TNAU

Chromatogram C56-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-005.qgd
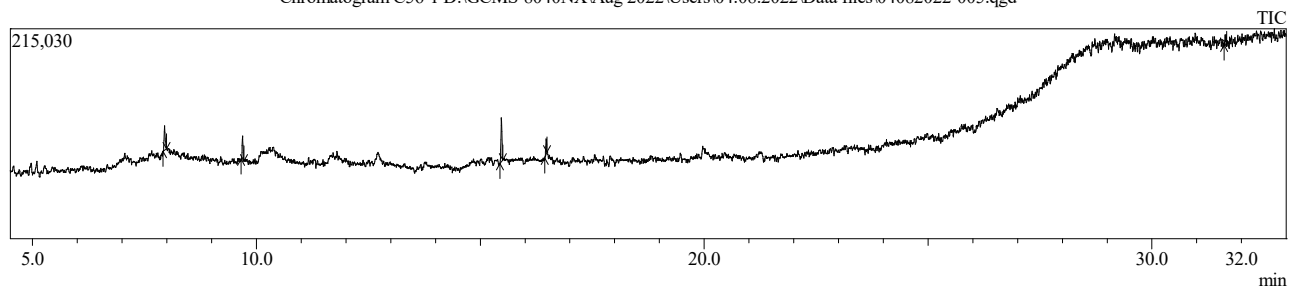
Peak Report TIC

| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.947	42296	22.59	25225	20.63	1.68	87	Undecane
2	9.690	35362	18.89	24739	20.24	1.43	87	Undecane
3	15.471	67096	35.83	44919	36.74	1.49	90	2,4-Di-tert-butylphenol
4	16.472	22864	12.21	15628	12.78	1.46	83	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
5	31.655	19619	10.48	11739	9.60	1.67	31	3,4-Dihydroxymandelic acid-4TMS
		187237	100.00	122250	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:259
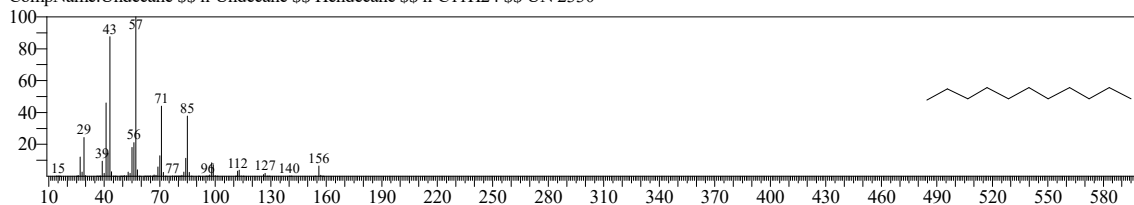RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(5974)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan
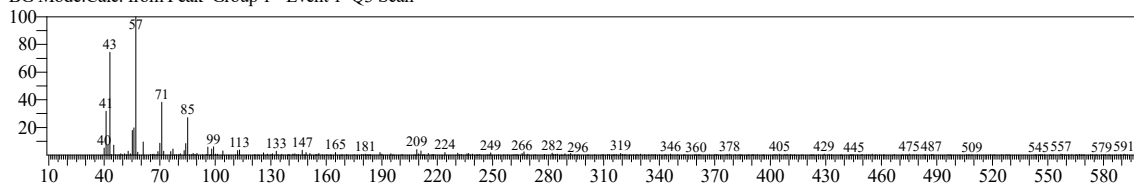
Hit#:1 Entry:12897 Library:NIST20R.lib
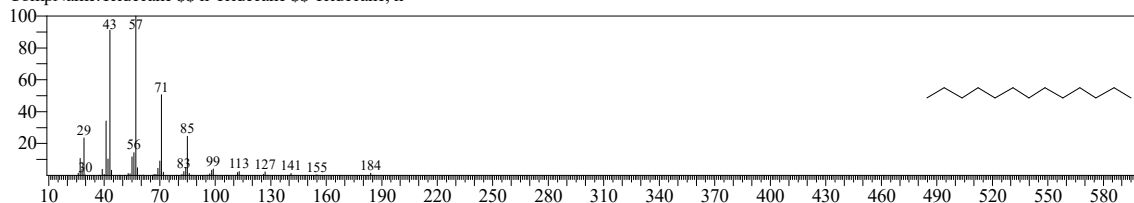SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:40226 Library:NIST20M1.lib
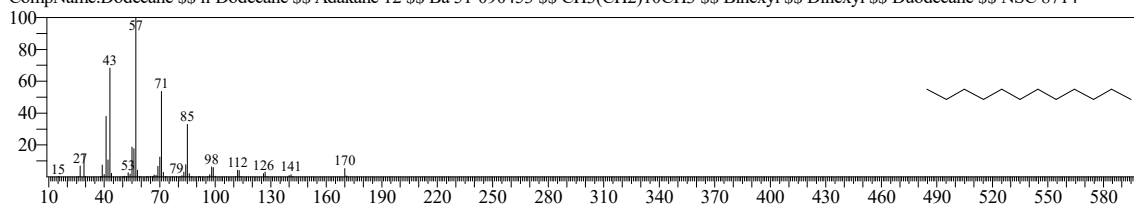SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:3 Entry:30057 Library:NIST20M1.lib
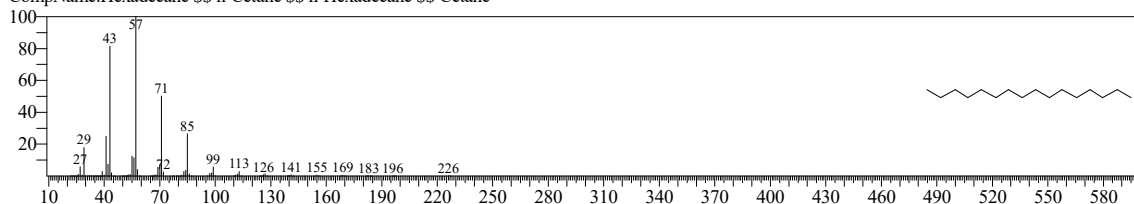SI:86 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:4 Entry:27737 Library:NIST20R.lib
SI:86 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
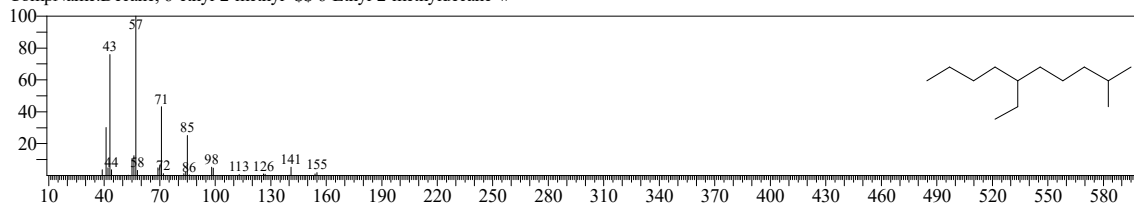CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

Hit#:5 Entry:40255 Library:NIST20M1.lib
SI:85 Formula:C13H28 CAS:62108-21-8 MolWeight:184 RetIndex:1185
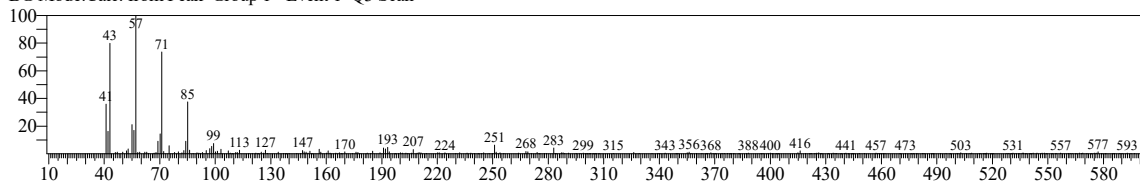CompName:Decane, 6-ethyl-2-methyl- $$ 6-Ethyl-2-methyldecane #

TNAU

<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:270
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(5077)
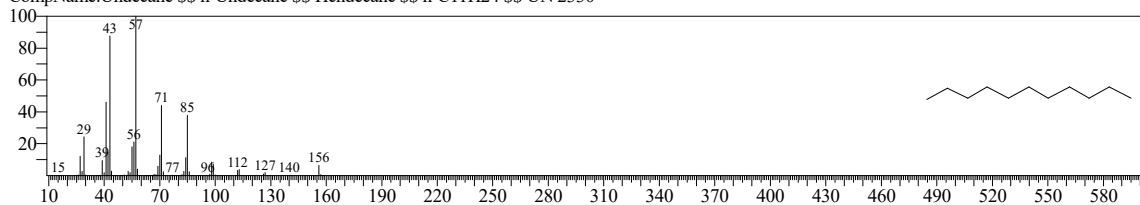BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:12897 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
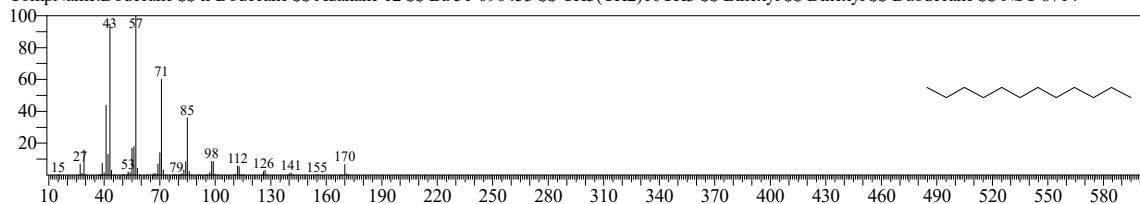CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:16191 Library:NIST20R.lib
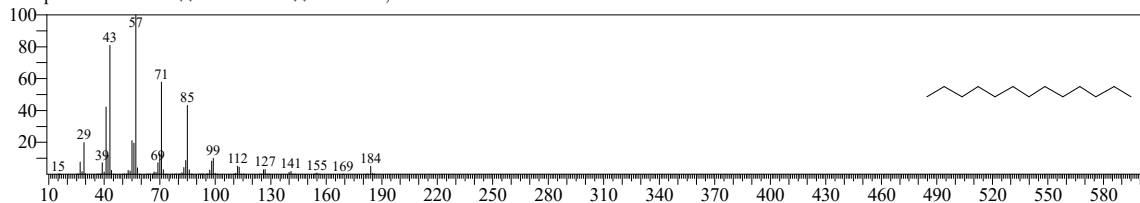SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:3 Entry:19410 Library:NIST20R.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
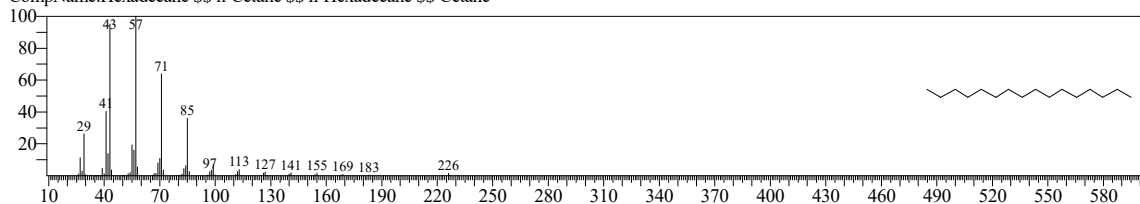CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:4 Entry:27736 Library:NIST20R.lib
SI:87 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
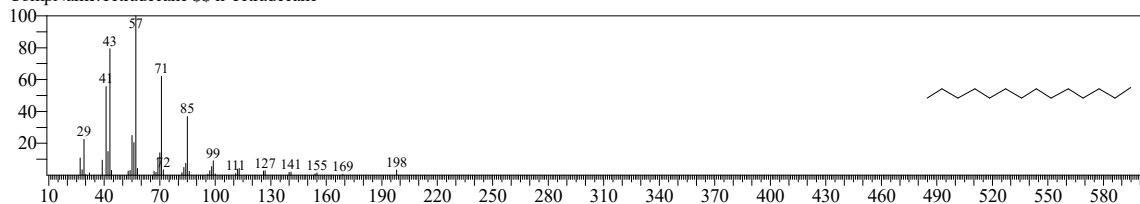CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

Hit#:5 Entry:22498 Library:NIST20R.lib
SI:87 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane
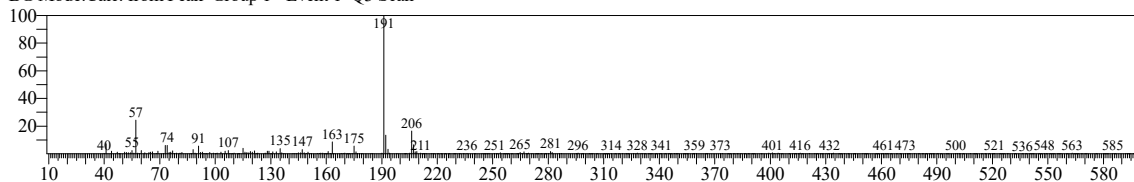
<< Target >>
Line#:3 R.Time:15.470(Scan#:2195) MassPeaks:323
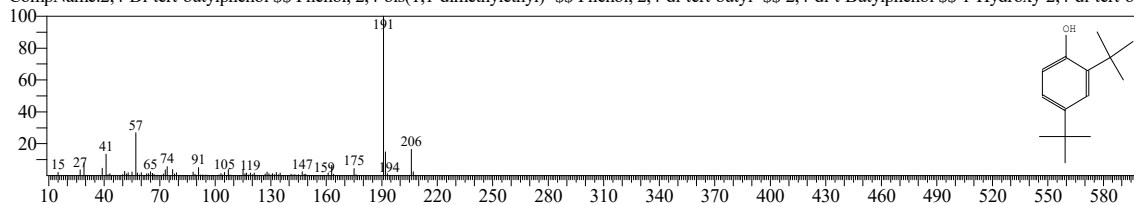RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.15(14616)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:24086 Library:NIST20R.lib
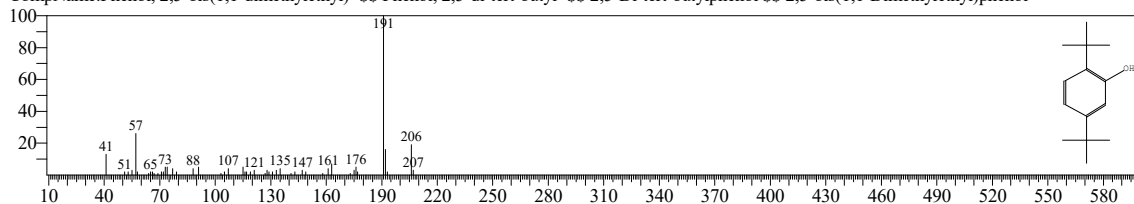SI:90 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu

Hit#:2 Entry:24098 Library:NIST20R.lib
SI:88 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
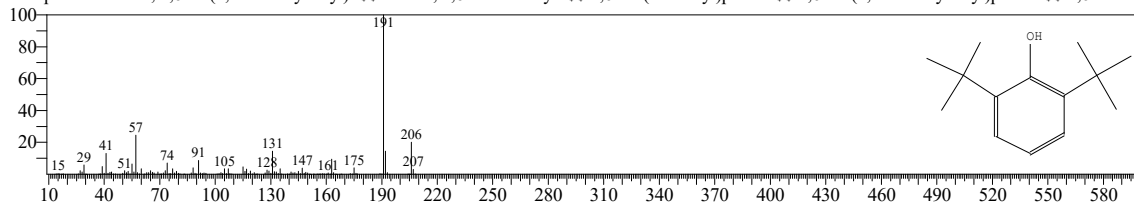CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol

Hit#:3 Entry:59031 Library:NIST20M1.lib
SI:88 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
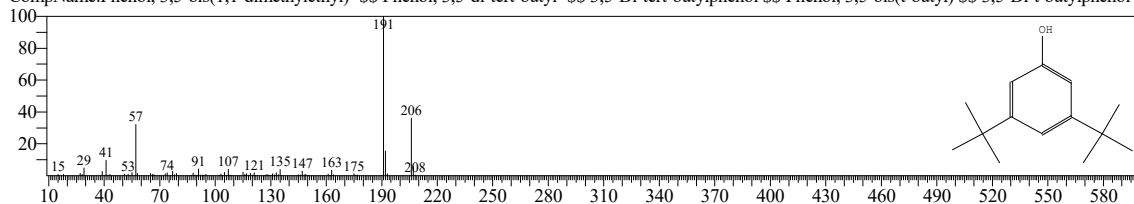CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

Hit#:4 Entry:24110 Library:NIST20R.lib
SI:87 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $

Hit#:5 Entry:170993 Library:NIST20M1.lib
SI:84 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255
CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters $$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #
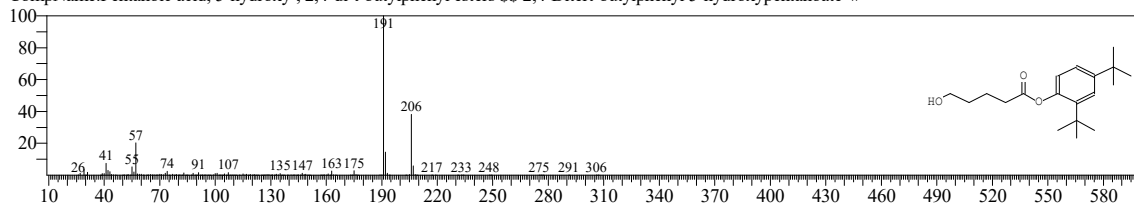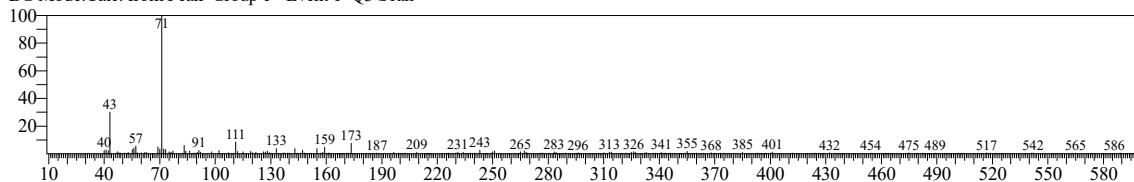
TNAU

<< Target >>
Line#:4 R.Time:16.470(Scan#:2395) MassPeaks:305
RawMode:Averaged 16.465-16.475(2394-2396) BasePeak:71.05(6785)
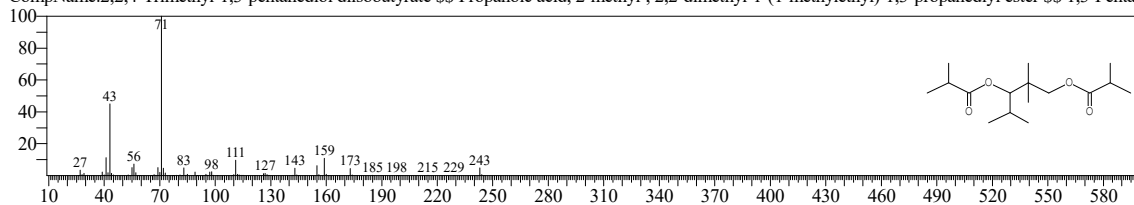BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34622 Library:NIST20R.lib
SI:83 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan

Hit#:2 Entry:68304 Library:NIST20M1.lib
SI:76 Formula:C11H20O4 CAS:7492-70-8 MolWeight:216 RetIndex:1385
CompName:Butanoic acid, 2-butoxy-1-methyl-2-oxoethyl ester $$ Butyric acid, ester with butyl lactate $$ Butyl butyryl lactate $$ Butyl butyrolactate $$ La
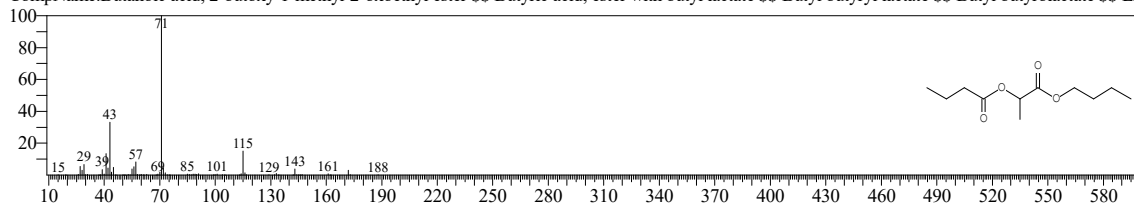
Hit#:3 Entry:6356 Library:NIST20R.lib
SI:76 Formula:C8H16O CAS:1004-29-1 MolWeight:128 RetIndex:948
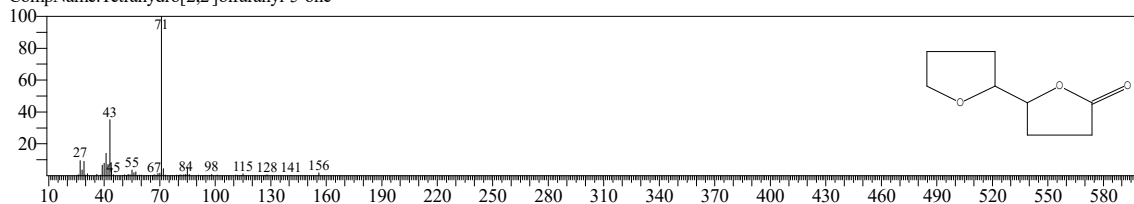CompName:Furan, 2-butyltetrahydro- $$ Octane, 1,4-epoxy- $$ 2-Butyltetrahydrofuran
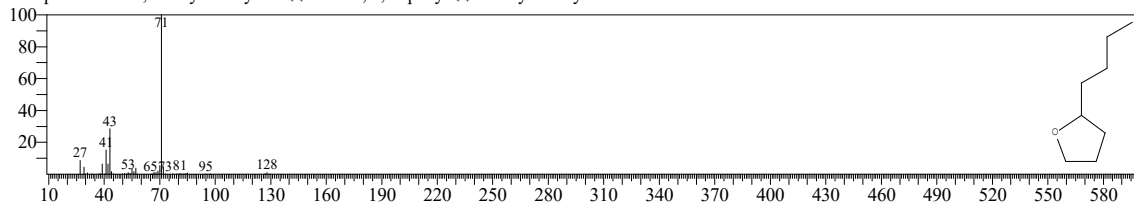
Hit#:4 Entry:20598 Library:NIST20M1.lib
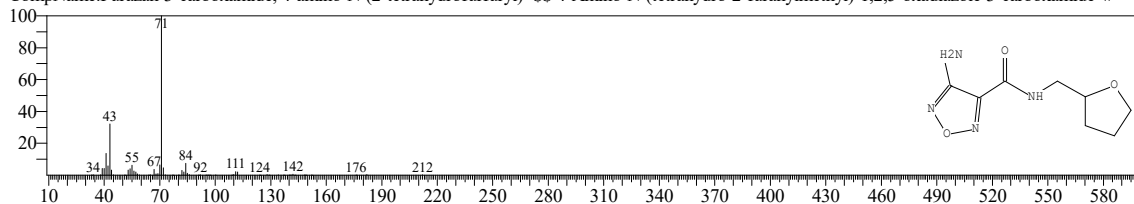SI:76 Formula:C8H12O3 CAS:19680-00-3 MolWeight:156 RetIndex:1316
CompName:Tetrahydro[2,2']bifuranyl-5-one

Hit#:5 Entry:64203 Library:NIST20M1.lib
SI:76 Formula:C8H12N4O3 CAS:309735-27-1 MolWeight:212 RetIndex:1980
CompName:Furazan-3-carboxamide, 4-amino-N-(2-tetrahydrofurfuryl)- $$ 4-Amino-N-(tetrahydro-2-furanylmethyl)-1,2,5-oxadiazole-3-carboxamide #
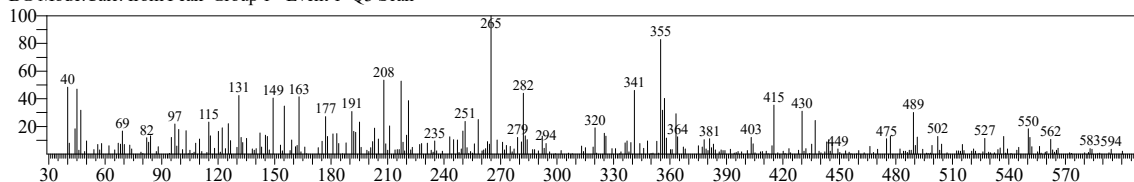
TNAU

<< Target >>
Line#:5   R.Time:31.655(Scan#:5432)   MassPeaks:319
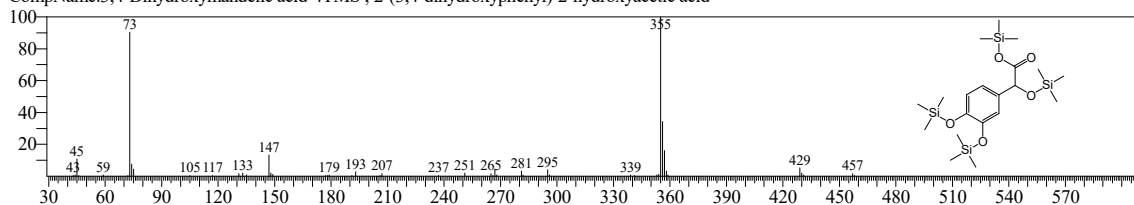RawMode:Averaged 31.650-31.660(5431-5433) BasePeak:264.95(819)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
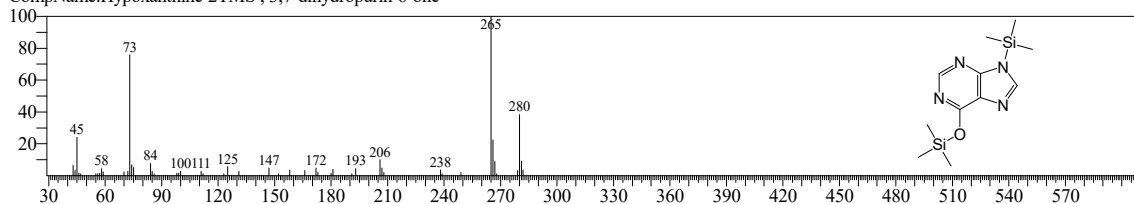SI:31 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
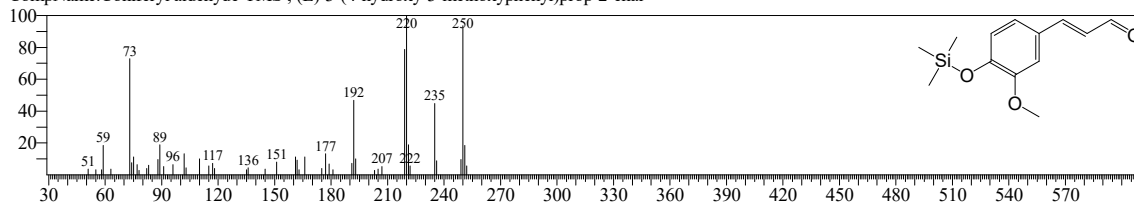CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:3 Entry:339 Library:OA_TMS_DB5_67min_V3.lib
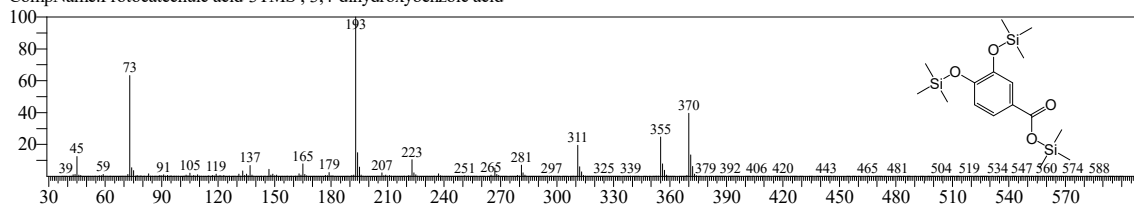SI:21 Formula:C13H18O3Si CAS:458-36-6 MolWeight:250 RetIndex:1859
CompName:Coniferyl aldehyde-TMS ; (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal

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

Hit#:5 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:18 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one