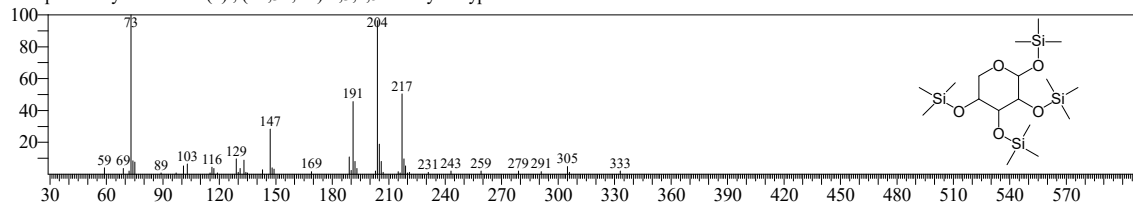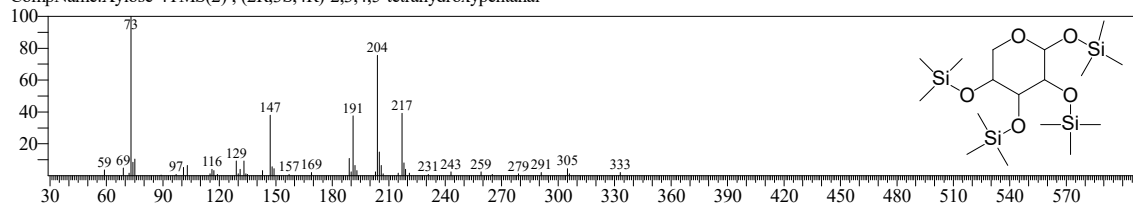SI:27 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:2 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:3 Entry:205 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1624
CompName:Lyxose-4TMS(1) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:4 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:5 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
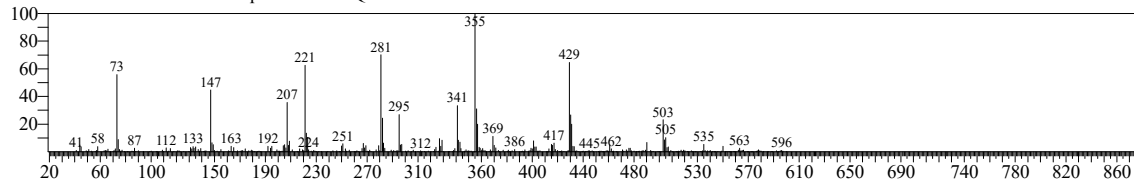CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

TNAU

<< Target >>
Line#:21 R.Time:28.705(Scan#:4842) MassPeaks:355
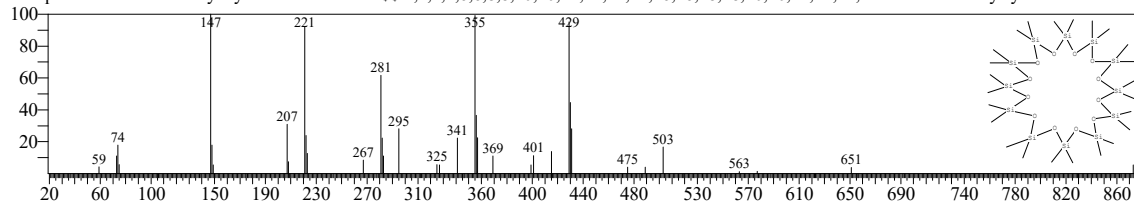RawMode:Averaged 28.700-28.710(4841-4843) BasePeak:355.05(5974)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
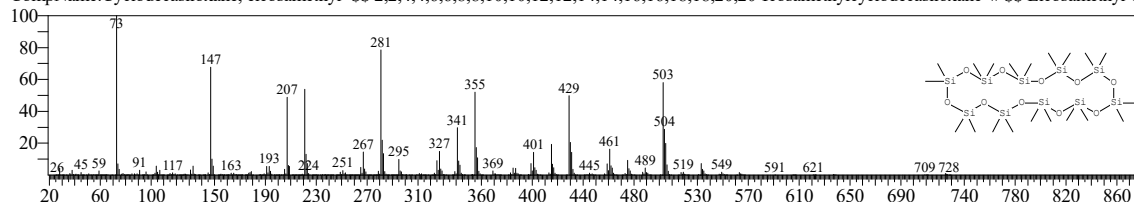SI:82 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:80 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:43658 Library:NIST20R.lib
SI:76 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
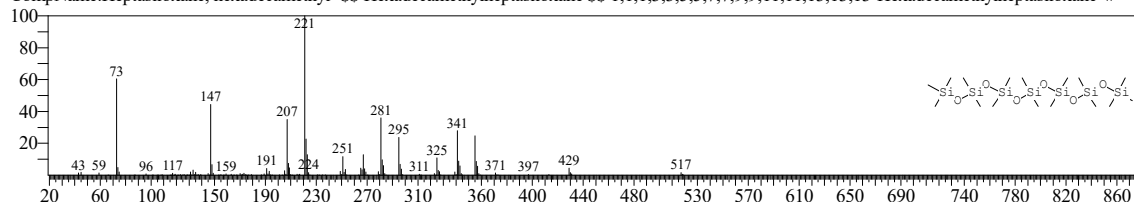SI:74 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:73 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
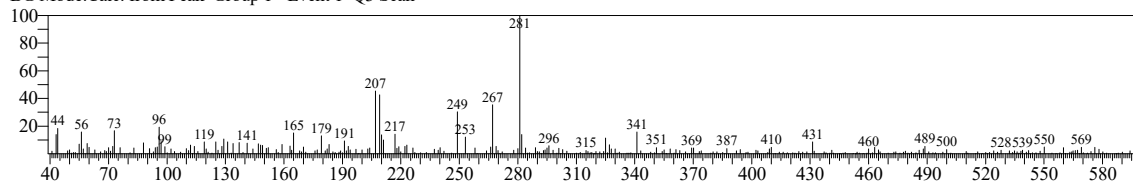
TNAU

<< Target >>
Line#:22   R.Time:29.205(Scan#:4942) MassPeaks:294
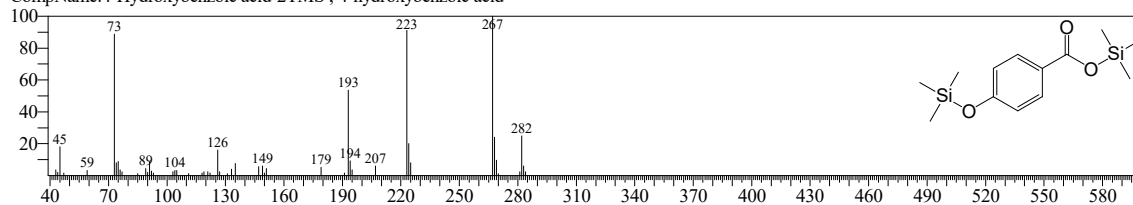RawMode:Averaged 29.200-29.210(4941-4943) BasePeak:281.05(1560)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
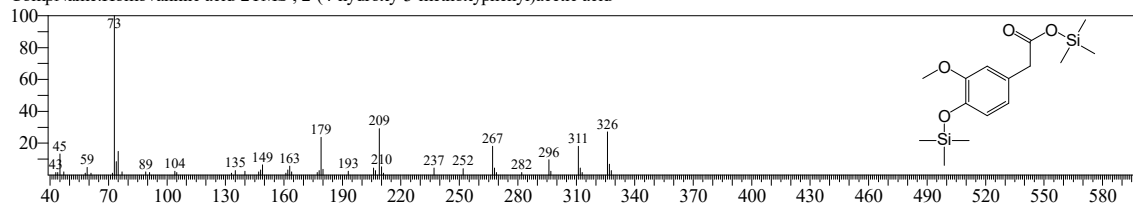SI:38 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:2 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
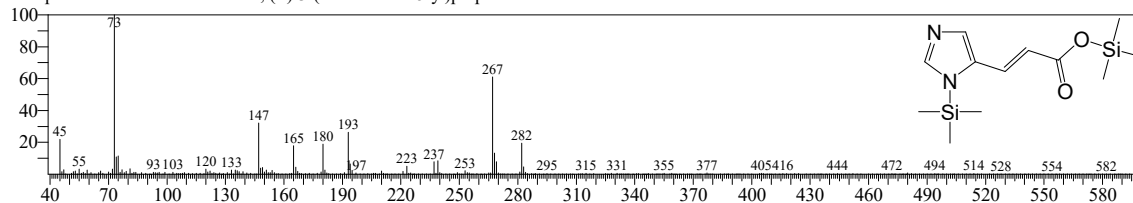SI:37 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:3 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

Hit#:4 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
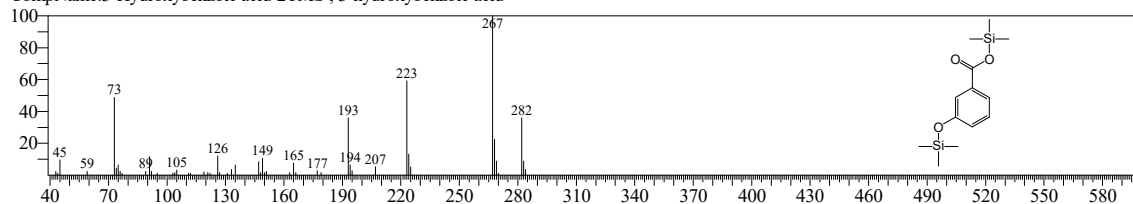SI:36 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

Hit#:5 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid
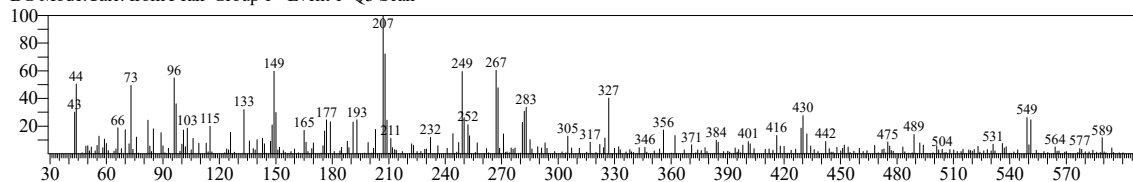
TNAU

<< Target >>
Line#:23 R.Time:29.490(Scan#:4999) MassPeaks:302
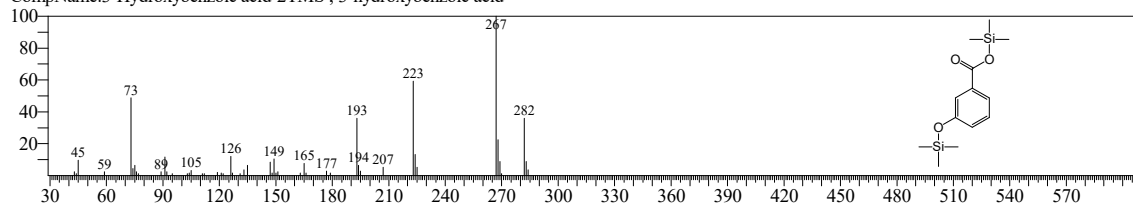RawMode:Averaged 29.485-29.495(4998-5000) BasePeak:207.05(858)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
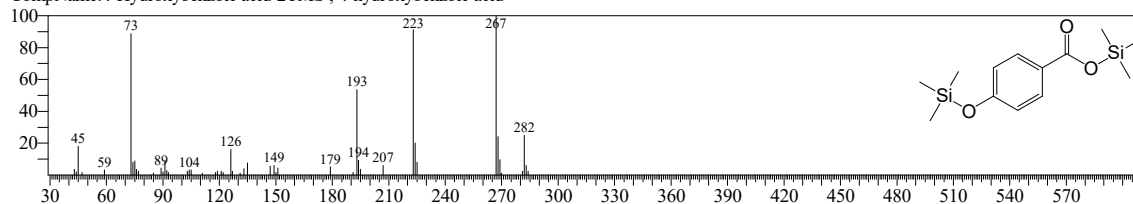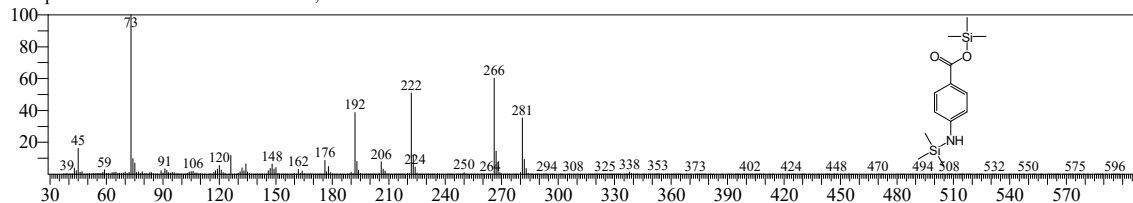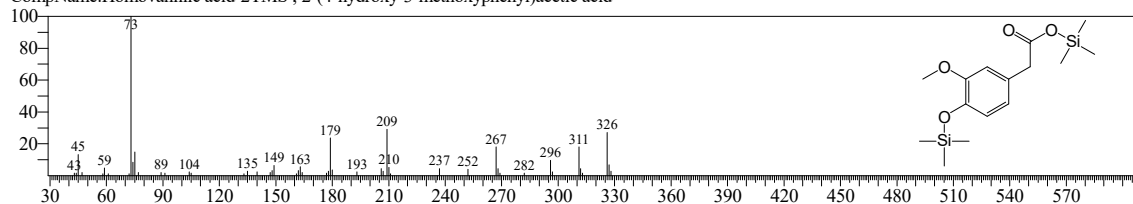CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:4 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
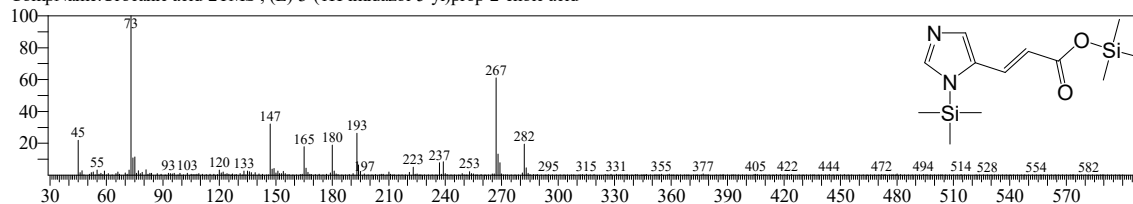CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:5 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid
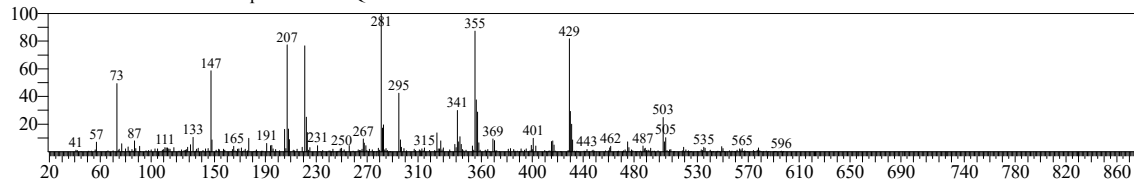
TNAU

<< Target >>
Line#:24 R.Time:29.720(Scan#:5045) MassPeaks:308
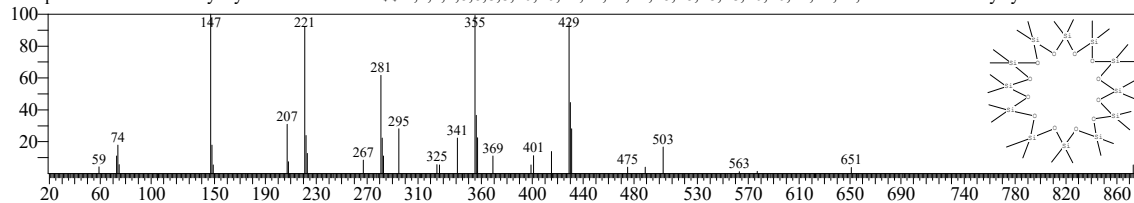RawMode:Averaged 29.715-29.725(5044-5046) BasePeak:281.05(3381)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
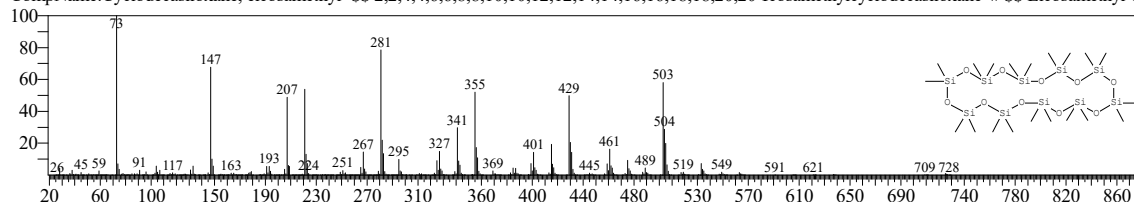SI:80 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:79 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
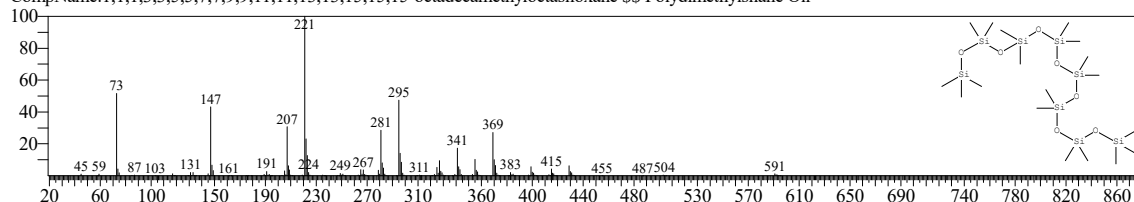SI:75 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
SI:72 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
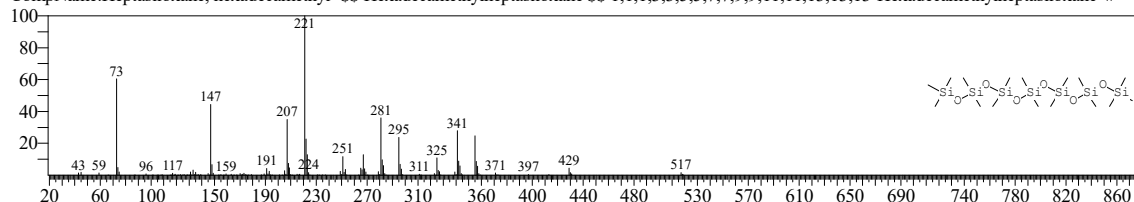CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:71 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
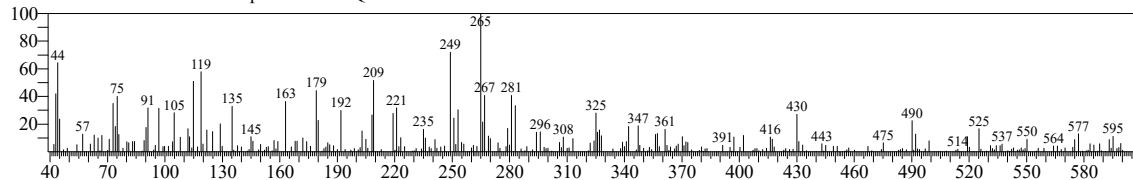
TNAU

<< Target >>
Line#:25 R.Time:30.270(Scan#:5155) MassPeaks:296
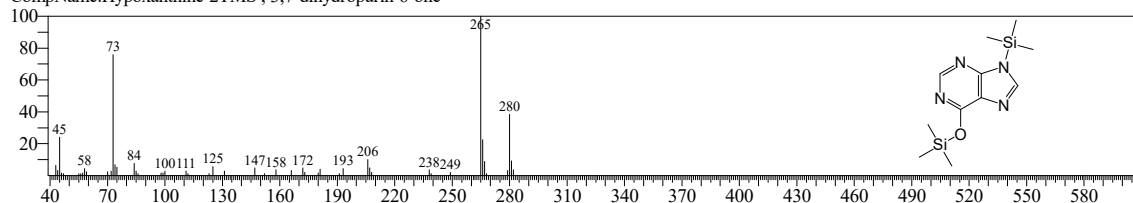RawMode:Averaged 30.265-30.275(5154-5156) BasePeak:265.00(767)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
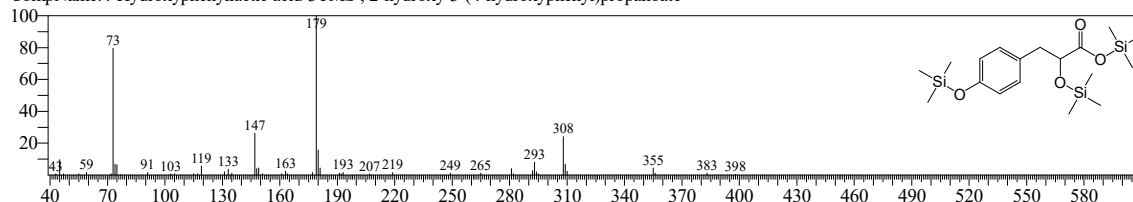SI:36 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:2 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
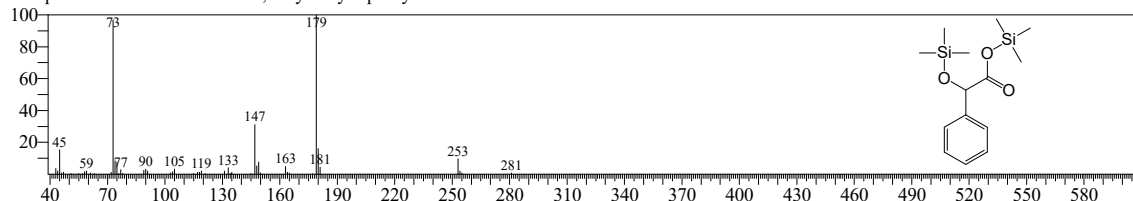SI:35 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

Hit#:3 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid

Hit#:4 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
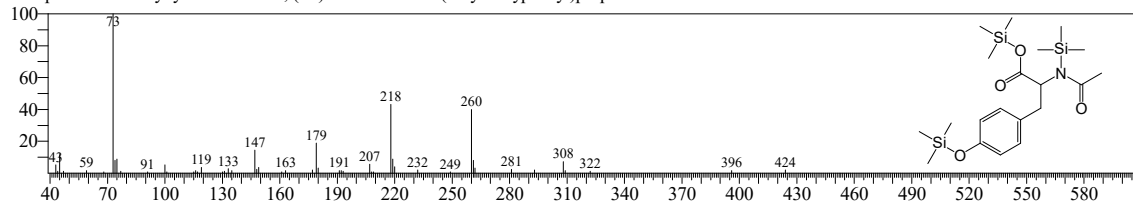SI:33 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:5 Entry:461 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C20H37NO4Si3 CAS:537-55-3 MolWeight:439 RetIndex:2119
CompName:N-Acetyltyrosine-3TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid
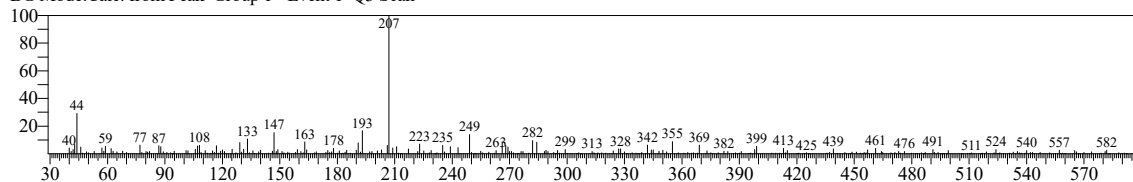
TNAU

<< Target >>
Line#:26 R.Time:30.305(Scan#:5162) MassPeaks:289
RawMode:Averaged 30.300-30.310(5161-5163) BasePeak:207.05(2727)
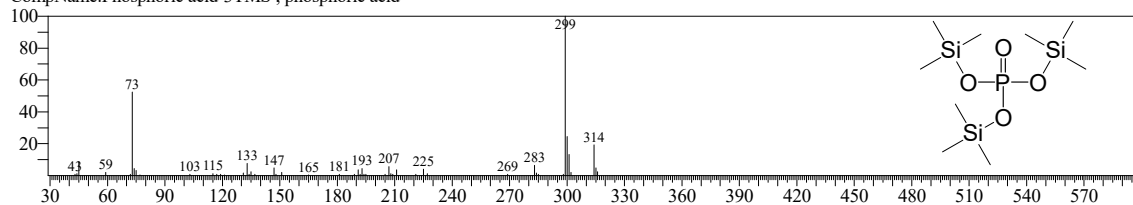BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:79 Library:OA_TMS_DB5_67min_V3.lib
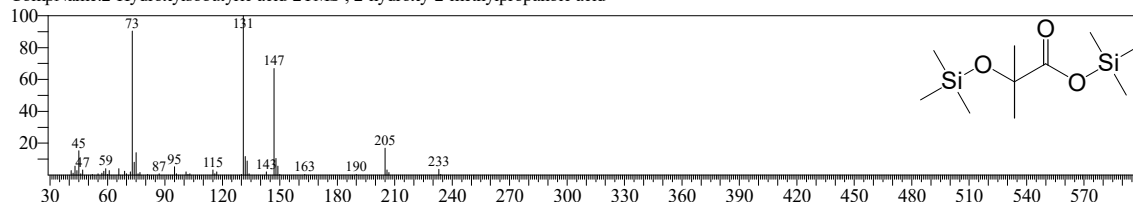SI:32 Formula:C9H27O4PSi3 CAS:7664-38-2 MolWeight:314 RetIndex:1280
CompName:Phosphoric acid-3TMS ; phosphoric acid

Hit#:2 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
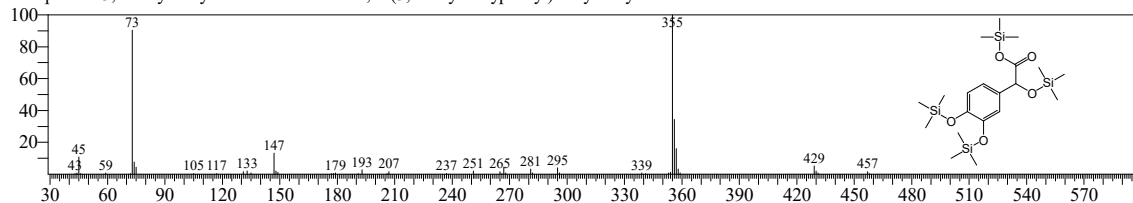SI:31 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid

Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
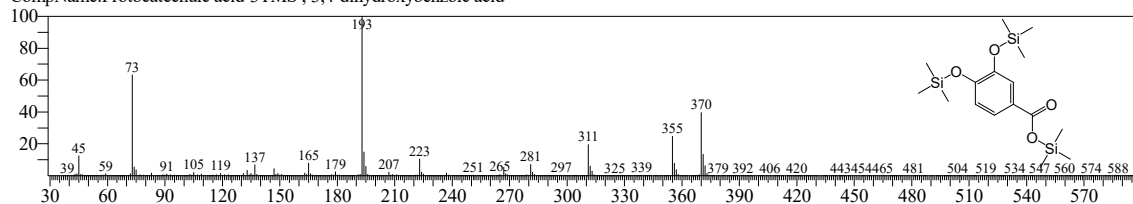CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:4 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
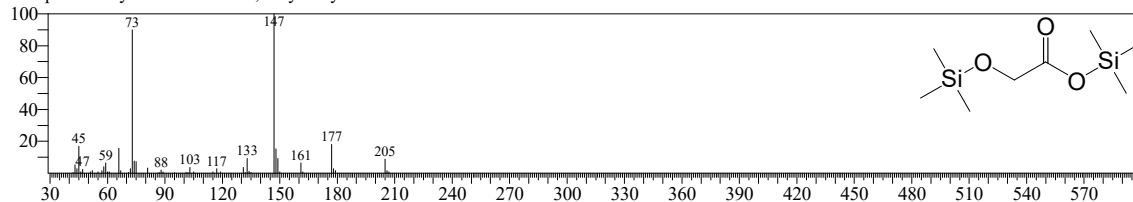CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

Hit#:5 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
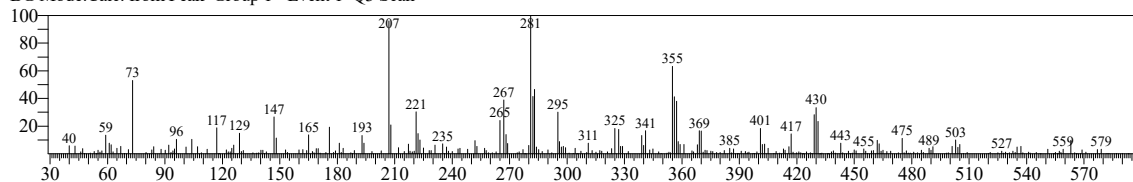CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

<< Target >>
Line#:27 R.Time:30.955(Scan#:5292) MassPeaks:294
RawMode:Averaged 30.950-30.960(5291-5293) BasePeak:281.05(1785)
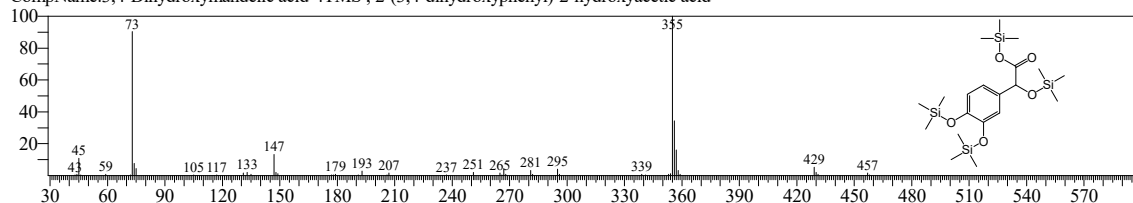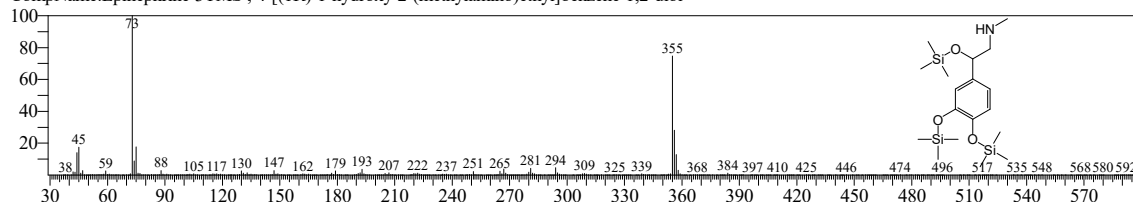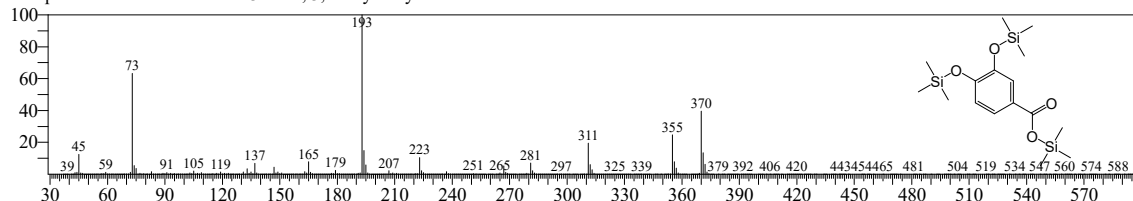BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:51 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:44 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#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
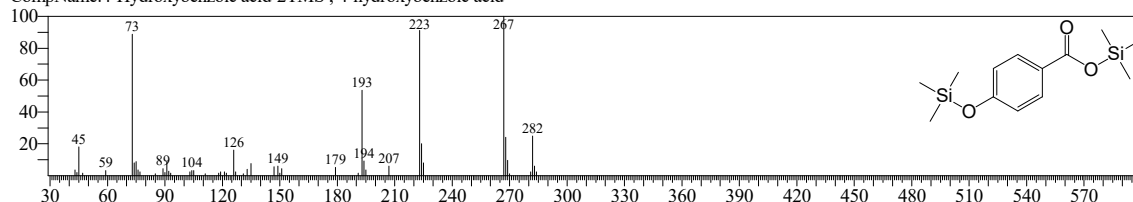SI:42 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
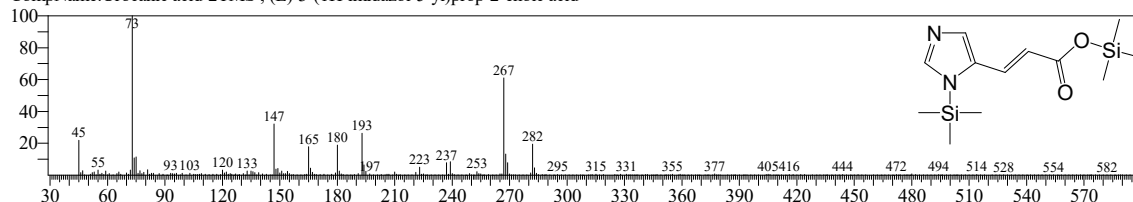SI:38 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:5 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
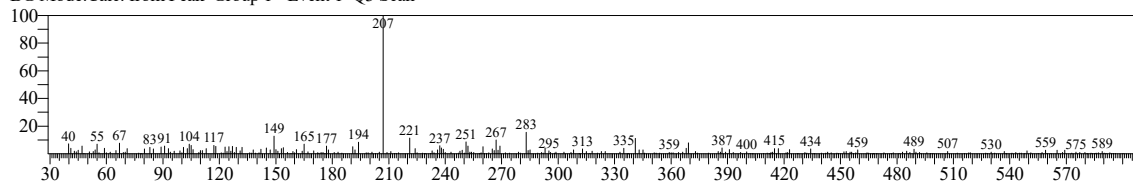CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

TNAU

<< Target >>
Line#:28 R.Time:30.990(Scan#:5299) MassPeaks:283
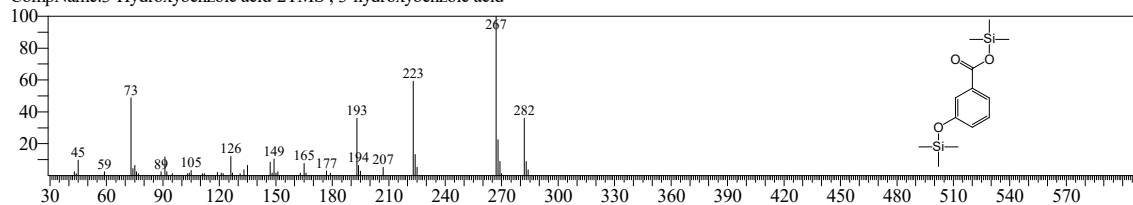RawMode:Averaged 30.985-30.995(5298-5300) BasePeak:207.00(2385)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
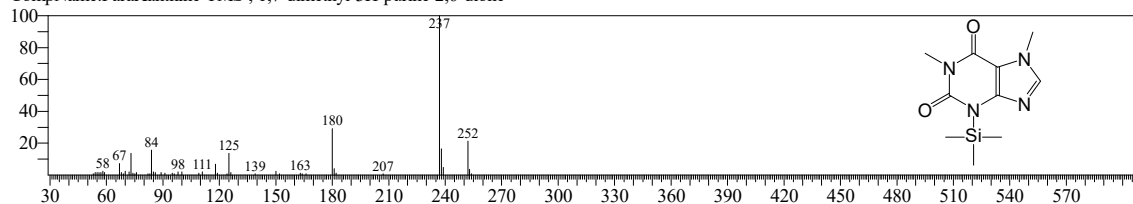SI:32 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:2 Entry:428 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C10H16N4O2Si CAS:611-59-6 MolWeight:252 RetIndex:1983
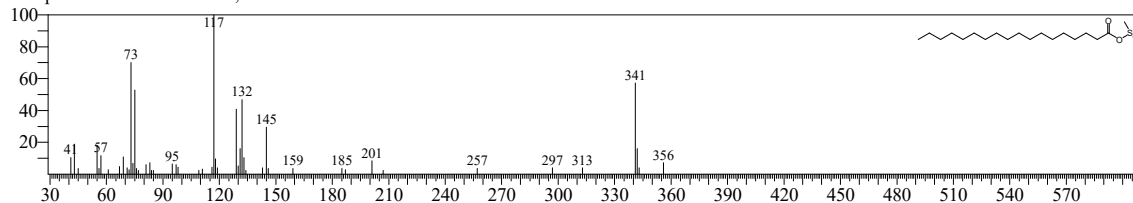CompName:ParaXanthine-TMS ; 1,7-dimethyl-3H-purine-2,6-dione

Hit#:3 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
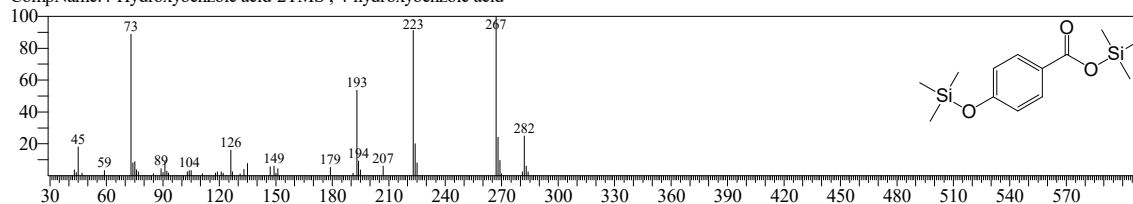CompName:Stearic acid-TMS ; octadecanoic acid

Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
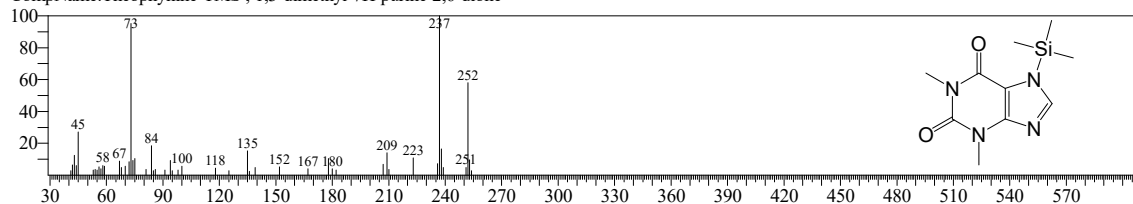SI:28 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:5 Entry:395 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C10H16N4O2Si CAS:58-55-9 MolWeight:252 RetIndex:1936
CompName:Theophylline-TMS ; 1,3-dimethyl-7H-purine-2,6-dione
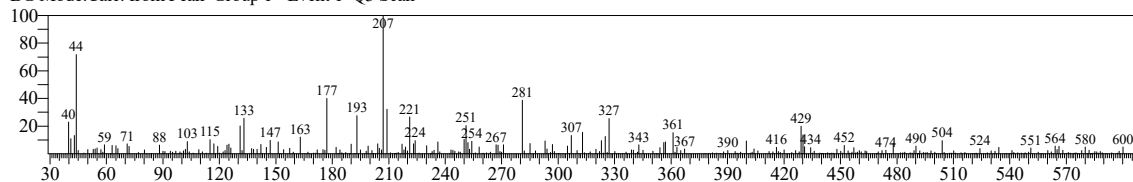
<< Target >>
Line#:29 R.Time:31.295(Scan#:5360) MassPeaks:299
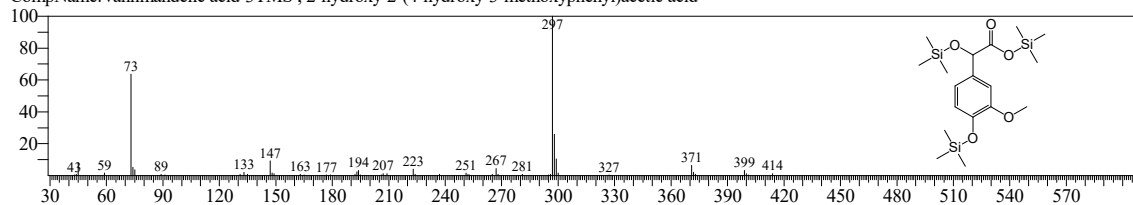RawMode:Averaged 31.290-31.300(5359-5361) BasePeak:207.05(1266)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:359 Library:OA_TMS_DB5_67min_V3.lib
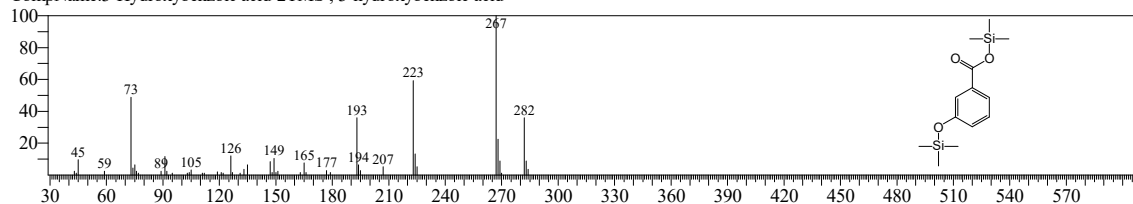SI:32 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
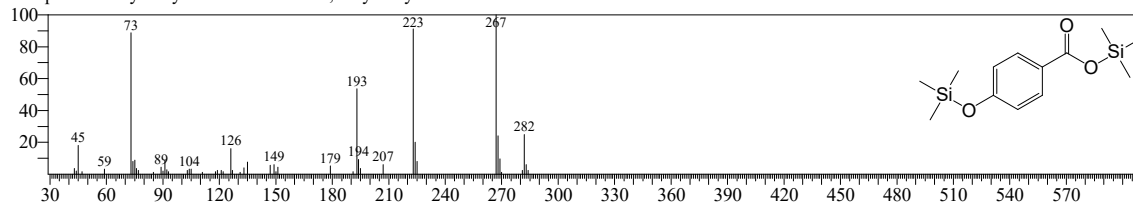SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
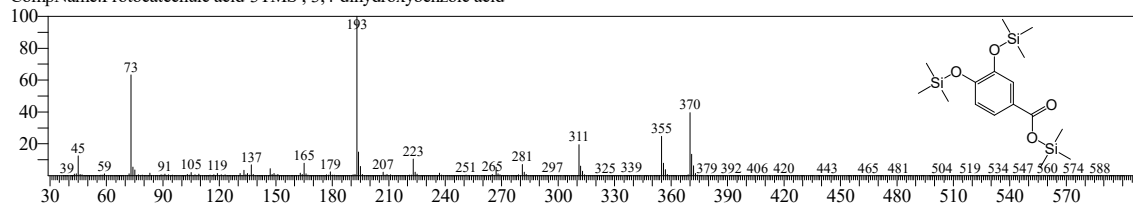SI:29 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:4 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
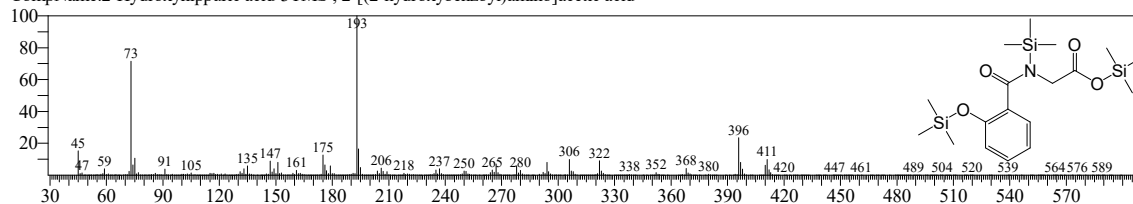SI:29 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

Hit#:5 Entry:420 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H33NO4Si3 CAS:487-54-7 MolWeight:411 RetIndex:1973
CompName:2-Hydroxyhippuric acid-3TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid
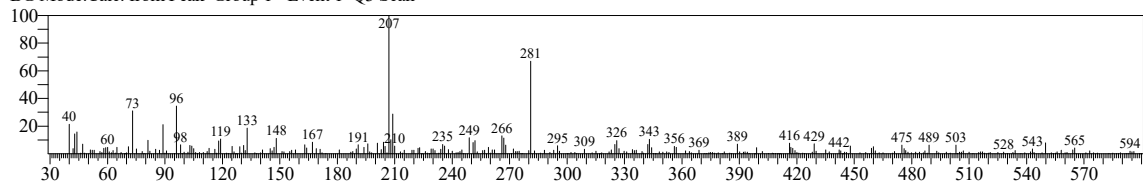
TNAU

<< Target >>
Line#:30 R.Time:31.430(Scan#:5387) MassPeaks:311
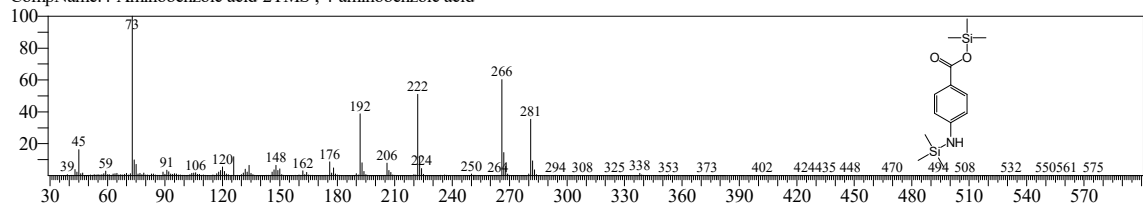RawMode:Averaged 31.425-31.435(5386-5388) BasePeak:207.05(1982)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
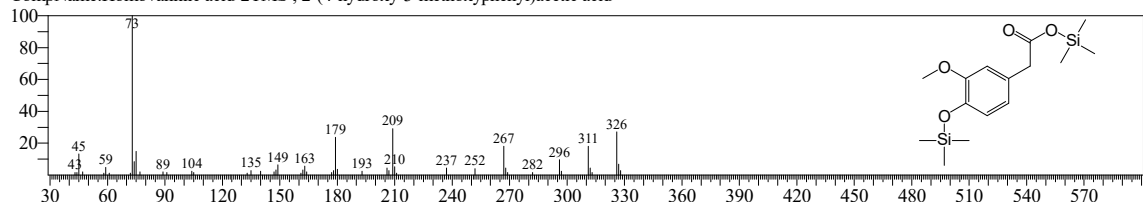CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:2 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
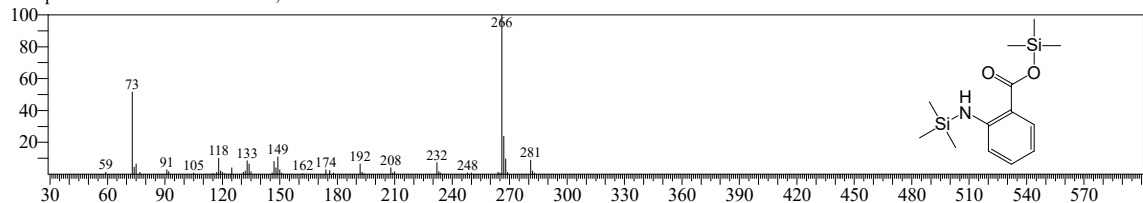SI:36 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:3 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
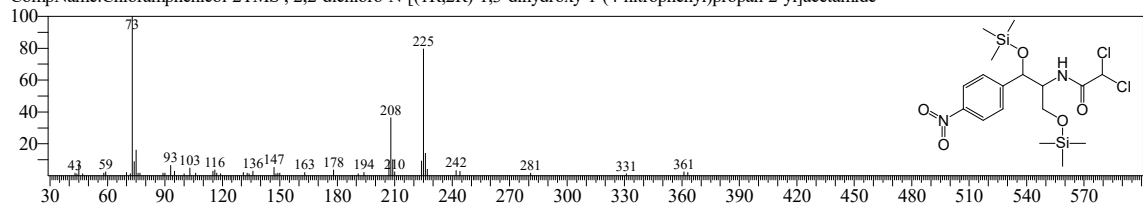SI:35 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

Hit#:4 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
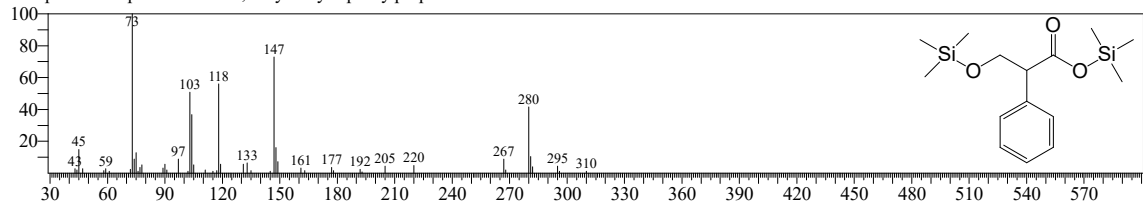SI:34 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide

Hit#:5 Entry:195 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid
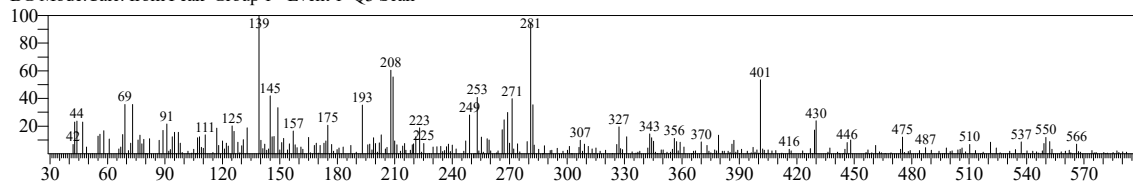
TNAU

<< Target >>
Line#:31   R.Time:31.900(Scan#:5481) MassPeaks:318
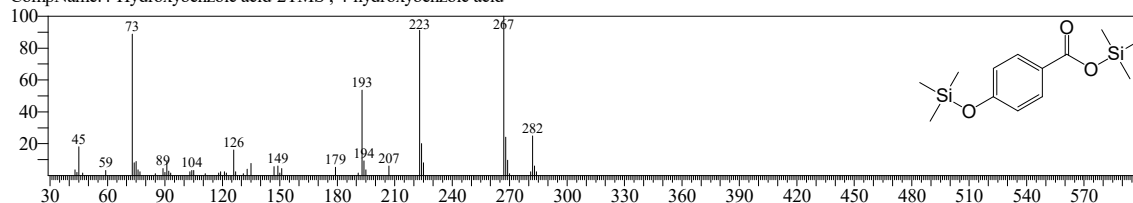RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:139.05(1036)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
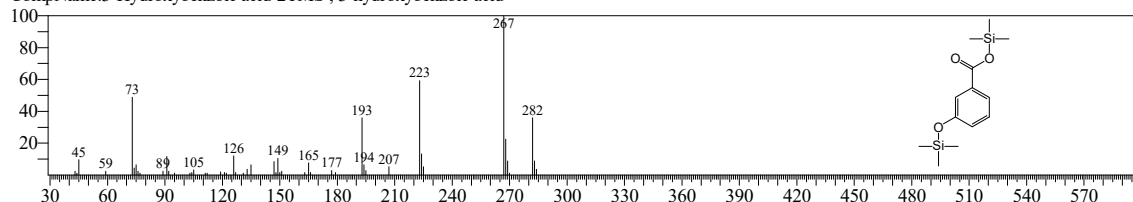CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
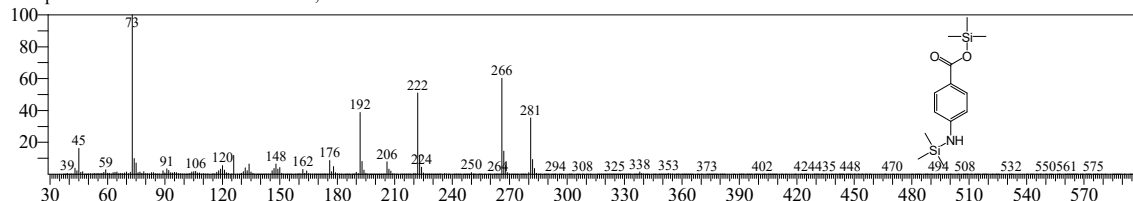CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
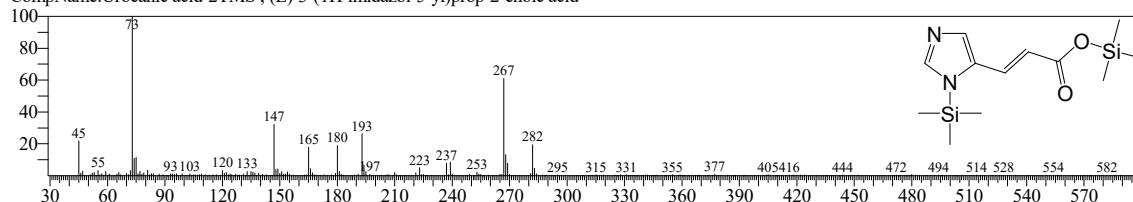CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:4 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
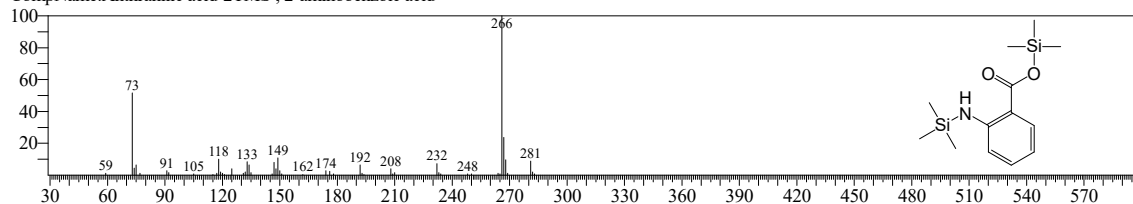CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid
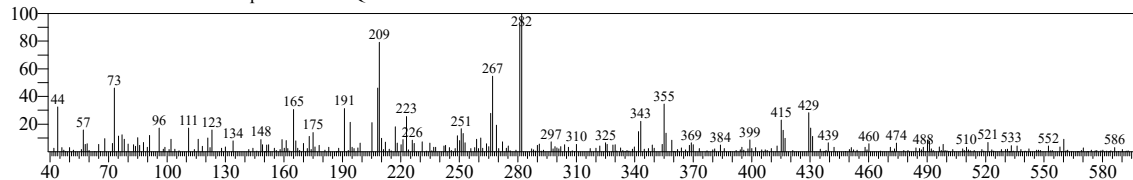
TNAU

<< Target >>
Line#:32 R.Time:32.005(Scan#:5502) MassPeaks:299
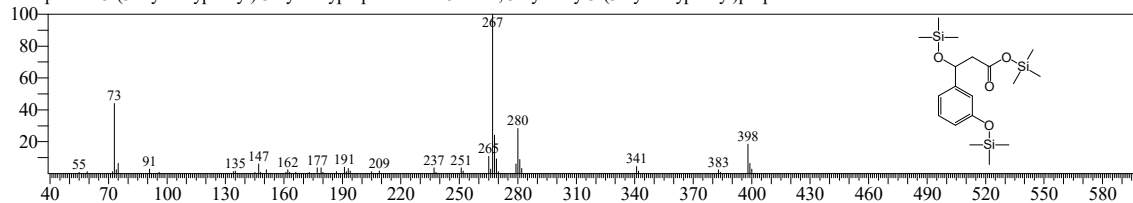RawMode:Averaged 32.000-32.010(5501-5503) BasePeak:282.05(986)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
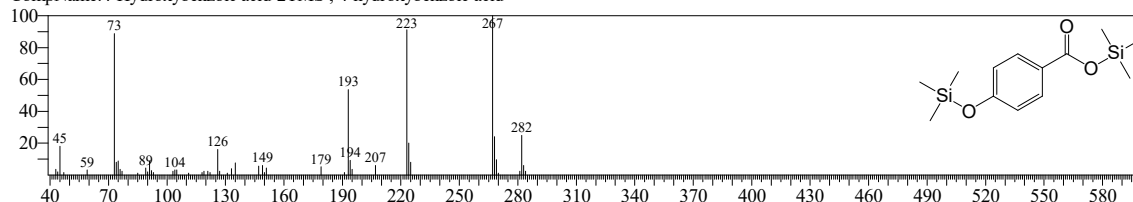SI:37 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
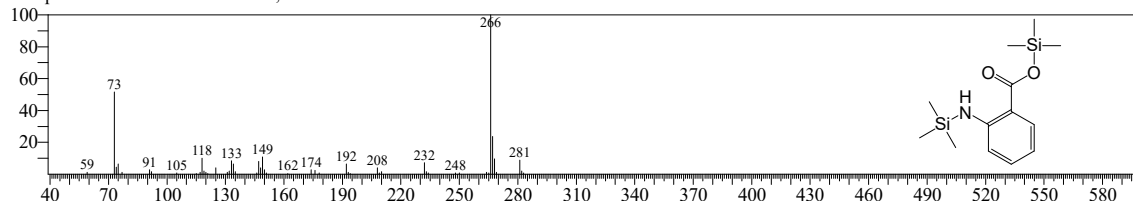SI:37 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:3 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
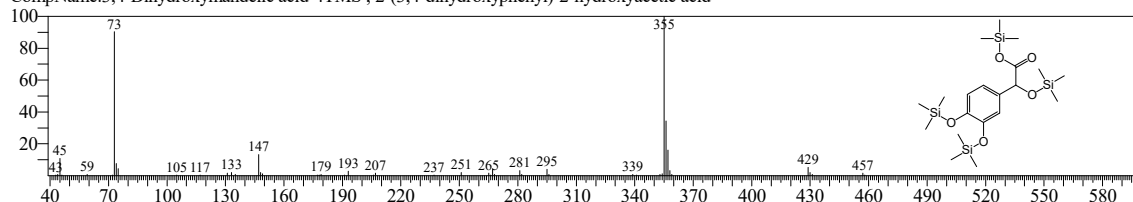SI:36 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
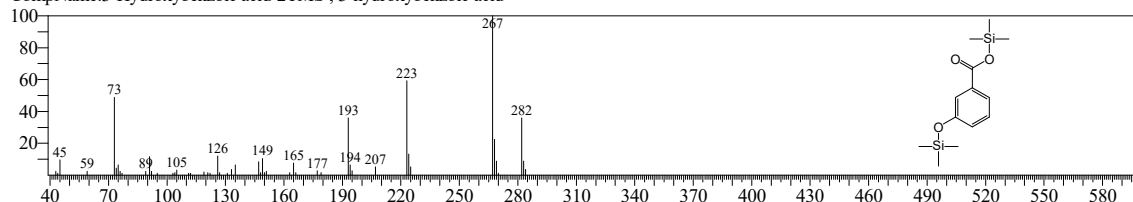SI:35 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:5 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
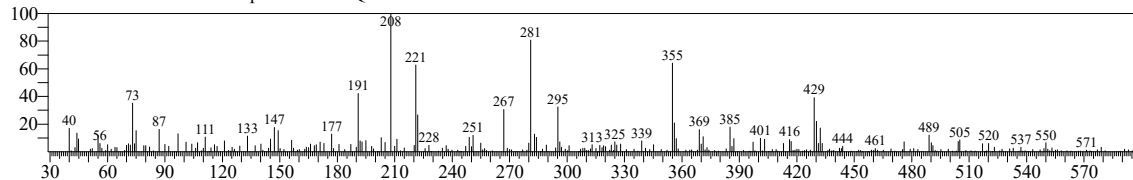
TNAU

<< Target >>
Line#:33   R.Time:32.485(Scan#:5598) MassPeaks:303
RawMode:Averaged 32.480-32.490(5597-5599) BasePeak:208.00(1585)
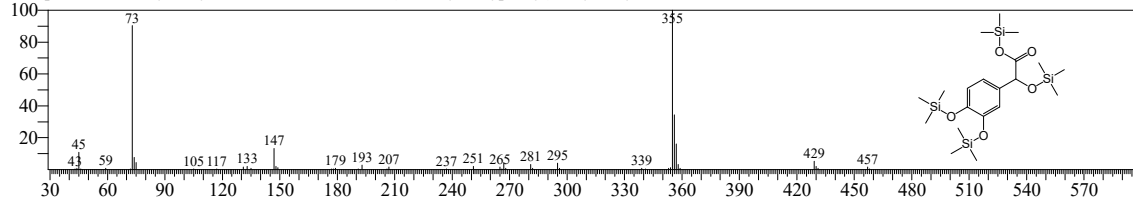BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
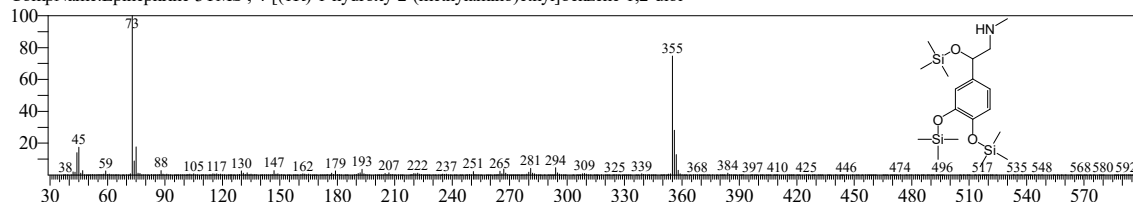SI:44 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

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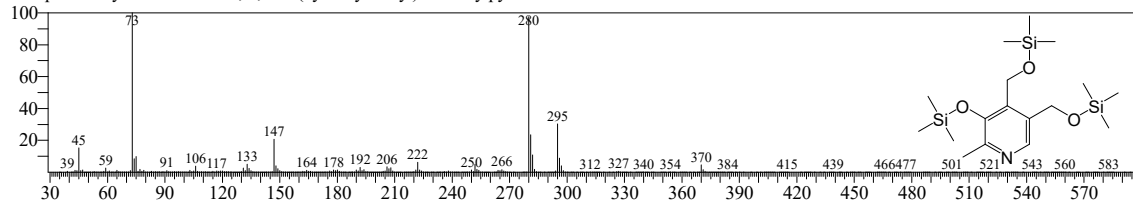CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:3 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
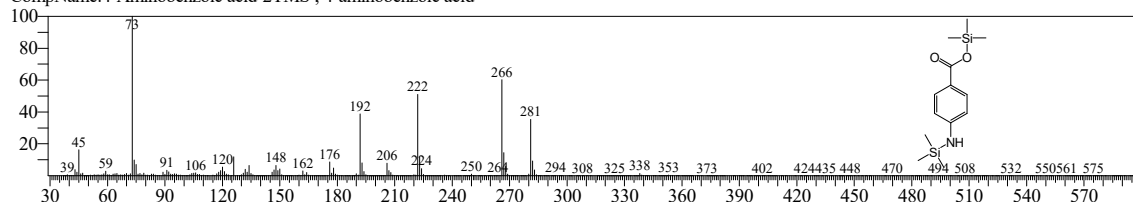CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

Hit#:4 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
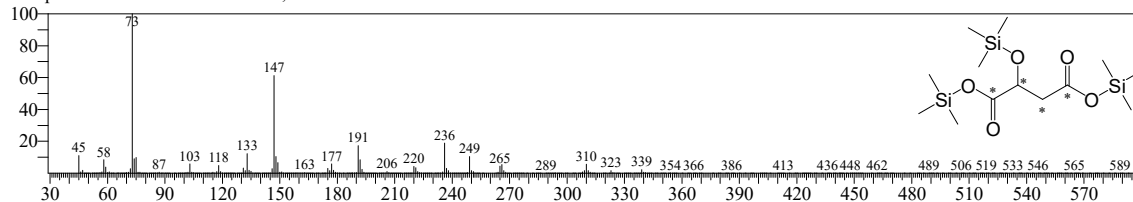SI:34 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:5 Entry:143 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula: CAS:0-00-0 MolWeight:354 RetIndex:1495
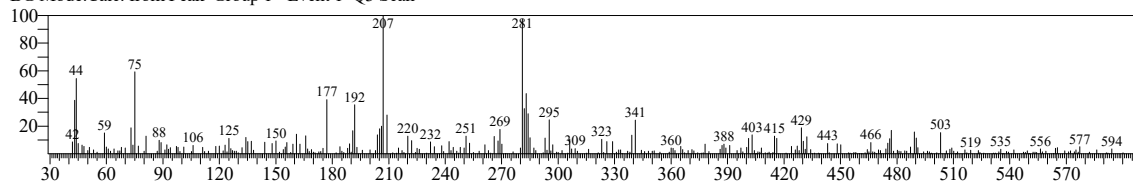CompName:Malic acid-13C4-3TMS ;

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<< Target >>
Line#:34 R.Time:32.810(Scan#:5663) MassPeaks:311
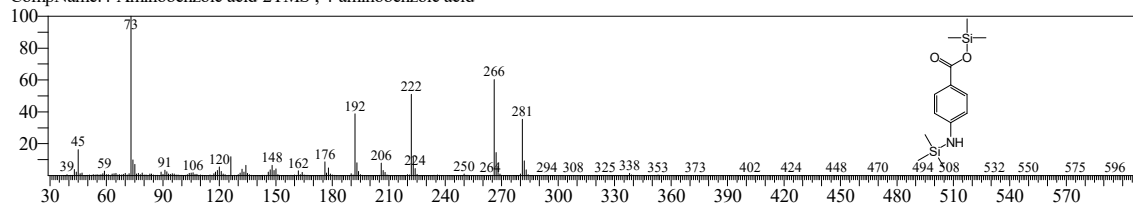RawMode:Averaged 32.805-32.815(5662-5664) BasePeak:207.05(1124)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
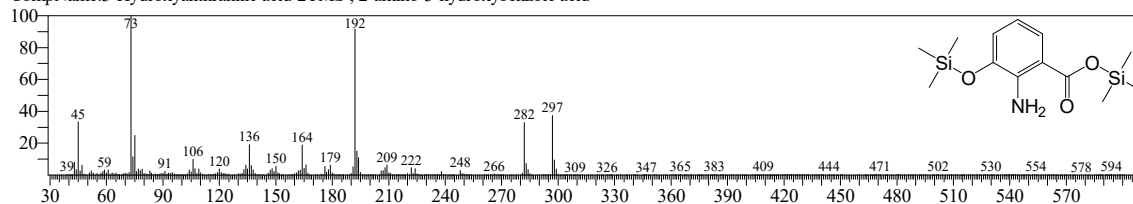SI:41 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:2 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
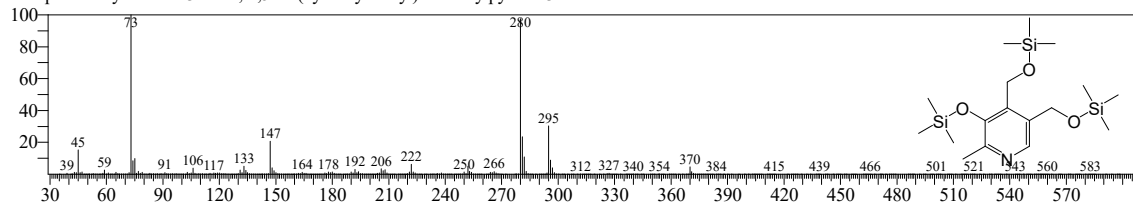CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:3 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
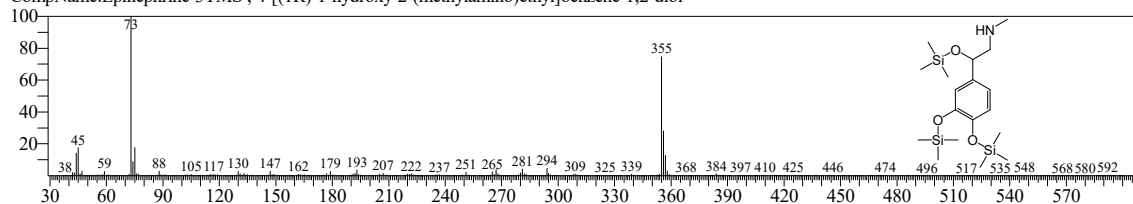SI:33 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

Hit#:4 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
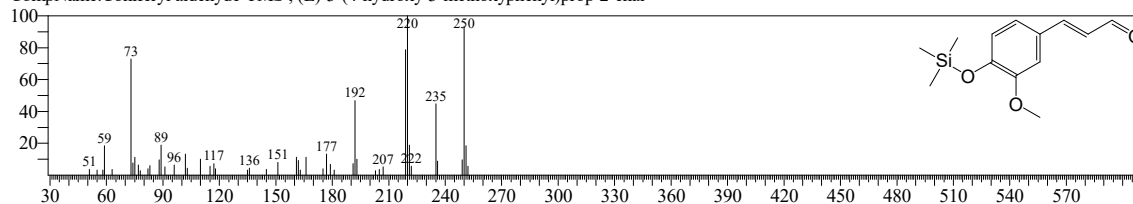CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:5 Entry:339 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H18O3Si CAS:458-36-6 MolWeight:250 RetIndex:1859
CompName:Coniferyl aldehyde-TMS ; (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal
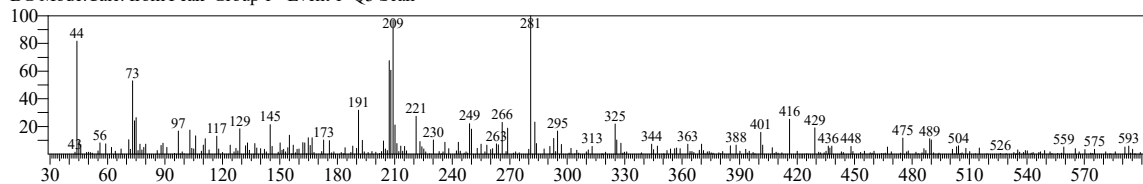
TNAU

<< Target >>
Line#:35 R.Time:32.930(Scan#:5687) MassPeaks:294
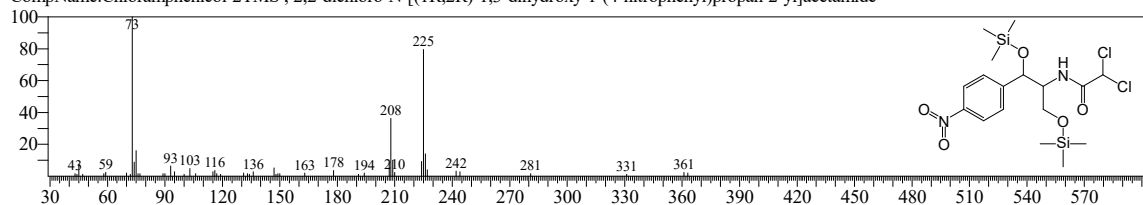RawMode:Averaged 32.925-32.935(5686-5688) BasePeak:281.00(1187)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
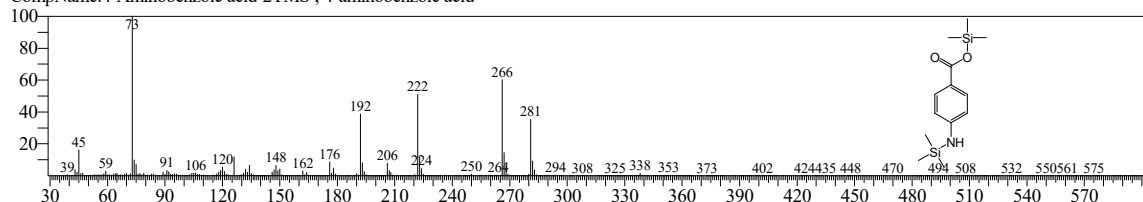CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide

Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
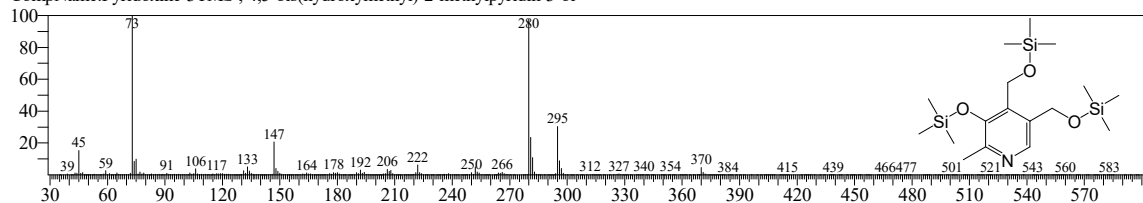SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:3 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
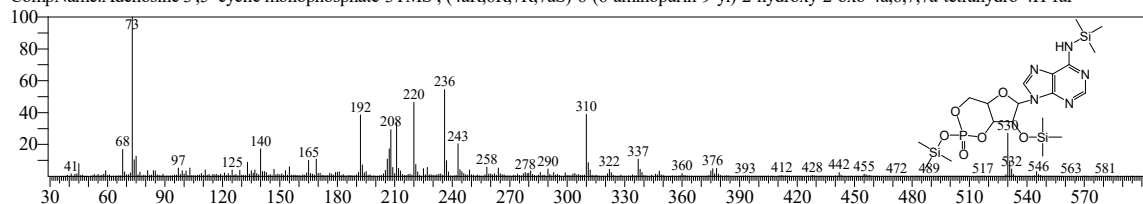SI:34 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

Hit#:4 Entry:566 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C19H36N5O6PSi3 CAS:60-92-4 MolWeight:545 RetIndex:3138
CompName:Adenosine 3',5'-cyclic monophosphate-3TMS ; (4aR,6R,7R,7aS)-6-(6-aminopurin-9-yl)-2-hydroxy-2-oxo-4a,6,7,7a-tetrahydro-4H-fur

Hit#:5 Entry:506 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C19H36N2O4Si3 CAS:2147-61-7 MolWeight:440 RetIndex:2375
CompName:3-Hydroxy-kynurenine-3TMS ; 2-amino-4-(2-amino-3-hydroxyphenyl)-4-oxobutanoic acid