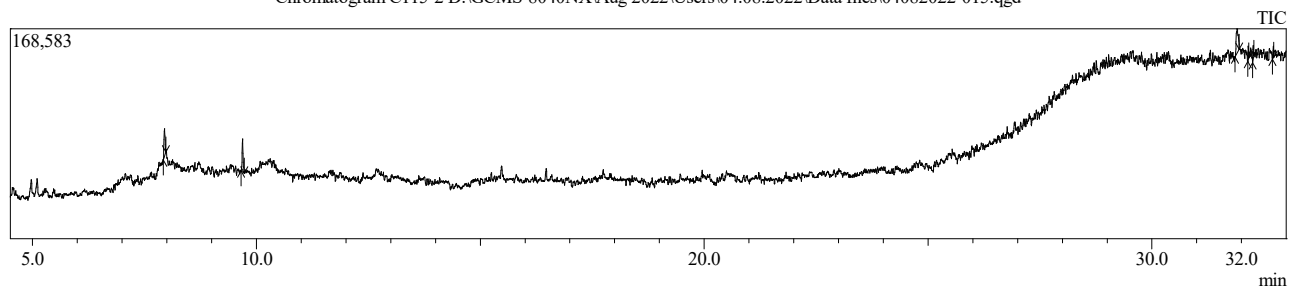


TNAU

Sample Information

Analyzed by : Admin
 Analyzed : 05-Aug-22 2:00:30 AM
 Sample Type : Unknown
 Level # : 1
 Sample Name : C115-2
 Sample ID : C115-2
 IS Amount : [1]=1
 Sample Amount : 1
 Dilution Factor : 1
 Vial # : 15
 Injection Volume : 1.00
 Data File : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-015.qgd
 Org Data File : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-015.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 4:31:31 PM

Chromatogram C115-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-015.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.945	37944	22.60	22449	22.51	1.69	85	Tridecane
2	9.690	40049	23.85	26464	26.54	1.51	89	Dodecane
3	31.902	62301	37.11	19421	19.47	3.21	31	Urocanic acid-2TMS
4	32.151	9737	5.80	10926	10.96	0.89	34	Epinephrine-4TMS
5	32.260	10526	6.27	11009	11.04	0.96	39	Epinephrine-3TMS
6	32.710	7339	4.37	9454	9.48	0.78	40	Hypoxanthine-2TMS
		167896	100.00	99723	100.00			

Library

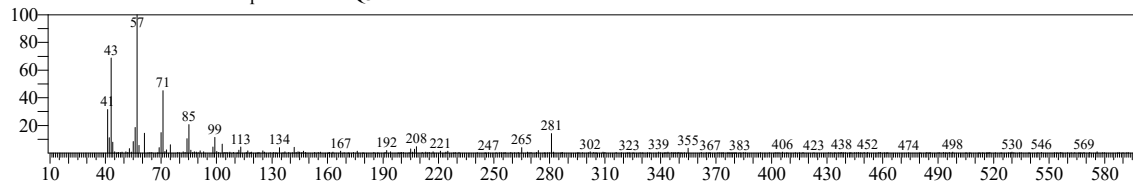
TNAU

<< Target >>

Line#:1 R.Time:7.945(Scan#:690) MassPeaks:268

RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(5090)

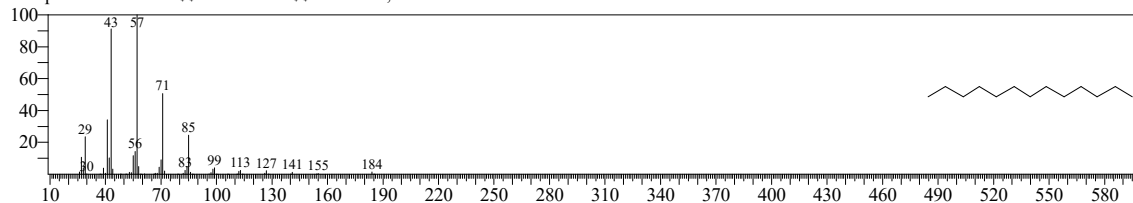
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:40226 Library:NIST20M1.lib

SI:85 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300

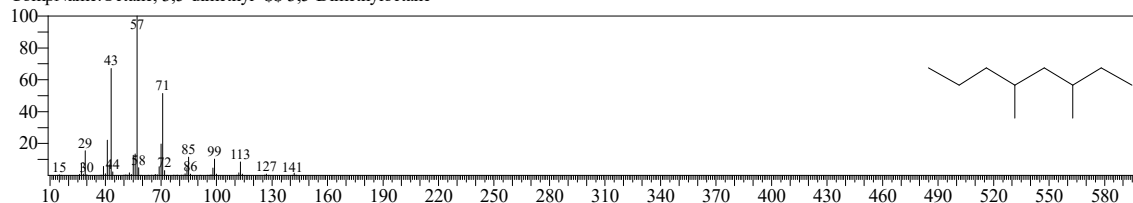
CompName:Tridecane \$\$ n-Tridecane \$\$ Tridecane, n-



Hit#:2 Entry:13631 Library:NIST20M1.lib

SI:84 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887

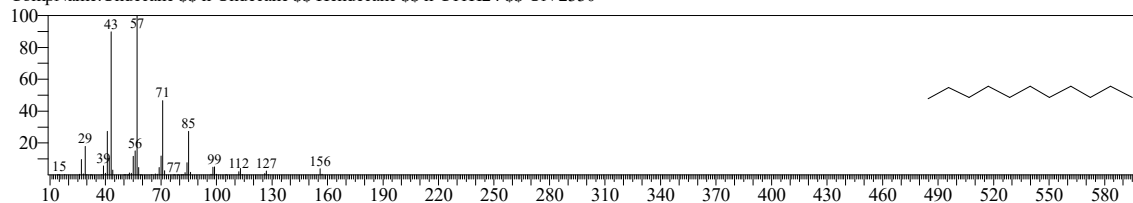
CompName:Octane, 3,5-dimethyl- \$\$ 3,5-Dimethyloctane



Hit#:3 Entry:21042 Library:NIST20M1.lib

SI:84 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100

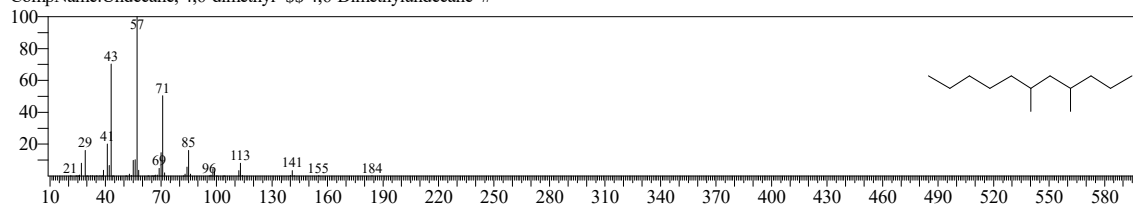
CompName:Undecane \$\$ n-Undecane \$\$ Hendecane \$\$ n-C11H24 \$\$ UN 2330



Hit#:4 Entry:40271 Library:NIST20M1.lib

SI:84 Formula:C13H28 CAS:17312-82-2 MolWeight:184 RetIndex:1185

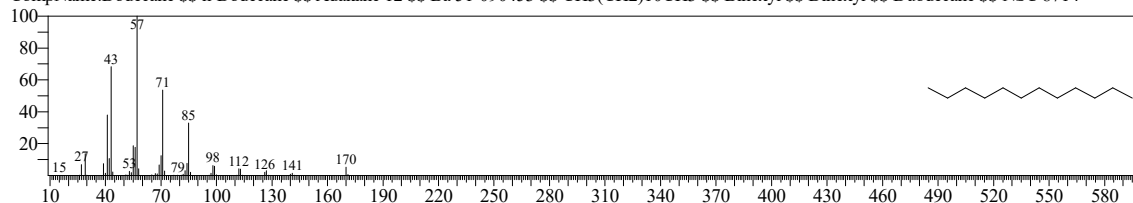
CompName:Undecane, 4,6-dimethyl- \$\$ 4,6-Dimethylundecane #



Hit#:5 Entry:30057 Library:NIST20M1.lib

SI:84 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



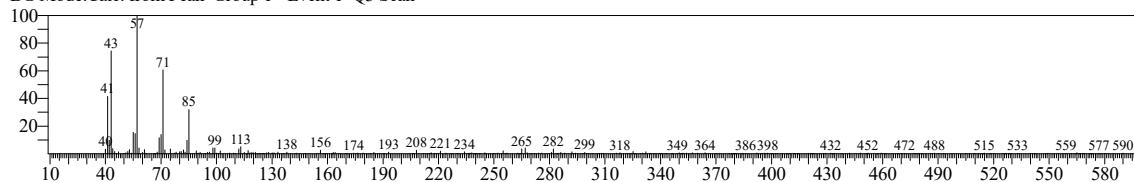
TNAU

<< Target >>

Line# 2 R.Time: 9.690 (Scan#: 1039) MassPeaks: 258

RawMode: Averaged 9.685-9.695 (1038-1040) BasePeak: 57.10 (5537)

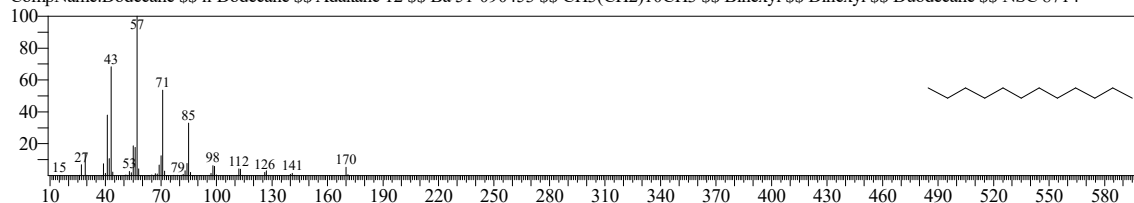
BG Mode: Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#: 1 Entry: 30057 Library: NIST20M1.lib

SI: 89 Formula: C₁₂H₂₆ CAS: 112-40-3 MolWeight: 170 RetIndex: 1200

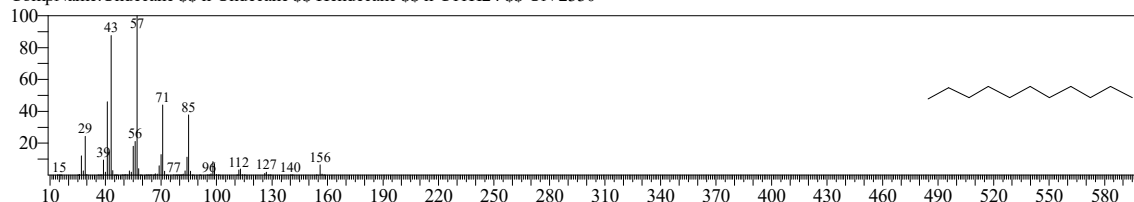
CompName: Dodecane \$\$ n-Dodecane \$\$ Adakane 12 \$\$ Ba 51-090453 \$\$ CH₃(CH₂)₁₀CH₃ \$\$ Bihexyl \$\$ Dihexyl \$\$ Duodecane \$\$ NSC 8714



Hit#: 2 Entry: 12897 Library: NIST20R.lib

SI: 89 Formula: C₁₁H₂₄ CAS: 1120-21-4 MolWeight: 156 RetIndex: 1100

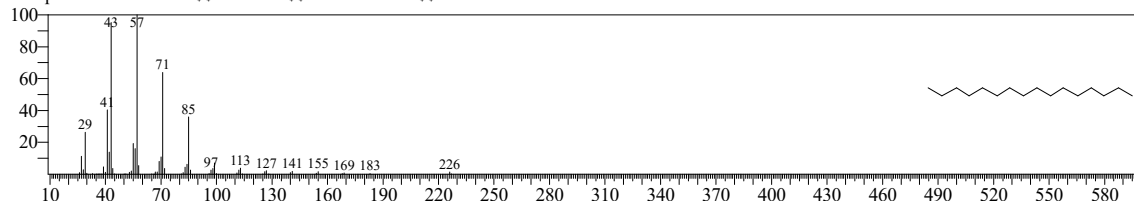
CompName: Undecane \$\$ n-Undecane \$\$ Hendecane \$\$ n-C₁₁H₂₄ \$\$ UN 2330



Hit#: 3 Entry: 27736 Library: NIST20R.lib

SI: 89 Formula: C₁₆H₃₄ CAS: 544-76-3 MolWeight: 226 RetIndex: 1600

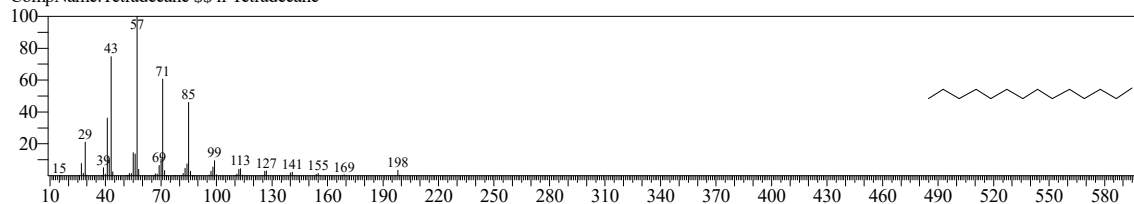
CompName: Hexadecane \$\$ n-Cetane \$\$ n-Hexadecane \$\$ Cetane



Hit#: 4 Entry: 22497 Library: NIST20R.lib

SI: 89 Formula: C₁₄H₃₀ CAS: 629-59-4 MolWeight: 198 RetIndex: 1400

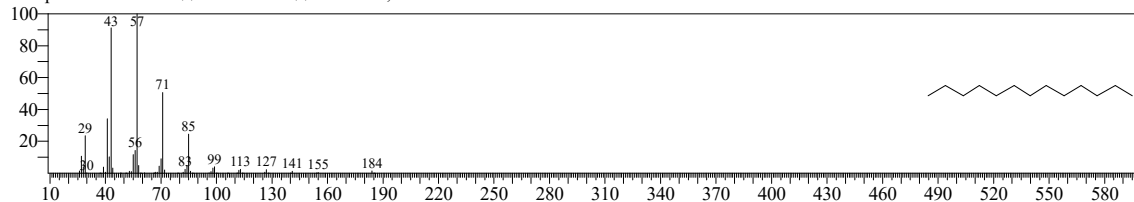
CompName: Tetradecane \$\$ n-Tetradecane



Hit#: 5 Entry: 40226 Library: NIST20M1.lib

SI: 89 Formula: C₁₃H₂₈ CAS: 629-50-5 MolWeight: 184 RetIndex: 1300

CompName: Tridecane \$\$ n-Tridecane \$\$ Tridecane, n-



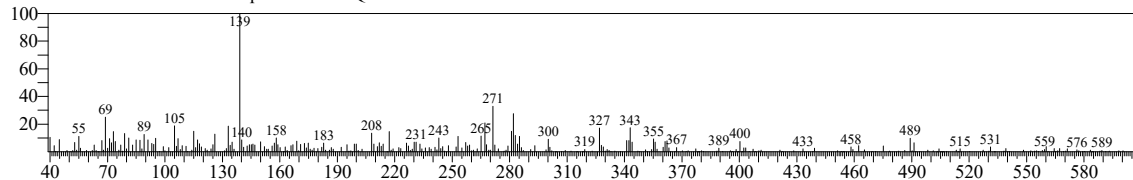
TNAU

<< Target >>

Line#3 R.Time:31.900(Scan#:5481) MassPeaks:307

RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:139.10(2633)

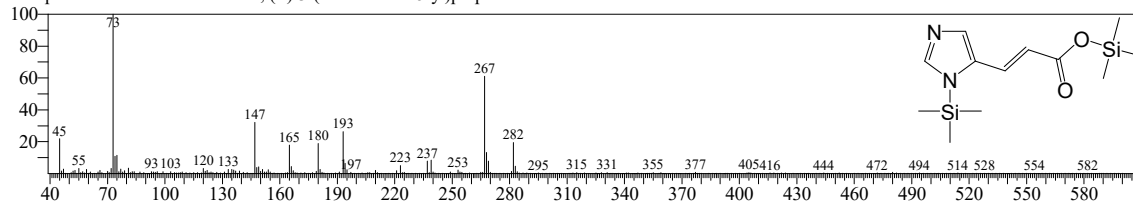
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#1 Entry:438 Library:OA TMS_DB5_67min_V3.lib

SI:31 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014

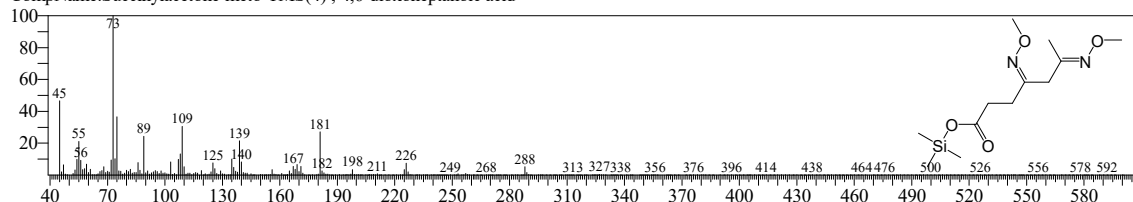
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#2 Entry:193 Library:OA TMS_DB5_67min_V3.lib

SI:31 Formula:C12H24N2O4Si CAS:51568-18-4 MolWeight:288 RetIndex:1599

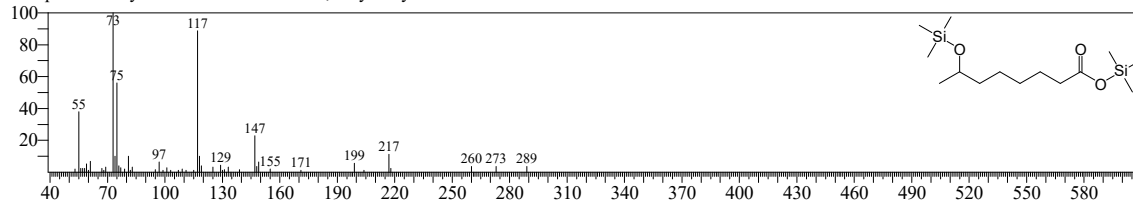
CompName:Succinylacetone-meto-TMS(4) ; 4,6-dioxoheptanoic acid



Hit#3 Entry:169 Library:OA TMS_DB5_67min_V3.lib

SI:31 Formula:C14H32O3Si2 CAS:17173-14-7 MolWeight:304 RetIndex:1551

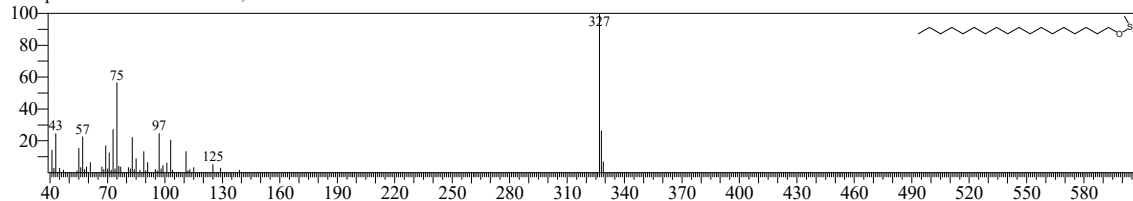
CompName:7-Hydroxooctanoic acid-2TMS ; 7-hydroxyoctanoic acid



Hit#4 Entry:477 Library:OA TMS_DB5_67min_V3.lib

SI:30 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156

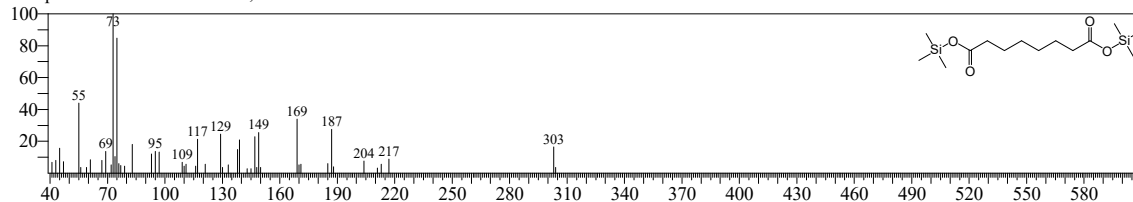
CompName:Octadecanol-TMS ; octadecan-1-ol



Hit#5 Entry:258 Library:OA TMS_DB5_67min_V3.lib

SI:30 Formula:C14H30O4Si2 CAS:505-48-6 MolWeight:318 RetIndex:1700

CompName:Suberic acid-2TMS ; octanedioic acid



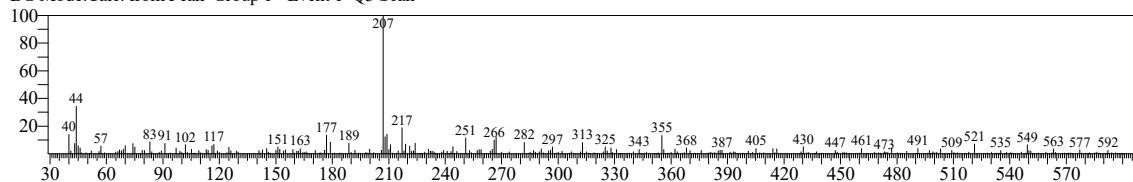
TNAU

<< Target >>

Line#:4 R.Time:32.150(Scan#:5531) MassPeaks:306

RawMode:Averaged 32.145-32.155(5530-5532) BasePeak:207.05(2479)

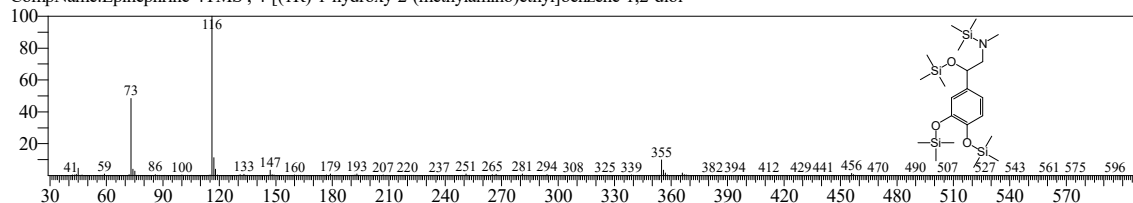
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:431 Library:OA_TMS_DB5_67min_V3.lib

SI:34 Formula:C₂₁H₄₅NO₃Si₄ CAS:51-43-4 MolWeight:471 RetIndex:1989

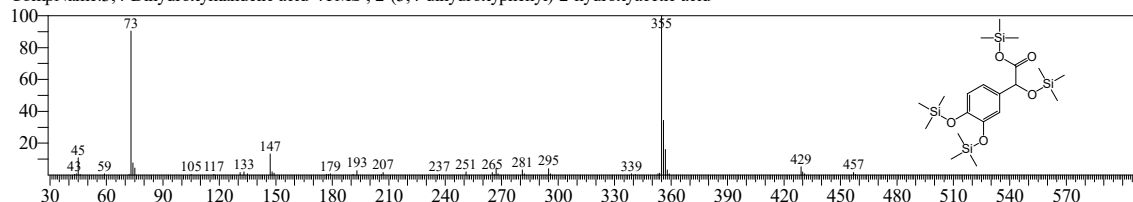
CompName:Epinephrine-4TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib

SI:30 Formula:C₂₀H₄₂O₄Si₄ CAS:775-01-9 MolWeight:458 RetIndex:1942

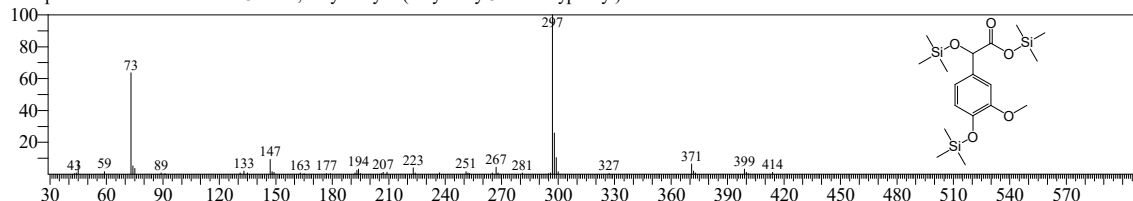
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:3 Entry:359 Library:OA_TMS_DB5_67min_V3.lib

SI:29 Formula:C₁₈H₁₃O₅Si₃ CAS:55-10-7 MolWeight:414 RetIndex:1894

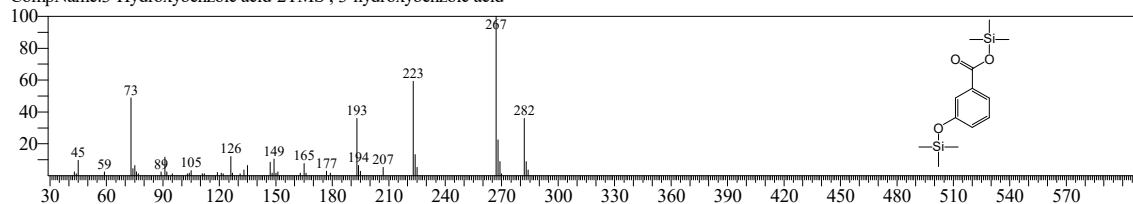
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid



Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib

SI:29 Formula:C₁₃H₂₂O₃Si₂ CAS:99-06-9 MolWeight:282 RetIndex:1572

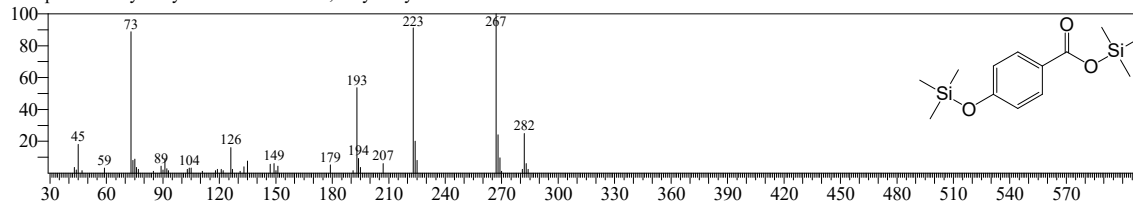
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib

SI:27 Formula:C₁₃H₂₂O₃Si₂ CAS:99-96-7 MolWeight:282 RetIndex:1636

CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



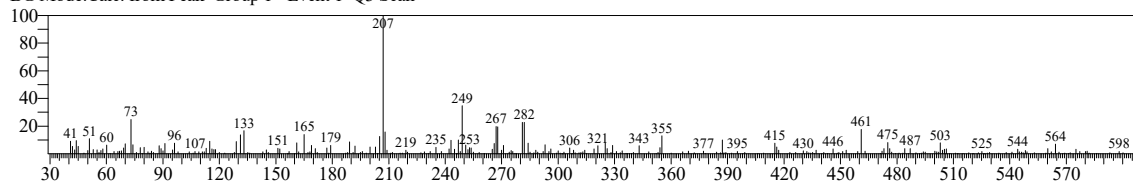
TNAU

<< Target >>

Line#:5 R.Time:32.260(Scan#:5553) MassPeaks:276

RawMode:Averaged 32.255-32.265(5552-5554) BasePeak:207.05(2096)

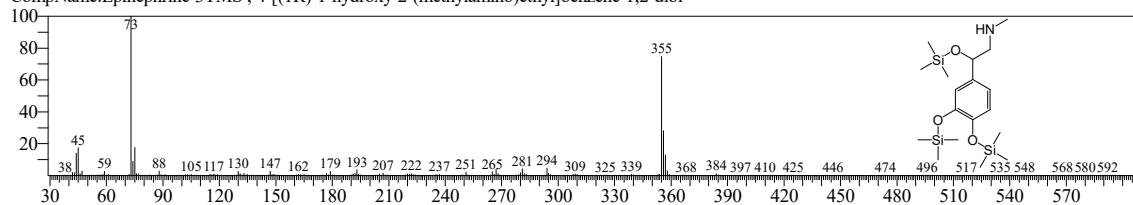
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib

SI:39 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868

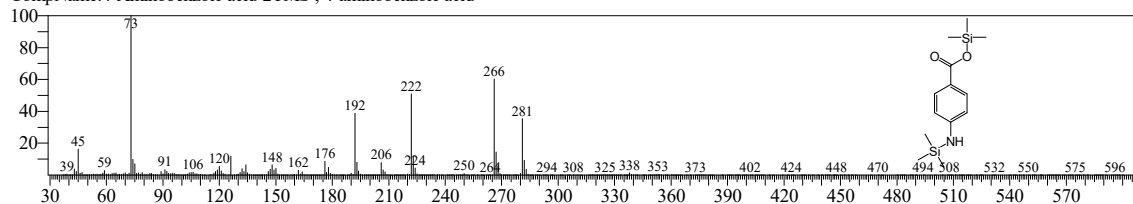
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib

SI:38 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845

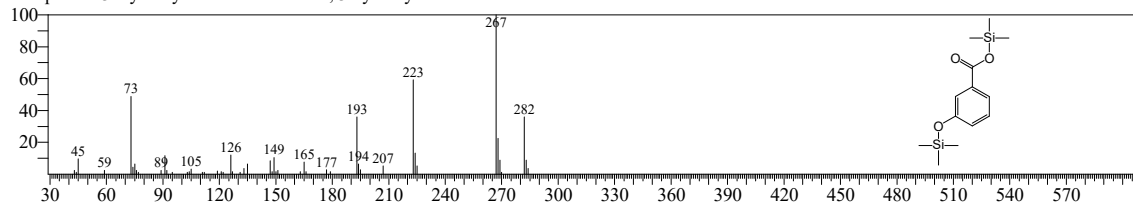
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib

SI:36 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572

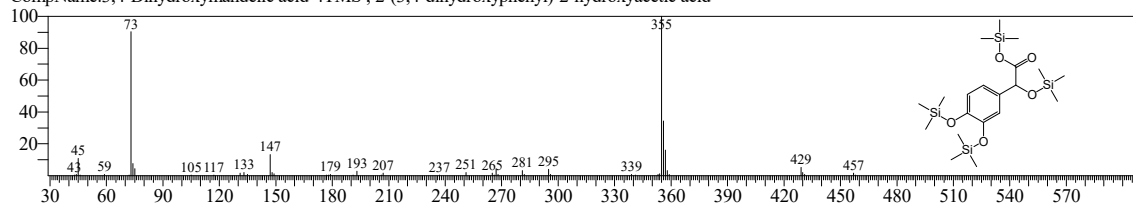
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib

SI:35 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942

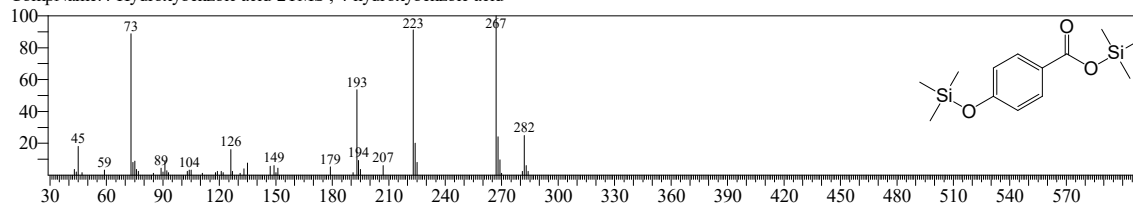
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:5 Entry: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



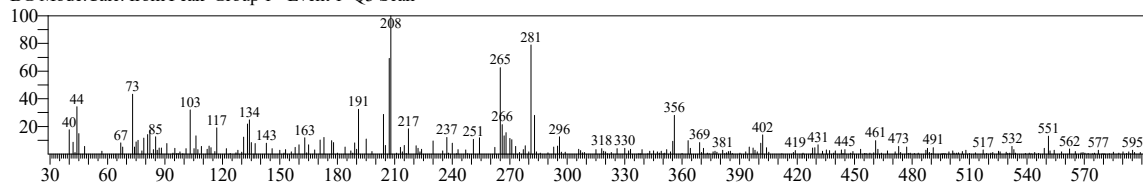
TNAU

<< Target >>

Line#6 R.Time:32.710(Scan#:5643) MassPeaks:274

RawMode:Averaged 32.705-32.715(5642-5644) BasePeak:208.00(1118)

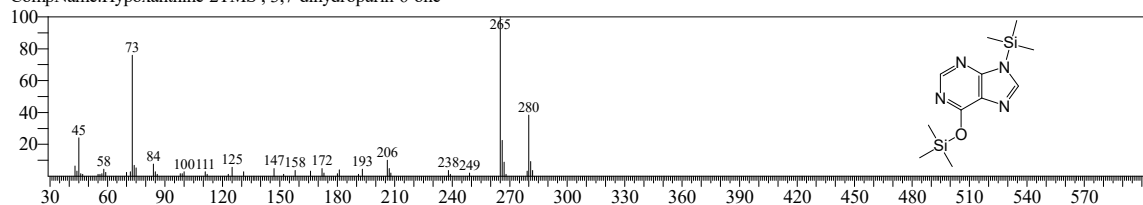
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#1 Entry:310 Library:OA TMS DB5_67min_V3.lib

SI:40 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822

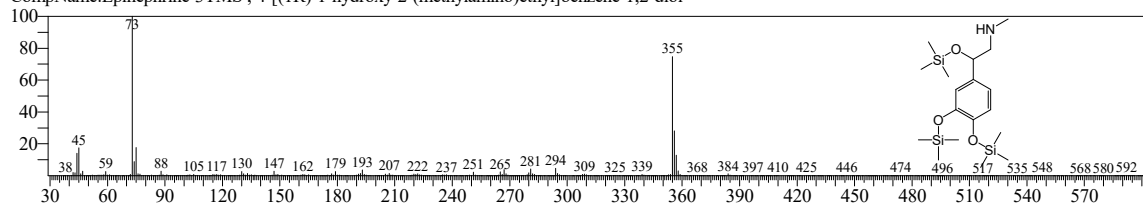
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#2 Entry:343 Library:OA TMS DB5_67min_V3.lib

SI:39 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868

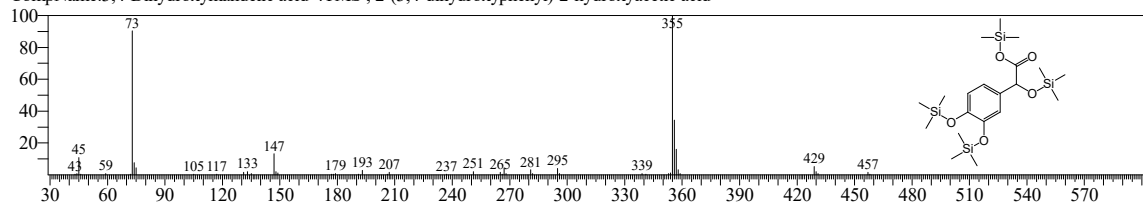
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#3 Entry:402 Library:OA TMS DB5_67min_V3.lib

SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942

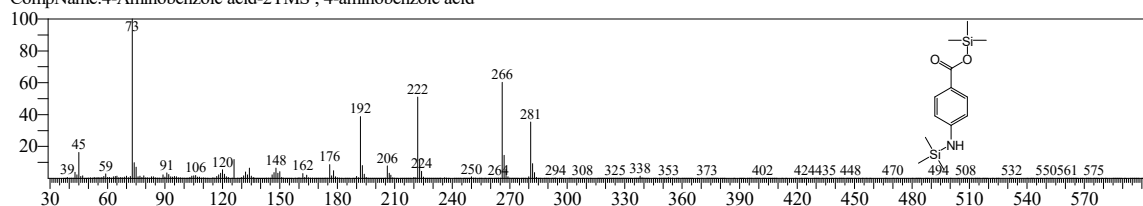
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#4 Entry: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#5 Entry:384 Library:OA TMS DB5_67min_V3.lib

SI:36 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919

CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

