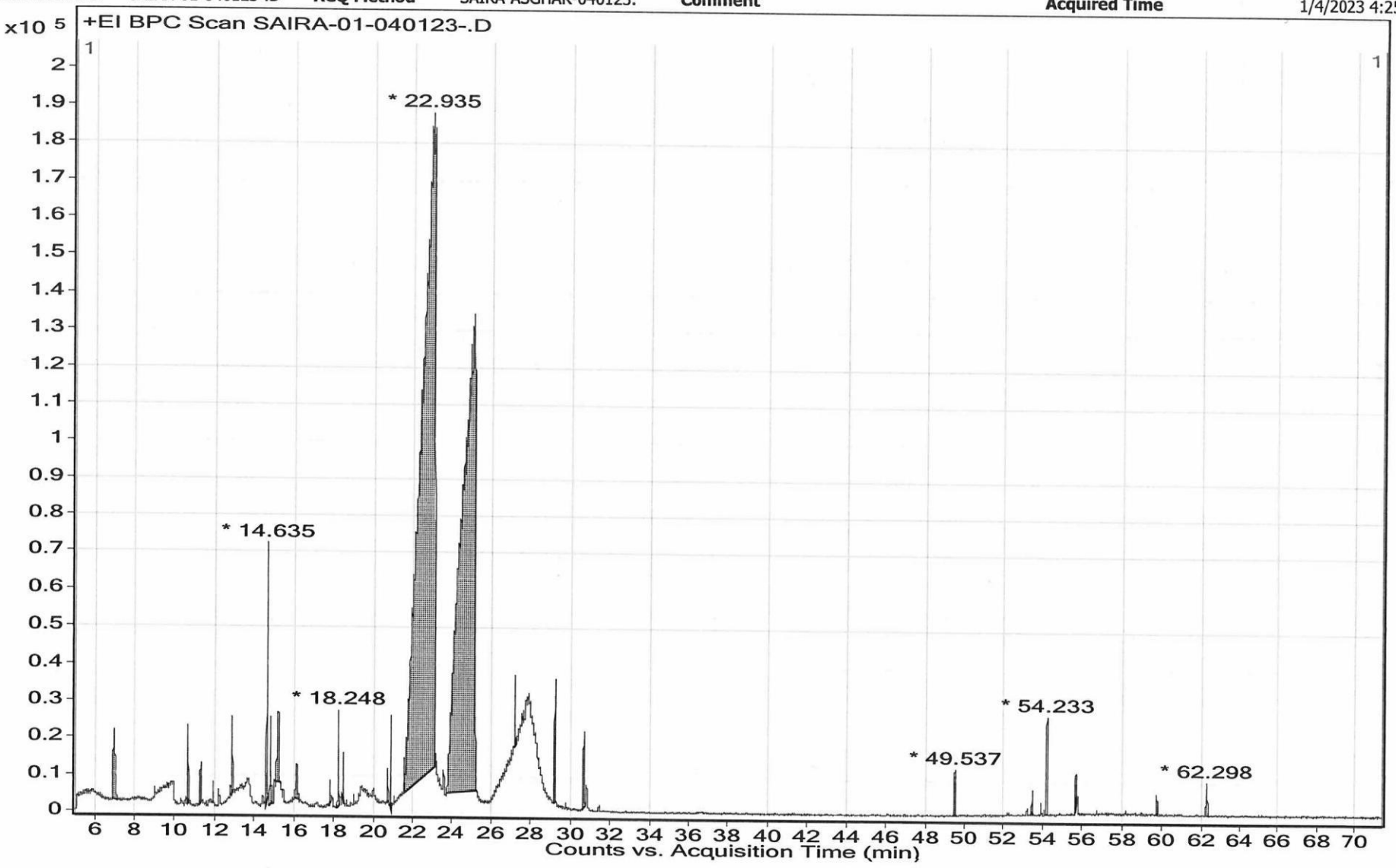
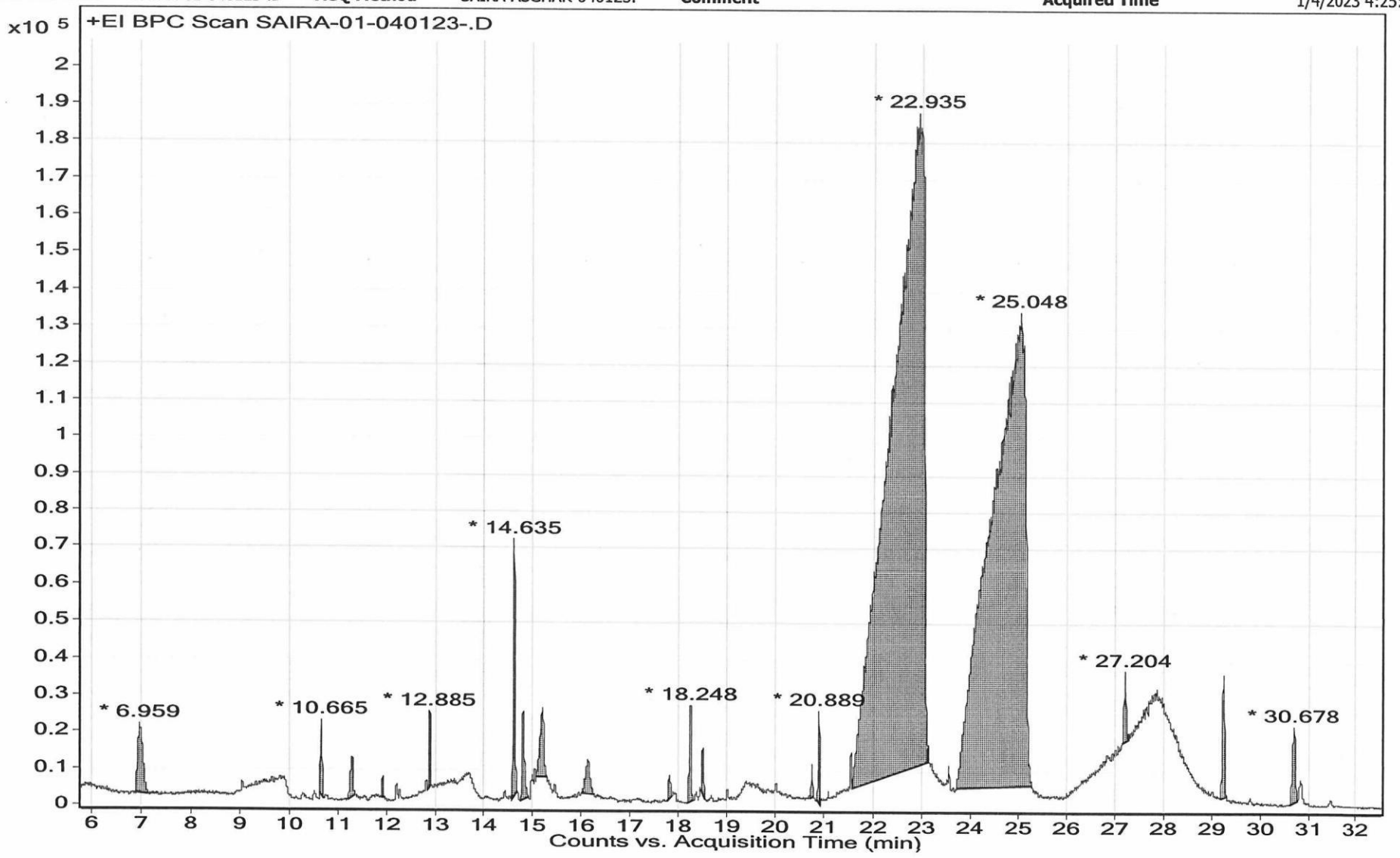
Sample Name	SAIRA-01-040123-	**Position**	13	**Instrument Name**	GCMS TQQQ	**User Name**	HEJ-G-104-03\Adminis
Inj Vol	2	**InjPosition**		**SampleType**		**IRM Calibration Status**	Not Applicable
Data Filename	SAIRA-01-040123-.D	**ACQ Method**	SAIRA-ASGHAR-040123.	**Comment**		**Acquired Time**	1/4/2023 4:25:32 PM

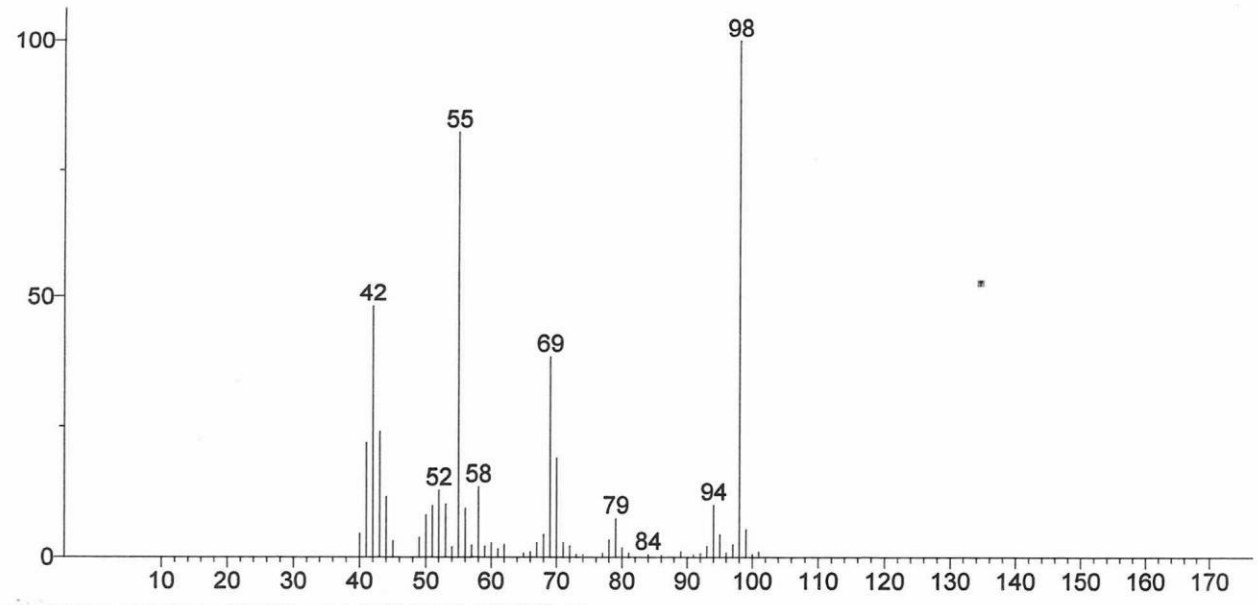


Sample Name	SAIRA-01-040123-	**Position**	13	**Instrument Name**	GCMS TQQQ	**User Name**	HEJ-G-104-03\Adminis
Inj Vol	2	**InjPosition**		**SampleType**		**IRM Calibration Status**	Not Applicable
Data Filename	SAIRA-01-040123-.D	**ACQ Method**	SAIRA-ASGHAR-040123.	**Comment**		**Acquired Time**	1/4/2023 4:25:32 PM



SAIRA-01

Peak Number	RT	Area	Area %	Height	Width	Area Sum %	Height %
1	6.959	130098	1.58	19044	0.246	0.83	10.79
2	10.665	42161	0.51	20527	0.089	0.27	11.63
3	11.303	39765	0.48	10952	0.146	0.25	6.2
4	11.93	10383	0.13	5916	0.068	0.07	3.35
5	12.885	43214	0.52	20705	0.071	0.28	11.73
6	14.635	159950	1.94	69644	0.107	1.02	39.44
7	14.817	80443	0.98	23984	0.175	0.51	13.58
8	15.209	107465	1.3	18806	0.228	0.68	10.65
9	16.146	55385	0.67	9428	0.249	0.35	5.34
10	17.817	19076	0.23	6419	0.1	0.12	3.64
11	18.248	73429	0.89	26145	0.128	0.47	14.81
12	18.498	33245	0.4	12525	0.086	0.21	7.09
13	20.743	14153	0.17	9234	0.078	0.09	5.23
14	20.889	46916	0.57	24817	0.071	0.3	14.05
15	22.935	8246571	100	176571	1.55	52.53	100
16	25.048	6154454	74.63	128610	1.568	39.2	72.84
17	27.204	46824	0.57	19009	0.118	0.3	10.77
18	29.235	113918	1.38	33427	0.139	0.73	18.93
19	30.678	87101	1.06	20565	0.171	0.55	11.65
20	49.537	50210	0.61	12450	0.192	0.32	7.05
21	53.482	11350	0.14	6057	0.078	0.07	3.43
22	54.233	60813	0.74	26269	0.096	0.39	14.88
23	55.68	18073	0.22	9394	0.061	0.12	5.32
24	59.757	16288	0.2	5291	0.135	0.1	3
25	62.298	38028	0.46	8748	0.196	0.24	4.95
						100	



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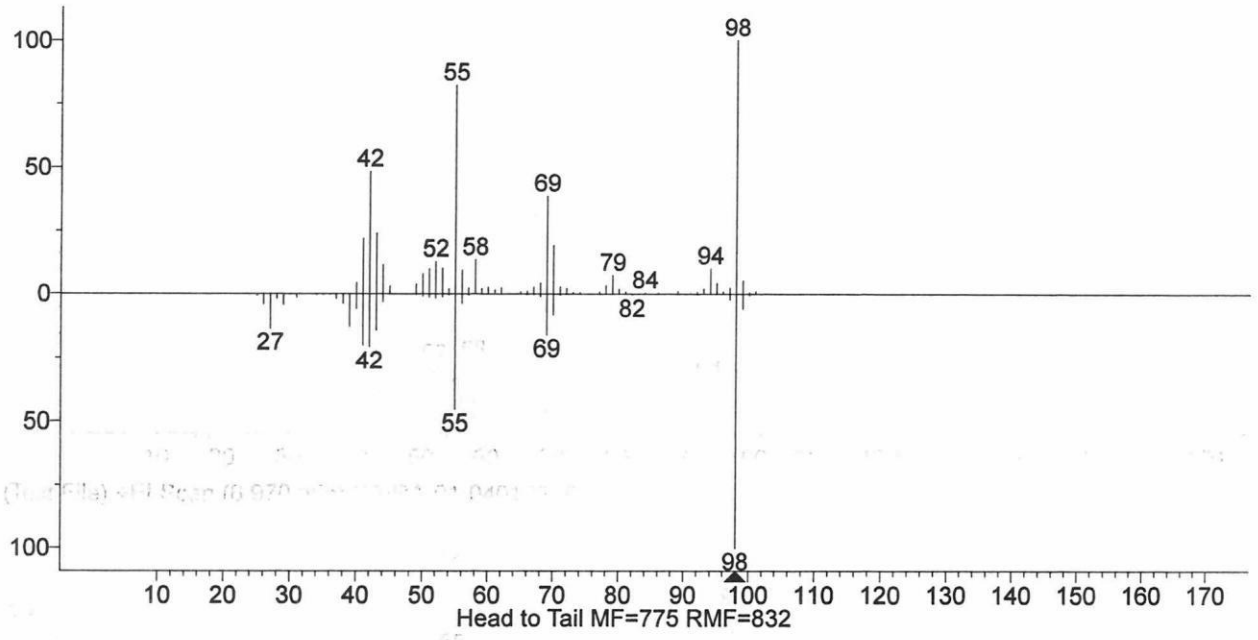
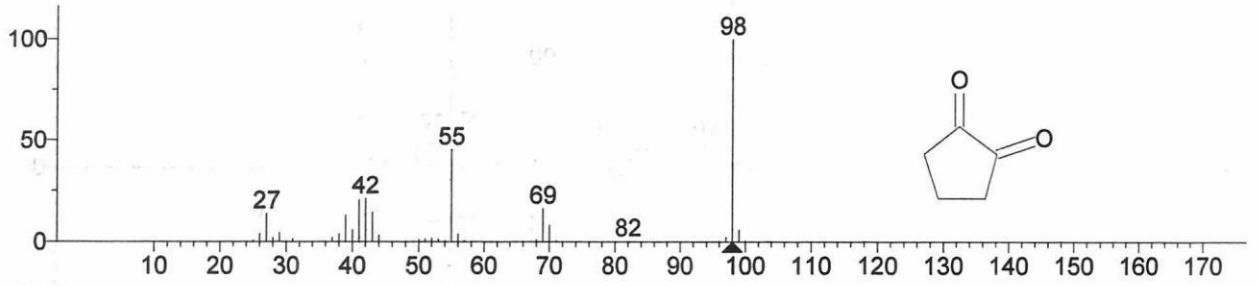


Head to Tail MF=775 RMF=832

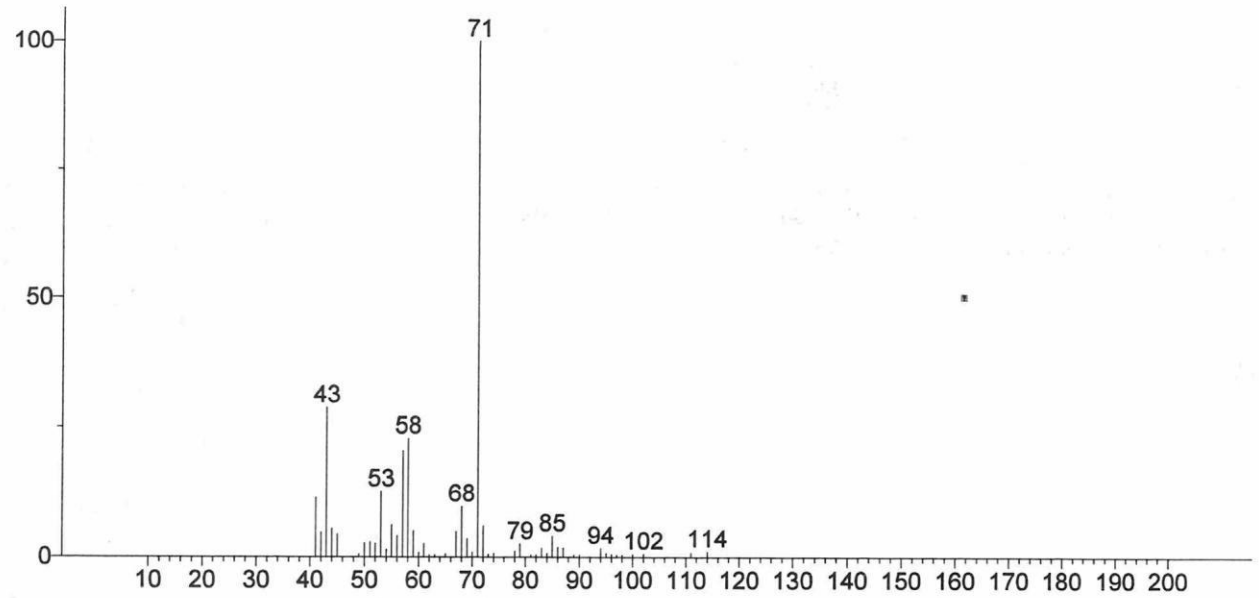


(mainlib) 1,2-Cyclopentanedione

Name: 1,2-Cyclopentanedione
Formula: $C_5H_6O_2$
MW: 98 CAS#: 3008-40-0 NIST#: 162182 ID#: 60722 DB: mainlib
Other DBs: HODOC
Contributor: Chemical Concepts
10 largest peaks:
98 999 | 55 452 | 42 209 | 41 203 | 69 161 | 43 142 | 27 136 | 39 128 | 70 82 | 40 57 |
Synonyms:
no synonyms.

Estimated non-polar retention index (n-alkane scale):
Value: 942 iu
Confidence interval (Ketones): 57(50%) 246(95%) iu

Retention index.
1. Value: 1741.6 iu
Column Type: Packed
Column Class: Standard polar
Active Phase: Carbowax 20M
-TPA
Column Length: 6 ft
Carrier Gas: He
Substrate: Gas Chrom P (60-80 mesh)
Data Type: Normal alkane
RI
Program Type: Ramp
Start T: 70 C
End T: 180 C
Heat Rate: 5 K/min
Source: Fiddler, W.; Doerr, R.C.;
Wasserman, A.E., Composition of an ether-soluble fraction of a liquid smoke solution, J. Agric. Food Chem., 18(2), 1970, 310-312.



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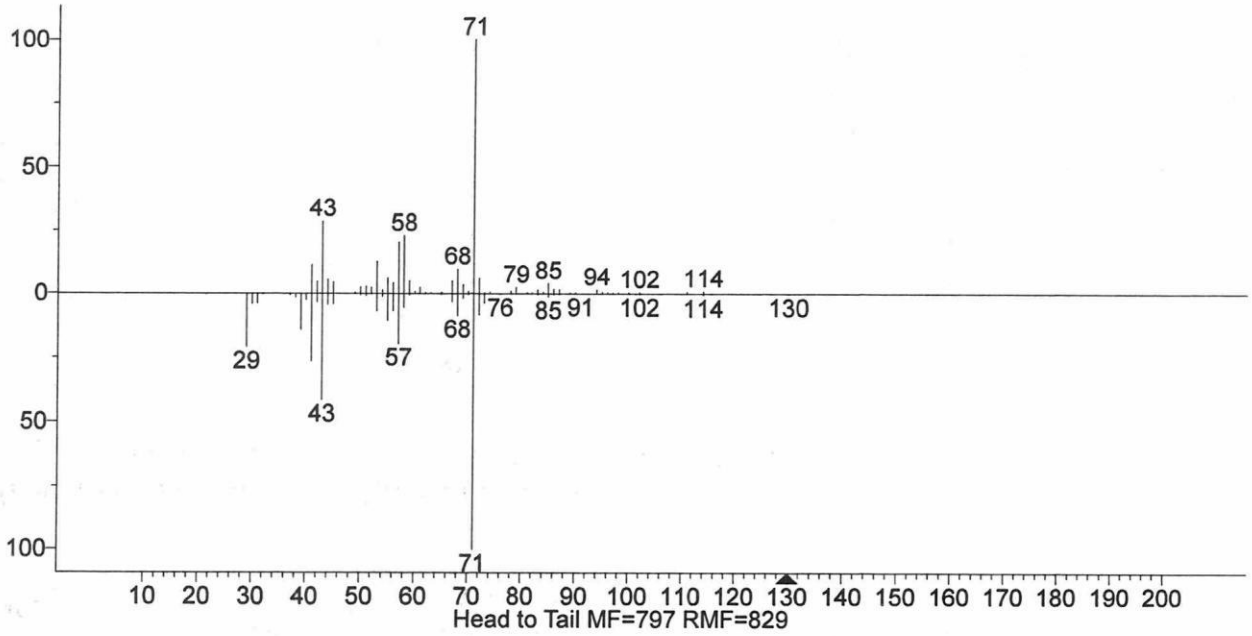
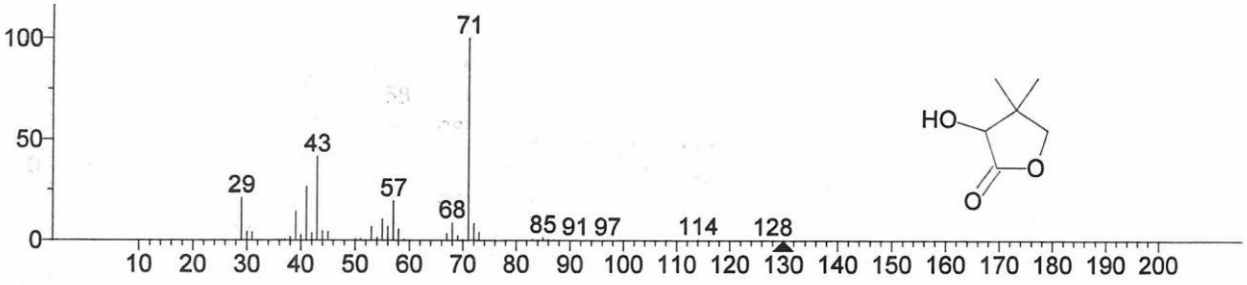


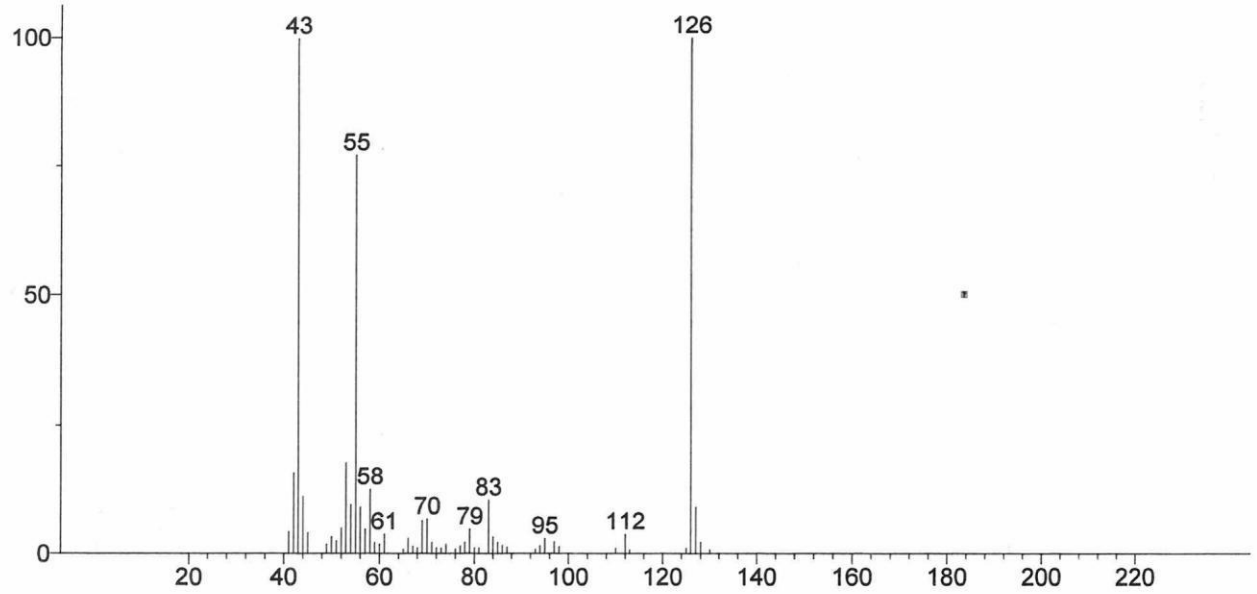
Head to Tail MF=797 RMF=829



(replib) Pantolactone

Name: Pantolactone
Formula: $C_6H_{10}O_3$
MW: 130 CAS#: 599-04-2 NIST#: 223057 ID#: 8012 DB: replib
Other DBs: Fine, TSCA, HODOC, EINECS
Contributor: Chemical Concepts
10 largest peaks:
71 999 | 43 414 | 41 263 | 29 209 | 57 194 | 39 141 | 55 106 | 68 86 | 72 83 | 53 68 |
Synonyms:
1.2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (R)-
2.2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, D-(-)-
3.(D)-Pantolactone
4.D-(-)-Pantolactone
5.D-(-)Pantoyl lactone
6.Pantolyl lactone
7.Pantothenic lactone
8.Pantoyl lactone
9.Pentoyl lactone
10.D-(-)-Pantolyl lactone
11.D-(-)-Pantoic acid lactone
12.D(-)-2-Hydroxy-3,3-dimethyl-γ-butyrolactone
13.D-1-Hydroxy-2,2-dimethyl-3-butyrolactone
14.(R)-(-)-Pantolactone
15.Pentoyl lactone clene
16.3-Hydroxy-4,4-dimethyldihydro-2(3H)-furanone #
Estimated non-polar retention index (n-alkane scale):
Value: 1148 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu
Retention index.
1. Value: 990 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-1
Column Length:
50 m
Carrier Gas: N2
Column Diameter: 0.32 mm
Phase Thickness: 0.52 um
Data Type: Normal alkane
RI
Program Type: Complex
Description: 40C => 2C/min =>130C =>4C/min => 250C
Source: Teai, T.; Claude
-Lafontaine, A.; Schippa, C.; Cozzolino, F., Volatile compounds in fresh pulp of pineapple (Ananas comosus [L.] Merr.) from French Polynesia, J. Essent. Oil Res., 13(5), 2001, 314-318.

2. Value: 931 iu
Column Type:
Capillary
Column Class: Semi-standard non-polar
Active Phase: Squalane
Carrier Gas: N2
Data Type: Kovats



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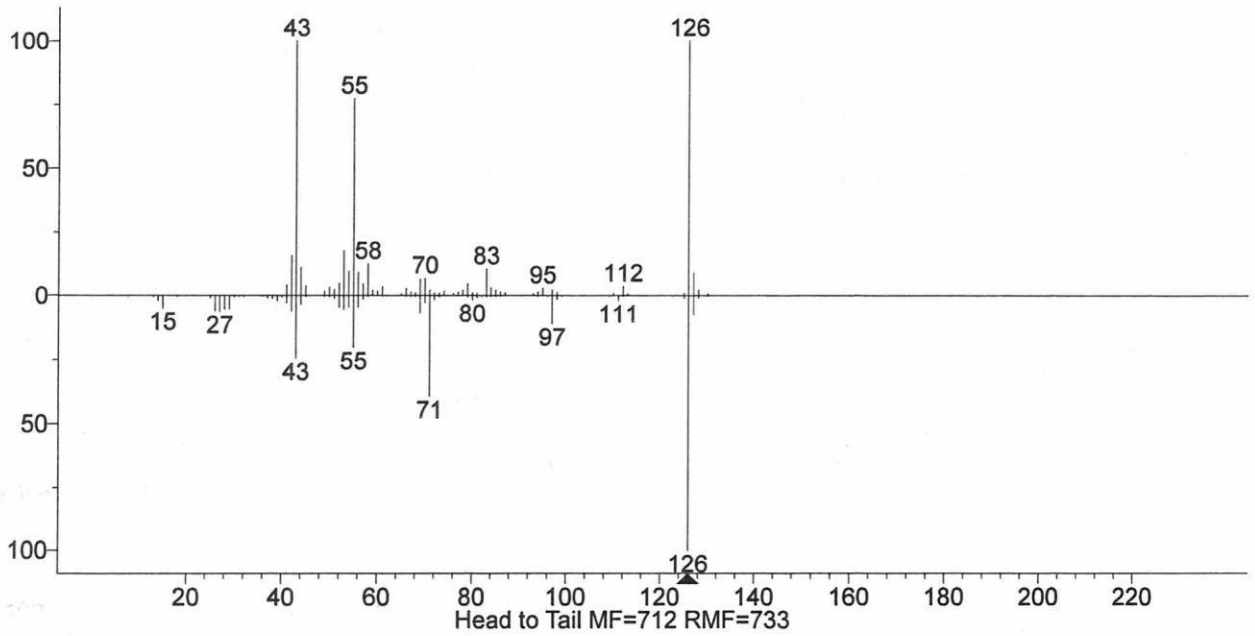
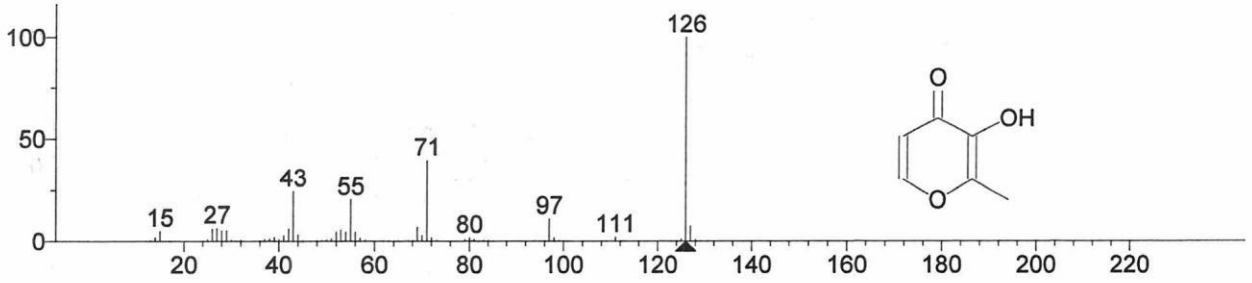


Head to Tail MF=712 RMF=733



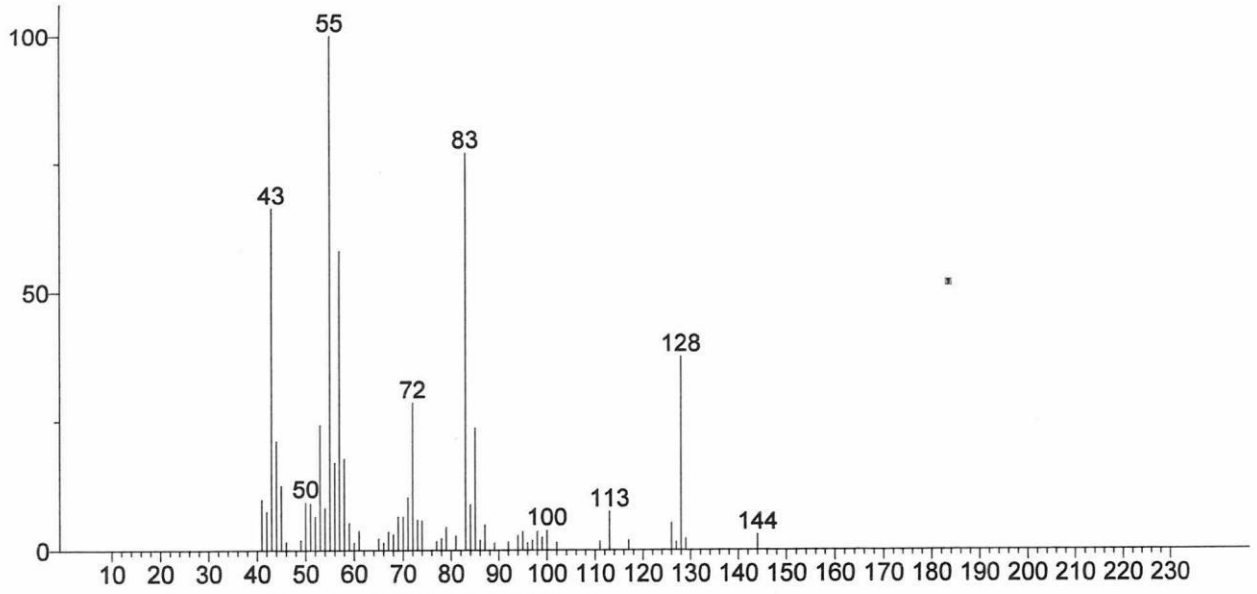
(replib) Maltol

Name: Maltol
Formula: $C_6H_6O_3$
MW: 126 CAS#: 118-71-8 NIST#: 2557 ID#: 17332 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS
10 largest peaks:
126 999 | 71 392 | 43 243 | 55 202 | 97 109 | 127 74 | 69 68 | 27 62 | 42 60 | 26 59 |
Synonyms:
1.4H-Pyran-4-one, 3-hydroxy-2-methyl-
2.Larixic acid
3.Larixinic acid
4.Palatone
5.2-Methyl-3-hydroxypyrone
6.3-Hydroxy-2-methyl-4-pyrone
7.3-Hydroxy-2-methylpyrone
8.3-Hydroxy-2-methyl-4-pyranone
9.3-Hydroxy-2-methyl-1,4-pyrone
10.Corps praline
11.Talmon
12.Vetol
13.2-Methyl pyromeconic acid
14.2-Methyl-3-hydroxy-4-pyrone
15.3-Hydroxy-2-methyl-γ-pyrone
16.3-Hydroxy-2-methyl-4H-pyran-4-one
17.2-Methyl-3-oxy-γ-pyrone
18.Veltol

Estimated non-polar retention index (n-alkane scale):
Value: 1063 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1092.2 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: SE-30
Column
Length: 40 m
Column Diameter: 0.35 mm
Phase Thickness: 0.35 um
Data Type: Kovats RI
Program Type:
Isothermal
Start T: 100 C
Source: Tudor, E., Temperature dependence of the retention index for perfumery compounds on a SE-30 glass capillary column. I. Linear equations, J. Chromatogr. A, 779, 1997, 287-297.

2.
Value: 1130 iu
Column Type: Packed
Column Class: Standard non-polar
Active Phase: SE-30
Column Length:
6 m
Carrier Gas: He



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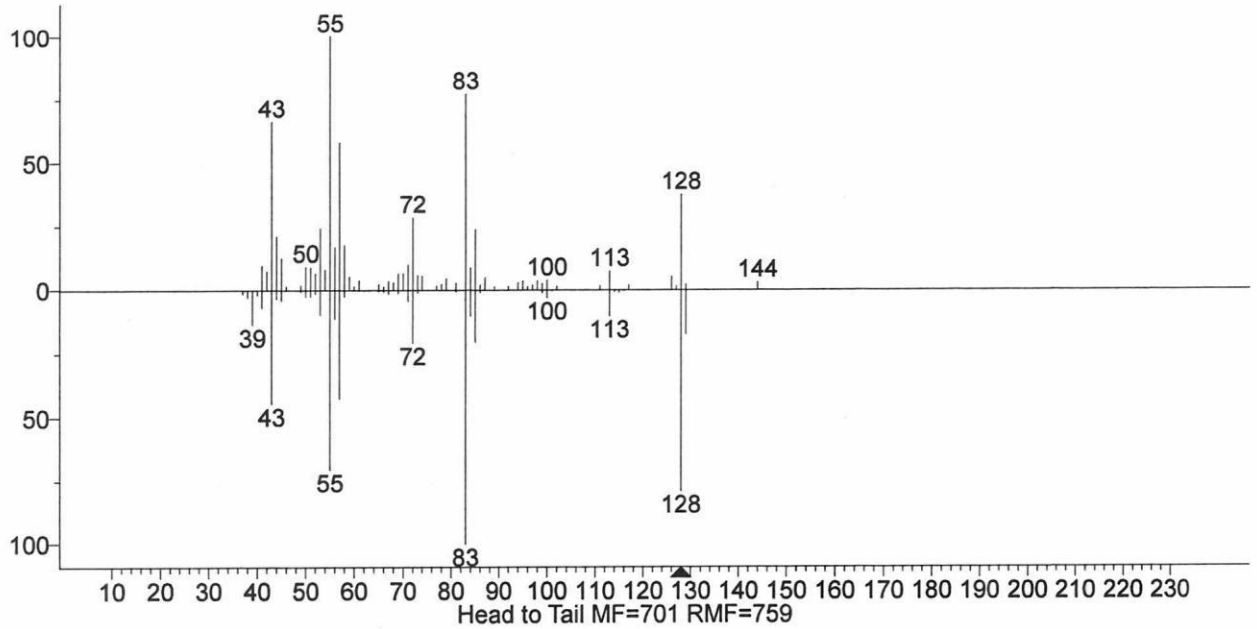
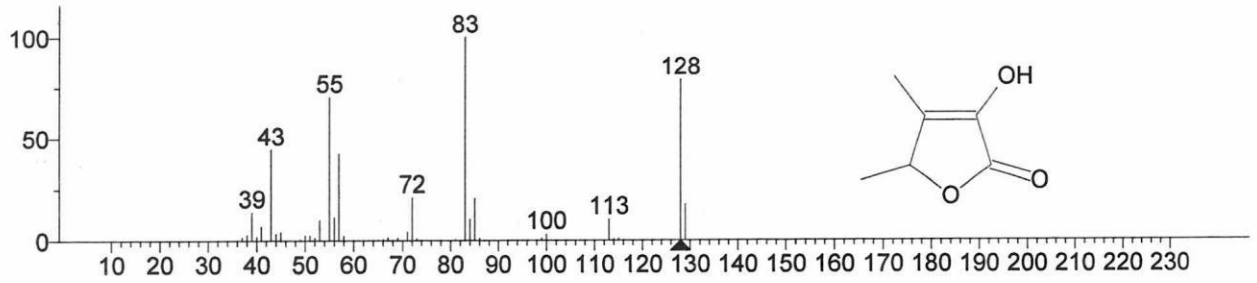


Head to Tail MF=701 RMF=759



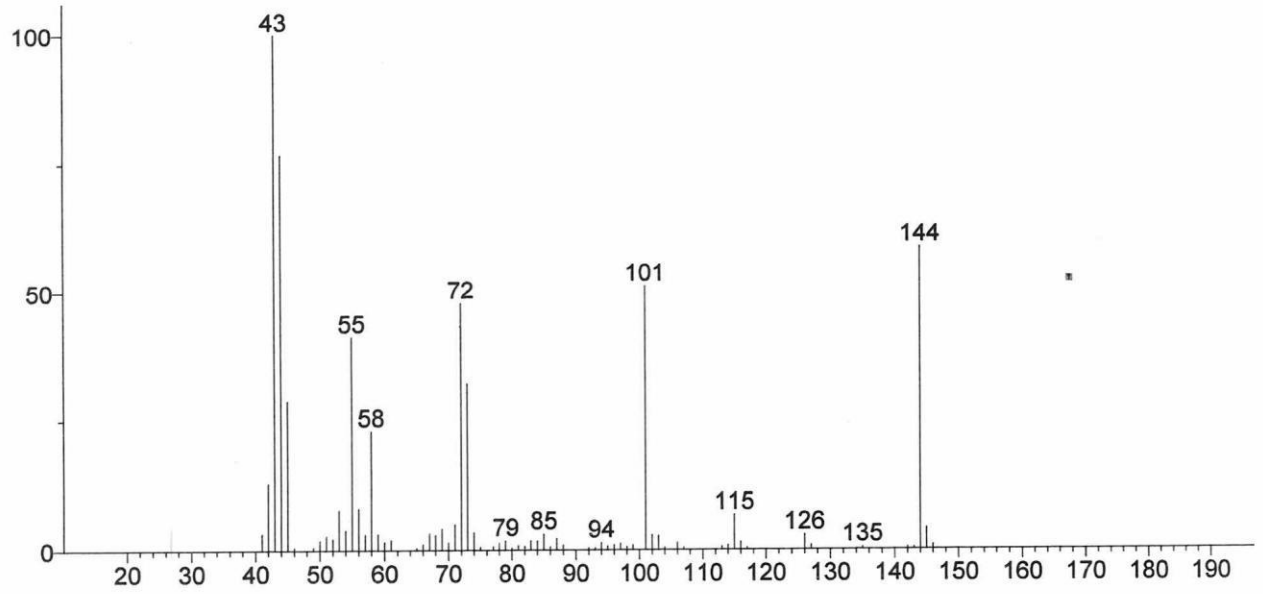
(mainlib) 2(5H)-Furanone, 3-hydroxy-4,5-dimethyl-

Name: 2(5H)-Furanone, 3-hydroxy-4,5-dimethyl-
Formula: $C_6H_8O_3$
MW: 128 CAS#: 28664-35-9 NIST#: 265961 ID#: 45390 DB: mainlib
Other DBs: EINECS
Contributor: A.A.Kutin, Moscow, Russia
10 largest peaks:
83 999 | 128 787 | 55 702 | 43 443 | 57 423 | 72 206 | 85 202 | 129 173 | 39 135 | 56 111 |
Synonyms:
1.Sotolone
2.4,5-Dimethyl-3-hydroxy-2(5H)-furanone
3.Furan-2(5H)-one, 3-hydroxy-4,5-dimethyl-
4.3-Hydroxy-4,5-dimethyl-2(5H)-furanone #

Estimated non-polar retention index (n-alkane scale):
Value: 1088 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1108 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: SPB-1
Column
Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 35 C
End T: 225 C
Heat Rate: 4 K/min
Start Time: 5 min
End Time: 20
min
Source: Chisholm, M.G.; Jell, J.A.; Cass, D.M., Jr., Characterization of the major odorants found in the peel oil of Citrus reticulata Blanco cv. Clementine using gas chromatography-olfactometry, Flavour Fragr. J., 18, 2003, 275-281.

2. Value: 1068 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5
CB
Column Length: 50 m
Carrier Gas: He
Column Diameter: 0.32 mm
Phase Thickness: 1.2 um
Data Type:
Normal alkane RI
Program Type: Complex
Description: 36C =>20C/min =>85C=>1C/min =>145C=>3C/min
=>250C



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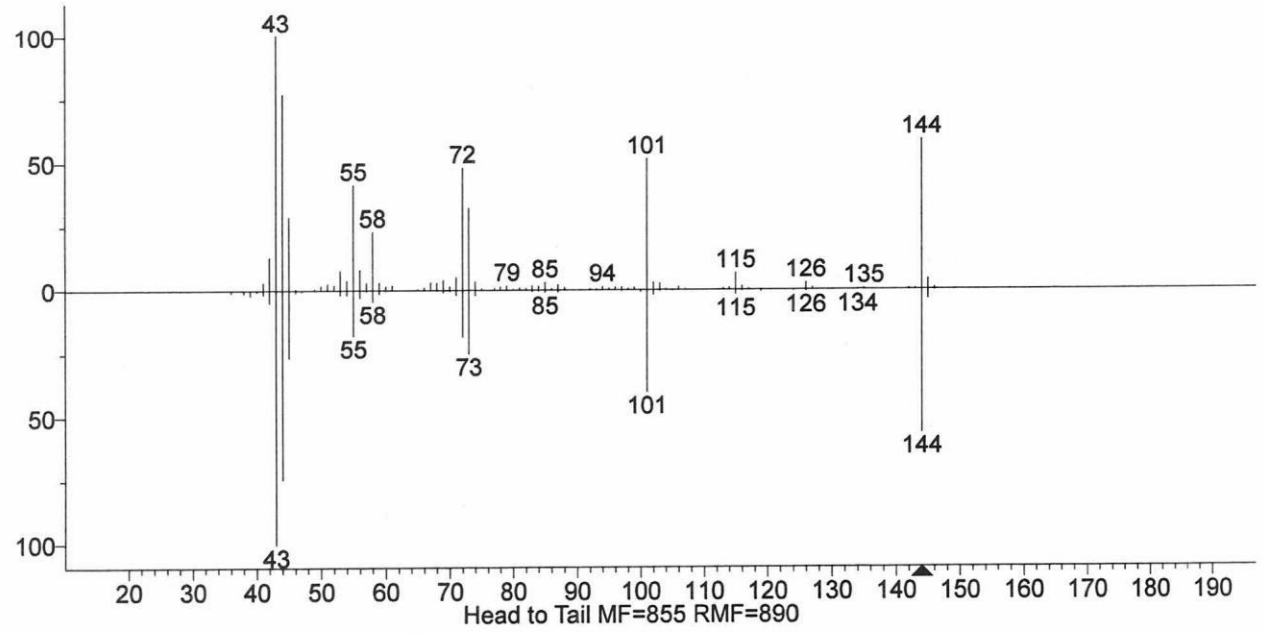
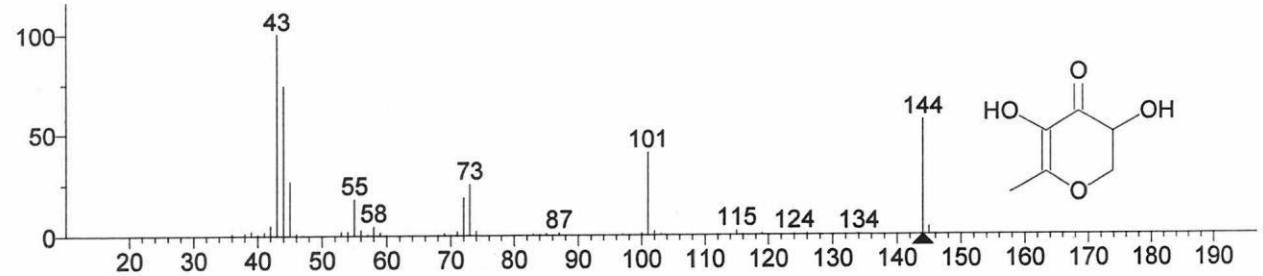


Head to Tail MF=855 RMF=890



(replib) 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-

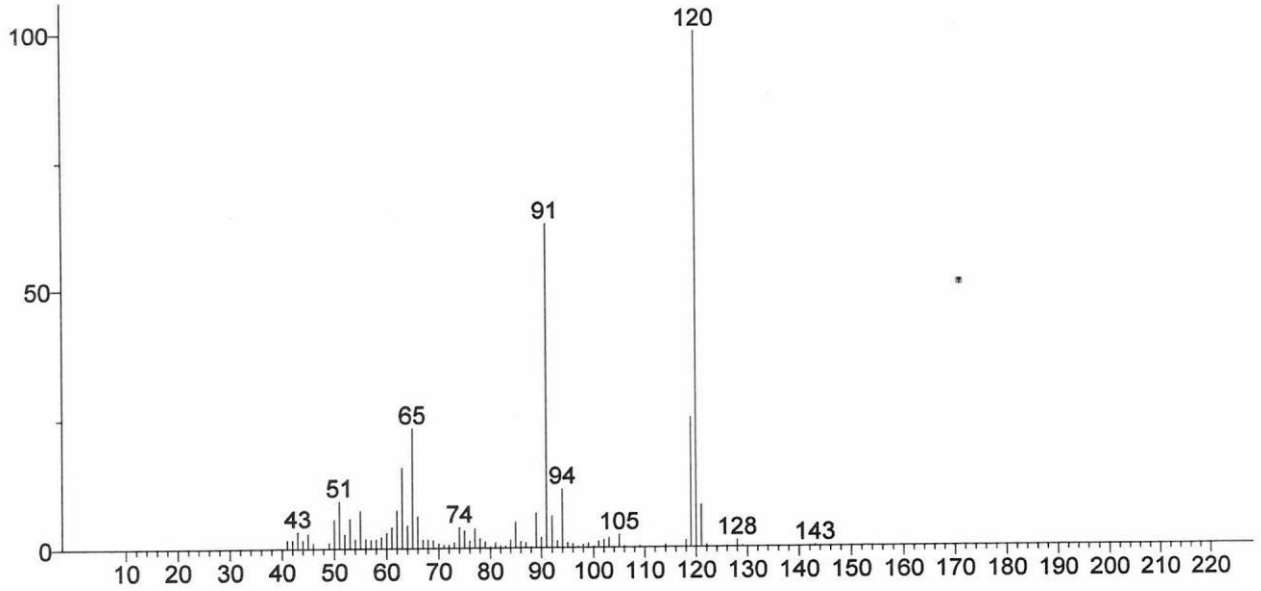
Name: 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
Formula: $C_6H_8O_4$
MW: 144 CAS#: 28564-83-2 NIST#: 108691 ID#: 1857 DB: replib
Other DBs: RTECS
Contributor: Philip Morris R&D
10 largest peaks:
43 999 | 44 742 | 144 563 | 101 402 | 45 264 | 73 249 | 72 182 | 55 177 | 42 48 | 58 43 |
Synonyms:
1.3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one #

Estimated non-polar retention index (n-alkane scale):
Value: 1269 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1119 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Complex
Description: -20C (5min) => 10C/min => 100C => 4C/min =>200C => 10C/min =>
280C
Source: Eri, S.; Khoo, B.K.; Lech, J.; Hartman, T.G., Direct thermal desorption-gas chromatography and gas chromatography-mass spectrometry profiling of hop (Humulus lupulus L.) essential oils in support of varietal characterization, J. Agric. Food Chem., 48, 2000, 1140-1149.

2. Value: 1107 iu
Column Type: Capillary
Column
Class: Standard non-polar
Active Phase: DB-1
Column Length: 60 m
Carrier Gas: N2
Column Diameter: 0.25
mm
Phase Thickness: 1 um
Data Type: Linear RI
Program Type: Ramp
Start T: 30 C
End T: 200 C
Heat
Rate: 5 K/min
End Time: 30 min
Source: Wu, C.-M.; Wang, Z.; Wu, Q.H., Volatile compounds produced from monosodium glutamate in common food cooking, J. Agric. Food Chem., 48, 2000, 2438-2442.

<...>



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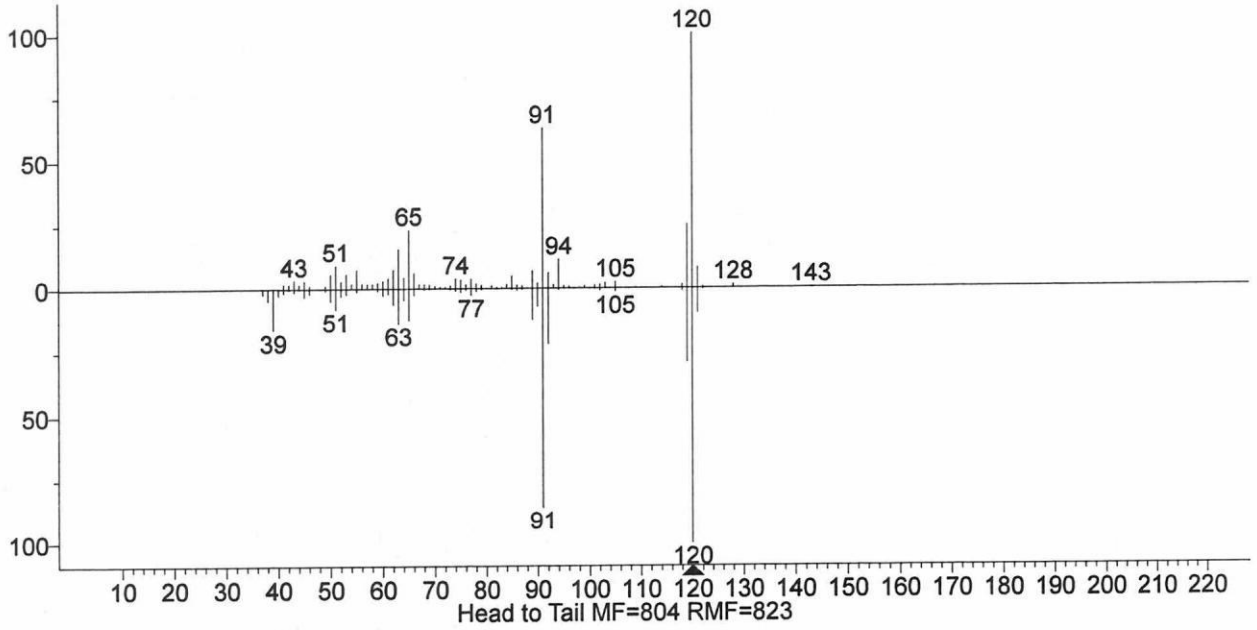
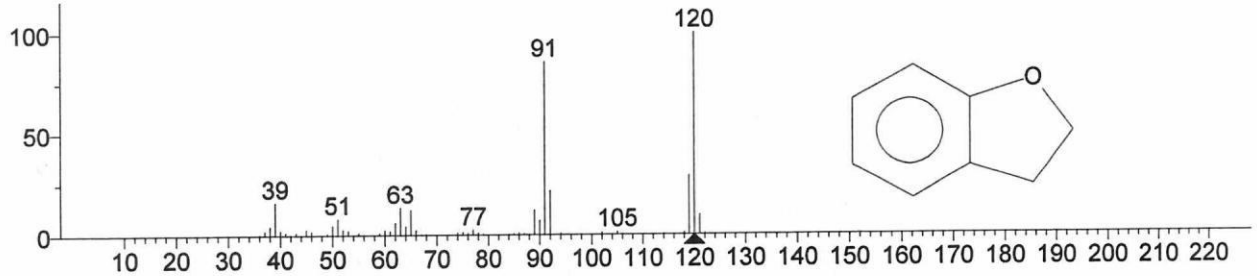


Head to Tail MF=804 RMF=823



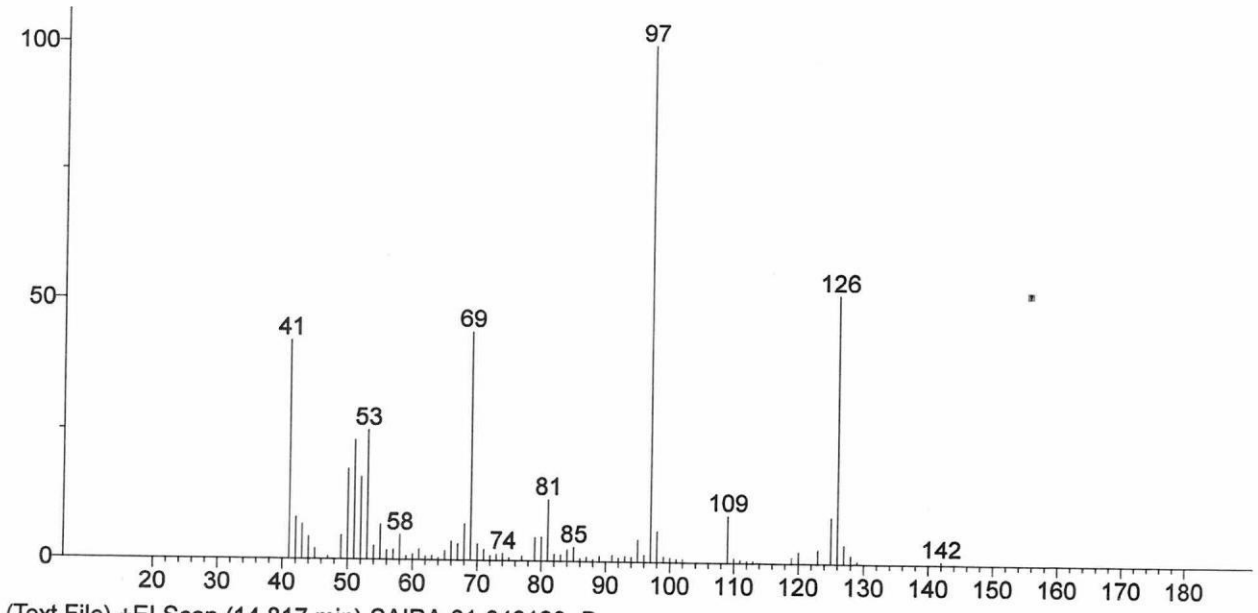
(replib) Benzofuran, 2,3-dihydro-

Name: Benzofuran, 2,3-dihydro-
Formula: C_8H_8O
MW: 120 CAS#: 496-16-2 NIST#: 109771 ID#: 16156 DB: replib
Other DBs: Fine, TSCA, EPA, HODOC, EINECS, IRDB
Contributor: Philip Morris R&D
10 largest peaks:
120 999 | 91 855 | 119 288 | 92 216 | 39 159 | 63 134 | 65 122 | 89 121 | 121 96 | 51 80 |
Synonyms:
1.Coumaran
2.Dihydrobenzofuran
3.Dihydrocoumarone
4.Kumaran
5.2,3-Dihydrobenzofuran
6.2,3-Dihydro-1-benzofuran #

Estimated non-polar retention index (n-alkane scale):
Value: 1036 iu
Confidence interval (Ethers): 68(50%) 293(95%) iu

Retention index.
1. Value: 1188 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 30 m
Carrier Gas: N2
Column Diameter: 0.32 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 150 C
End T: 280 C
Heat Rate: 3 K/min
Source: Coen, M.; Engel, R.;
Nahrstedt, A., Chavicol .beta.-D-glucoside, a phenylpropanoid heteroside, benzyl-.beta.-D-glucoside and glycosidically bound volatiles from subspecies of Cedronella canariensis, Phytochemistry, 40(1), 1995, 149-155.

2. Value: 1187 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: SPB-1
Column
Length: 50 m
Carrier Gas: He
Column Diameter: 0.20 mm
Data Type: Kovats RI
Program Type: Ramp
Start T:
35 C
End T: 200 C
Heat Rate: 3 K/min



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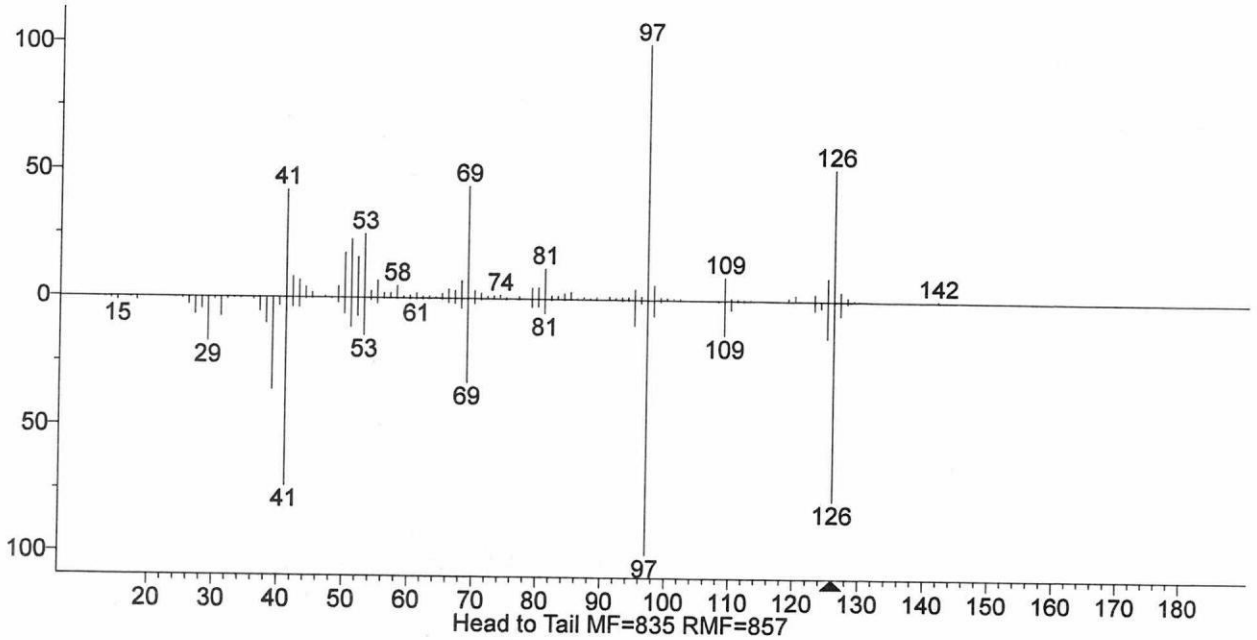
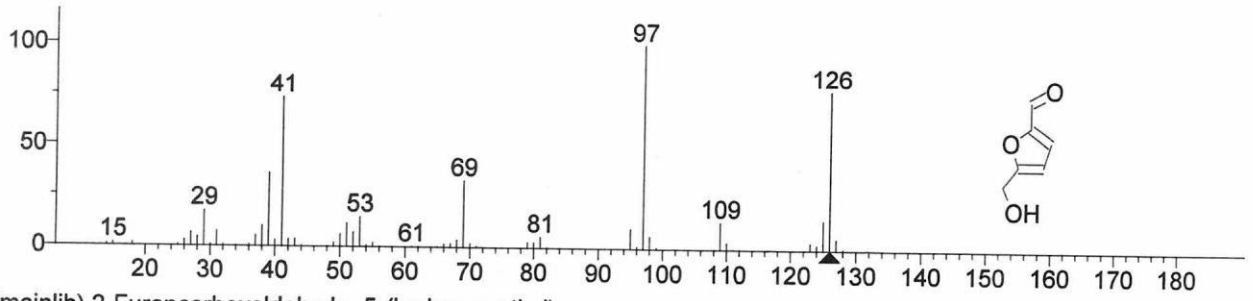


Head to Tail MF=835 RMF=857



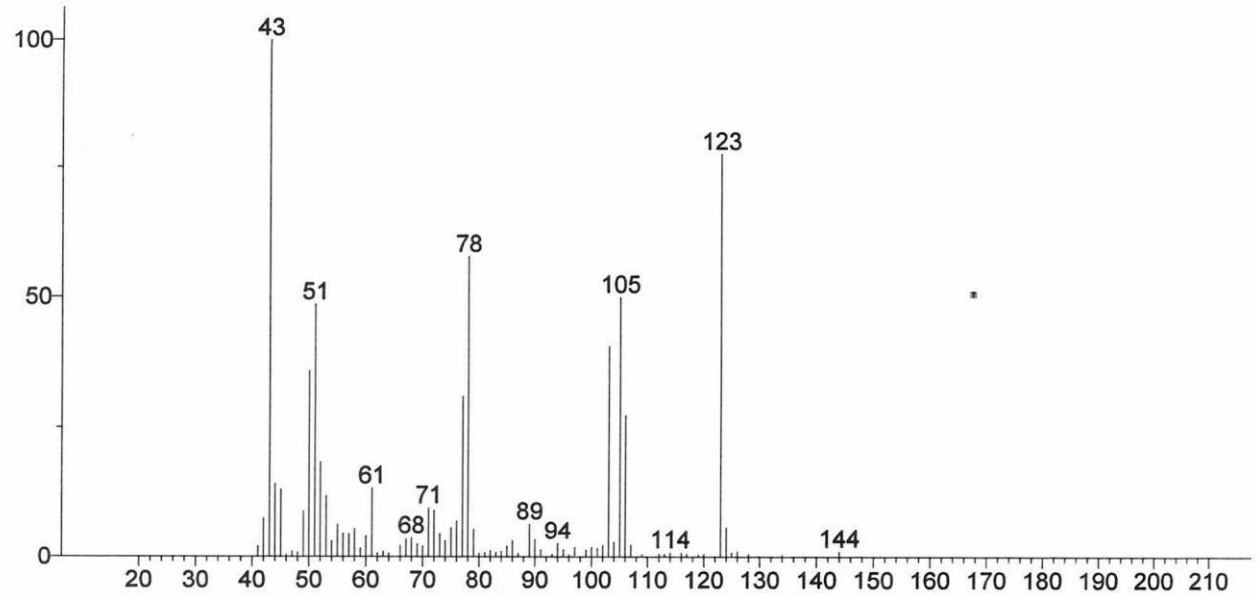
(mainlib) 2-Furancarboxaldehyde, 5-(hydroxymethyl)-

Name: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
Formula: $C_6H_6O_3$
MW: 126 CAS#: 67-47-0 NIST#: 231276 ID#: 60271 DB: mainlib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-4745
10 largest peaks:
97 999 | 126 779 | 41 732 | 39 358 | 69 326 | 29 171 | 53 145 | 125 145 | 109 134 | 51 115 |
Synonyms:
1.2-Furaldehyde, 5-(hydroxymethyl)-
2.5-Hydrxoymethylfurfural
3.Hydroxymethylfurfurole
4.HMF
5.5-(Hyddroxymethyl)Furfurole
6.5-(Hydroxymethyl)-2-formylfuran
7.5-(Hydroxymethyl)-2-furaldehyde
8.5-(Hydroxymethyl)-2-furancarbonal
9.5-(Hydroxymethyl)-2-furfural
10.5-(Hydroxymethyl)-2-furfuraldehyde
11.5-(Hydroxymethyl)furan-2-aldehyde
12.5-(Hydroxymethyl)furfural
13.5-Hydroxymethylfuraldehyde
14.5-Oxymethylfurfurole
15.5-Hydroxymethylfurfuraldehyde
16.5-Hydroxymethyl-2-furancarbaldehyde
17.Hydroxymethylfurfuraldehyde
18.5-(Hydroxymethyl)-2-furancarboxaldehyde
19.2-Hydroxymethyl-5-furfural

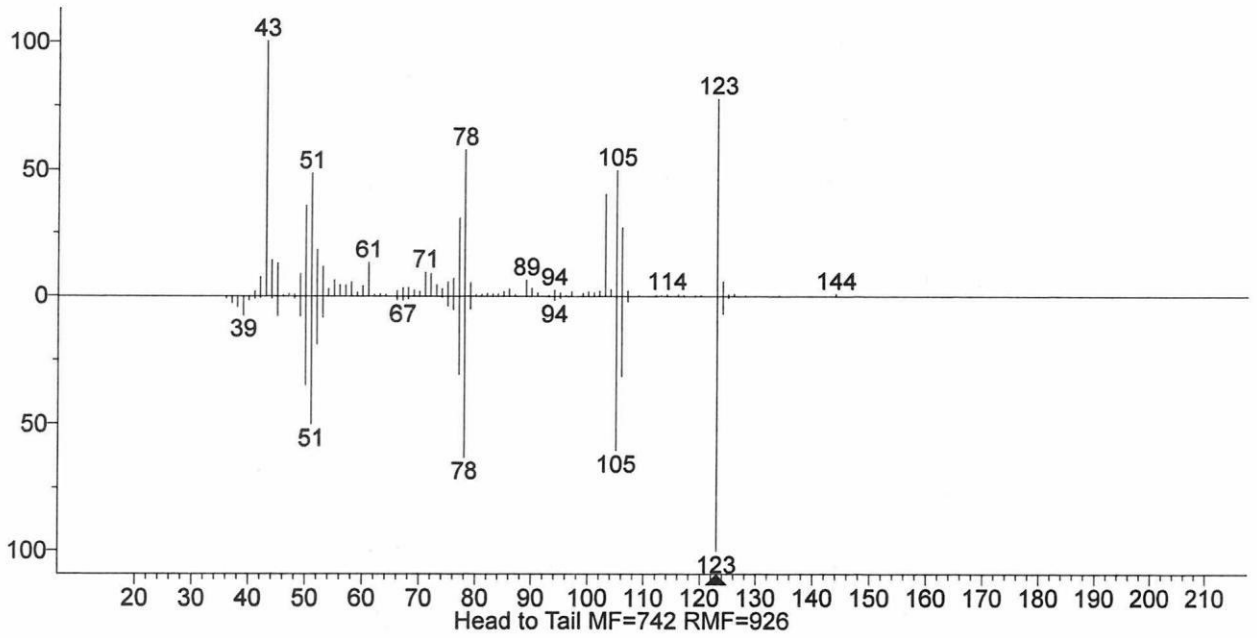
Estimated non-polar retention index (n-alkane scale):
Value: 1163 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1176 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 60 m
Carrier Gas: N2
Column Diameter: 0.25 mm
Phase Thickness: 1 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 30 C
End T: 200 C
Heat Rate: 5 K/min
End Time: 30 min
Source: Wu, C.-M.;
Wang, Z.; Wu, Q.H., Volatile compounds produced from monosodium glutamate in common food cooking, J. Agric. Food Chem., 48, 2000, 2438-2442.

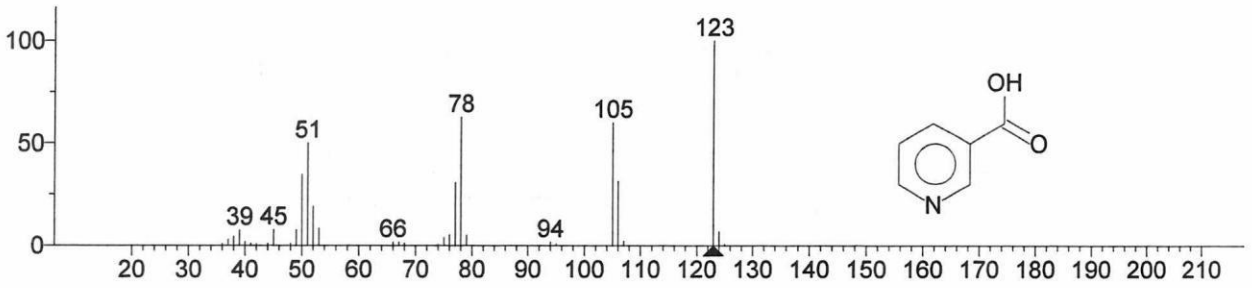
2. Value: 1208 iu



(Text File) +EI Scan (15.202 min) SAIRA-01-040123-.D

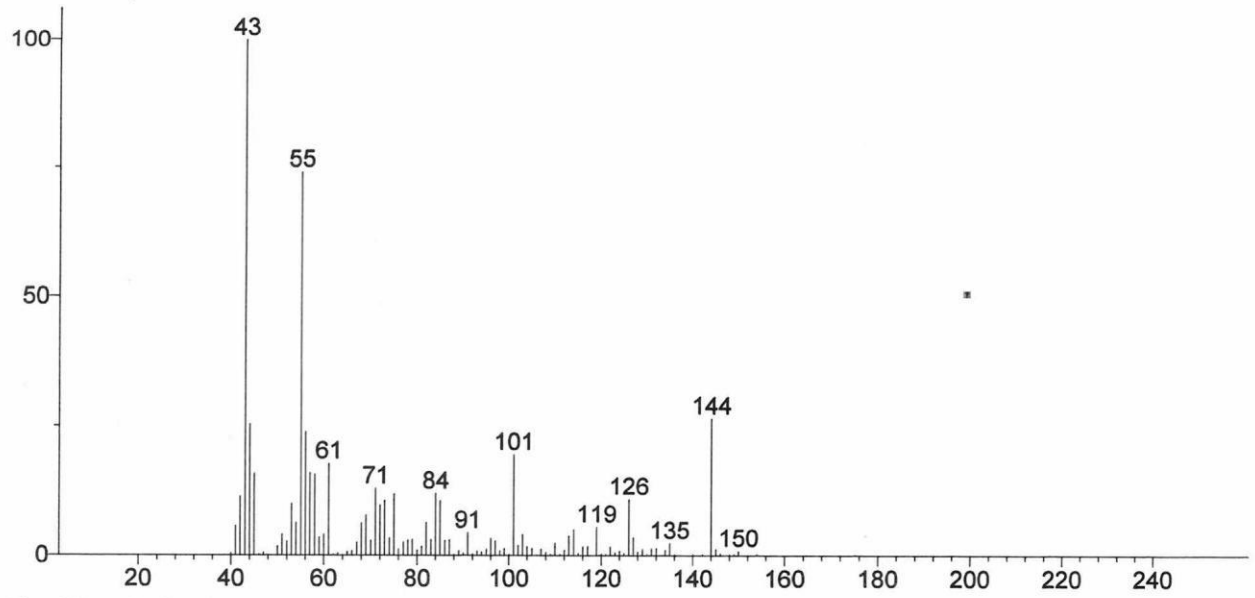


Head to Tail MF=742 RMF=926

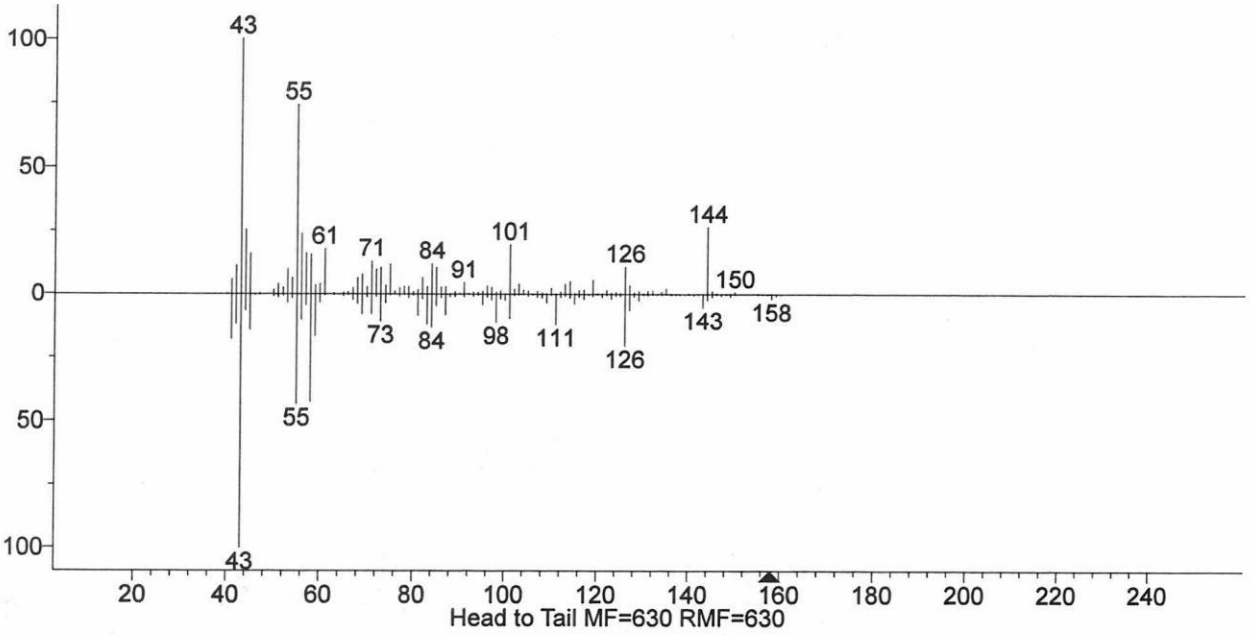


(replib) Niacin

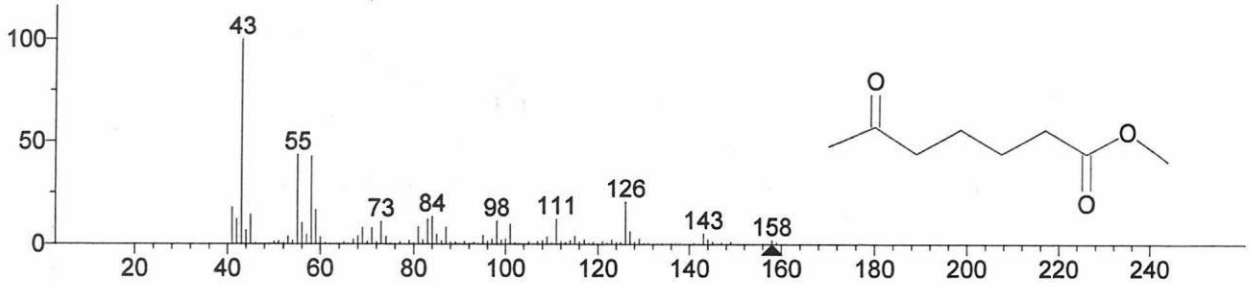
Name: Niacin
Formula: $C_6H_5NO_2$
MW: 123 CAS#: 59-67-6 NIST#: 312948 ID#: 16856 DB: replib
Other DBs: Fine, TSCA, RTECS, USP, HODOC, NIH, EINECS, IRDB
Contributor: Dr. P.K. Shah, NYC Police Laboratory, NY
10 largest peaks:
123 999 | 78 626 | 105 600 | 51 500 | 50 347 | 106 315 | 77 307 | 52 189 | 53 83 | 49 77 |
Synonyms:
1.3-Pyridinecarboxylic acid
2.Nicotinic acid
3.Akotin
4.Apelagrin
5.Daskil
6.Efacin
7.Linic
8.Nicacid
9.Nicangin
10.Nico-Span
11.Nicodelmine
12.Nicolar
13.Niconacid
14.Nicosan 3
15.Nicotinipca
16.Nicyl
17.Nyclin
18.Pellagrin
19.Pelonin
20.Pyridine-β-carboxylic acid
21.Vitamin B
22.3-Carboxylpyridine
23.3-Carboxypyridine
24.anti-Pellagra vitamin
25.Acidum nicotinicum
26.Bionic
27.Davitamon PP
28.Diacin
29.Direktan
30.Naotin
31.Niac
32.Nicamin
33.Nico-400
34.Nicobid
35.Nicocap
36.Nicocidin
37.Nicocrisina
38.Nicodan
39.Nicodon
40.Niconat
41.Niconazid
42.Nicorol
43.Nicoside
44.Nicosyl
45.Nicotamin
46.Nicotene



(Text File) +EI Scan (16.125-16.178 min, 16 Scans) SAIRA-01-040123-.D



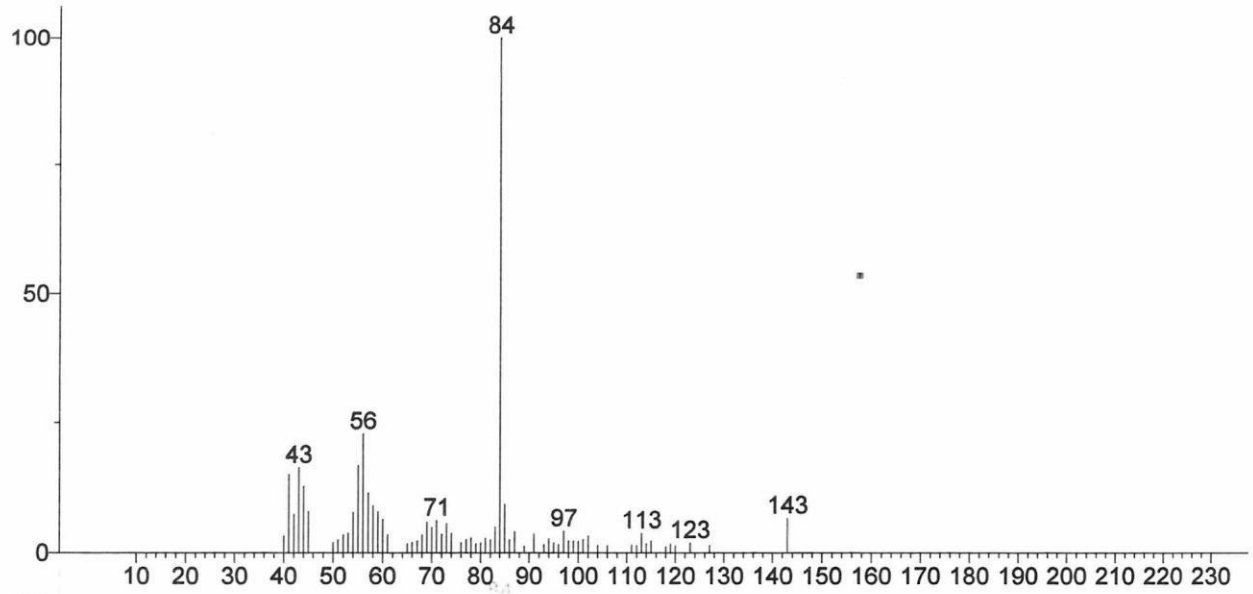
Head to Tail MF=630 RMF=630



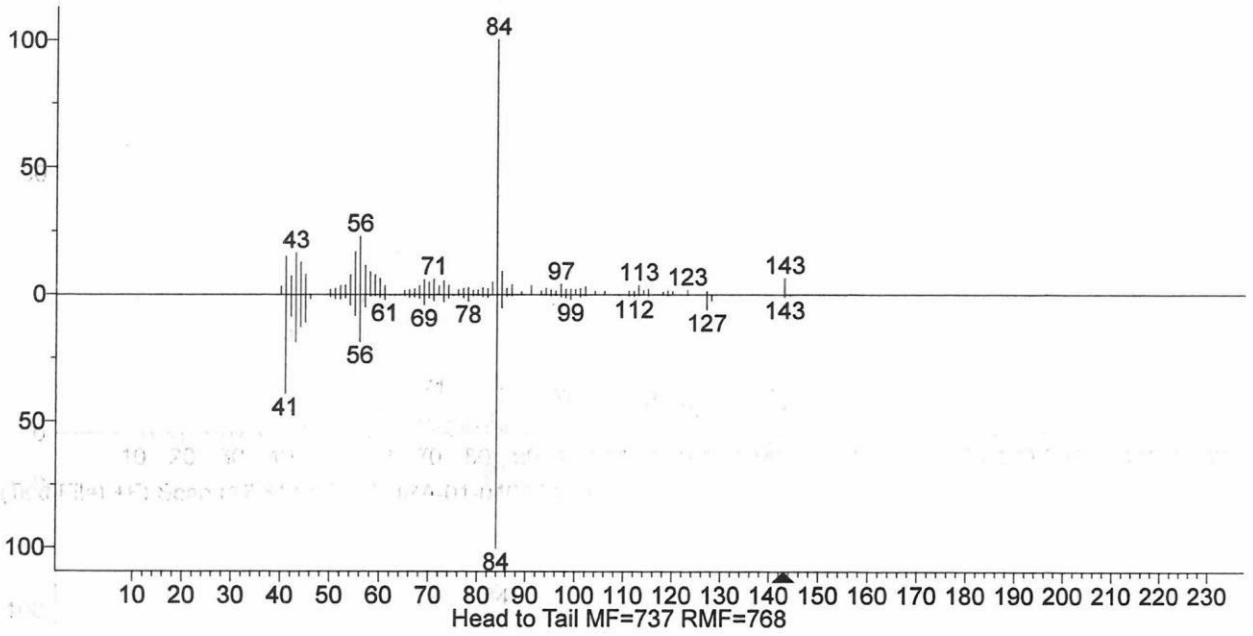
(mainlib) Methyl 6-oxoheptanoate

Name: Methyl 6-oxoheptanoate
Formula: $C_8H_{14}O_3$
MW: 158 CAS#: 2046-21-1 NIST#: 116666 ID#: 6770 DB: mainlib
Other DBs: None
Contributor: K. Jacobson, LBC, NIDDK, NIH, Bethesda, MD 20892
10 largest peaks:
43 999 | 55 433 | 58 425 | 126 205 | 41 177 | 59 164 | 45 142 | 84 132 | 111 121 | 42 120 |
Synonyms:
1.5-Acetylvaleric acid, methyl ester

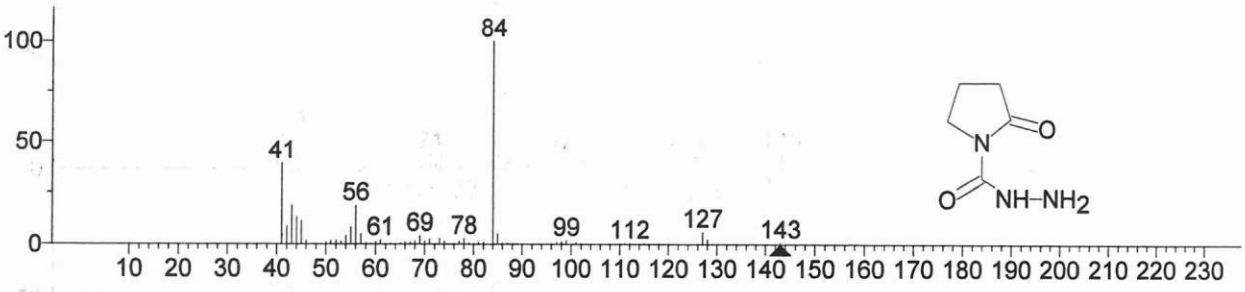
Estimated non-polar retention index (n-alkane scale):
Value: 1120 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (17.814 min) SAIRA-01-040123-.D



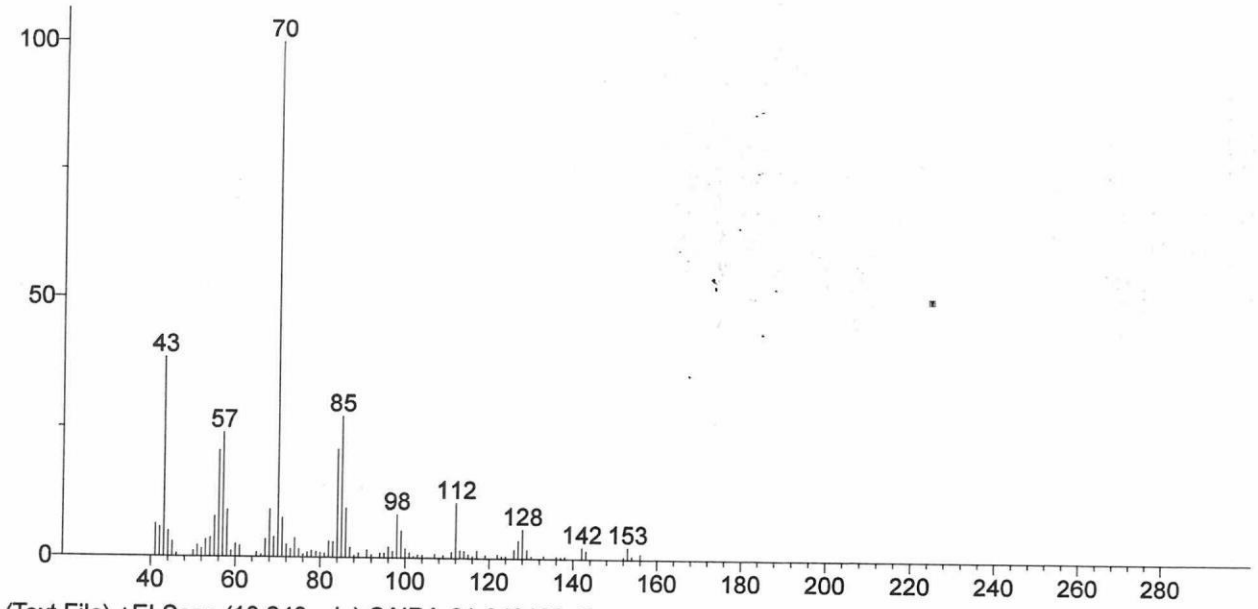
Head to Tail MF=737 RMF=768



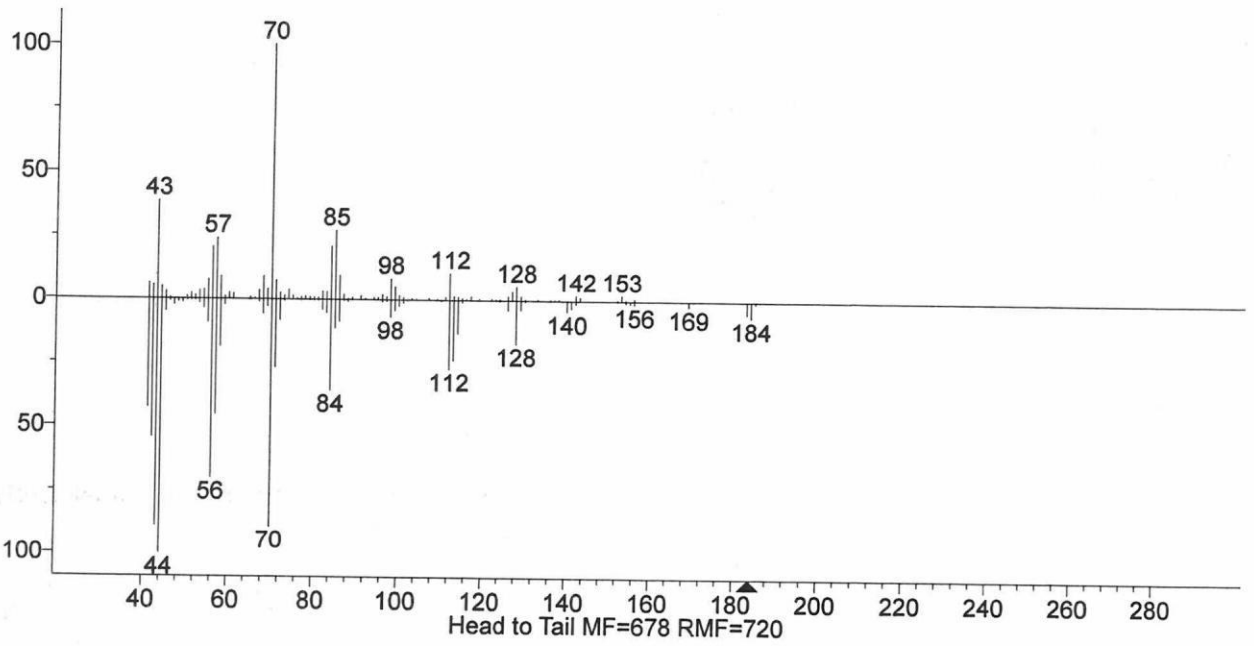
(mainlib) l-Pyrrolid-2-one, N-carboxyhydrazide

Name: l-Pyrrolid-2-one, N-carboxyhydrazide
Formula: $C_5H_9N_3O_2$
MW: 143 NIST#: 130586 ID#: 45666 DB: mainlib
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892
10 largest peaks:
84 999 | 41 390 | 43 186 | 56 184 | 44 129 | 45 111 | 42 86 | 55 82 | 127 59 | 85 52 |
Synonyms:
no synonyms.

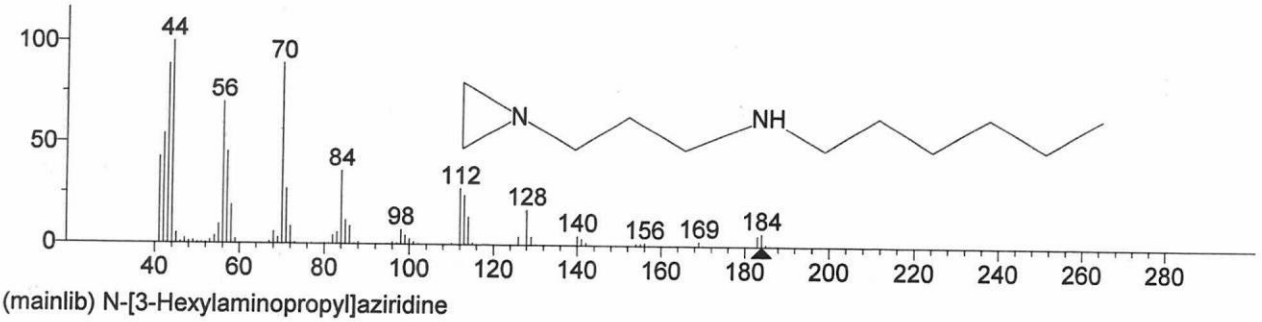
Estimated non-polar retention index (n-alkane scale):
Value: 1563 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu



(Text File) +EI Scan (18.248 min) SAIRA-01-040123-.D



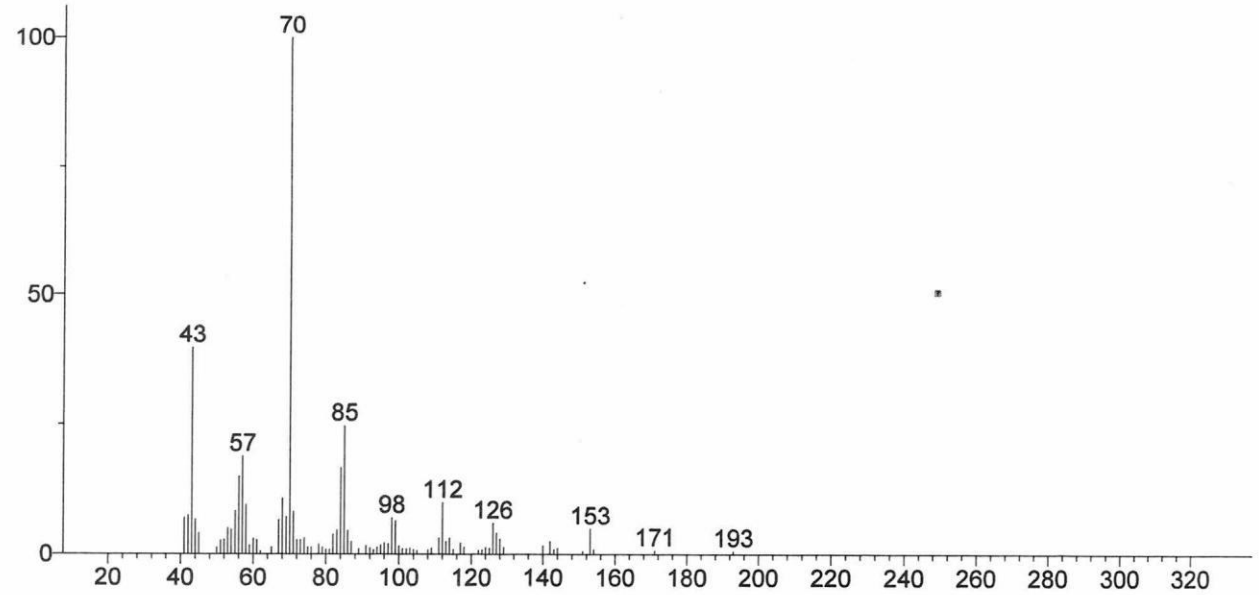
Head to Tail MF=678 RMF=720



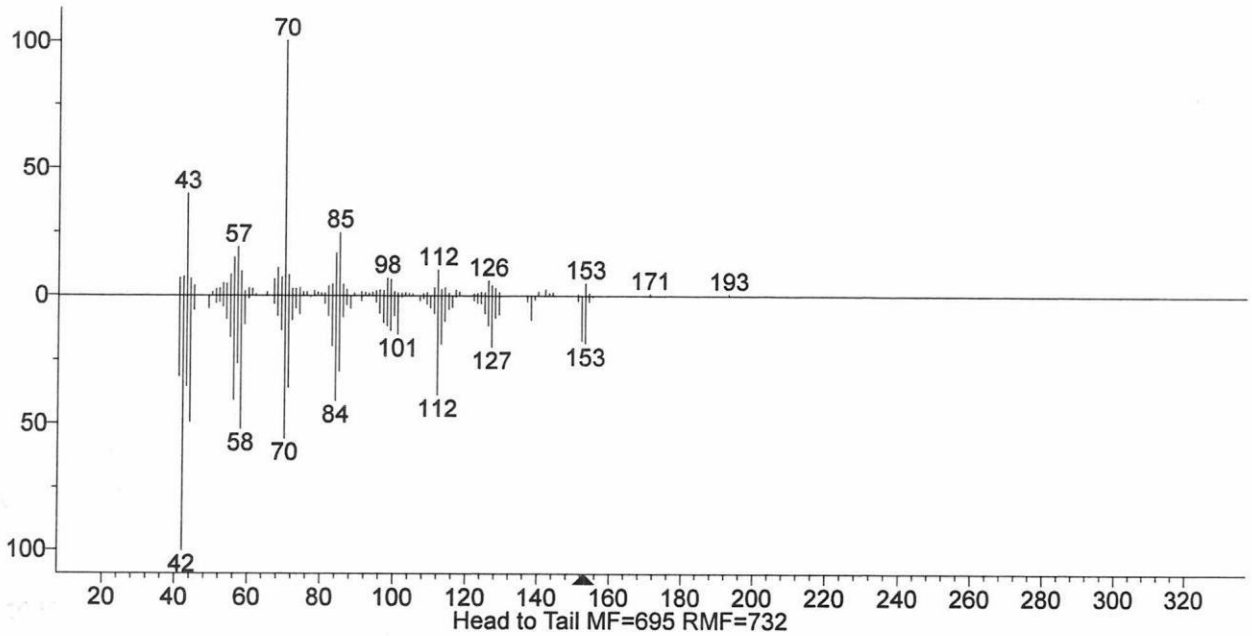
(mainlib) N-[3-Hexylaminopropyl]aziridine

Name: N-[3-Hexylaminopropyl]aziridine
Formula: $C_{11}H_{24}N_2$
MW: 184 NIST#: 256197 ID#: 14285 DB: mainlib
Contributor: Div. of Experiment Therapeutics WRAIR, WRAMC, Washington DC 20307
10 largest peaks:
44 999 | 70 891 | 43 886 | 56 699 | 42 541 | 57 454 | 41 427 | 84 359 | 112 274 | 71 268 |
Synonyms:
no synonyms.

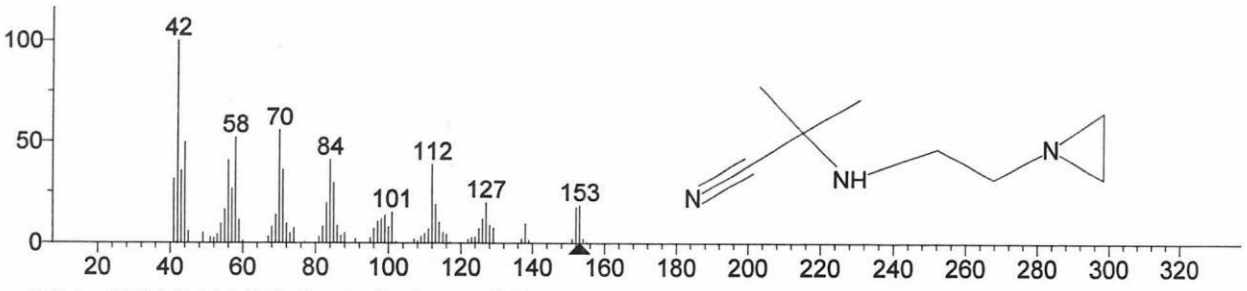
Estimated non-polar retention index (n-alkane scale):
Value: 1467 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu



(Text File) +EI Scan (18.498 min) SAIRA-01-040123-.D



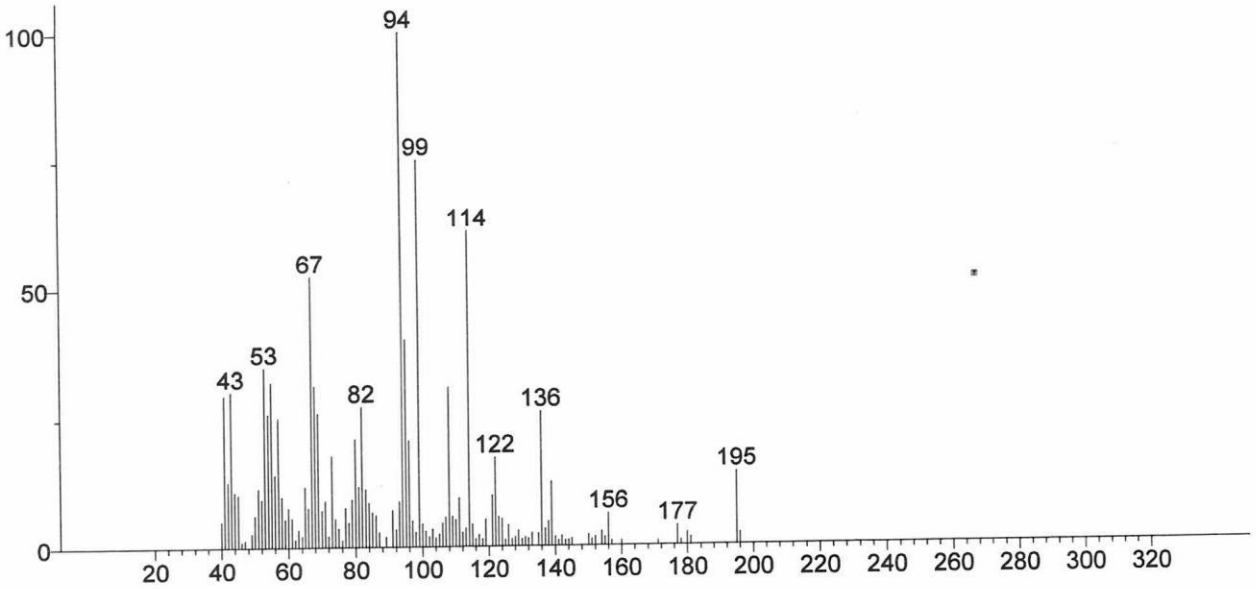
Head to Tail MF=695 RMF=732



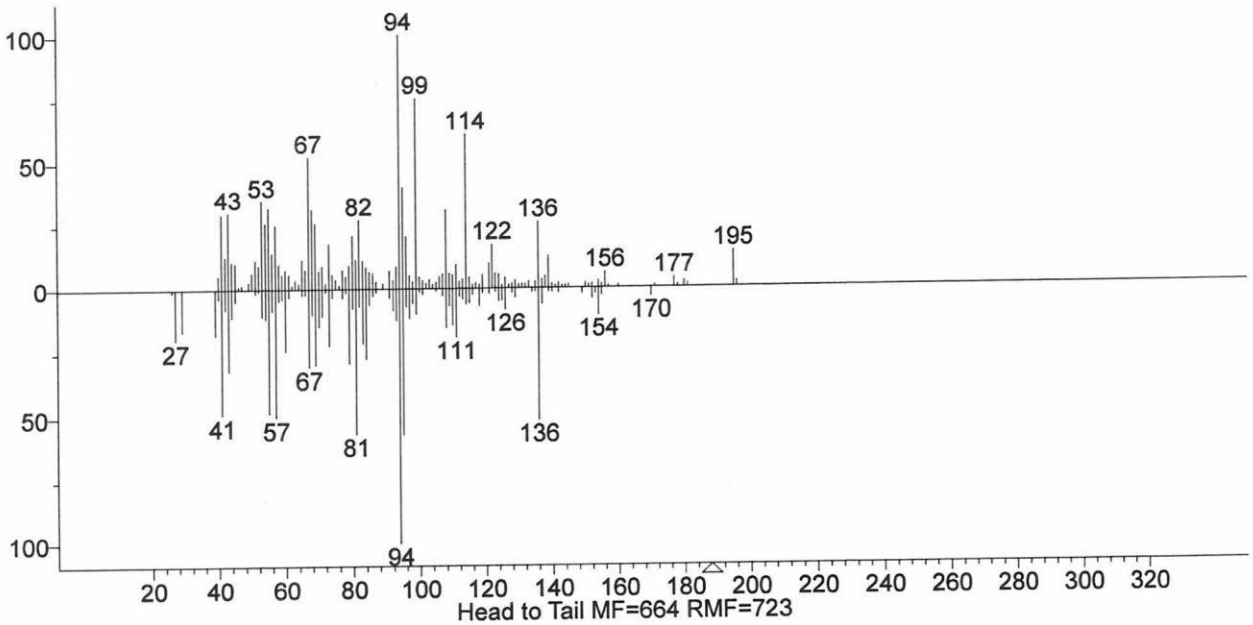
(mainlib) α-[2-[N-Aziridyl]ethylamino]isobutyronitrile

Name: α-[2-[N-Aziridyl]ethylamino]isobutyronitrile
Formula: $C_8H_{15}N_3$
MW: 153 NIST#: 256198 ID#: 4530 DB: mainlib
Contributor: Div. of Experiment Therapeutics WRAIR, WRAMC, Washington DC 20307
10 largest peaks:
42 999 | 70 555 | 58 518 | 44 493 | 84 409 | 56 406 | 112 386 | 71 358 | 43 353 | 41 315 |
Synonyms:
no synonyms.

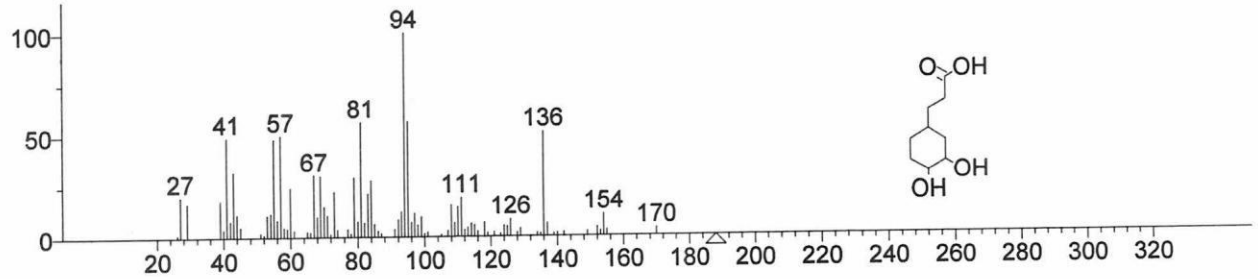
Estimated non-polar retention index (n-alkane scale):
Value: 1329 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu



(Text File) +EI Scan (20.747 min) SAIRA-01-040123-.D



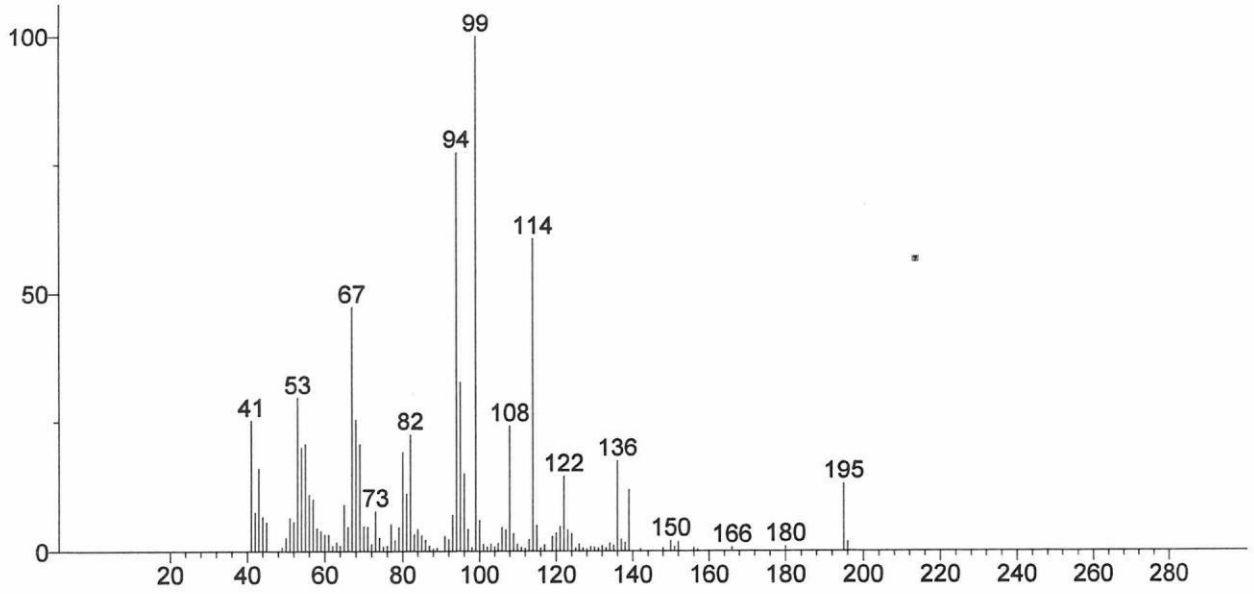
Head to Tail MF=664 RMF=723



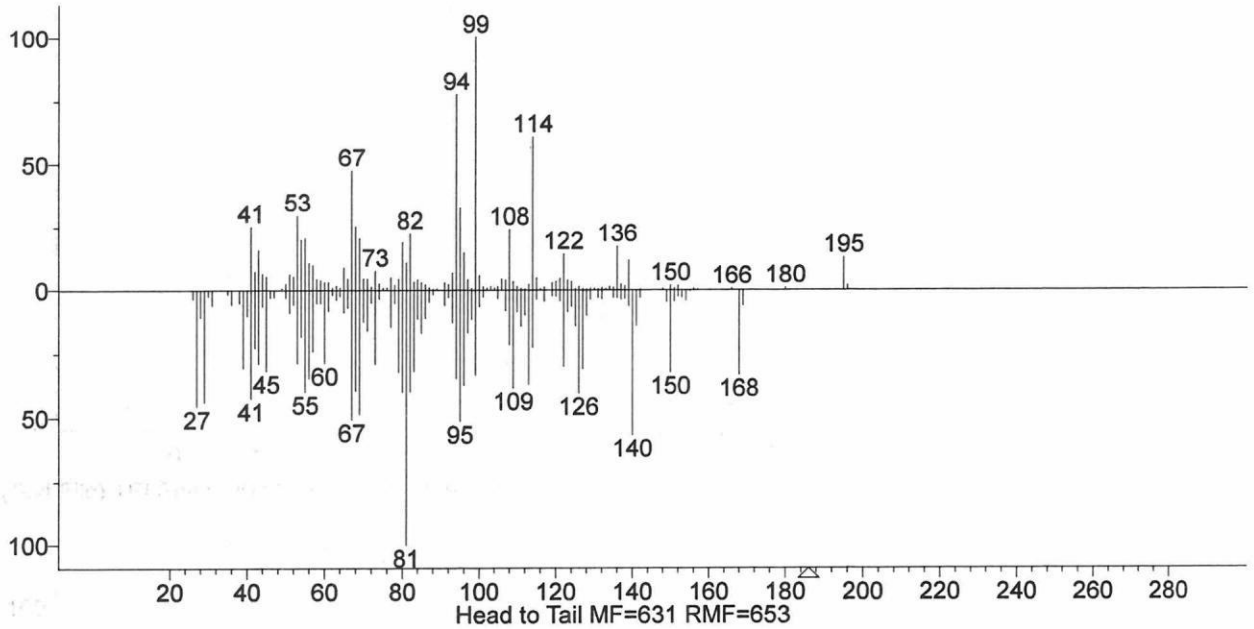
(mainlib) Cyclohexanepropanoic acid, 3,4-dihydroxy-

Name: Cyclohexanepropanoic acid, 3,4-dihydroxy-
Formula: $C_9H_{16}O_4$
MW: 188 CAS#: 57231-21-7 NIST#: 68756 ID#: 57609 DB: mainlib
Other DBs: None
Contributor: R.SELF FOOD RESEARCH INSTITUTE, NORWICH, U.K.
10 largest peaks:
94 999 | 95 565 | 81 562 | 136 513 | 57 498 | 41 488 | 55 481 | 43 319 | 67 303 | 69 296 |
Synonyms:
1.3-(3,4-Dihydroxycyclohexyl)propanoic acid #

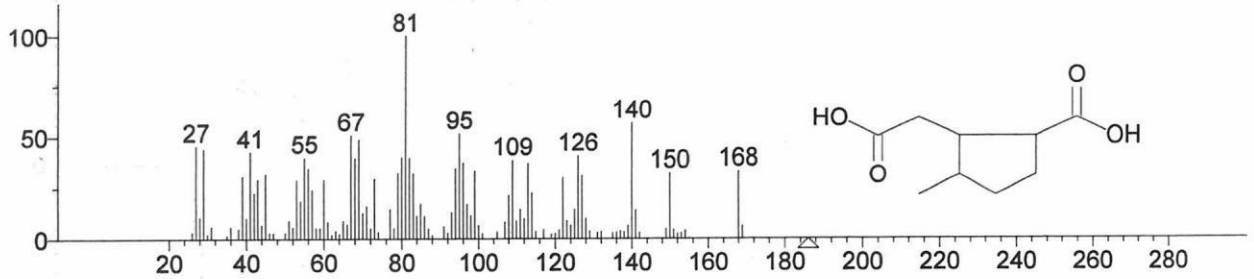
Estimated non-polar retention index (n-alkane scale):
Value: 1712 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (20.893 min) SAIRA-01-040123-.D



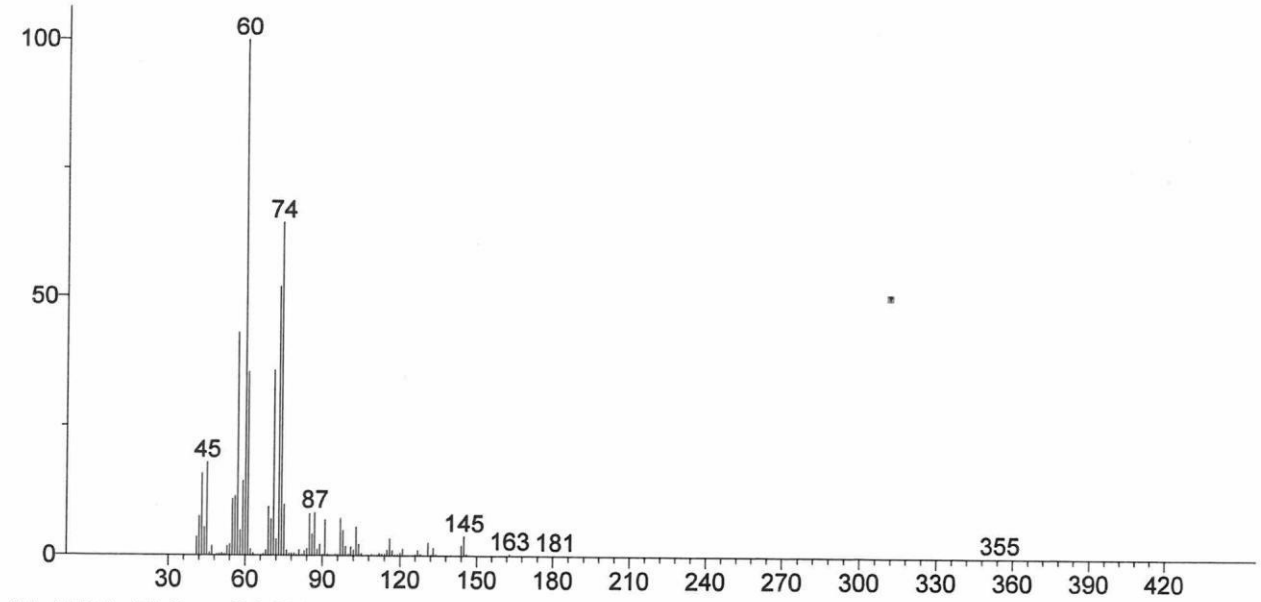
Head to Tail MF=631 RMF=653



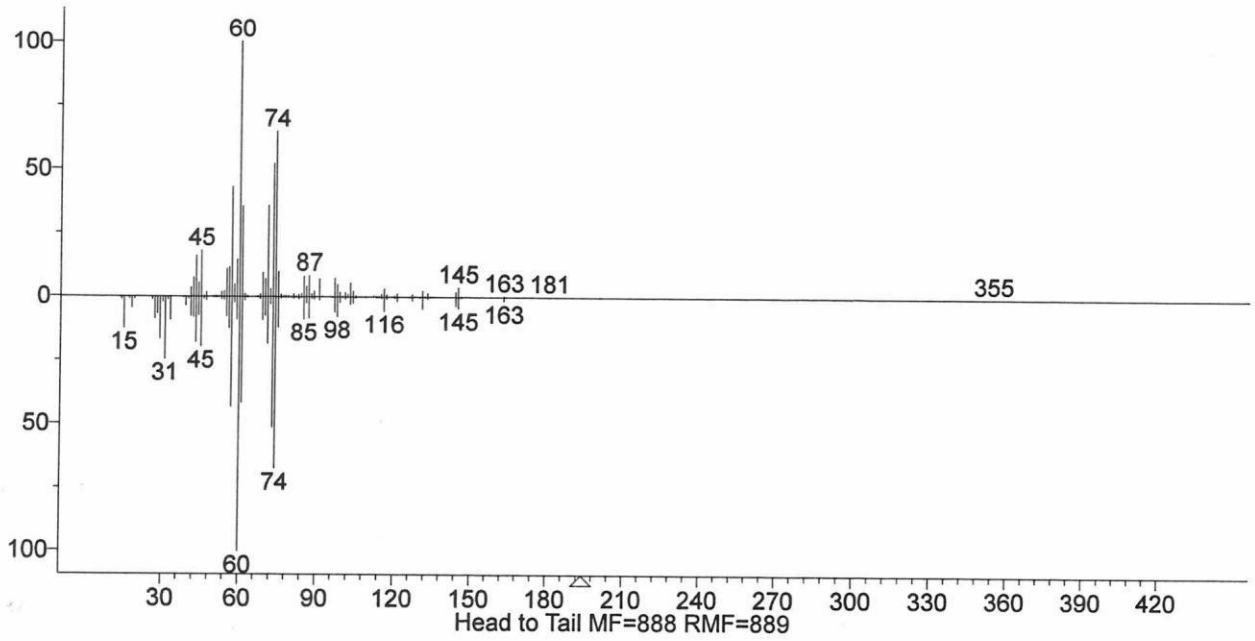
(mainlib) 2-Carboxymethyl-3-methyl-cyclopentanecarboxylic acid

Name: 2-Carboxymethyl-3-methyl-cyclopentanecarboxylic acid
Formula: $C_9H_{14}O_4$
MW: 186 NIST#: 186612 ID#: 43577 DB: mainlib
Contributor: Chemical Concepts
10 largest peaks:
81 999 | 140 565 | 95 513 | 67 505 | 69 485 | 27 454 | 29 438 | 41 424 | 126 404 | 80 398 |
Synonyms:
no synonyms.

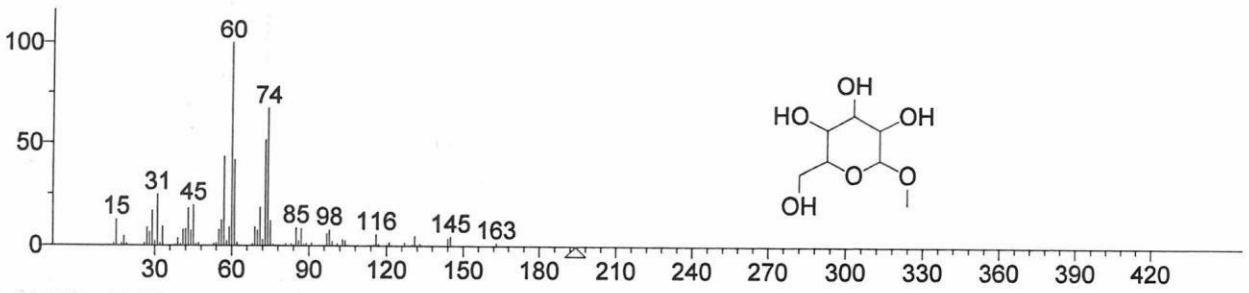
Estimated non-polar retention index (n-alkane scale):
Value: 1595 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu



(Text File) +EI Scan (22.920 min) SAIRA-01-040123-.D



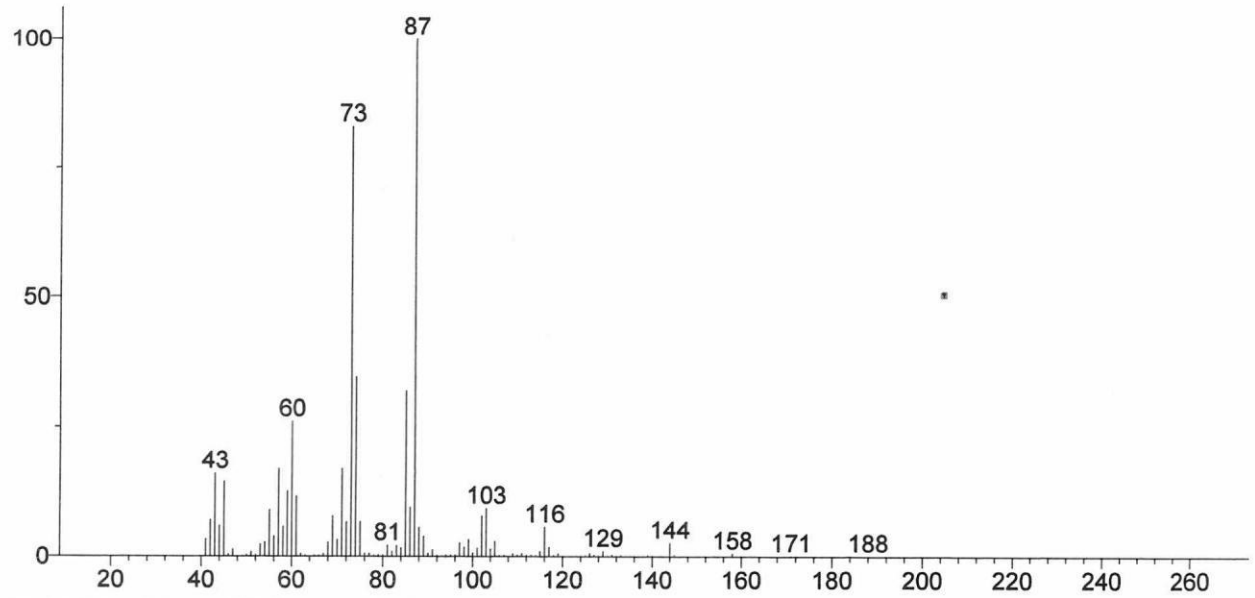
Head to Tail MF=888 RMF=889



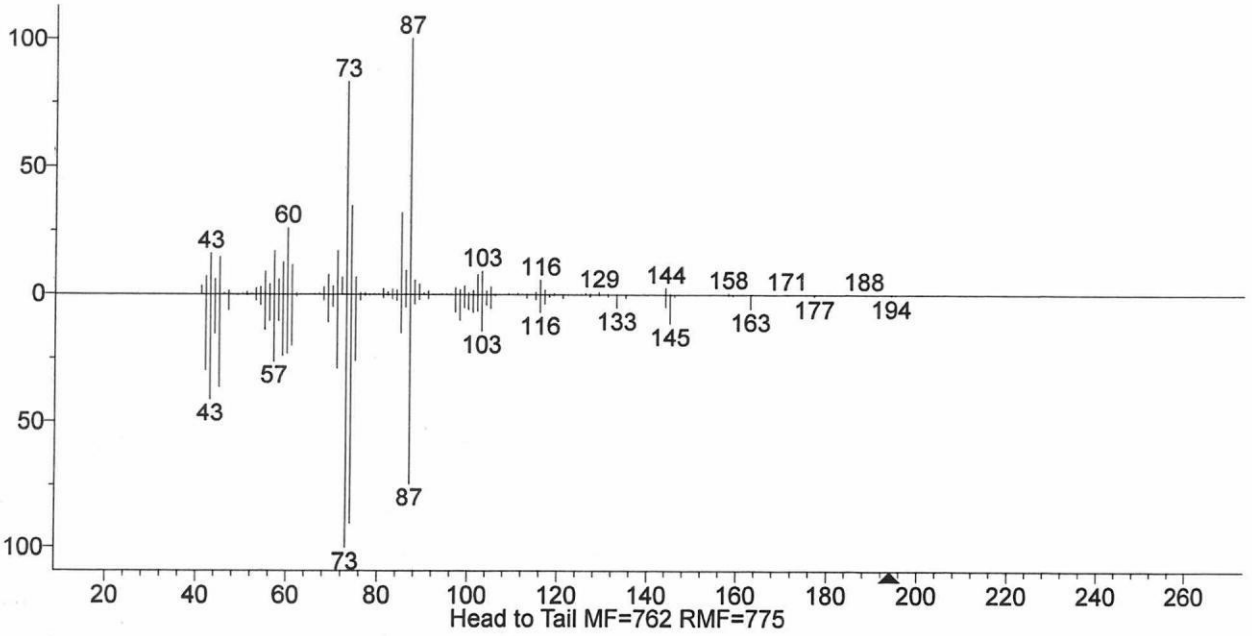
(mainlib) α-D-Glucopyranoside, methyl

Name: α-D-Glucopyranoside, methyl
Formula: $C_7H_{14}O_6$
MW: 194 CAS#: 97-30-3 NIST#: 229366 ID#: 27200 DB: mainlib
Other DBs: TSCA, HODOC, NIH, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW- 635
10 largest peaks:
60 999 | 74 671 | 73 512 | 57 432 | 61 416 | 31 245 | 45 195 | 71 185 | 43 179 | 29 167 |
Synonyms:
1.Glucopyranoside, methyl, α-D-
2.α-Methylglucoside
3.Methyl α-D-glucopyranoside
4.Methyl α-D-glucoside
5.α-d-Methylglucopyranoside
6.α-Methyl D-glucose ether
7.Methyl hexopyranoside #

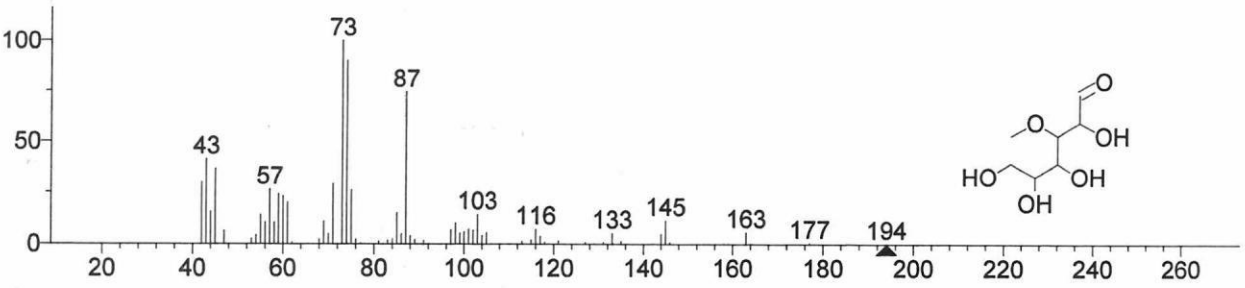
Estimated non-polar retention index (n-alkane scale):
Value: 1714 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (25.051 min) SAIRA-01-040123-.D



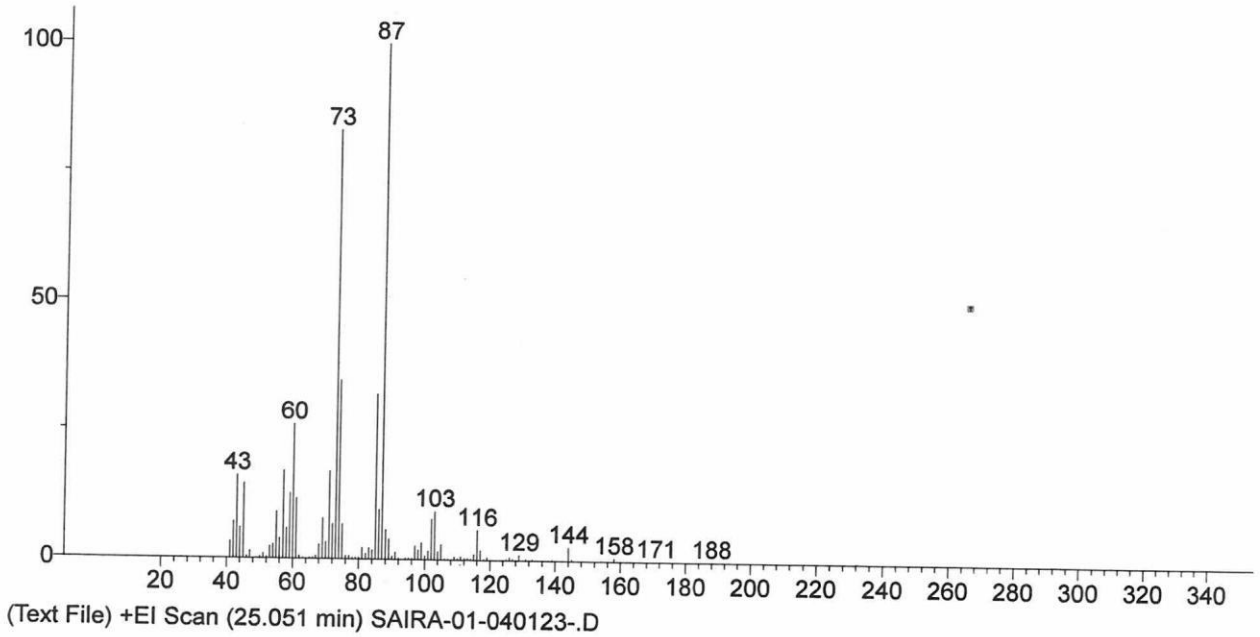
Head to Tail MF=762 RMF=775



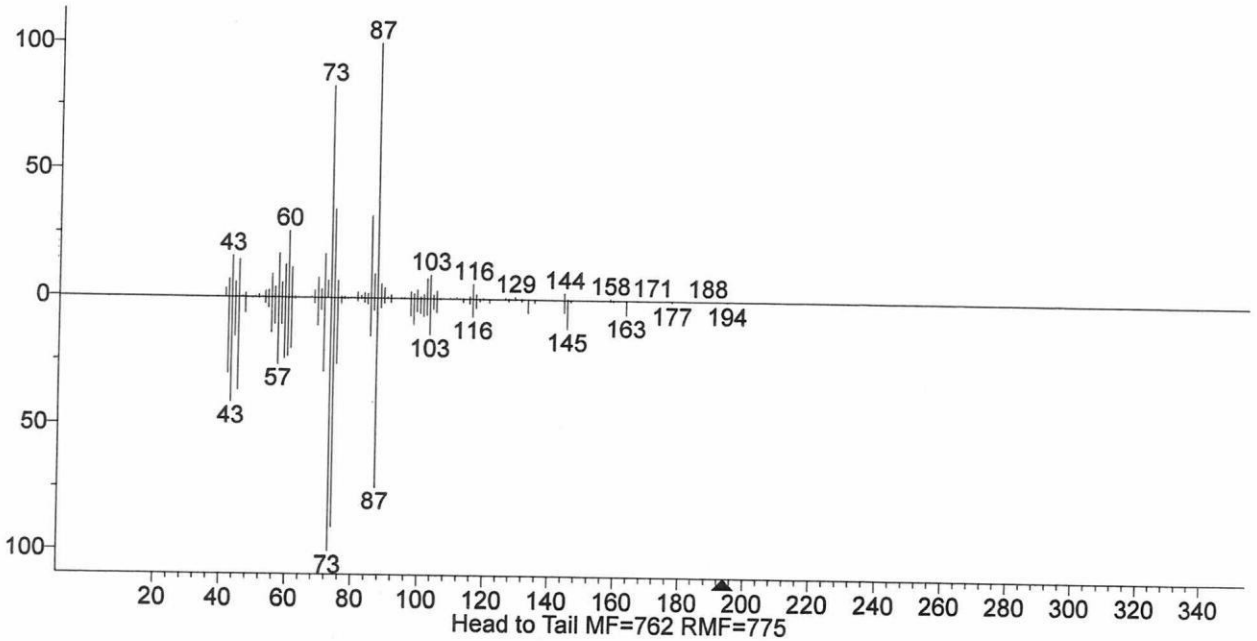
(mainlib) 3-O-Methyl-d-glucose

Name: 3-O-Methyl-d-glucose
Formula: $C_7H_{14}O_6$
MW: 194 NIST#: 127259 ID#: 35456 DB: mainlib
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892
10 largest peaks:
73 999 | 74 900 | 87 743 | 43 411 | 45 363 | 42 298 | 71 290 | 57 262 | 75 259 | 59 239 |
Synonyms:
no synonyms.

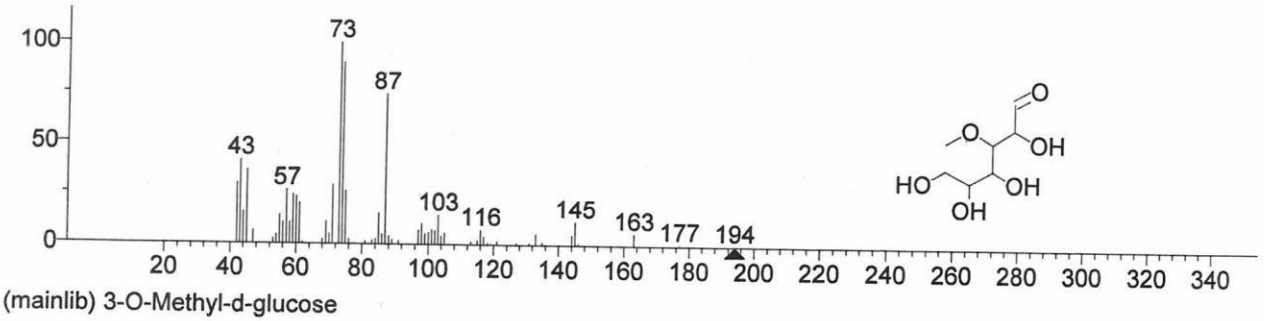
Estimated non-polar retention index (n-alkane scale):
Value: 1647 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (25.051 min) SAIRA-01-040123-.D



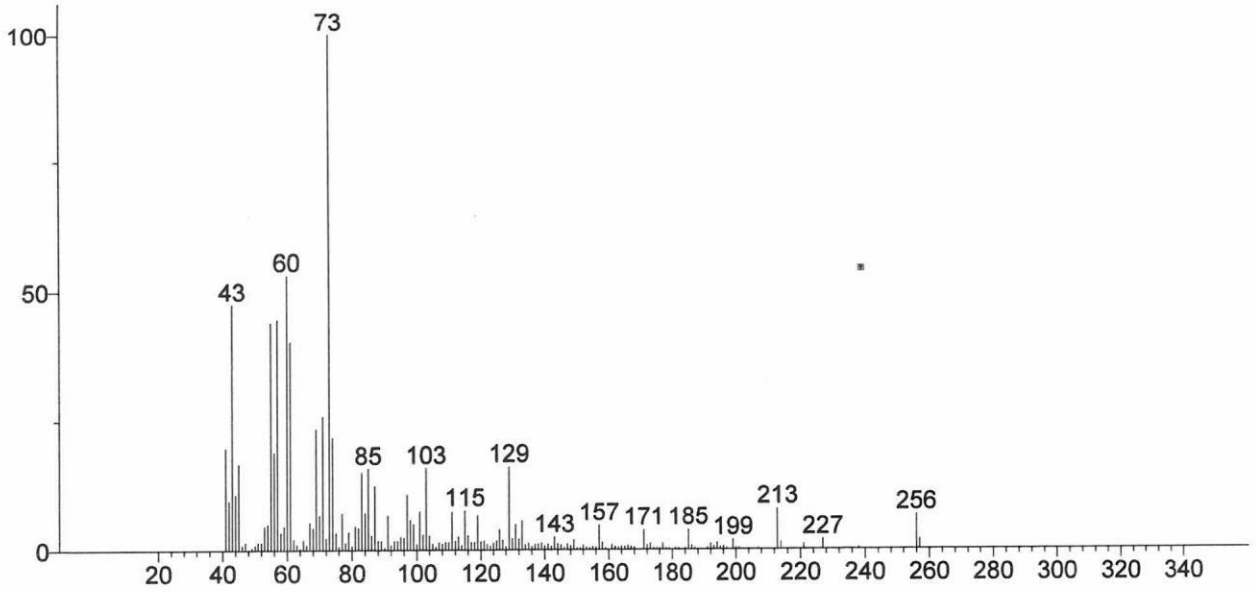
Head to Tail MF=762 RMF=775



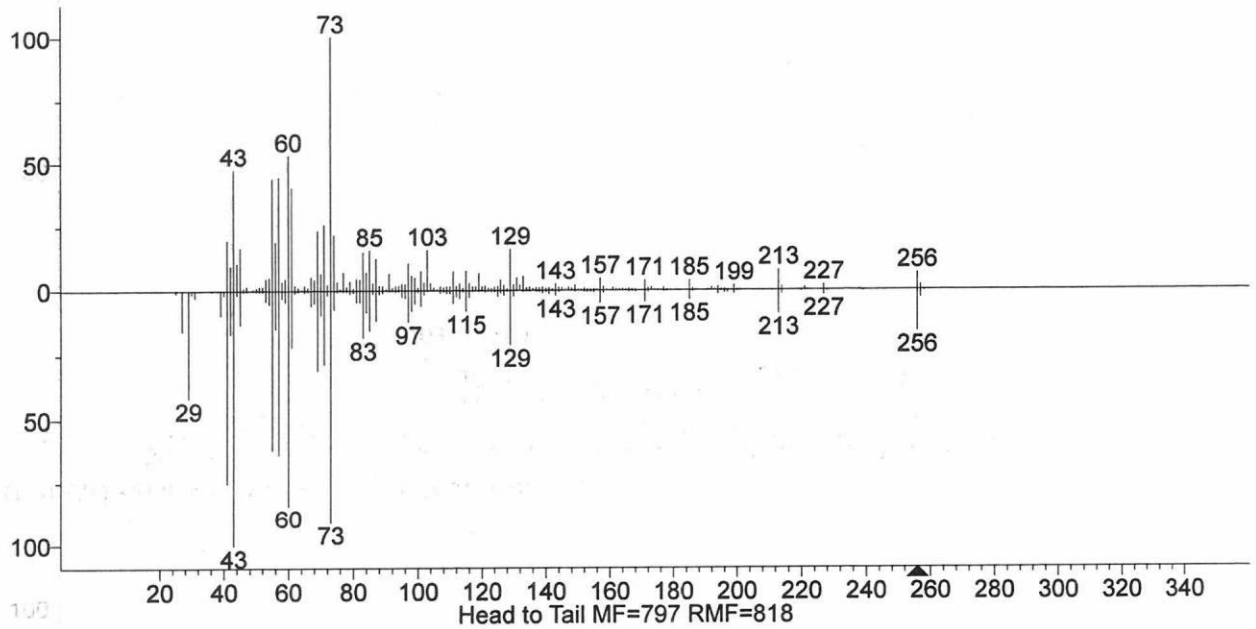
(mainlib) 3-O-Methyl-d-glucose

Name: 3-O-Methyl-d-glucose
Formula: $C_7H_{14}O_6$
MW: 194 NIST#: 127259 ID#: 35456 DB: mainlib
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892
10 largest peaks:
73 999 | 74 900 | 87 743 | 43 411 | 45 363 | 42 298 | 71 290 | 57 262 | 75 259 | 59 239 |
Synonyms:
no synonyms.

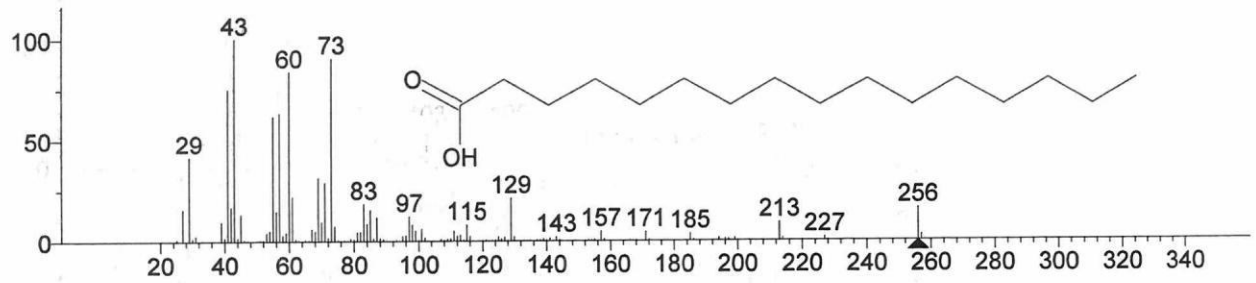
Estimated non-polar retention index (n-alkane scale):
Value: 1647 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (27.208 min) SAIRA-01-040123-.D



Head to Tail MF=797 RMF=818



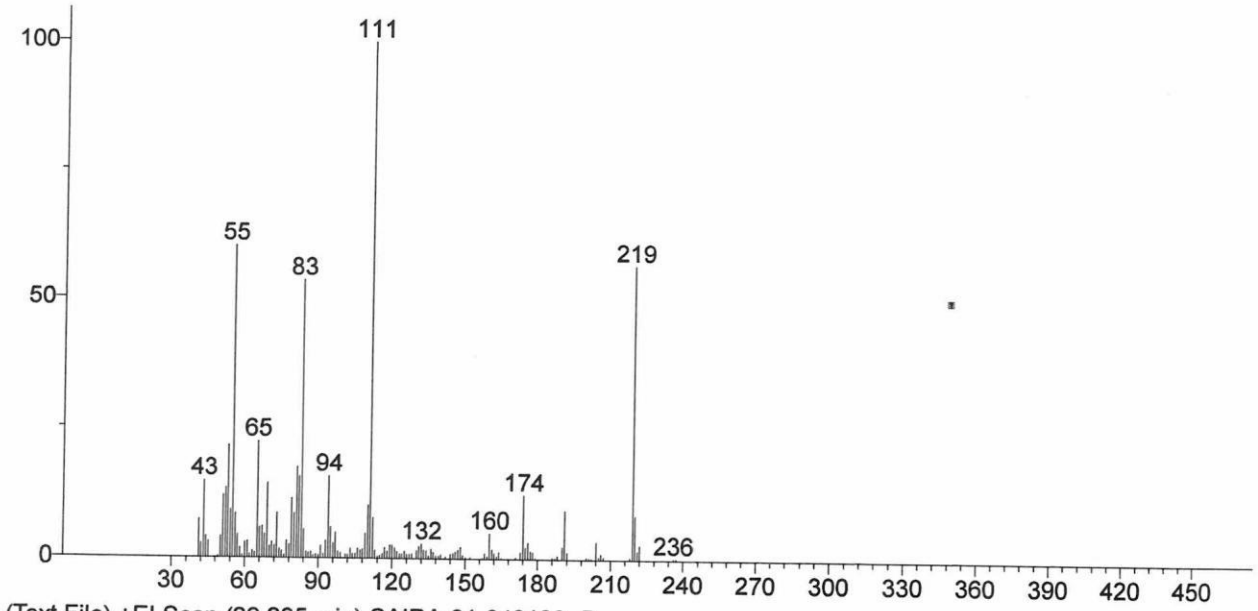
(mainlib) n-Hexadecanoic acid

Name: n-Hexadecanoic acid
Formula: $C_{16}H_{32}O_2$
MW: 256 CAS#: 57-10-3 NIST#: 151973 ID#: 8479 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Chemical Concepts
10 largest peaks:
43 999 | 73 905 | 60 838 | 41 749 | 57 634 | 55 616 | 29 414 | 69 310 | 71 285 | 61 218 |
Synonyms:
1.Hexadecanoic acid
2.n-Hexadecoic acid
3.Palmitic acid
4.Pentadecanecarboxylic acid
5.1-Pentadecanecarboxylic acid
6.Cetylic acid
7.Emersol 140
8.Emersol 143
9.Hexadecylic acid
10.Hydrofol
11.Hystrene 8016
12.Hystrene 9016
13.Industrene 4516
14.Prifrac 2960
15.Glycon P-45
16.Prifac 2960
17.Univol U332

Estimated non-polar retention index (n-alkane scale):
Value: 1968 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.
1. Value: 1942 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: RTX-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.22 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C
End T: 230 C
Heat Rate: 2 K/min
End Time: 35 min
Source: Paolini, J.;
Muselli, A.; Bernardini, A.-F.; Bighelli, A.; Casanova, J.; Costa, J., Thymol derivatives from essential oil of Doronicum corsicum L., Flavour Fragr. J., 22, 2007, 479-487.

2. Value: 1972 iu
Column Type: Capillary
Column



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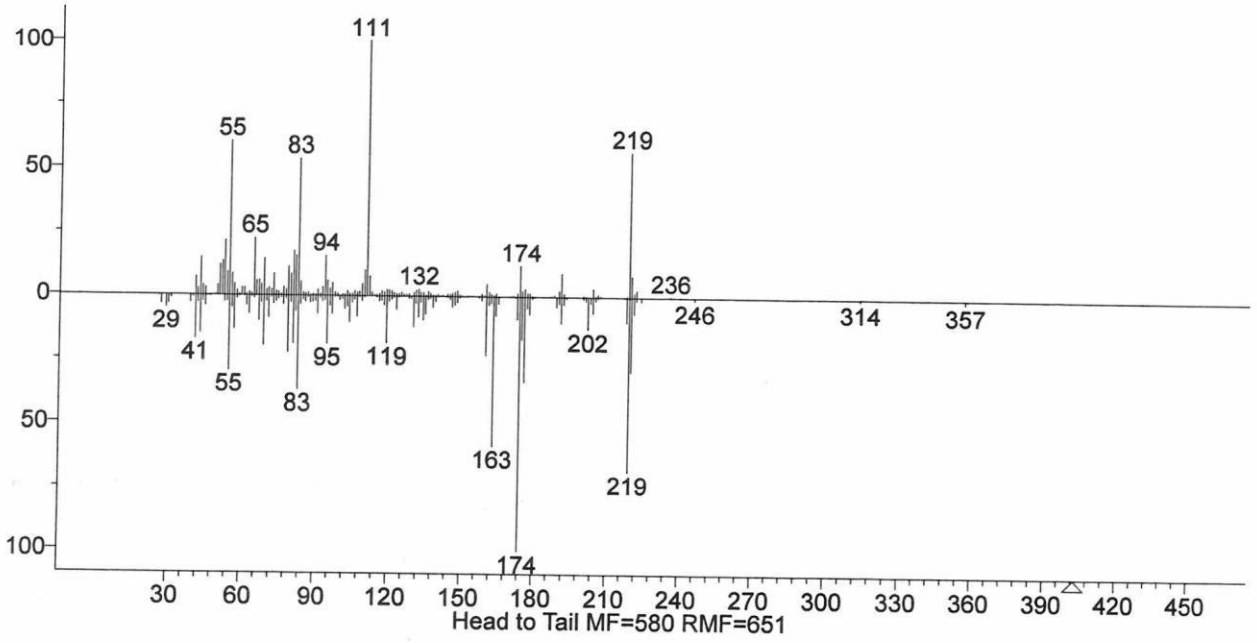
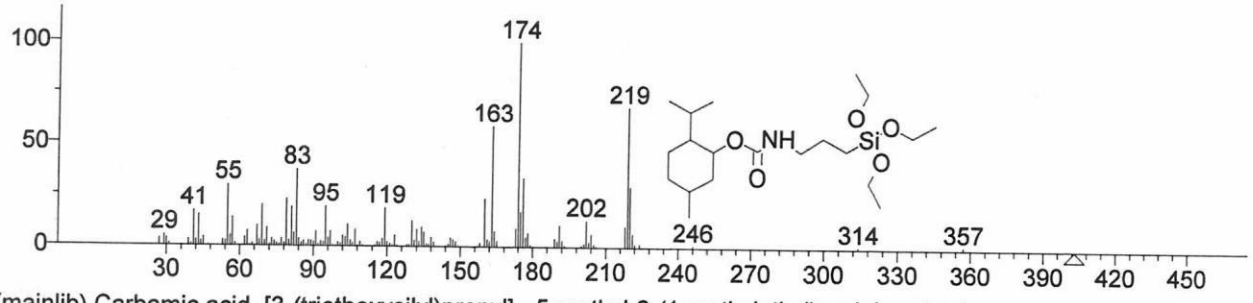


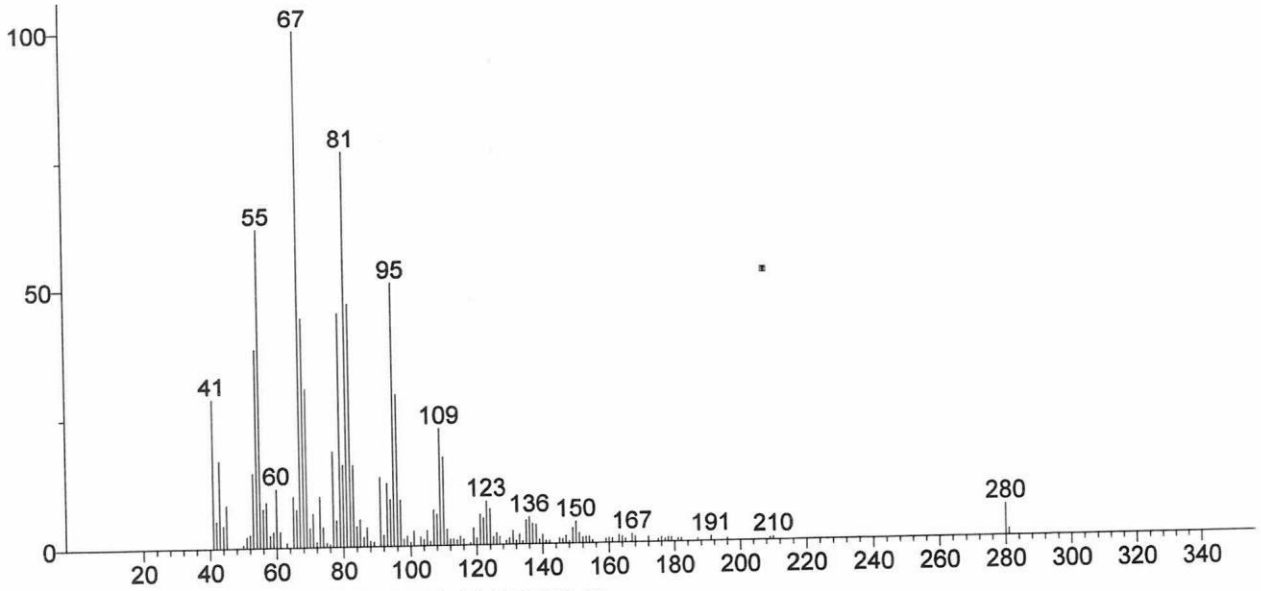
Head to Tail MF=580 RMF=651



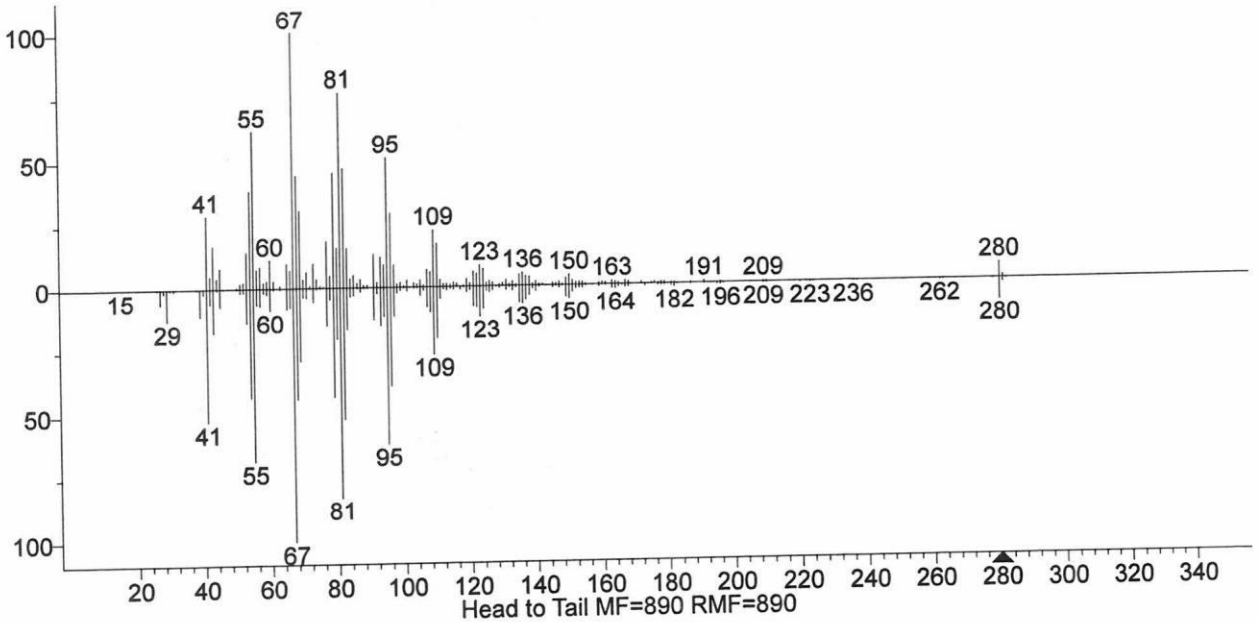
(mainlib) Carbamic acid, [3-(triethoxysilyl)propyl]-, 5-methyl-2-(1-methylethyl)cyclohexyl ester

Name: Carbamic acid, [3-(triethoxysilyl)propyl]-, 5-methyl-2-(1-methylethyl)cyclohexyl ester
Formula: $C_{20}H_{41}NO_5Si$
MW: 403 CAS#: 68479-61-8 NIST#: 73759 ID#: 129958 DB: mainlib
Other DBs: TSCA, EINECS
Contributor: RADIAN CORP
10 largest peaks:
174 999 | 219 681 | 163 584 | 83 369 | 176 333 | 55 295 | 220 295 | 160 230 | 79 224 | 69 197 |
Synonyms:
1.Menthyl N-(3-triethoxysilylpropyl)carbamate
2.2-Isopropyl-5-methylcyclohexyl 3-(triethoxysilyl)propylcarbamate #

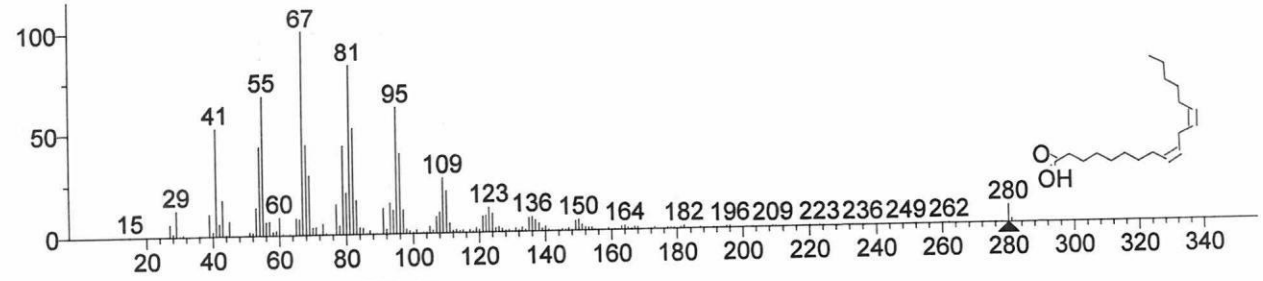
Estimated non-polar retention index (n-alkane scale):
Value: 2436 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (30.686 min) SAIRA-01-040123-.D



Head to Tail MF=890 RMF=890



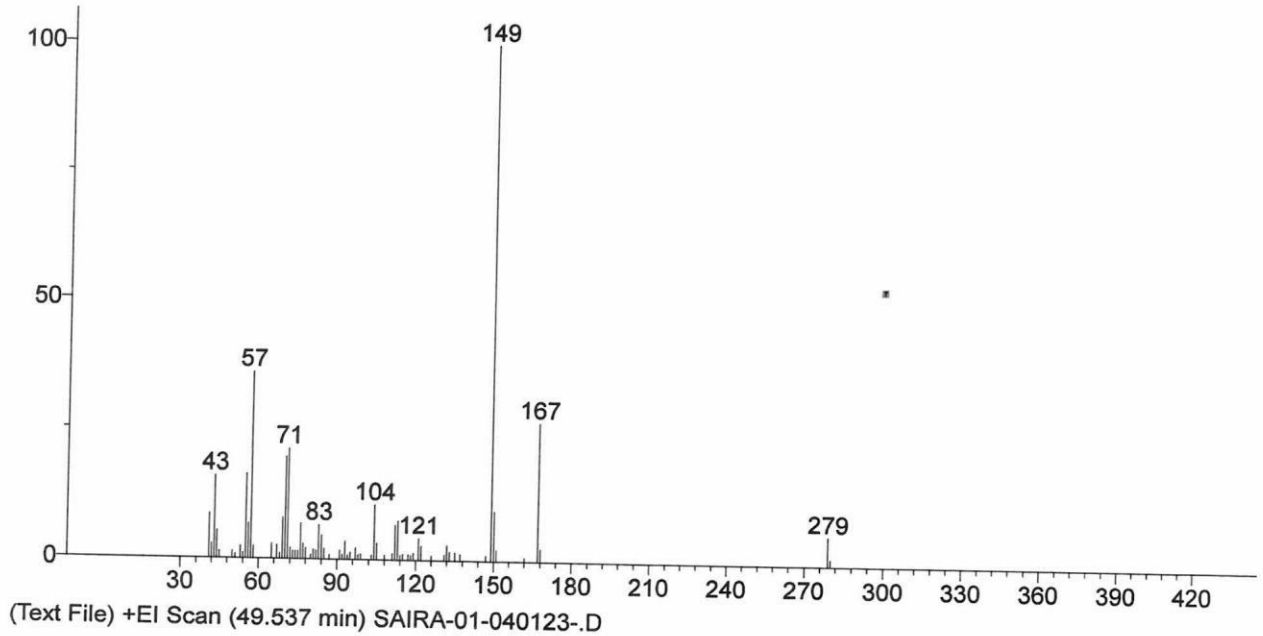
(replib) 9,12-Octadecadienoic acid (Z,Z)-

Name: 9,12-Octadecadienoic acid (Z,Z)-
Formula: $C_{18}H_{32}O_2$
MW: 280 CAS#: 60-33-3 NIST#: 333207 ID#: 7212 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
67 999 | 81 827 | 55 680 | 95 617 | 41 523 | 82 516 | 68 437 | 79 430 | 54 429 | 96 388 |
Synonyms:
1.cis-9,cis-12-Octadecadienoic acid
2.cis,cis-Linoleic acid
3.Grape seed oil
4.Linoleic
5.Linoleic acid
6.Linolic acid
7.Polylin No. 515
8.Telfairic acid
9.Unifac 6550
10.9,12-Octadecadienoic acid
11.Leinoleic acid
12.9,12-Linoleic acid
13.cis,cis-9,12-octadecadienoic acid
14.Linoelaidic acid
15.Linoleic acid 95
16.Emersol 310
17.Emersol 315
18.Vespula pensylvanica b708568k063
19.Pamolyn
20.Pamolyn 125
21.Pamolyn 200, 240
22.Pamolyn 380

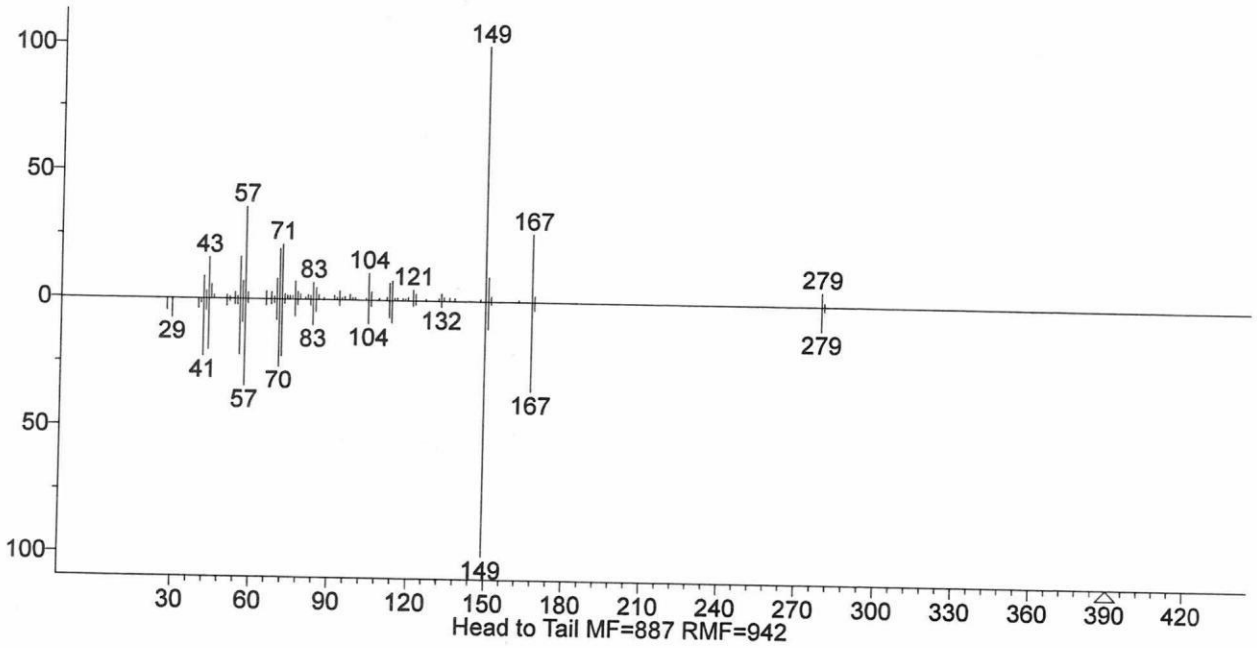
Estimated non-polar retention index (n-alkane scale):
Value: 2183 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.
1. Value: 2095 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column
Length: 25 m
Carrier Gas: H2
Column Diameter: 0.25 mm
Data Type: Linear RI
Program Type: Ramp
Start T:
80 C
End T: 270 C
Heat Rate: 10 K/min
Source: Ziegenbein, F.C.; Hanssen, H.-P.; König, W.A., Secondary
metabolites from Ganoderma lucidum and Spongiporus leucomallellus, Phytochemistry, 67, 2006, 202-211.

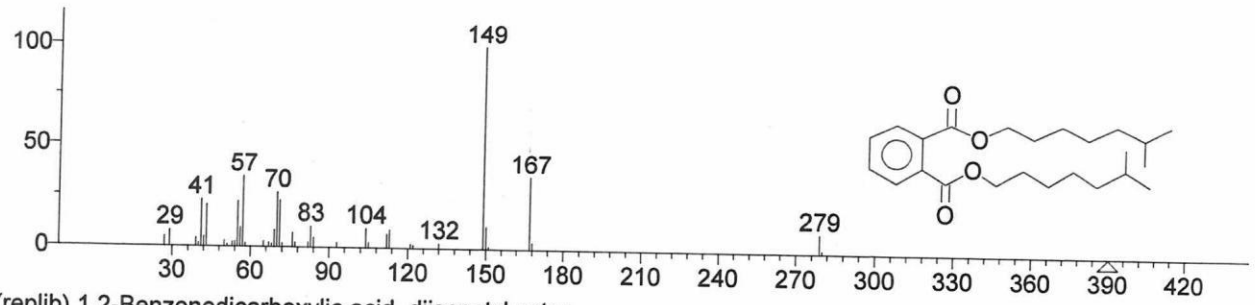
2.



(Text File) +EI Scan (49.537 min) SAIRA-01-040123-.D



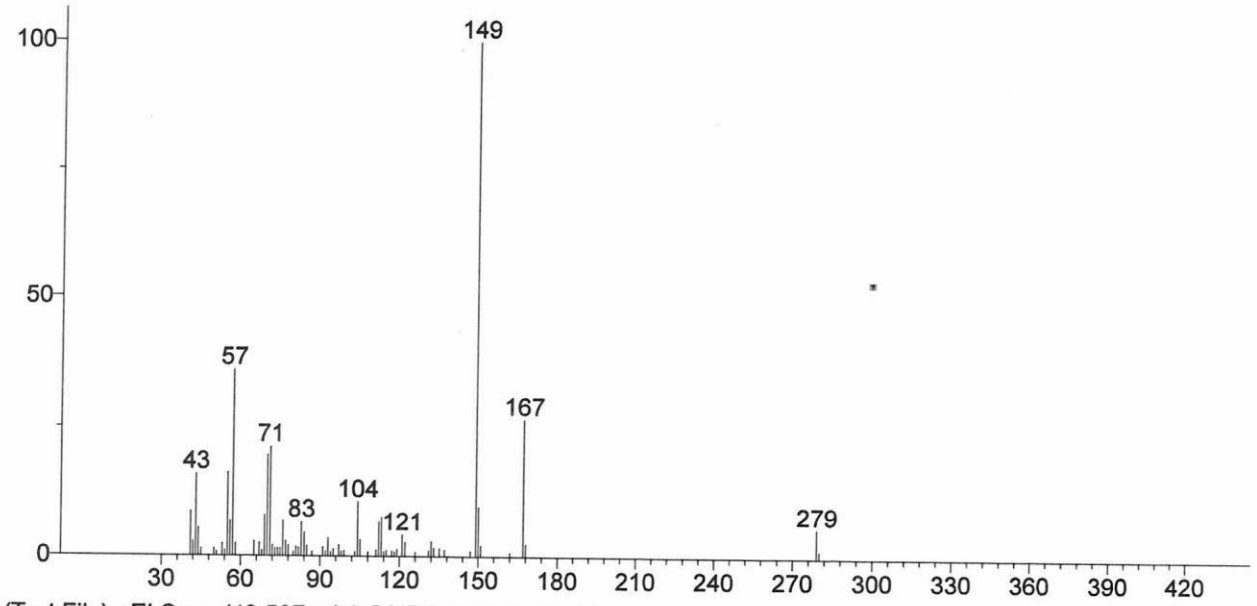
Head to Tail MF=887 RMF=942



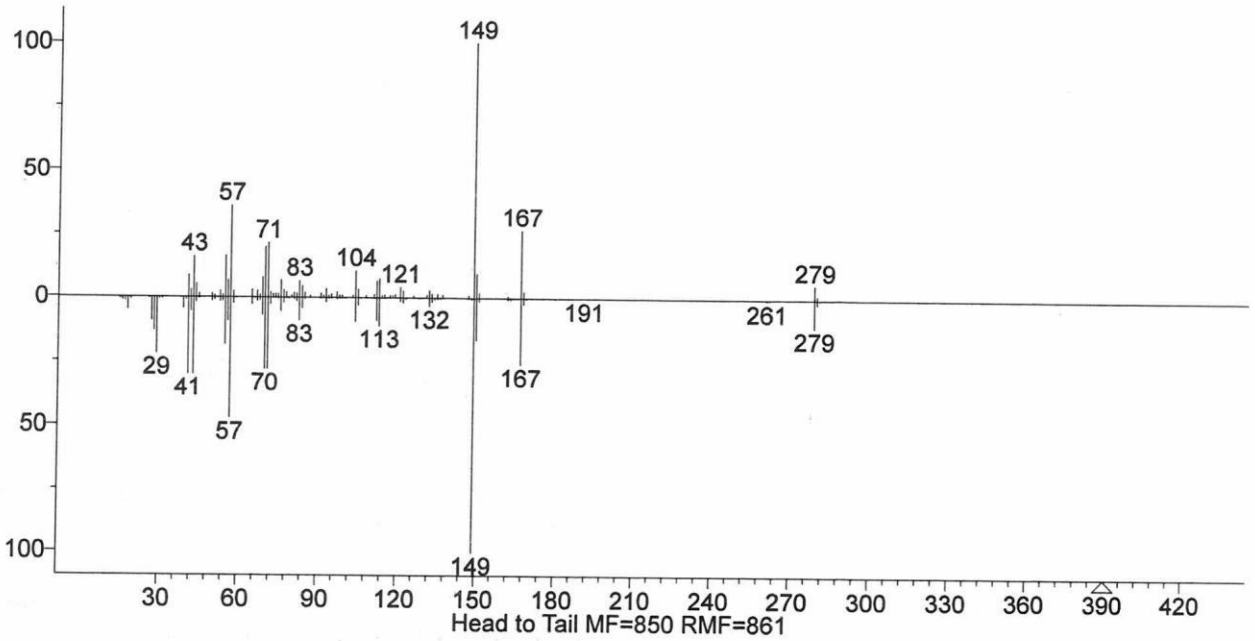
(replib) 1,2-Benzenedicarboxylic acid, diisooctyl ester

Name: 1,2-Benzenedicarboxylic acid, diisooctyl ester
Formula: $C_{24}H_{38}O_4$
MW: 390 CAS#: 27554-26-3 NIST#: 113206 ID#: 20061 DB: replib
Other DBs: Fine, TSCA, RTECS, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
149 999 | 167 350 | 57 341 | 70 264 | 41 225 | 71 224 | 55 218 | 43 200 | 150 107 | 83 100 |
Synonyms:
1.Diisooctyl phthalate
2.Hexaplas M/O
3.Isooctyl phthalate
4.Corflex 880
5.DIOP
6.Flexol plasticizer diop
7.Morflex 100
8.Palatinol D10
9.Phthalic acid, bis(6-methylheptyl) ester
10.Phthalic acid, diisooctyl ester
11.Witcizer 313
12.Bis(6-methylheptyl) phthalate #

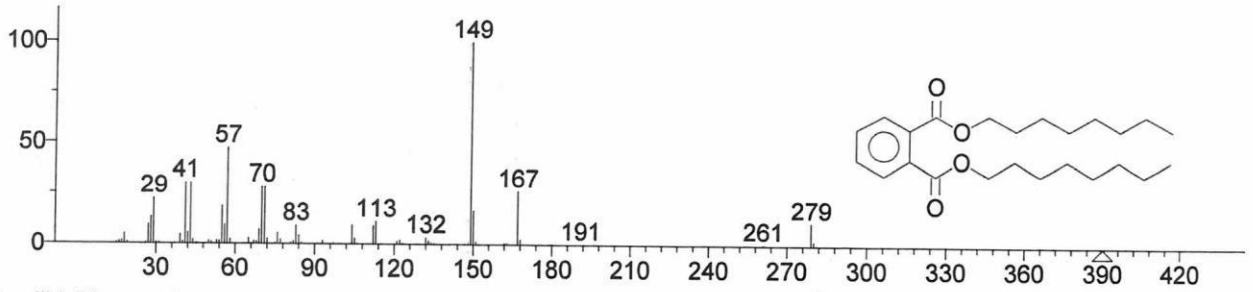
Estimated non-polar retention index (n-alkane scale):
Value: 2704 iu
Confidence interval (Esters): 47(50%) 201(95%) iu



(Text File) +EI Scan (49.537 min) SAIRA-01-040123-.D



Head to Tail MF=850 RMF=861



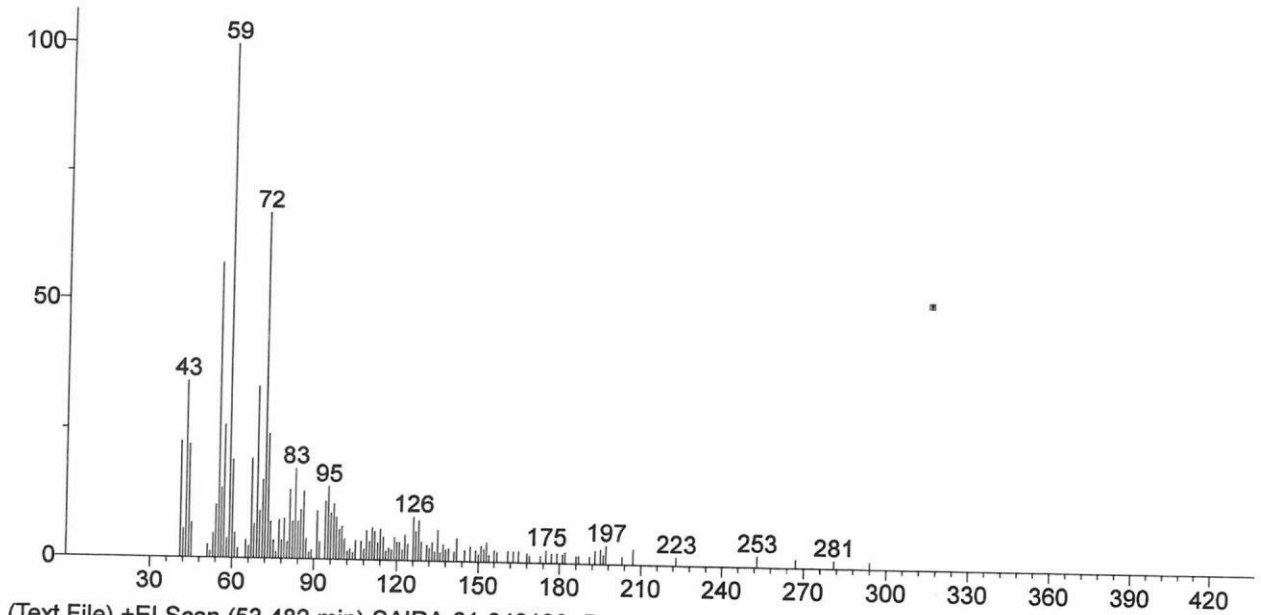
(replib) Di-n-octyl phthalate

Name: Di-n-octyl phthalate
Formula: $C_{24}H_{38}O_4$
MW: 390 CAS#: 117-84-0 NIST#: 23606 ID#: 19967 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
10 largest peaks:
149 999 | 57 470 | 41 300 | 43 300 | 70 280 | 71 280 | 167 260 | 29 220 | 55 185 | 150 165 |
Synonyms:
1.1,2-Benzenedicarboxylic acid, dioctyl ester
2.Phthalic acid, dioctyl ester
3.n-Octyl phthalate
4.Dinopol NOP
5.Dioctyl o-benzenedicarboxylate
6.Dioctyl phthalate
7.Octyl phthalate
8.Polycizer 162
9.1,2-Benzenedicarbonic acid, dioctyl ester
10.Dicapryl phthalate
11.Dioctyl 1,2-benzenedicarboxylate
12.Vinicizer 85
13.o-Benzenedicarboxylic acid, dioctyl ester
14.Celluflex dop
15.Dioktylester kyseliny ftalove
16.Dnop
17.PX-138
18.Rcra waste number U107
19.Dioctyl o-phthalate

Estimated non-polar retention index (n-alkane scale):
Value: 2832 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 2682 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: OV-101
Column
Length: 50 m
Carrier Gas: H2
Column Diameter: 0.3 mm
Phase Thickness: 0.35 um
Data Type: Kovats
RI
Program Type: Isothermal
Start T: 230 C
Source: Friocourt, M.P.; Berthou, F.; Picart, D.; Dreano, Y.; Floch, H.
H., Glass Capillary Column Gas Chromatography of Phthalate Esters, J. Chromatogr., 172, 1979, 261-271.

2.
Value: 2685 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: SE-30
Column Length:



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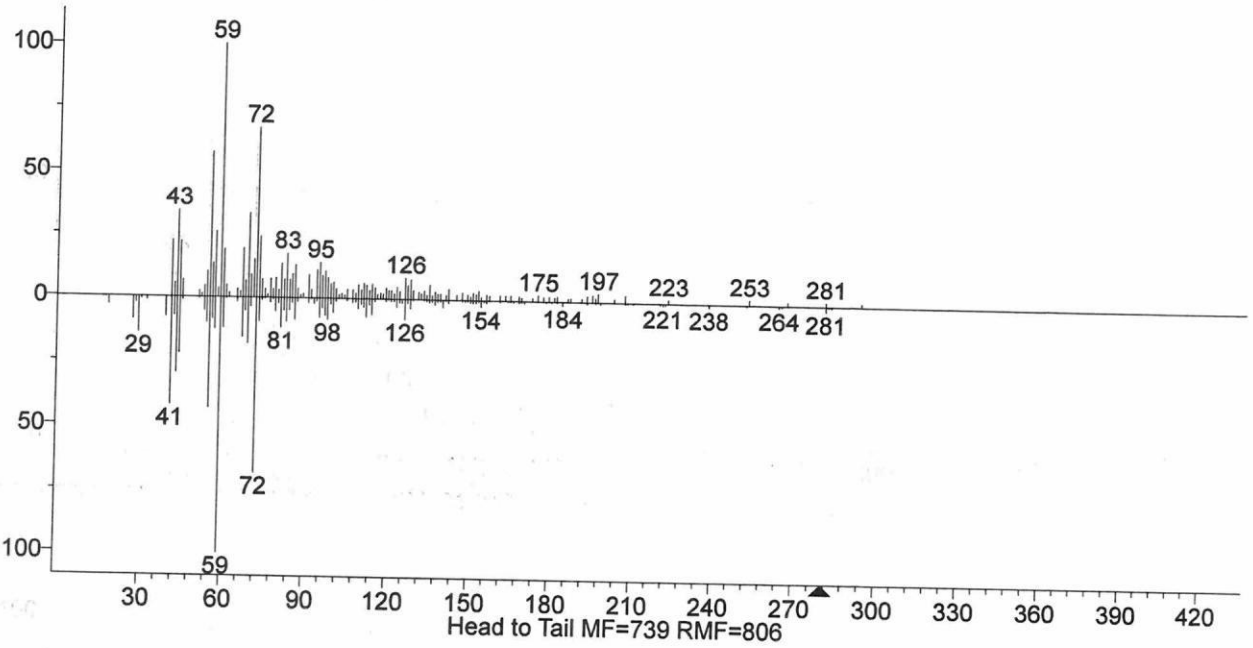
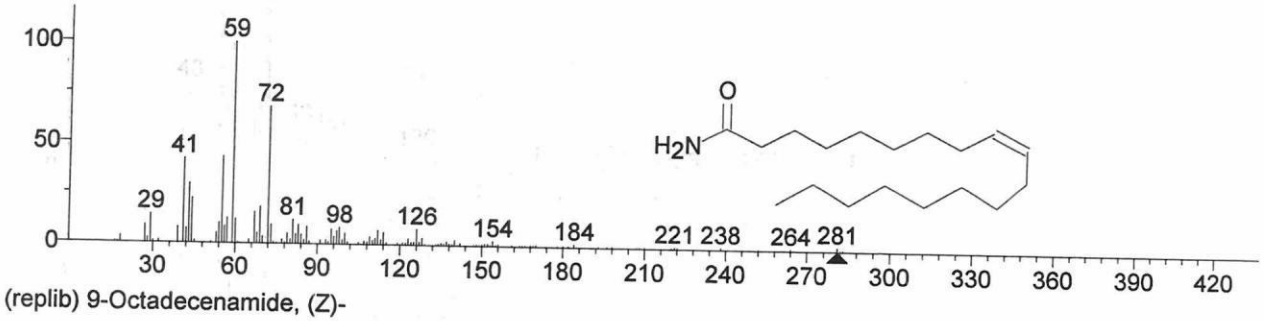


Head to Tail MF=739 RMF=806

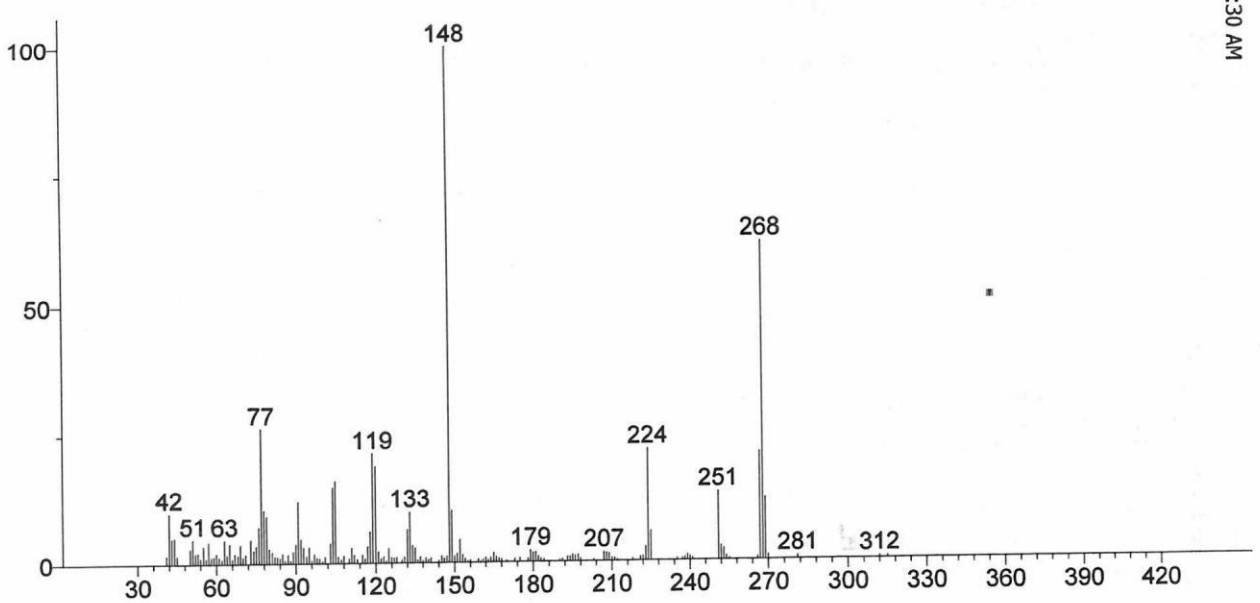


(replib) 9-Octadecenamide, (Z)-

Name: 9-Octadecenamide, (Z)-
Formula: $C_{18}H_{35}NO$
MW: 281 CAS#: 301-02-0 NIST#: 334156 ID#: 6574 DB: replib
Other DBs: Fine, TSCA, HODOC, NIH, EINECS
Contributor: Frank Antolasic, RMIT Applied Chemistry Department, Victoria Australia 3001
10 largest peaks:
59 999 | 72 680 | 55 430 | 41 419 | 43 295 | 44 220 | 69 181 | 67 154 | 29 140 | 57 125 |
Synonyms:
1.Adogen 73
2.Oleamide
3.Oleic acid amide
4.Oleyl amide
5.Slip-eze
6.Armoslip CP
7.Crodamide O
8.Crodamide OR
9.Amide O
10.Diamide O 200
11.Diamit O 200
12.(Z)-9-Octadecenamide
13.Aliphatic amide
14.Armid O
15.cis-9,10-Octadecenoamide
16.Crodamide O, OR
17.Kemamide O
18.Octadecene amide
19.Petrac Slip-Eze
20.Polydis TR 121
21.Unislip 1759
22.(9Z)-9-Octadecenamide #
23.9-Octadecenamide

Estimated non-polar retention index (n-alkane scale):
Value: 2228 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu

Retention index.
1. Value: 2397 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: HP-5
Column
Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Normal
alkane RI
Program Type: Complex
Description: 60C(5min) =>3C/min =>120C (2min) =>2C/min =>200C (2min)
=>3C/min =>320C
Source: Yasar, A.; Üçüncü, O.; Güleç, C.; Inceer, H.; Ayaz, S.; Yayh, N., GC-MS analysis of
chloroform extracts in flowers, stems, and roots of Tripleurospermum callosum, Pharm. Biol., 43(2), 2005, 108-112.



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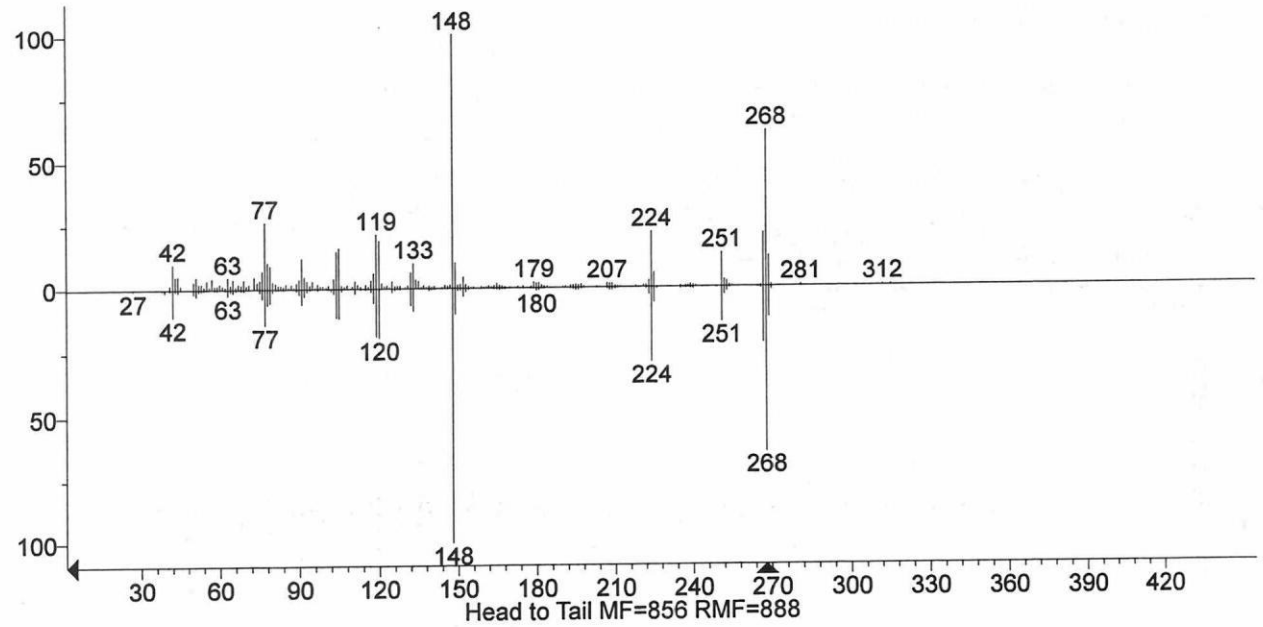
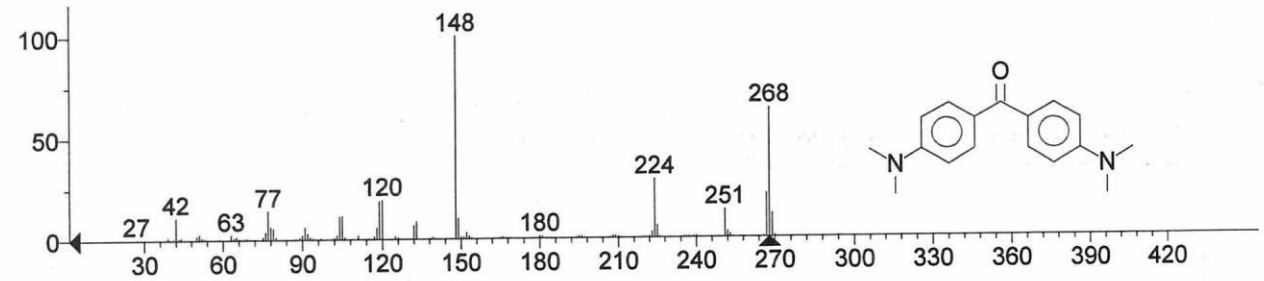


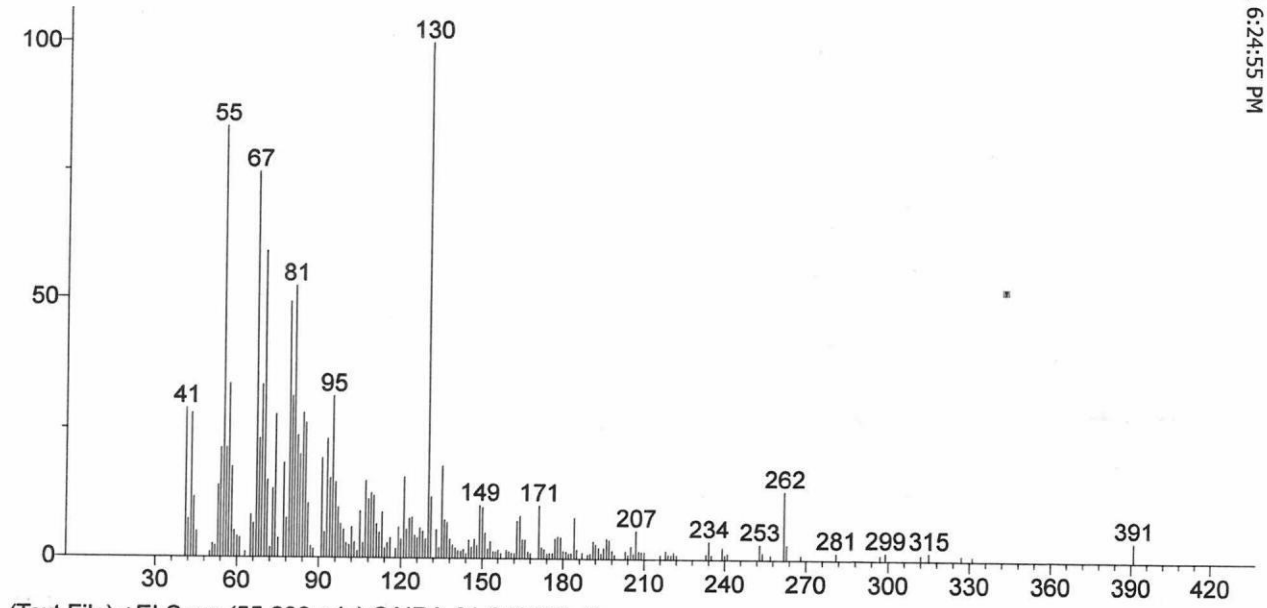
Head to Tail MF=856 RMF=888



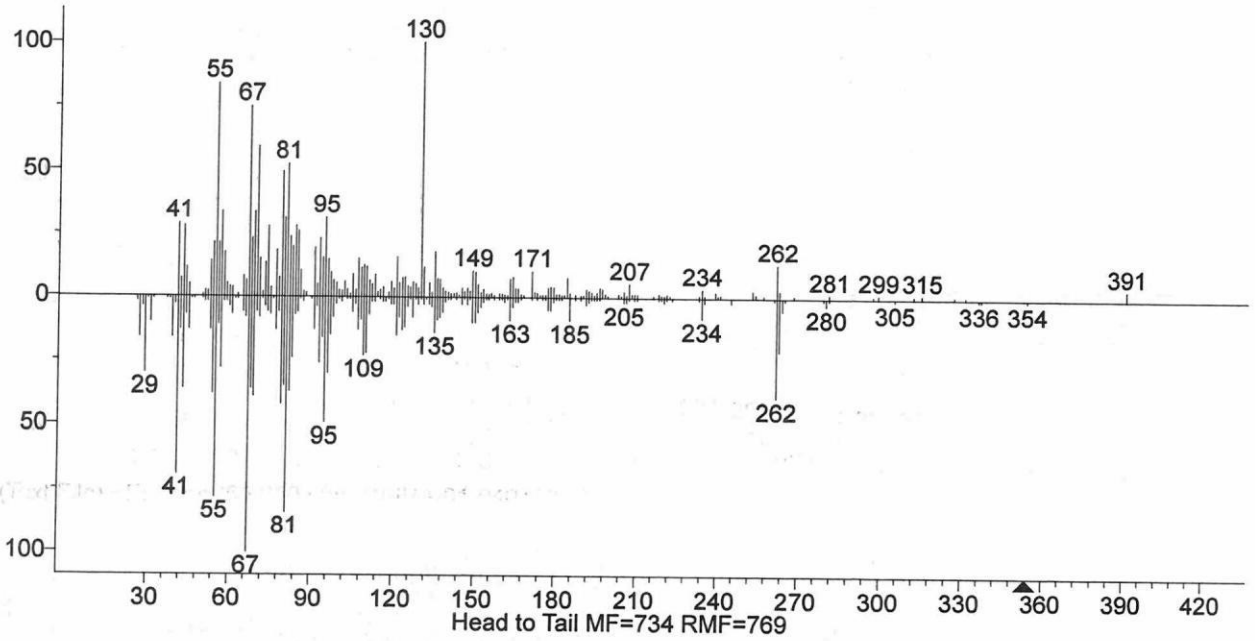
(mainlib) Methanone, bis[4-(dimethylamino)phenyl]-

Name: Methanone, bis[4-(dimethylamino)phenyl]-
Formula: $C_{17}H_{20}N_2O$
MW: 268 CAS#: 90-94-8 NIST#: 290948 ID#: 109402 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS
Contributor: NIST Mass Spectrometry Data Center, 1998.
10 largest peaks:
148 999 | 268 637 | 224 288 | 267 216 | 120 191 | 119 186 | 77 140 | 251 135 | 269 117 | 105 114 |
Synonyms:
1.Benzophenone, 4,4'-bis(dimethylamino)-
2.p,p'-bis(Dimethylamino)benzophenone
3.Bis[p-(N,N-dimethylamino)phenyl] ketone
4.Michler's ketone
5.N,N,N',N'-Tetramethyl-4,4'-diaminobenzophenone
6.4,4'-Bis(dimethylamino)benzophenone
7.4,4'-di(Dimethylamino)benzophenone
8.Michlers ketone
9.p,p'-Tetramethyl-4,4'-diaminobenzophenone
10.(Tetramethyldiamino)benzophenone
11.p,p'-Bis(N,N-dimethylamino)benzophenone
12.p,p'-Michler's ketone
13.Michler ketone
14.NCI-C02006
15.Bis(4-(dimethylamino)phenyl)methanone
16.N,N'-Bisdimethylamino;benzophenone
17.Ketone base
18.Bis-4,4'-(dimethylamino)-benzophenon (michlers keton)
19.4,4'-Bis(dimethylamino)-benzophenone

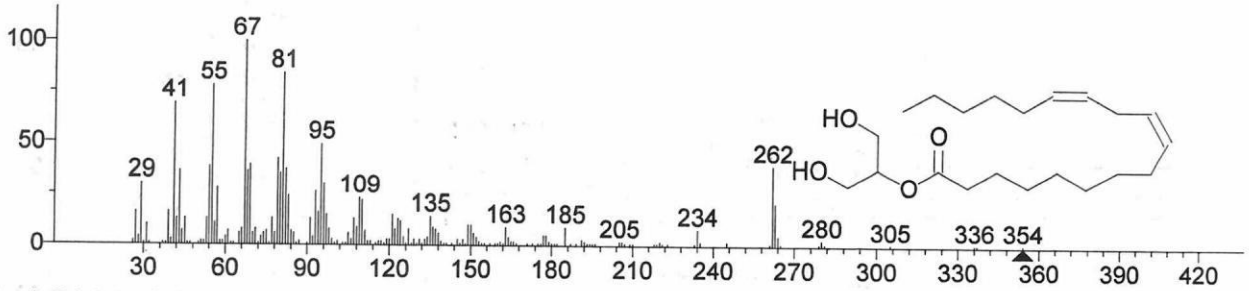
Estimated non-polar retention index (n-alkane scale):
Value: 2126 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (55.680 min) SAIRA-01-040123-.D



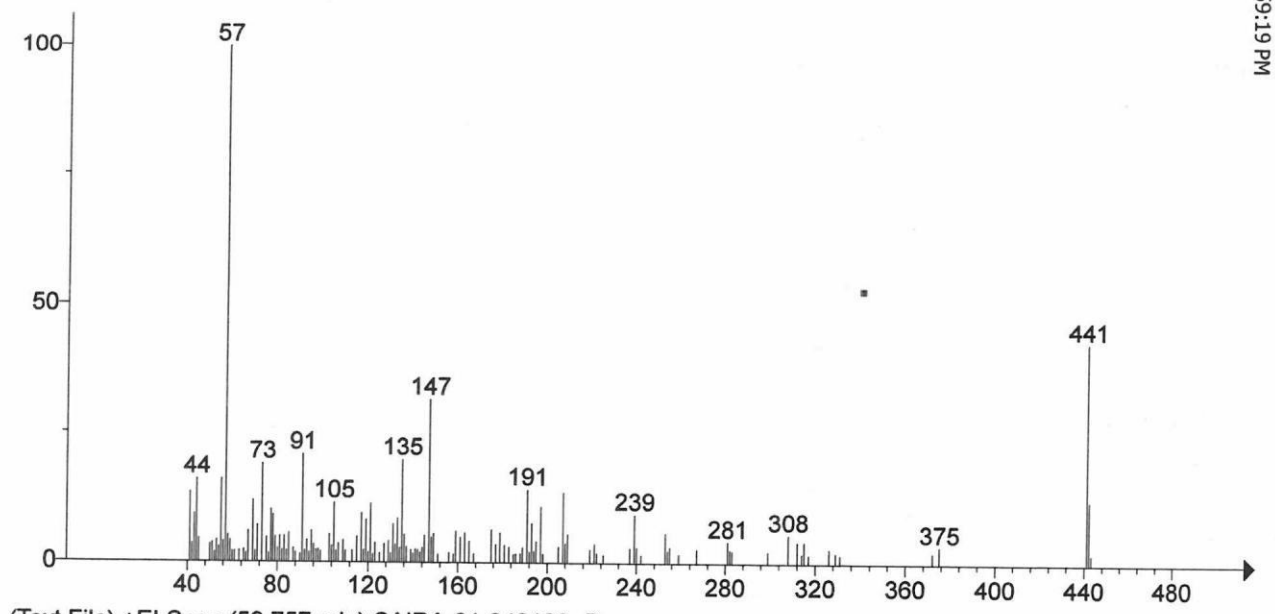
Head to Tail MF=734 RMF=769



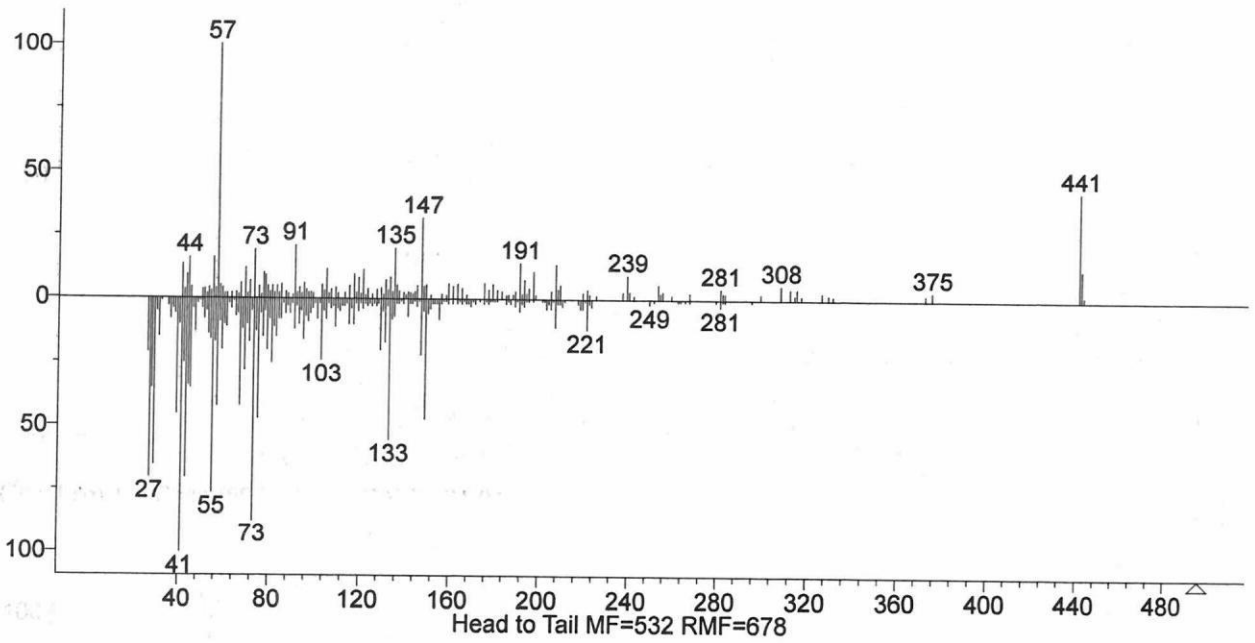
(mainlib) 9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Name: 9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester
Formula: $C_{21}H_{38}O_4$
MW: 354 CAS#: 3443-82-1 NIST#: 16013 ID#: 28833 DB: mainlib
Other DBs: None
10 largest peaks:
67 999 | 81 840 | 55 780 | 41 690 | 95 490 | 79 420 | 69 390 | 262 390 | 54 380 | 82 370 |
Synonyms:
1.Linolein, 2-mono-
2.β-Monolinolein
3.2-Hydroxy-1-(hydroxymethyl)ethyl (9Z,12Z)-9,12-octadecadienoate #

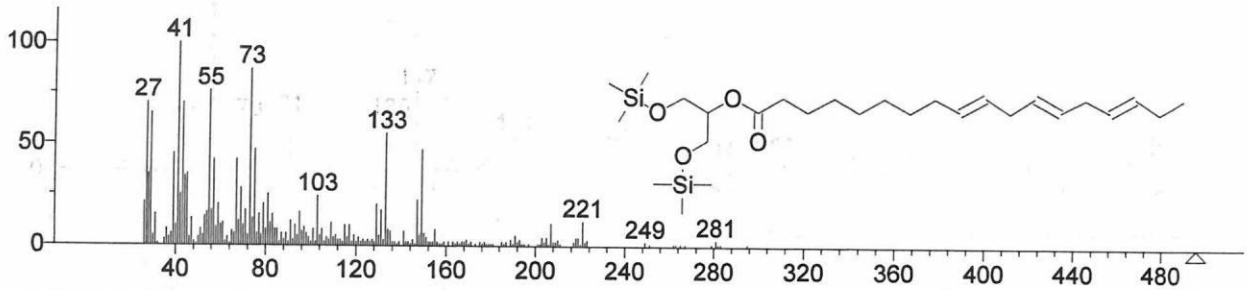
Estimated non-polar retention index (n-alkane scale):
Value: 2713 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (59.757 min) SAIRA-01-040123-.D



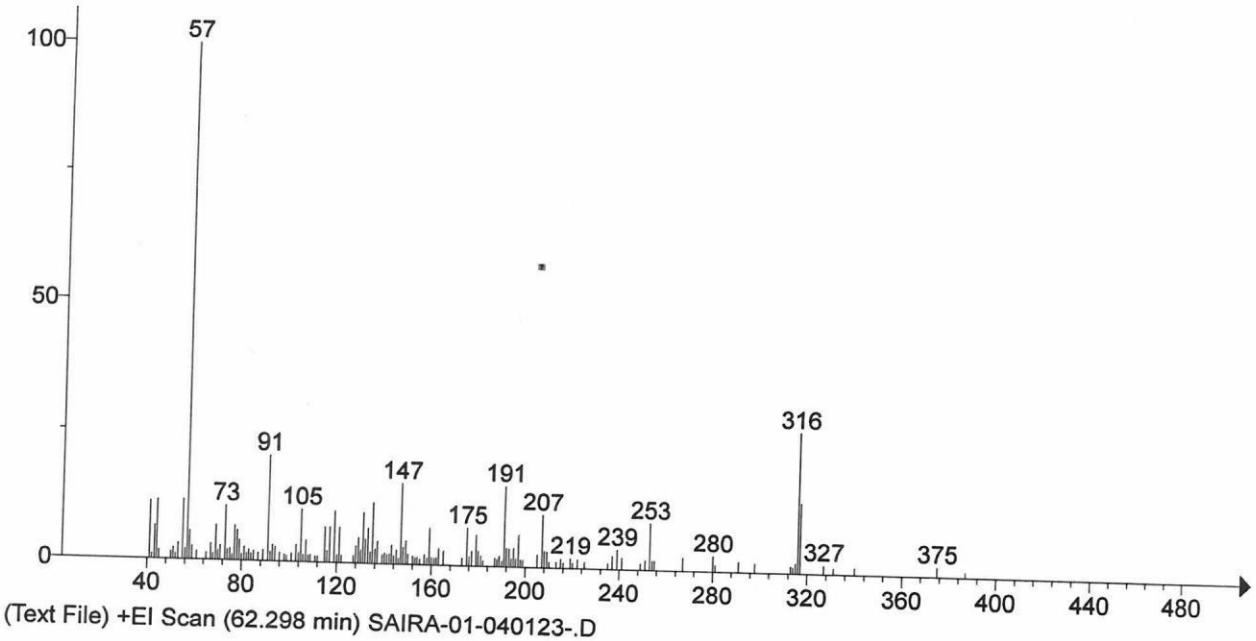
Head to Tail MF=532 RMF=678



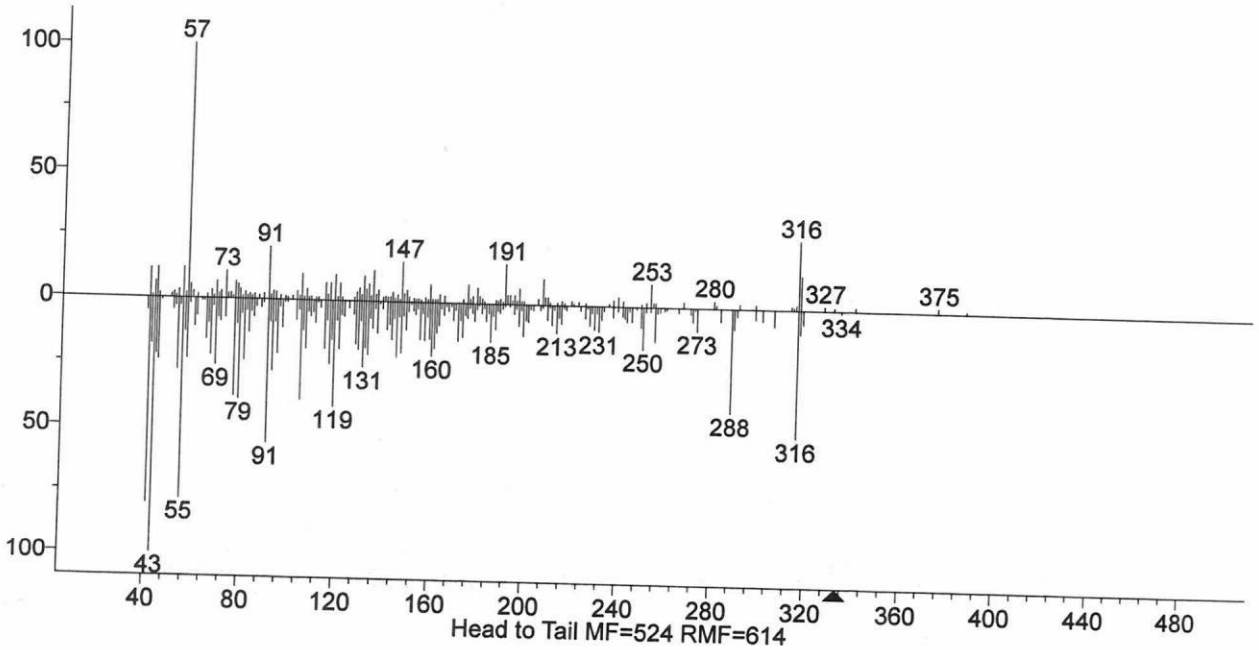
(mainlib) 9,12,15-Octadecatrienoic acid, 2-[(trimethylsilyl)oxy]-1-[[(trimethylsilyl)oxy]methyl]ethyl ester, (Z,Z,Z)-

Name: 9,12,15-Octadecatrienoic acid, 2-[(trimethylsilyl)oxy]-1-[[(trimethylsilyl)oxy]methyl]ethyl ester, (Z,Z,Z)-
Formula: $C_{27}H_{52}O_4Si_2$
MW: 496 CAS#: 55521-23-8 NIST#: 18114 ID#: 3312 DB: mainlib
Other DBs: None
10 largest peaks:
41 999 | 73 870 | 55 760 | 27 700 | 43 700 | 29 650 | 133 550 | 75 470 | 149 470 | 39 450 |
Synonyms:
1.2-[(Trimethylsilyl)oxy]-1-([(trimethylsilyl)oxy]methyl)ethyl (9E,12E,15E)-9,12,15-octadecatrienoate #

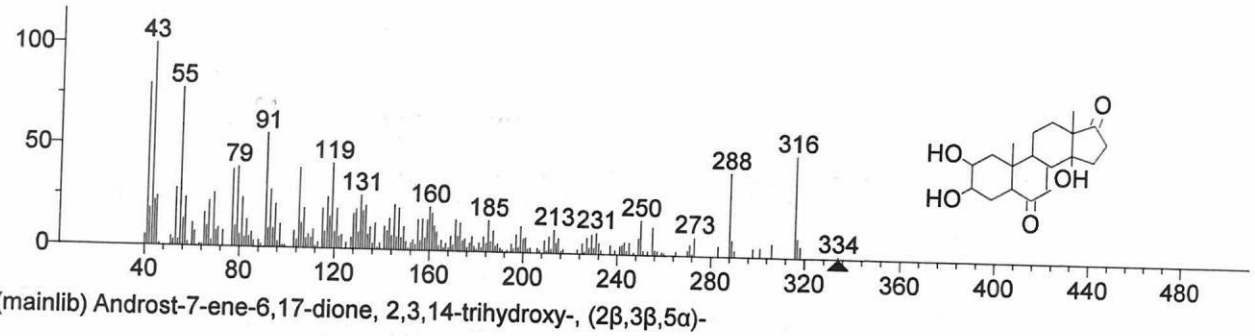
Estimated non-polar retention index (n-alkane scale):
Value: 2804 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) +EI Scan (62.298 min) SAIRA-01-040123-.D



Head to Tail MF=524 RMF=614



(mainlib) Androst-7-ene-6,17-dione, 2,3,14-trihydroxy-, (2β,3β,5α)-

Name: Androst-7-ene-6,17-dione, 2,3,14-trihydroxy-, (2β,3β,5α)-
Formula: $C_{19}H_{26}O_5$
MW: 334 CAS#: 55191-58-7 NIST#: 15527 ID#: 5584 DB: mainlib
Other DBs: None
Contributor: G.SCHULZ SCHERING AG, BERLIN, E.GERMANY.
10 largest peaks:
43 999 | 41 800 | 55 780 | 91 560 | 316 500 | 119 415 | 288 408 | 79 390 | 105 390 | 77 378 |
Synonyms:
1.2,3,14-Trihydroxyandrost-7-ene-6,17-dione #

Estimated non-polar retention index (n-alkane scale):
Value: 2649 iu
Confidence interval (Low reliability): 174(50%) 752(95%) iu