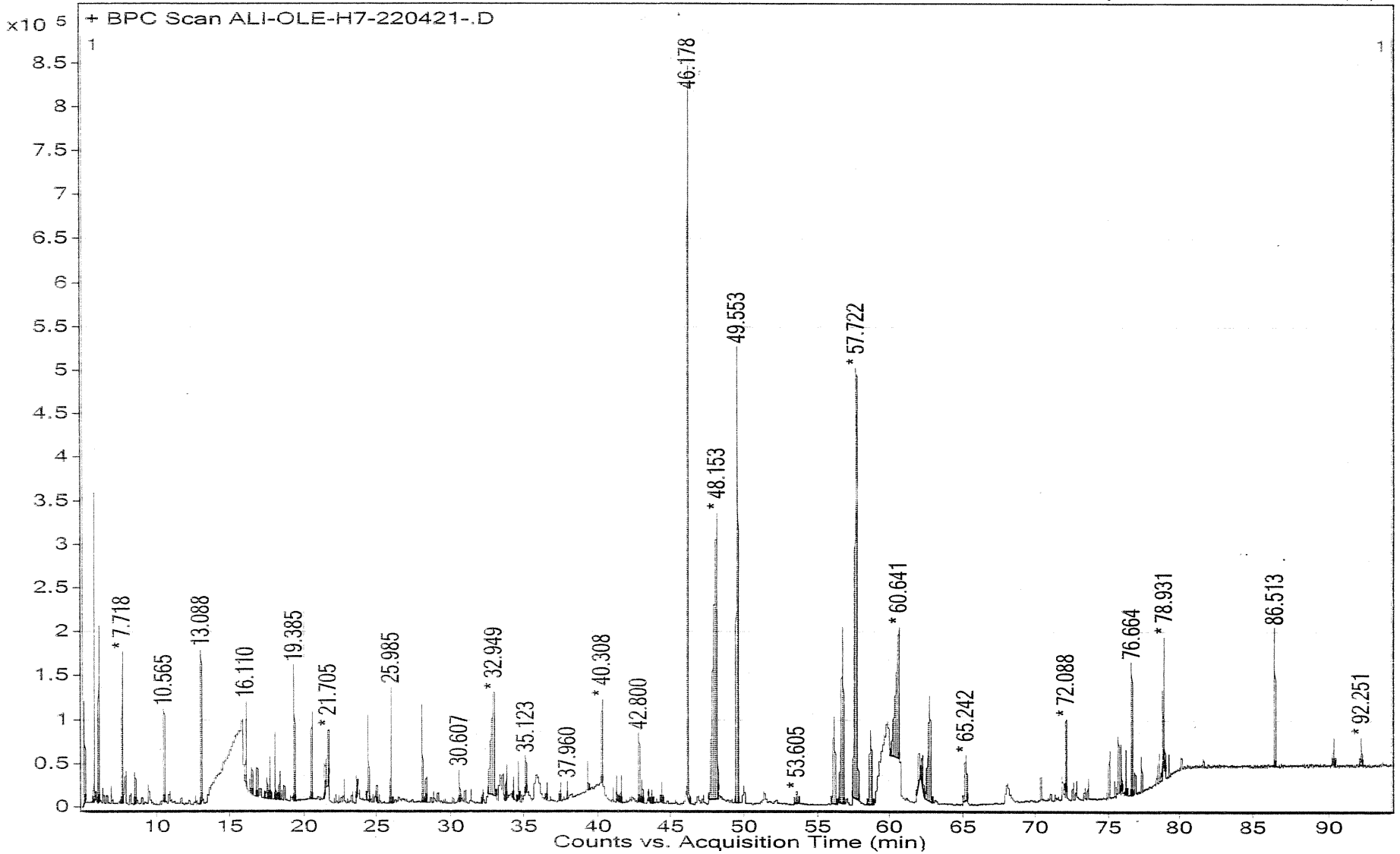
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **Sample Name** | ALI-OLE-H7-220421- | **Position** | 12 | **Instrument Name** | GCMS TQQQ | **User Name** | HEJ-G-104-03\Agile |
| **Inj Vol** | 3 | **InjPosition** | | **SampleType** | | **IRM Calibration Status** | Not Applicable |
| **Data Filename** | ALI-OLE-H7-220421-.D | **ACQ Method** | ALI-IMRAN-140421.M | **Comment** | | **Acquired Time** | 4/22/2021 3:25:56 |



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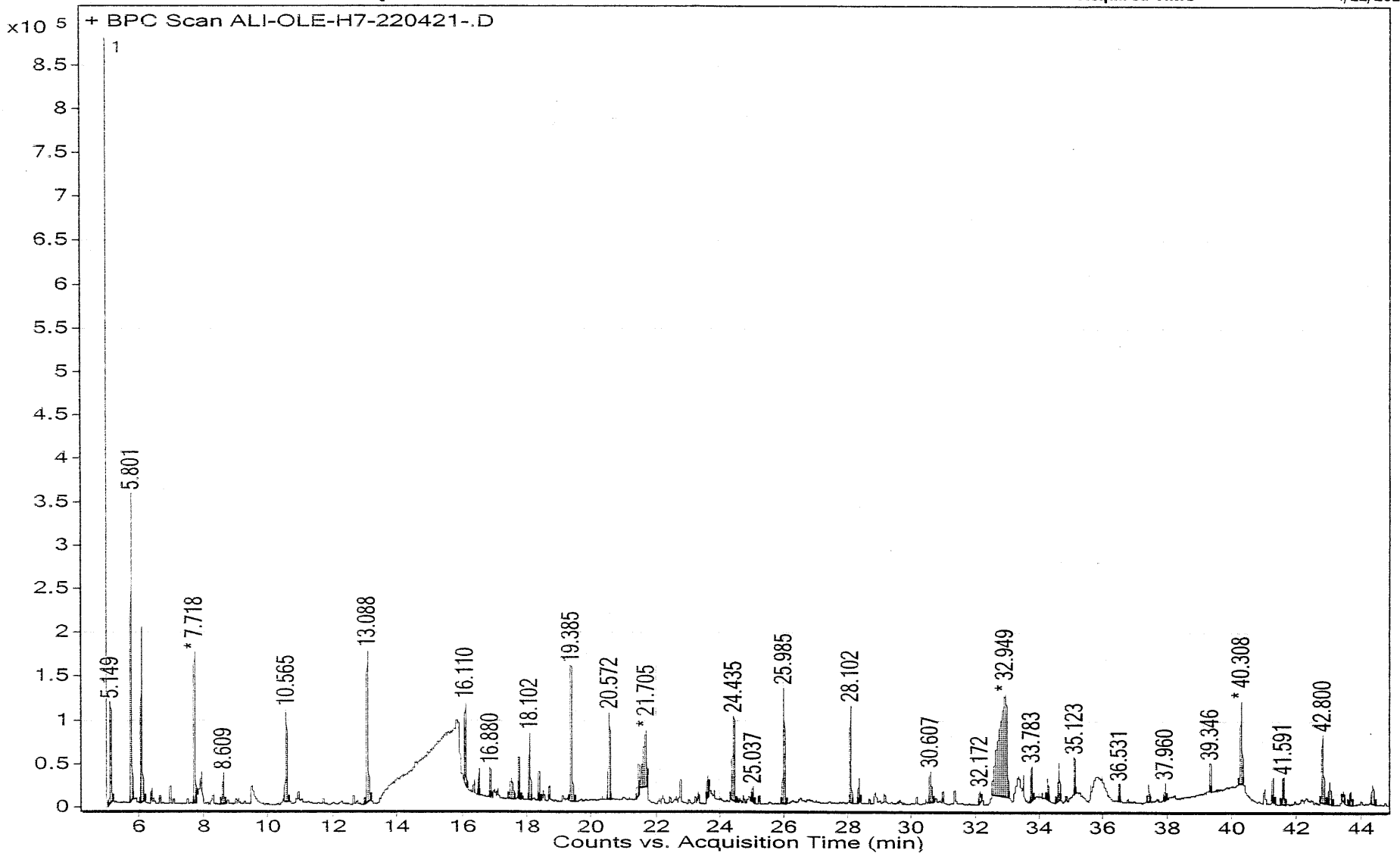
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **Sample Name** | ALI-OLE-H7-220421- | **Position** | 12 | **Instrument Name** | GCMS TQQQ | **User Name** | HEJ-G-104-03\Agile |
| **Inj Vol** | 3 | **InjPosition** | | **SampleType** | | **IRM Calibration Status** | Not Applicable |
| **Data Filename** | ALI-OLE-H7-220421-.D | **ACQ Method** | ALI-IMRAN-140421.M | **Comment** | | **Acquired Time** | 4/22/2021 3:25:56 I |



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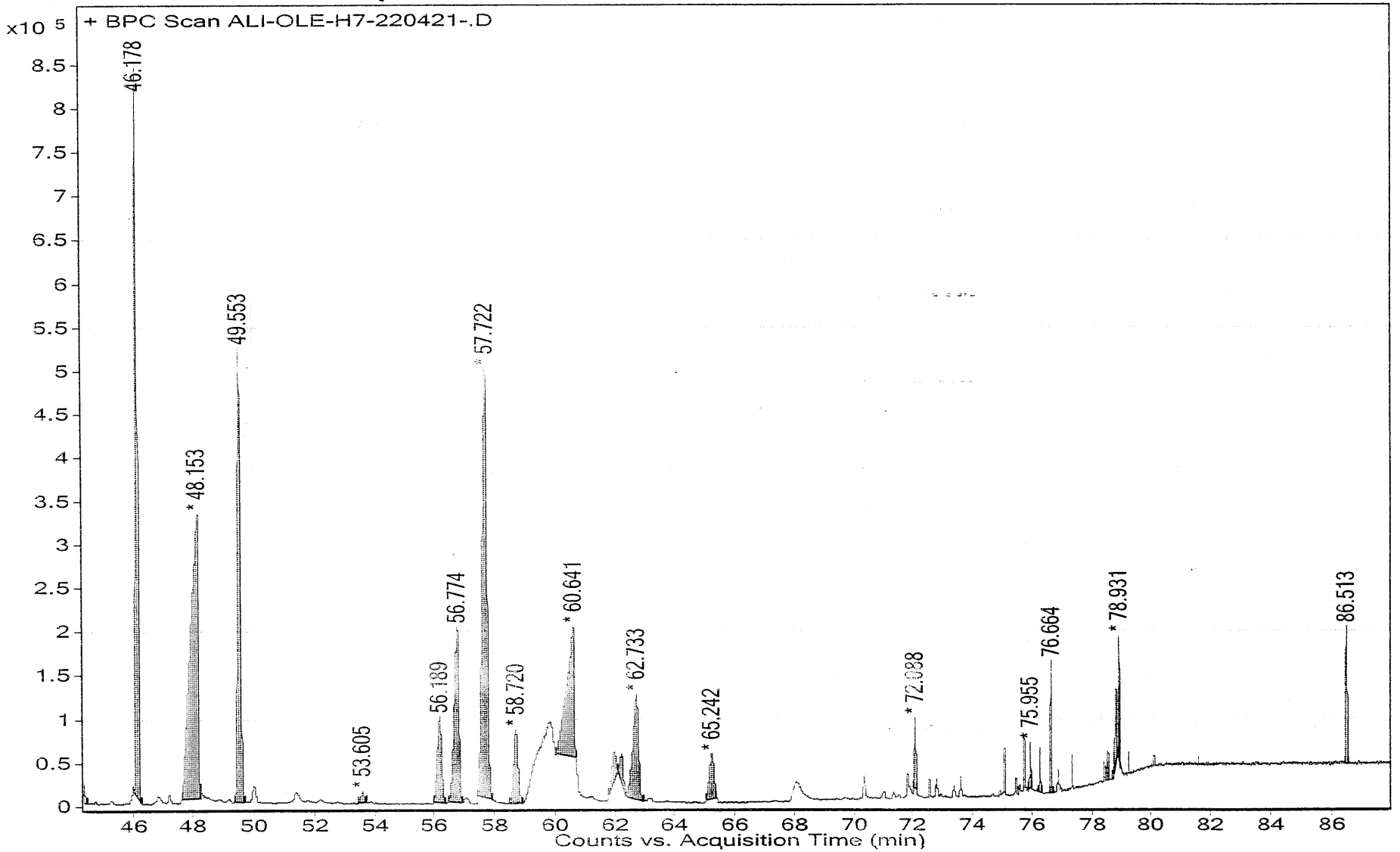
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **Sample Name** | ALI-OLE-H7-220421- | **Position** | 12 | **Instrument Name** | GCMS TQQQ | **User Name** | HEJ-G-104-03\Agile |
| **Inj Vol** | 3 | **InjPosition** | | **SampleType** | | **IRM Calibration Status** | Not Applicable |
| **Data Filename** | ALI-OLE-H7-220421-.D | **ACQ Method** | ALI-IMRAN-140421.M | **Comment** | | **Acquired Time** | 4/22/2021 3:25:56 I |



nt

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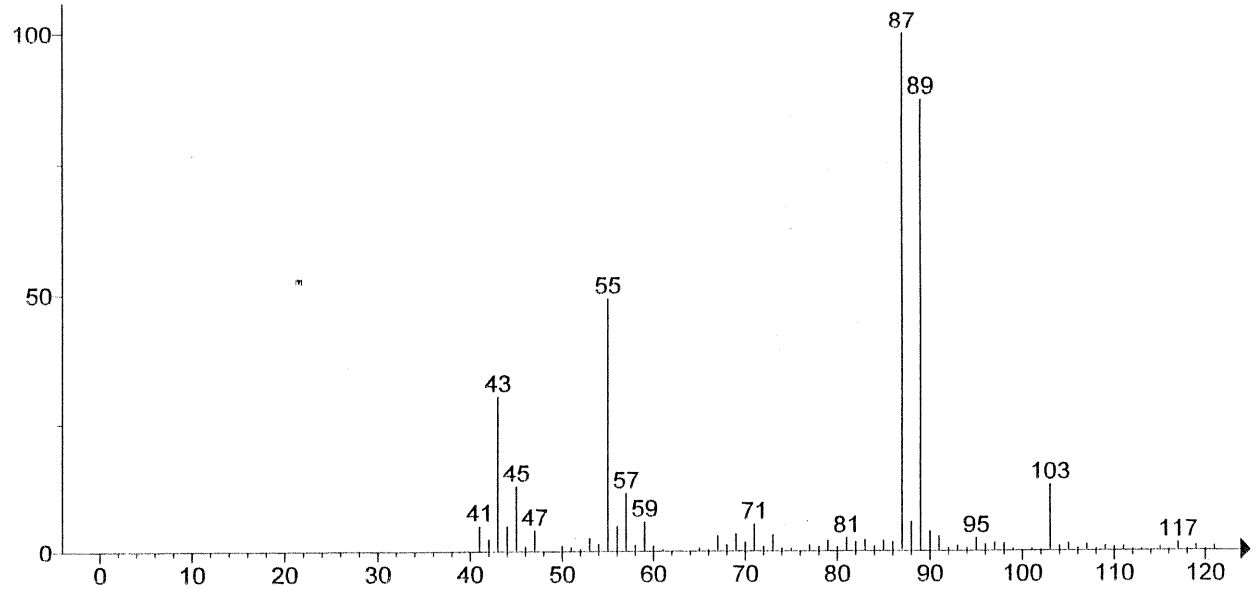
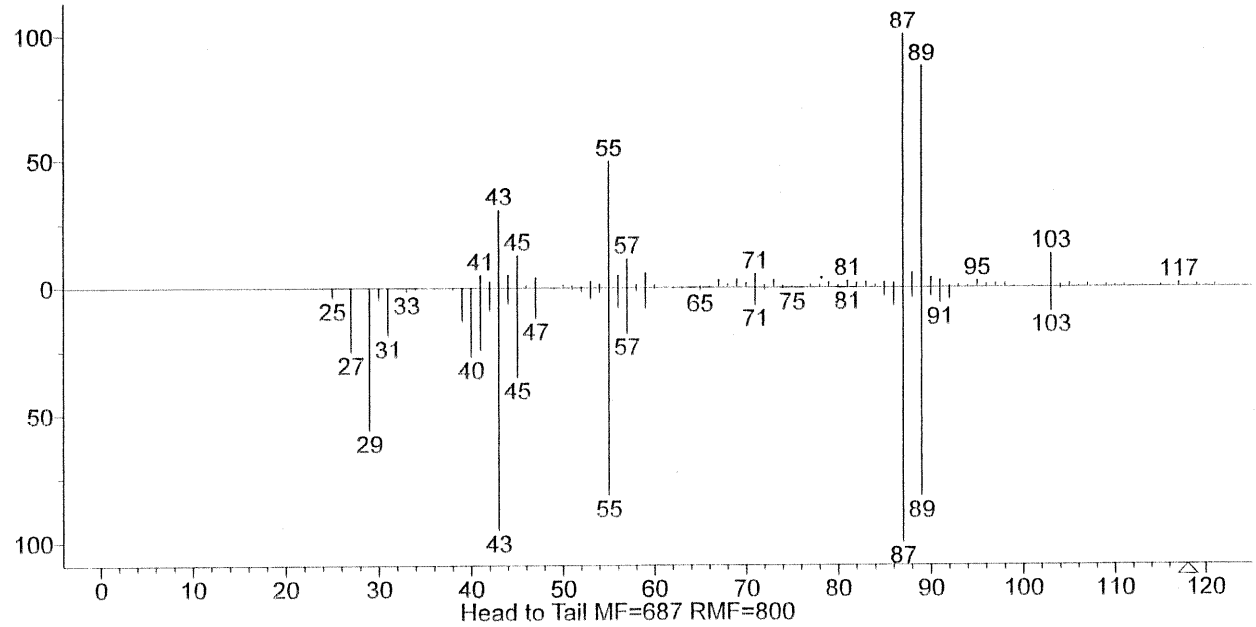
# OLE-H7

| Peak Number | RT | Area | Area % | Height | Width | Area Sum % | Height % |
|---|---|---|---|---|---|---|---|
| 1 | 5.149 | 410717 | 6.84 | 116555 | 0.171 | 0.94 | 13.91 |
| 2 | 5.801 | 946984 | 15.77 | 352576 | 0.132 | 2.17 | 42.08 |
| 3 | 6.111 | 535451 | 8.92 | 201475 | 0.146 | 1.22 | 24.05 |
| 4 | 7.718 | 481259 | 8.01 | 172052 | 0.103 | 1.1 | 20.53 |
| 5 | 8.609 | 114071 | 1.9 | 35734 | 0.171 | 0.26 | 4.26 |
| 6 | 10.565 | 350011 | 5.83 | 105624 | 0.157 | 0.8 | 12.61 |
| 7 | 13.088 | 580500 | 9.67 | 173624 | 0.185 | 1.33 | 20.72 |
| 8 | 16.11 | 274501 | 4.57 | 94551 | 0.096 | 0.63 | 11.28 |
| 9 | 16.534 | 75490 | 1.26 | 31203 | 0.071 | 0.17 | 3.72 |
| 10 | 16.88 | 79231 | 1.32 | 33785 | 0.071 | 0.18 | 4.03 |
| 11 | 17.543 | 159584 | 2.66 | 23930 | 0.203 | 0.36 | 2.86 |
| 12 | 17.767 | 131423 | 2.19 | 47755 | 0.1 | 0.3 | 5.7 |
| 13 | 18.102 | 241267 | 4.02 | 76368 | 0.128 | 0.55 | 9.11 |
| 14 | 18.398 | 88855 | 1.48 | 32953 | 0.103 | 0.2 | 3.93 |
| 15 | 19.385 | 529896 | 8.82 | 154480 | 0.189 | 1.21 | 18.44 |
| 16 | 20.572 | 342596 | 5.71 | 99582 | 0.143 | 0.78 | 11.89 |
| 17 | 21.47 | 114981 | 1.91 | 35696 | 0.1 | 0.26 | 4.26 |
| 18 | 21.705 | 517610 | 8.62 | 64345 | 0.235 | 1.18 | 7.68 |
| 19 | 23.623 | 81349 | 1.35 | 25498 | 0.078 | 0.19 | 3.04 |
| 20 | 24.435 | 411901 | 6.86 | 97849 | 0.189 | 0.94 | 11.68 |
| 21 | 25.037 | 48147 | 0.8 | 17408 | 0.089 | 0.11 | 2.08 |
| 22 | 25.985 | 404538 | 6.74 | 132529 | 0.146 | 0.92 | 15.82 |
| 23 | 28.102 | 329360 | 5.49 | 110821 | 0.128 | 0.75 | 13.23 |
| 24 | 28.366 | 72137 | 1.2 | 28120 | 0.089 | 0.16 | 3.36 |
| 25 | 30.607 | 165311 | 2.75 | 36361 | 0.178 | 0.38 | 4.34 |
| 26 | 32.172 | 48007 | 0.8 | 14413 | 0.103 | 0.11 | 1.72 |
| 27 | 32.949 | 2080576 | 34.65 | 116905 | 0.552 | 4.76 | 13.95 |
| 28 | 33.783 | 122075 | 2.03 | 40033 | 0.1 | 0.28 | 4.78 |
| 29 | 34.275 | 62809 | 1.05 | 23908 | 0.082 | 0.14 | 2.85 |
| 30 | 34.638 | 149877 | 2.5 | 42947 | 0.16 | 0.34 | 5.13 |
| 31 | 35.123 | 100688 | 1.68 | 41594 | 0.078 | 0.23 | 4.96 |
| 32 | 36.531 | 48951 | 0.82 | 19967 | 0.075 | 0.11 | 2.38 |
| 33 | 37.45 | 60431 | 1.01 | 20607 | 0.096 | 0.14 | 2.46 |
| 34 | 37.96 | 48287 | 0.8 | 19800 | 0.075 | 0.11 | 2.36 |
| 35 | 39.346 | 69926 | 1.16 | 32429 | 0.082 | 0.16 | 3.87 |
| 36 | 40.308 | 368077 | 6.13 | 93655 | 0.153 | 0.84 | 11.18 |
| 37 | 41.292 | 78239 | 1.3 | 27569 | 0.086 | 0.18 | 3.29 |
| 38 | 41.591 | 118170 | 1.97 | 30911 | 0.135 | 0.27 | 3.69 |
| 39 | 42.8 | 321397 | 5.35 | 77885 | 0.178 | 0.73 | 9.3 |
| 40 | 43.024 | 99800 | 1.66 | 25638 | 0.164 | 0.23 | 3.06 |
| 41 | 43.445 | 41353 | 0.69 | 11947 | 0.107 | 0.09 | 1.43 |
| 42 | 43.676 | 63220 | 1.05 | 15146 | 0.171 | 0.14 | 1.81 |
| 43 | 44.382 | 102381 | 1.71 | 23168 | 0.171 | 0.23 | 2.77 |
| 44 | 46.178 | 4770040 | 79.44 | 837860 | 0.235 | 10.91 | 100 |
| 45 | 48.153 | 6004681 | 100 | 326469 | 0.62 | 13.73 | 38.96 |
| 46 | 49.553 | 3648713 | 60.76 | 522211 | 0.314 | 8.34 | 62.33 |
| 47 | 53.605 | 94429 | 1.57 | 13173 | 0.264 | 0.22 | 1.57 |
| 48 | 56.189 | 989765 | 16.48 | 99146 | 0.396 | 2.26 | 11.83 |
| 49 | 56.774 | 2158750 | 35.95 | 201324 | 0.442 | 4.94 | 24.03 |
| 50 | 57.722 | 5687920 | 94.72 | 492581 | 0.495 | 13.01 | 58.79 |

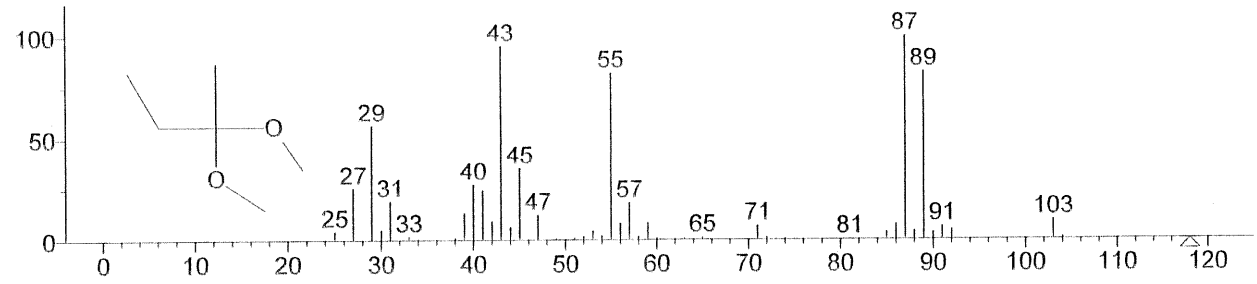
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 51 | 58.72 | 882814 | 14.7 | 84871 | 0.41 | 2.02 | 10.13 |
| 52 | 60.641 | 2653154 | 44.18 | 149019 | 0.659 | 6.07 | 17.79 |
| 53 | 61.999 | 314189 | 5.23 | 33652 | 0.296 | 0.72 | 4.02 |
| 54 | 62.241 | 269887 | 4.49 | 34077 | 0.246 | 0.62 | 4.07 |
| 55 | 62.733 | 1545203 | 25.73 | 120801 | 0.592 | 3.53 | 14.42 |
| 56 | 65.242 | 564707 | 9.4 | 51598 | 0.356 | 1.29 | 6.16 |
| 57 | 72.088 | 298458 | 4.97 | 81216 | 0.114 | 0.68 | 9.69 |
| 58 | 75.955 | 144881 | 2.41 | 52270 | 0.1 | 0.33 | 6.24 |
| 59 | 76.286 | 121572 | 2.02 | 50804 | 0.089 | 0.28 | 6.06 |
| 60 | 76.664 | 406628 | 6.77 | 151098 | 0.111 | 0.93 | 18.03 |
| 61 | 78.824 | 392137 | 6.53 | 84821 | 0.125 | 0.9 | 10.12 |
| 62 | 78.931 | 360383 | 6 | 142187 | 0.111 | 0.82 | 16.97 |
| 63 | 86.513 | 677962 | 11.29 | 157009 | 0.139 | 1.55 | 18.74 |
| 64 | 90.376 | 128620 | 2.14 | 29812 | 0.164 | 0.29 | 3.56 |
| 65 | 92.251 | 147538 | 2.46 | 31199 | 0.171 | 0.34 | 3.72 |
| | | | | | | 99.96 | |




(Text File) +EI Scan (5.149 min) ALI-OLE-H7-220421-.D




Head to Tail MF=687 RMF=800



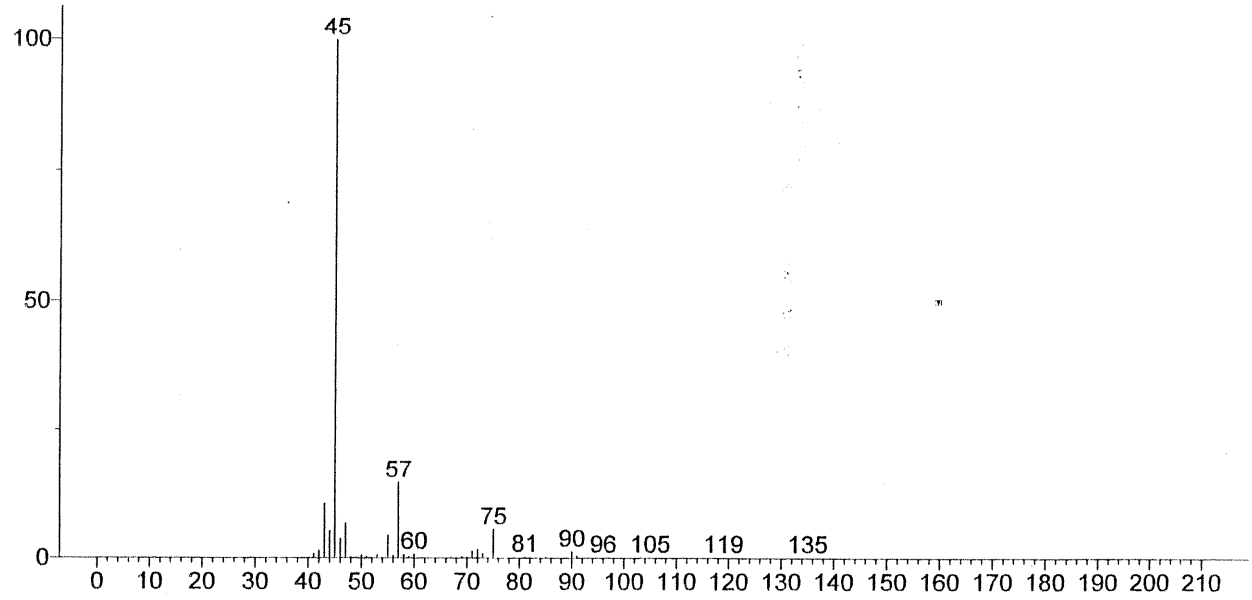

(mainlib) 2,2-Dimethoxybutane

Name: 2,2-Dimethoxybutane
Formula: $C_6H_{14}O_2$
MW: 118 CAS#: 3453-99-4 NIST#: 250250 ID#: 48775 DB: mainlib
Other DBs: None
Contributor: TNO Volatile Compounds in Food - Chemical Concepts
10 largest peaks:
87 999 | 43 950 | 89 822 | 55 817 | 29 560 | 45 351 | 40 270 | 27 251 | 41 242 | 31 188 |
Synonyms:
no synonyms.

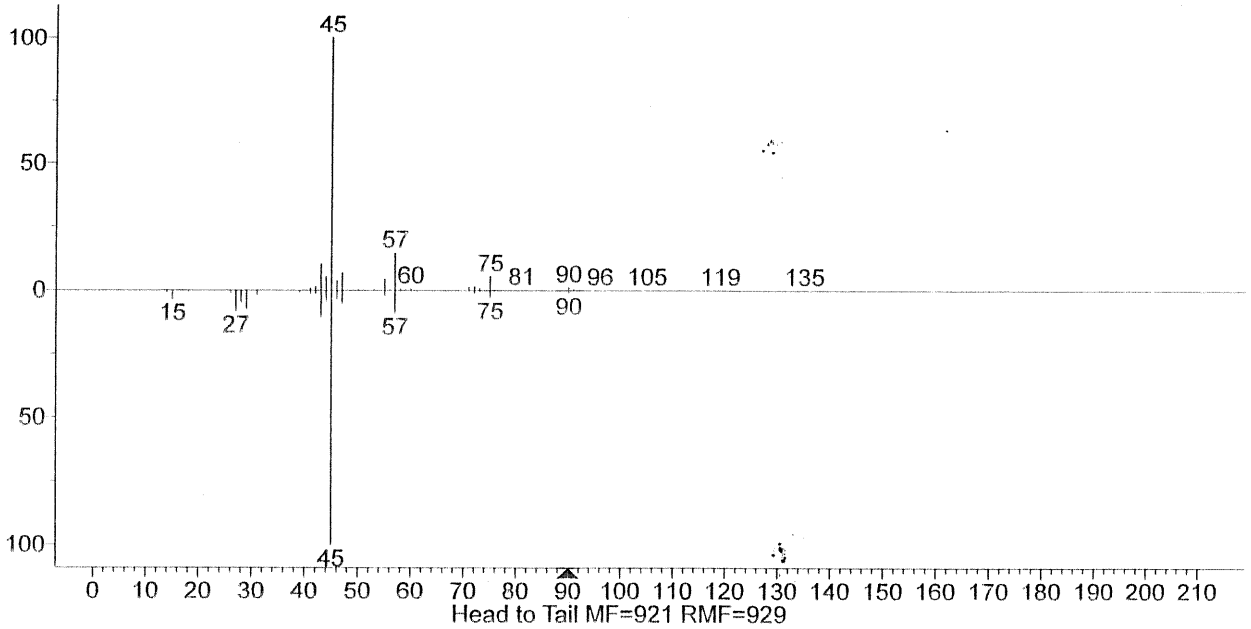
Estimated non-polar retention index (n-alkane scale):
Value: 685 iu
Confidence interval (Ethers): 68(50%) 293(95%) iu

Retention index.
1. Value: 748.5 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: SE-54
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: 40C(5min) =>4C/min => 230C(20min)=> 5C/min => 280C (5min)

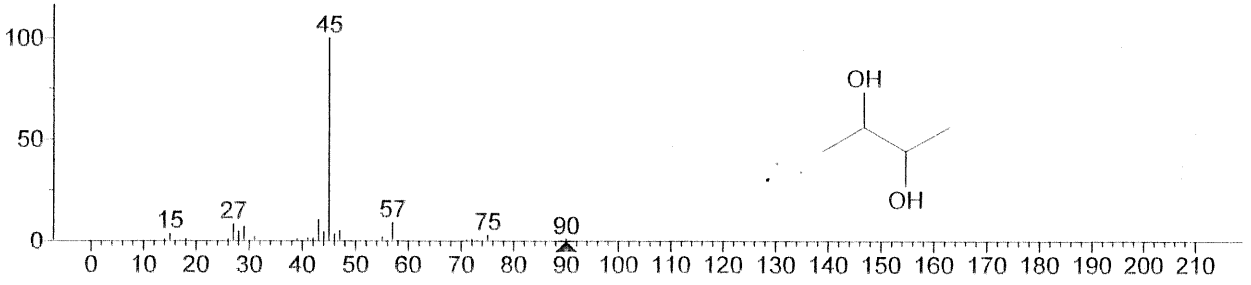
Source: Gao, H.; Zhao, T.; Kong, Q.; Chen, X.; Hu, Z., Analysis of unknown organic pollutants in sewage by solid -phase extraction combined with gas chromatography-mass spectrometry, J. Chromatogr. Sci., 42, 2004, 91-99.




(Text File) +EI Scan (5.804 min) ALI-OLE-H7-220421-.D



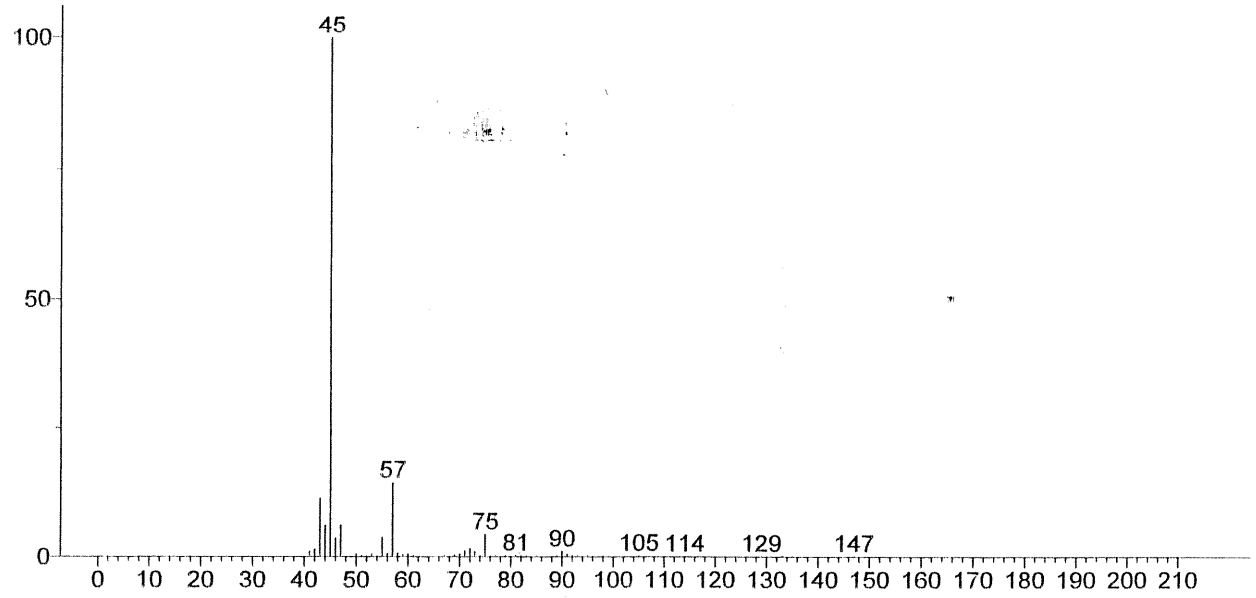

Head to Tail MF=921 RMF=929



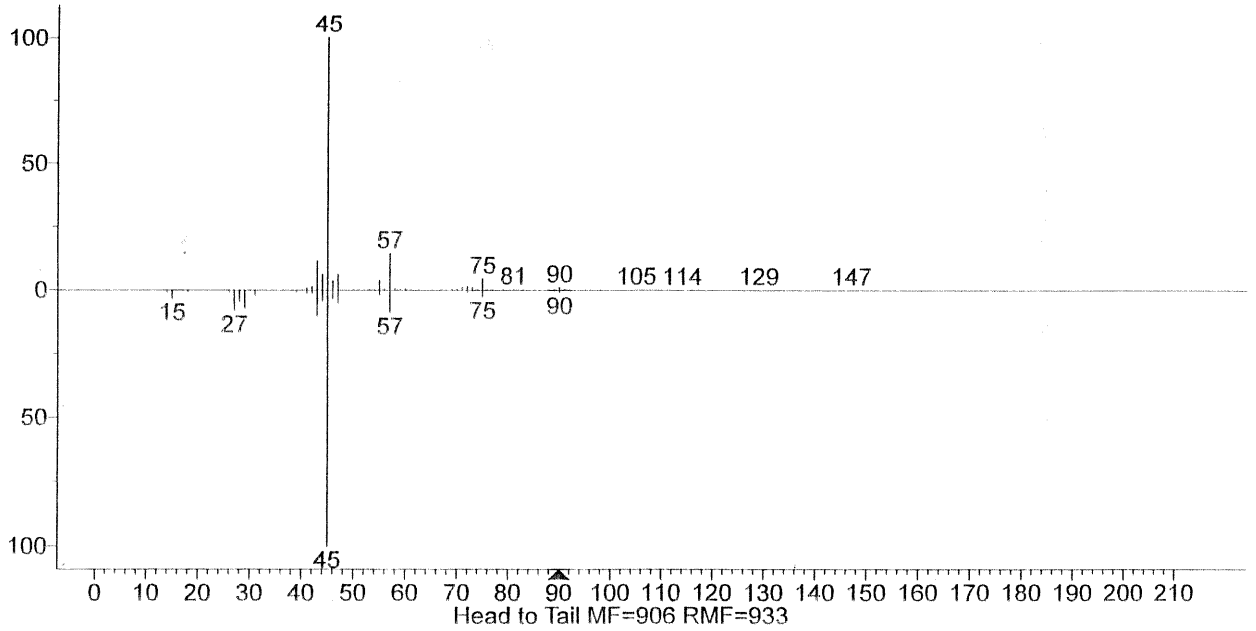

(mainlib) 2,3-Butanediol, [R-(R*,R*)]-

Name: 2,3-Butanediol, [R-(R*,R*)]-
Formula: $C_4H_{10}O_2$
MW: 90 CAS#: 24347-58-8 NIST#: 235815 ID#: 15312 DB: mainlib
Other DBs: HODOC, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-6416
10 largest peaks:
45 999 | 43 104 | 57 89 | 27 82 | 29 71 | 47 51 | 28 46 | 44 45 | 15 35 | 46 34 |
Synonyms:
1.2,3-Butanediol #

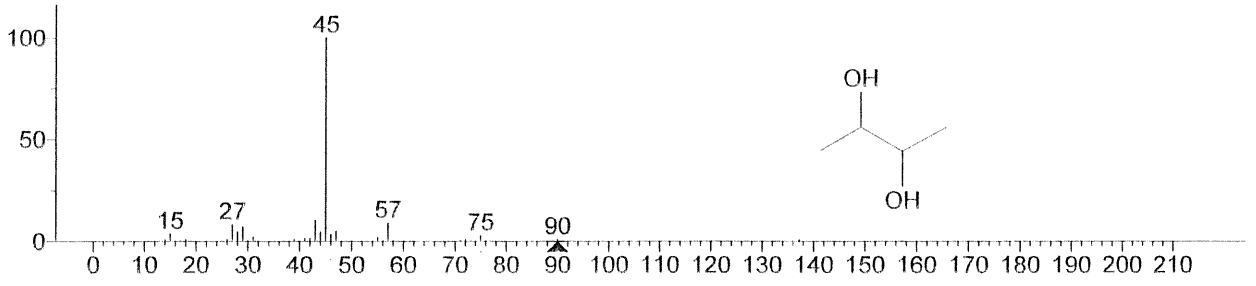
Estimated non-polar retention index (n-alkane scale):
Value: 743 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu




(Text File) +EI Scan (6.111 min) ALI-OLE-H7-220421-.D



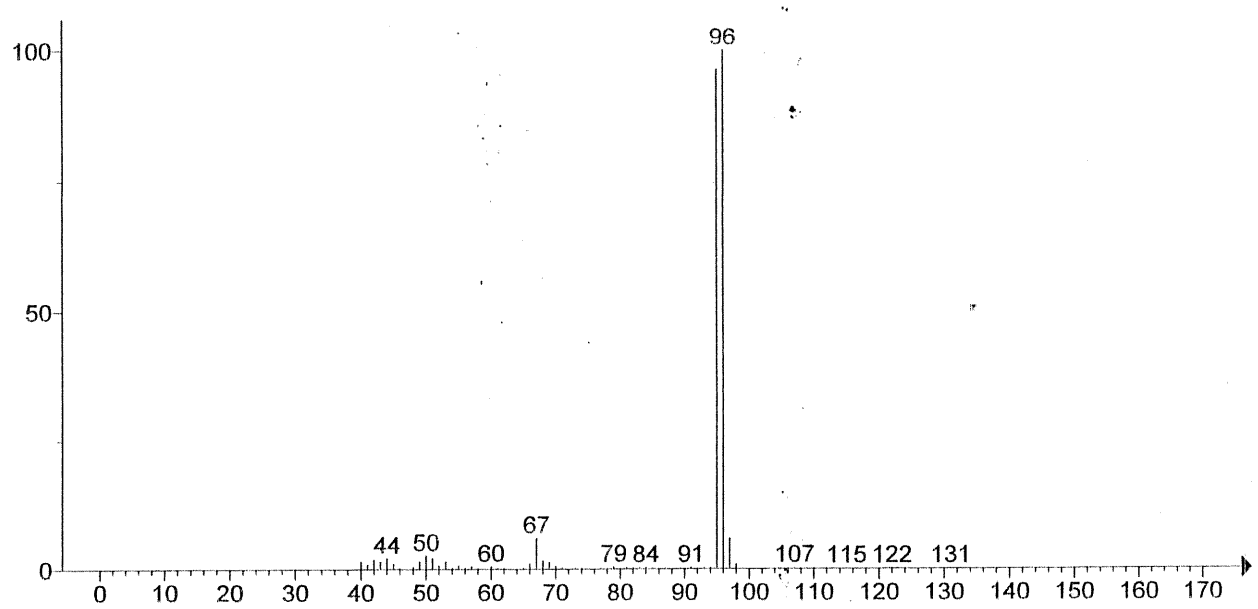

Head to Tail MF=906 RMF=933



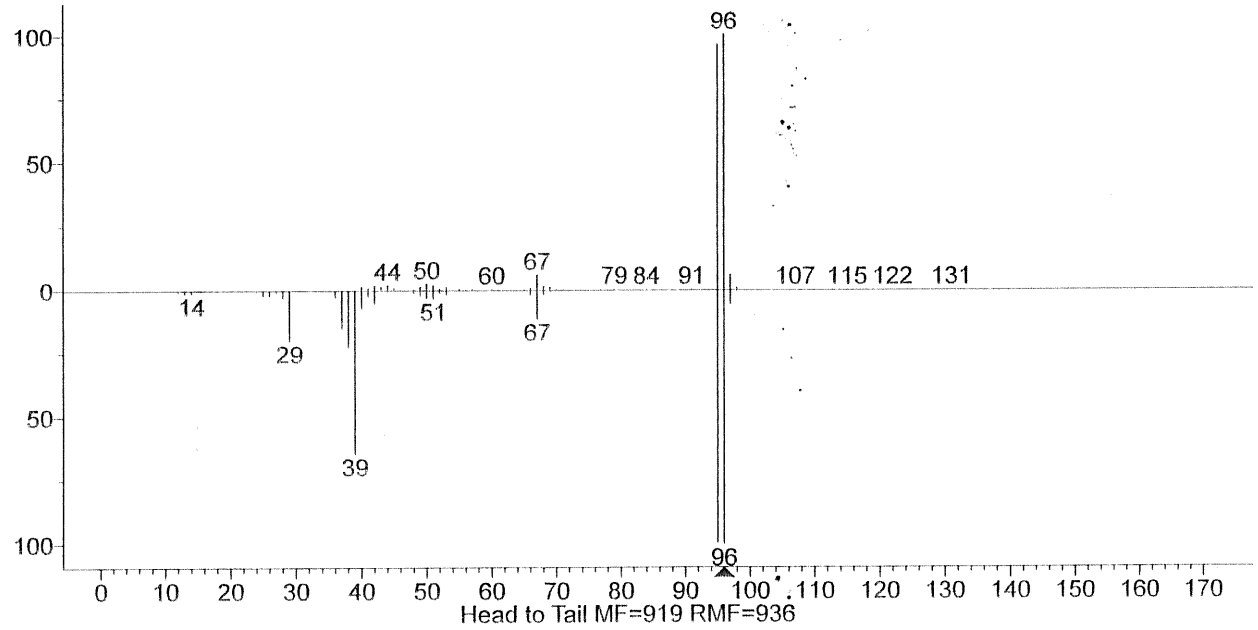

(mainlib) 2,3-Butanediol, [R-(R*,R*)]-

Name: 2,3-Butanediol, [R-(R*,R*)]-
Formula: $C_4H_{10}O_2$
MW: 90 CAS#: 24347-58-8 NIST#: 235815 ID#: 15312 DB: mainlib
Other DBs: HODOC, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-6416
10 largest peaks:
45 999 | 43 104 | 57 89 | 27 82 | 29 71 | 47 51 | 28 46 | 44 45 | 15 35 | 46 34 |
Synonyms:
1.2,3-Butanediol #

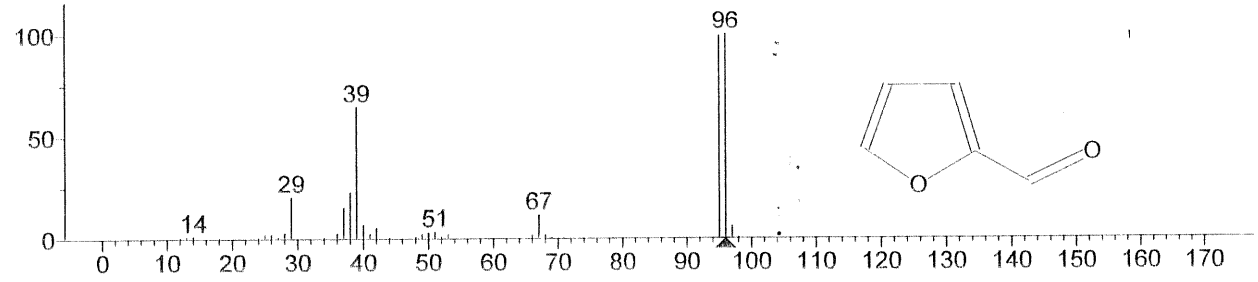
Estimated non-polar retention index (n-alkane scale):
Value: 743 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu




(Text File) +EI Scan (7.718 min) ALI-OLE-H7-220421-.D




Head to Tail MF=919 RMF=936

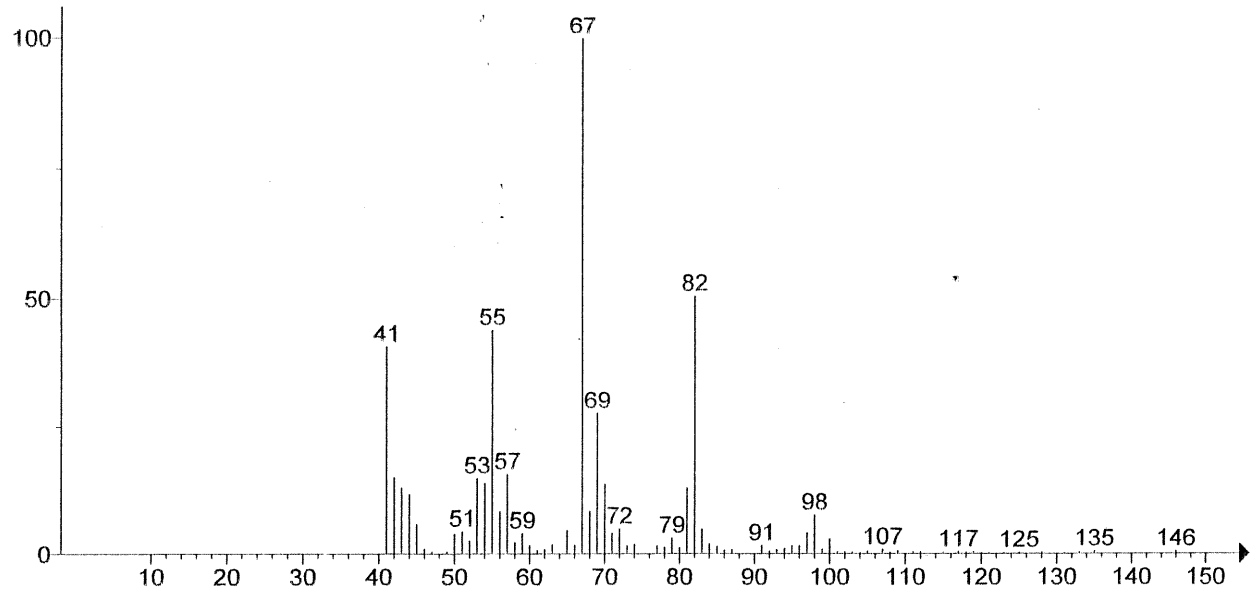



(mainlib) Furfural

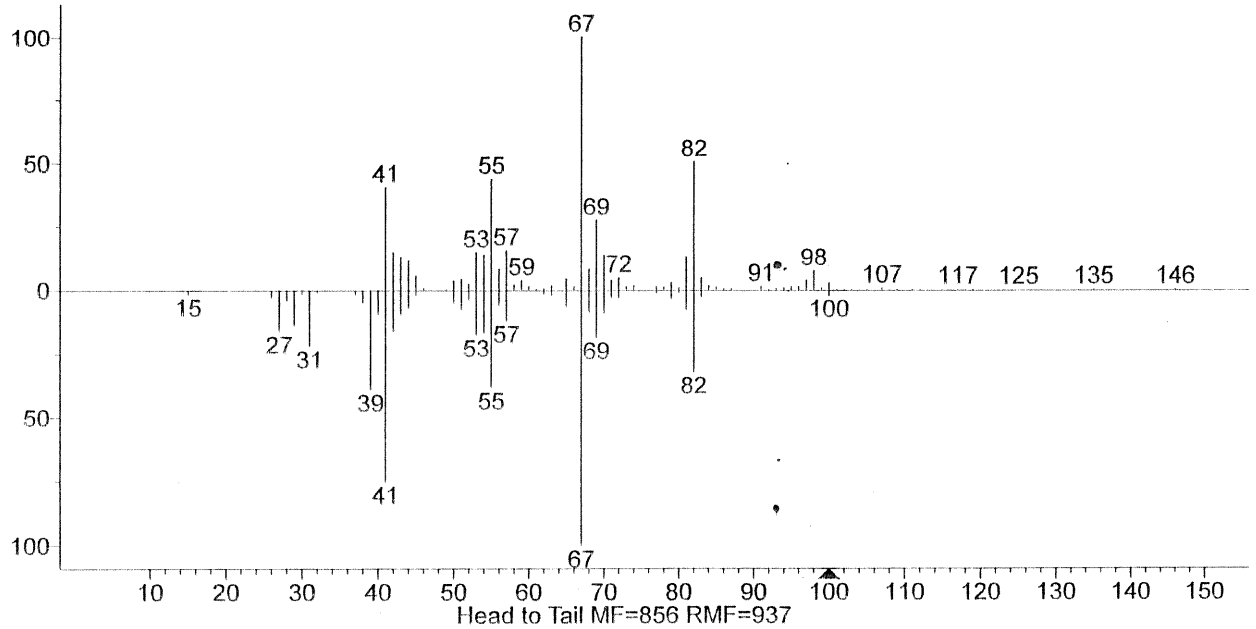
Name: Furfural
Formula: $C_5H_4O_2$
MW: 96 CAS#: 98-01-1 NIST#: 118785 ID#: 59378 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
96 999 | 95 991 | 39 644 | 38 226 | 29 201 | 37 151 | 67 114 | 40 69 | 97 57 | 42 53 |
Synonyms:
1.2-Furancarboxaldehyde
2.2-Furaldehyde
3.α-Furole
4.Artificial ant oil
5.Fural
6.Furaldehyde
7.Furale
8.Furancarbonal
9.Furfuraldehyde
10.Furfurole
11.Furfurylaldehyde
12.Furole
13.Pyromucic aldehyde
14.2-Formylfuran
15.2-Furanaldehyde
16.2-Furancarbonal
17.2-Furfural
18.2-Furfuraldehyde
19.2-Furylaldehyde
20.Furol
21.2-Furylmethanal
22.Artificial oil of ants
23.Furfurale
24.Furfurol
25.Nci-C56177
26.2-Furil-metanale
27.2-Furankarbaldehyd
28.Furfuralu
29.Rcra waste number U125
30.UN 1199
31.2-Furylaldehyde xypropane
32.2-Furylcarboxaldehyde
33.Cyclic aldehyde
34.Qo furfural

Estimated non-polar retention index (n-alkane scale):
Value: 831 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

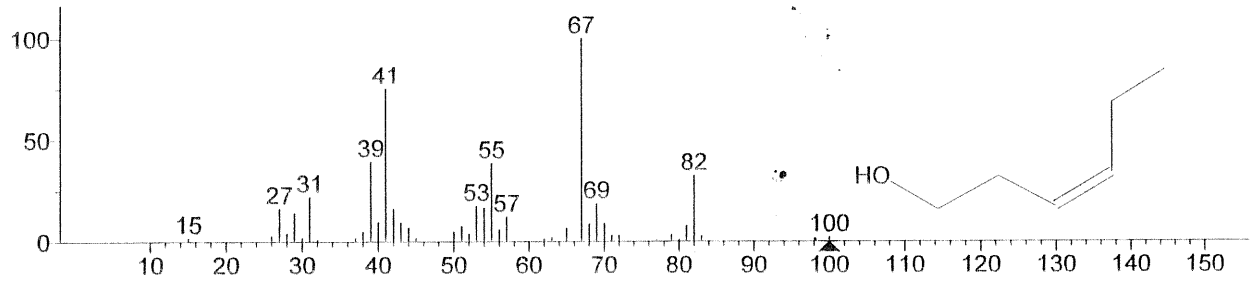
Retention index.
1. Value: 794 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column
Length: 60 m




(Text File) +EI Scan (8.609 min) ALI-OLE-H7-220421-.D




Head to Tail MF=856 RMF=937



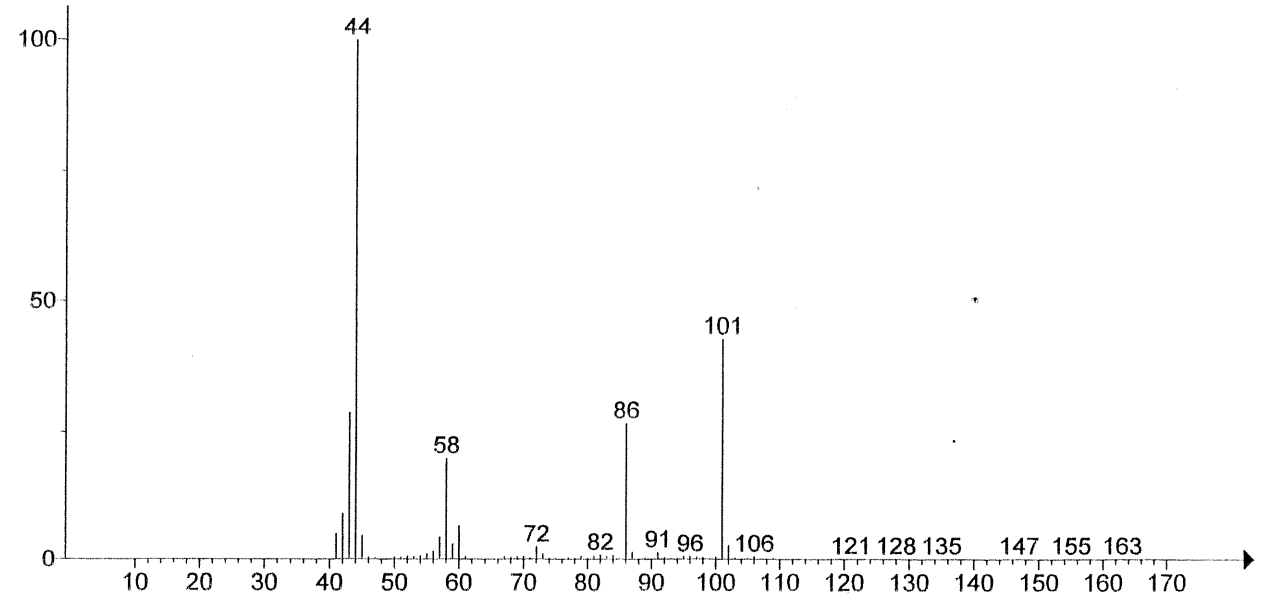

(mainlib) 3-Hexen-1-ol, (Z)-

Name: 3-Hexen-1-ol, (Z)-
Formula: $C_6H_{12}O$
MW: 100 CAS#: 928-96-1 NIST#: 114154 ID#: 28426 DB: mainlib
Other DBs: TSCA, RTECS, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
67 999 | 41 750 | 39 390 | 55 382 | 82 321 | 31 218 | 69 184 | 53 174 | 54 164 | 27 161 |
Synonyms:
1.(Z)-Hex-3-en-1-ol
2.cis-3-Hexen-1-ol
3.cis-3-Hexene-1-ol
4.cis-3-Hexenol
5.Blatteralkohol (German)
6.Leaf alcohol
7.Z-3-Hexenol
8.3-(Z)-Hexenol
9.β,γ-Hexenol
10.Blatteralkohol
11.Hexen-30L-1
12.3-Hexen-1-ol
13.3-Hexen-1-ol, cis-
14.3-Hexenol, cis-
15.(3Z)-3-Hexen-1-ol #

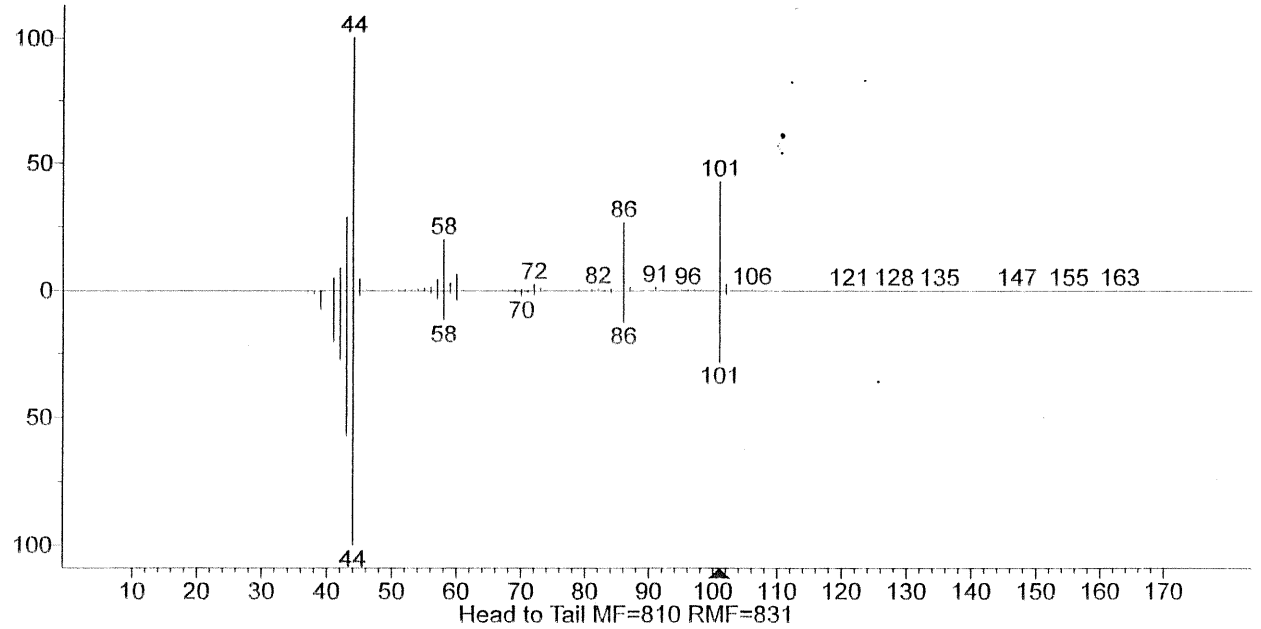
Estimated non-polar retention index (n-alkane scale):
Value: 868 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

Retention index.
1. Value: 838 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-101
Column
Length: 25 m
Carrier Gas: He
Column Diameter: 0.2 mm
Phase Thickness: 0.2 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 70 C
End T: 200 C
Heat Rate: 3 K/min
Start Time: 2 min
End Time: 15
min
Source: Politeo, O.; Jukic, M.; Milos, M., Chemical composition and antioxidant capacity of free volatile aglycones from basil (Ocimum basilicum L.) compared with its essential oil, Food Chem., 101, 2007, 379-385.

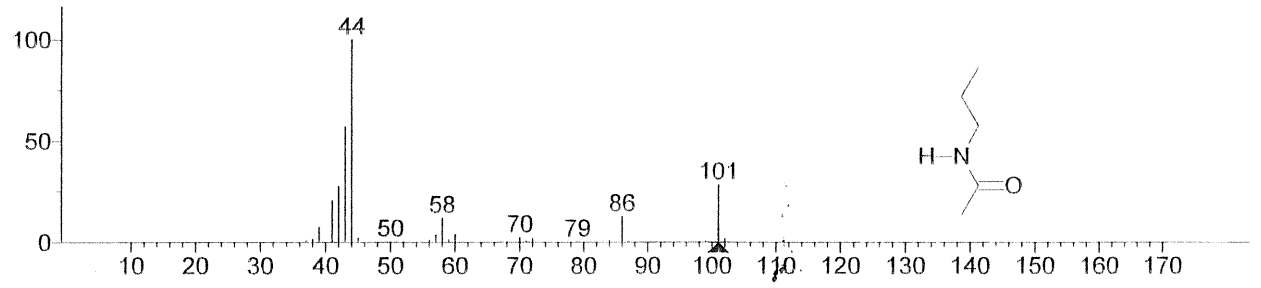
2.
Value: 872 iu
Column Type: Capillary
Column Class: Standard non-polar




(Text File) +EI Scan (10.562 min) ALI-OLE-H7-220421-.D




Head to Tail MF=810 RMF=831




(mainlib) N-(n-Propyl)acetamide

Name: N-(n-Propyl)acetamide
Formula: $C_5H_{11}NO$
MW: 101 CAS#: 5331-48-6 NIST#: 223038 ID#: 13993 DB: mainlib
Other DBs: Fine, EINECS
Contributor: Chemical Concepts
10 largest peaks:
44 999 | 43 571 | 101 283 | 42 274 | 41 203 | 86 126 | 58 118 | 39 74 | 60 39 | 57 35 |
Synonyms:
1.Acetamide, N-propyl-
2.N-Propylacetamide
3.Acetamide, N-n-propyl-,

Estimated non-polar retention index (n-alkane scale):
Value: 918 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu

Retention index.
1. Value: 974 iu
Column Type: Packed
Column Class: Standard non-polar
Active Phase: SE-30
Column Length:
1 m
Carrier Gas: N2
Substrate: Chromosorb W AW
Data Type: Kovats RI
Program Type: Isothermal
Start T:
180 C
Source: Krawczyk, W.; Piotrowski, G.T., Relationships Between Structure and Retention Index for N
-Substituted Amides of Aliphatic Acids on a Non-Polar Column, J. Chromatogr., 463, 1989, 297-304.

2. Value: 974
iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: Polydimethyl siloxanes
Data Type:
Normal alkane RI
Program Type: Ramp
Source: Zenkevich, I.G.; Chupalov, A.A., New Possibilities of Chromato
Mass Pectrometric Identification of Organic Compounds Using Increments of Gas Chromatographic Retention
Indices of Molecular Structural Fragments, Zh. Org. Khim. (Rus.), 32(5), 1996, 656-666, In original 656-666.

<...
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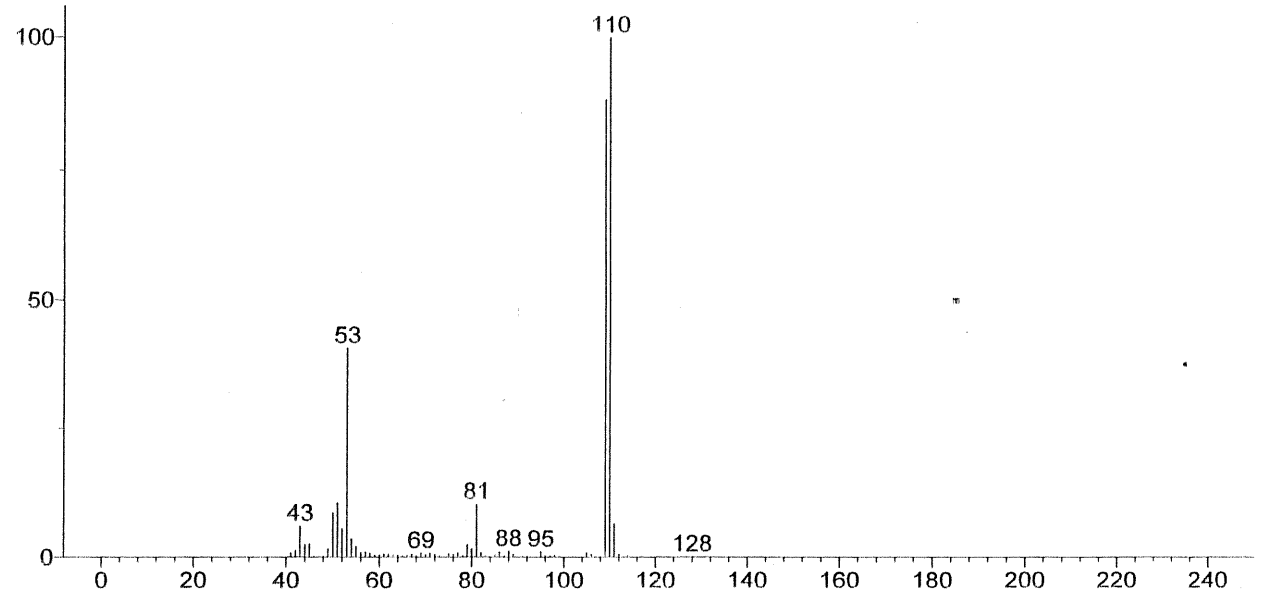
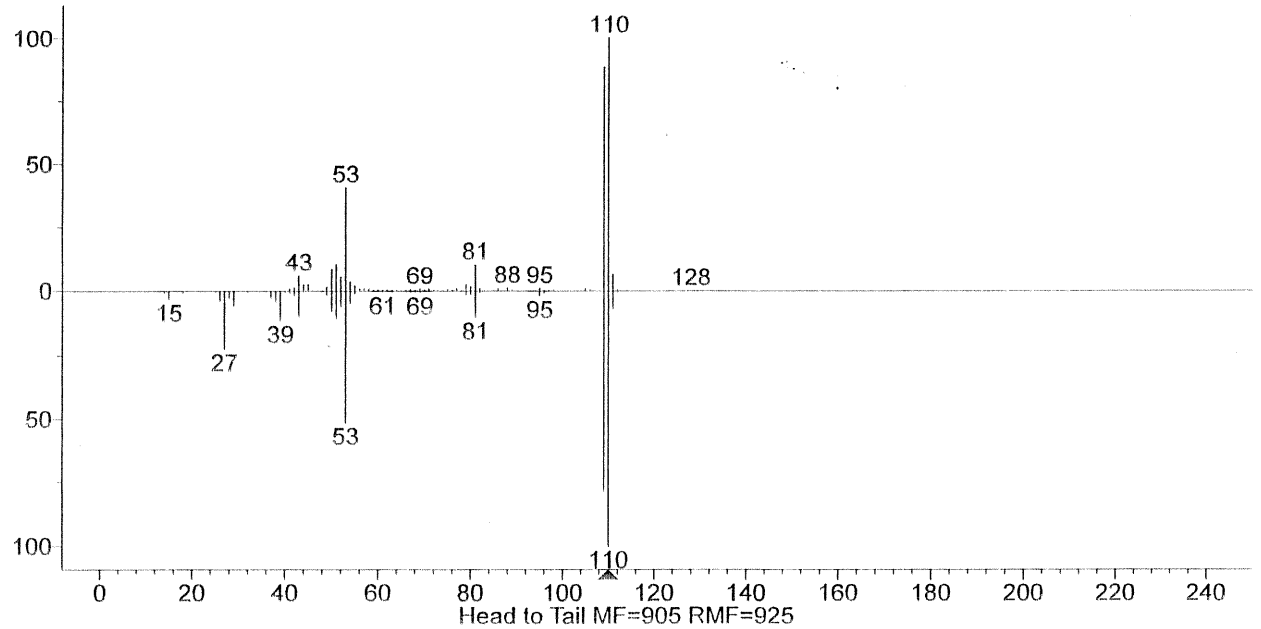
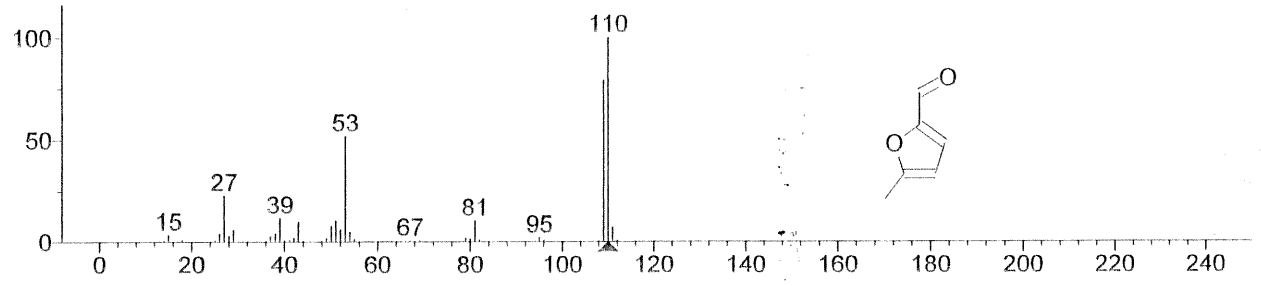



(Text File) +EI Scan (13.092 min) ALI-OLE-H7-220421-.D




Head to Tail MF=905 RMF=925



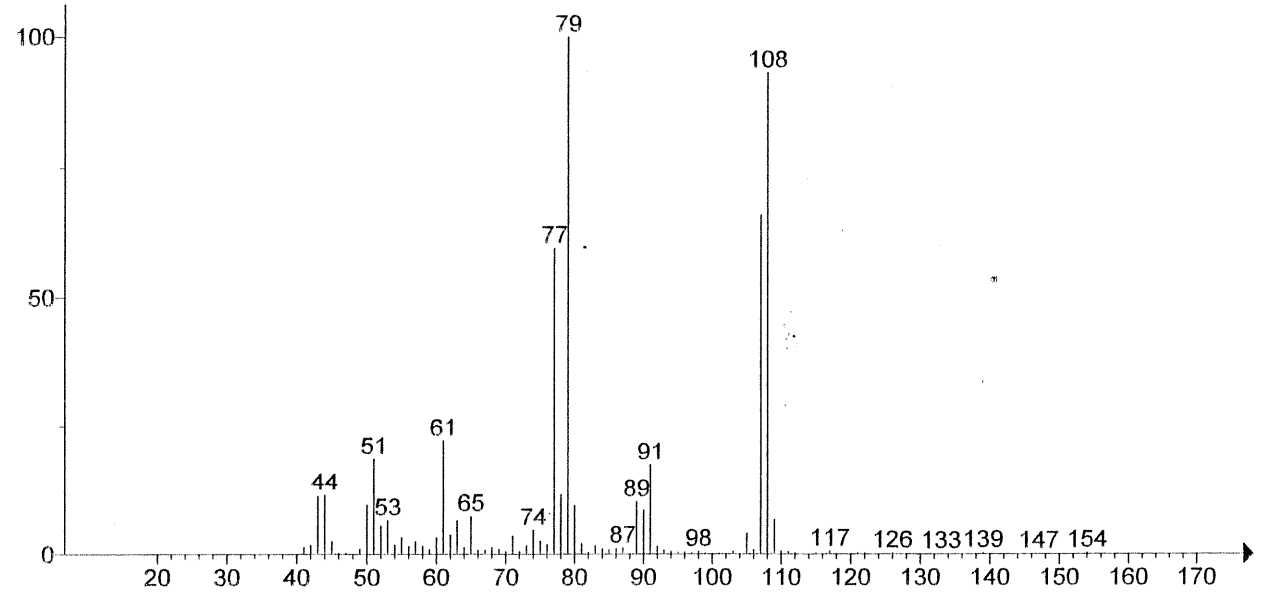

(mainlib) 2-Furancarboxaldehyde, 5-methyl-

Name: 2-Furancarboxaldehyde, 5-methyl-
Formula: $C_6H_6O_2$
MW: 110 CAS#: 620-02-0 NIST#: 233793 ID#: 74019 DB: mainlib
Other DBs: Fine, TSCA, RTECS, HODOC, EINECS, IRDB
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-1340
10 largest peaks:
110 999 | 109 788 | 53 515 | 27 225 | 39 115 | 51 104 | 81 102 | 43 97 | 50 77 | 111 69 |
Synonyms:
1.2-Furaldehyde, 5-methyl-
2.Furfural, 5-methyl-
3.2-Formyl-5-methylfuran
4.2-Methyl-5-formylfuran
5.5-Methyl-2-furaldehyde
6.5-Methyl-2-furancarboxaldehyde
7.5-Methyl-2-furfural
8.5-Methylfurfural
9.5-Methylfurfuraldehyde
10.5-Methyl furfural

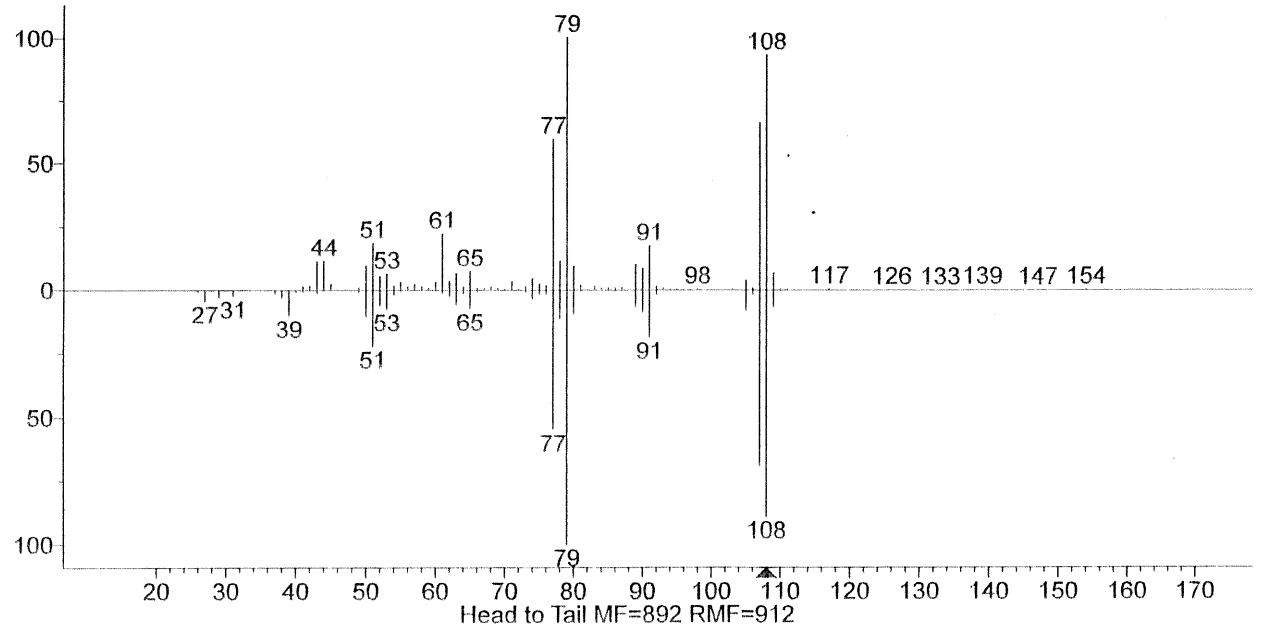
Estimated non-polar retention index (n-alkane scale):
Value: 920 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 924 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: 0.4 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C
End T: 280 C
Heat Rate: 3 K/min
Start Time: 10 min
End Time: 60
min
Source: Pino, J.A.; Marbot, R.; Vázquez, C., Characterization of volatile in Cosa Rican Guava [Psidium friedrichsthalianum (Berg) Niedenzu] fruit, J. Agric. Food Chem., 50, 2002, 6023-6026.

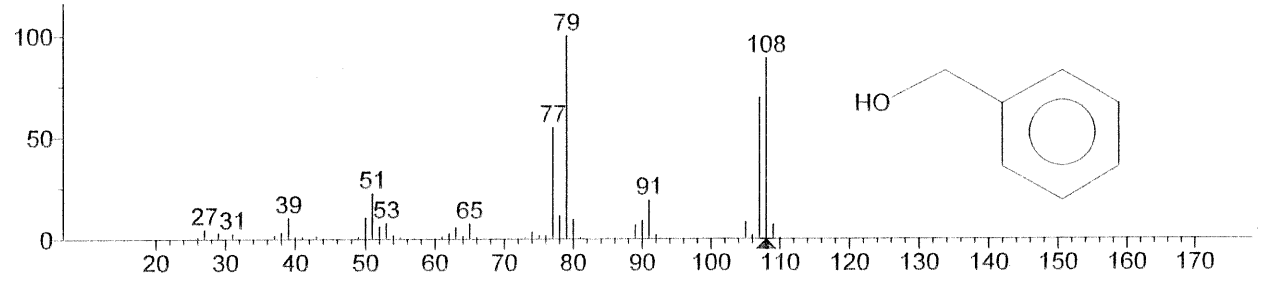
2. Value: 926 iu
Column
Type: Capillary
Column Class: Standard non-polar
Active Phase: SPB-1
Column Length: 60 m
Carrier Gas:
N2
Column Diameter: 0.32 mm




(Text File) +EI Scan (16.110 min) ALI-OLE-H7-220421-.D




Head to Tail MF=892 RMF=912



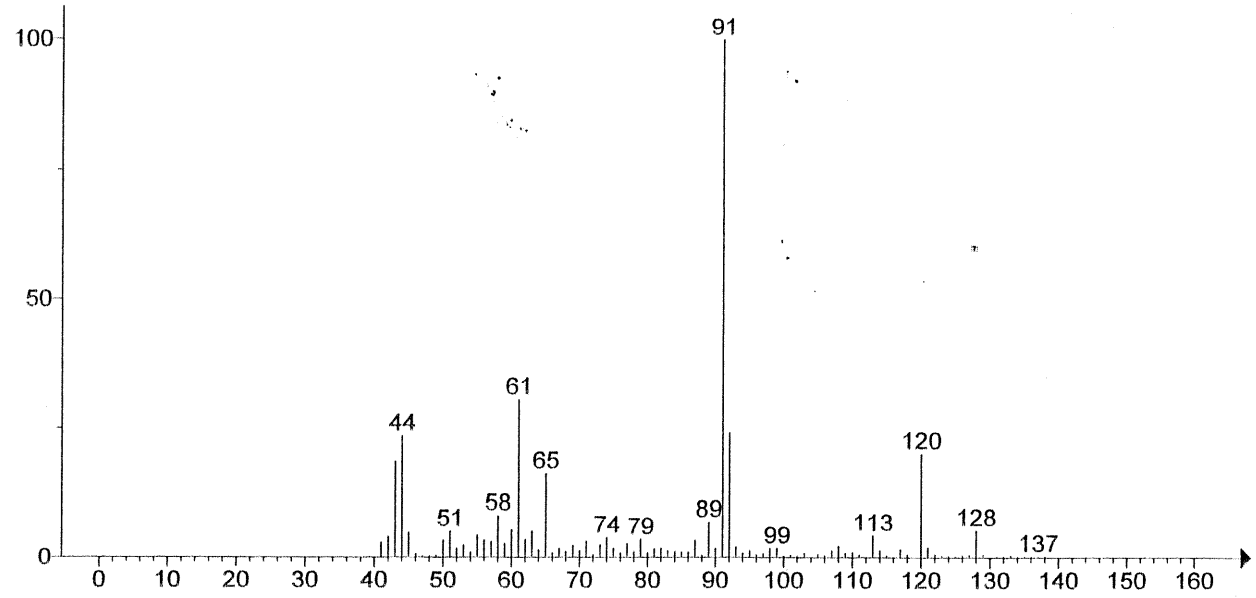

(mainlib) Benzyl Alcohol

Name: Benzyl Alcohol
Formula: $C_7H_8O$
MW: 108 CAS#: 100-51-6 NIST#: 151560 ID#: 42192 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB
Contributor: Chemical Concepts
10 largest peaks:
79 999 | 108 890 | 107 692 | 77 547 | 51 222 | 91 187 | 78 113 | 50 104 | 39 102 | 80 95 |
Synonyms:
1.Benzenemethanol
2.α-Hydroxytoluene
3.α-Toluenol
4.(Hydroxymethyl)benzene
5.Benzenecarbinol
6.Phenylcarbinol
7.Phenylmethanol
8.Phenylmethyl alcohol
9.Methanol, phenyl-
10.NCI-C06111
11.Hydroxytoluene
12.Benzylalcohol
13.Bentalol
14.Benzoyl alcohol

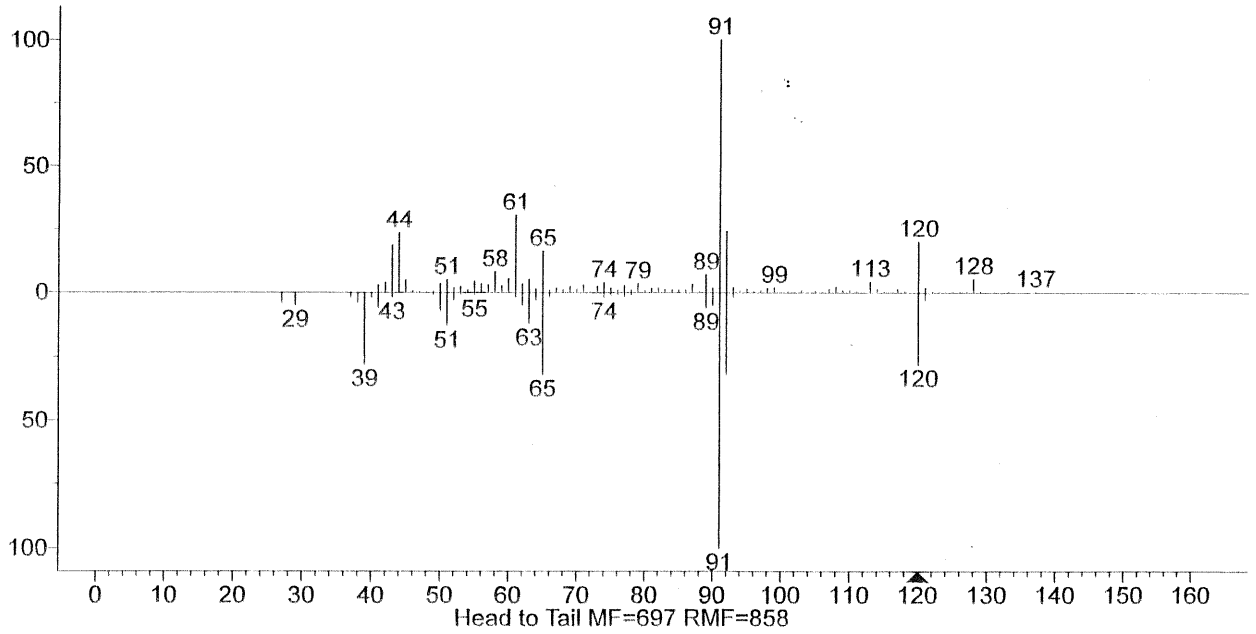
Estimated non-polar retention index (n-alkane scale):
Value: 1036 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

Retention index.
1. Value: 1005.7 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-Petro
Column
Length: 50 m
Column Diameter: 0.2 mm
Phase Thickness: 0.5 um
Data Type: Linear RI
Program Type:
Ramp
Start T: 50 C
End T: 270 C
Heat Rate: 2 K/min
Source: Pang T.; Zhu S.; Lu X.; Xu G., Identification of
unknown compounds on the basis of retention index data in comprehensive two-dimensional gas chromatography,
J. Sep. Sci., 30, 2007, 868-874.

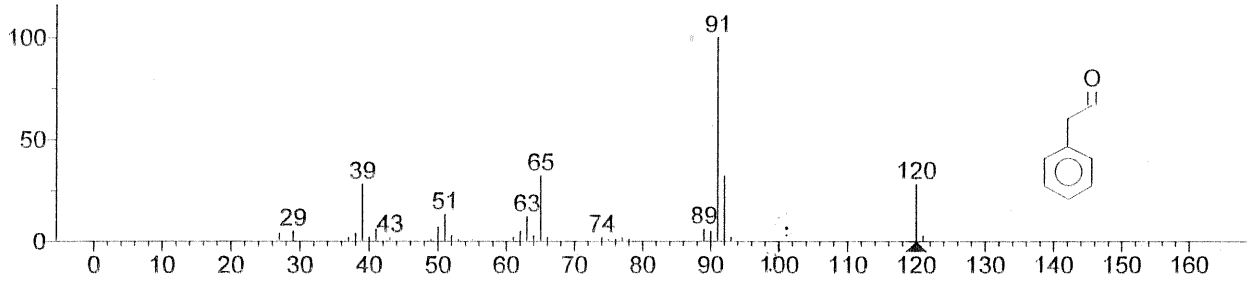
2. Value: 1005.7 iu
Column Type: Capillary
Column Class: Standard non
-polar
Active Phase: DB-Petro
Column Length: 50 m
Column Diameter: 0.2 mm
Phase Thickness: 0.5 um




(Text File) +EI Scan (16.534 min) ALI-OLE-H7-220421-.D




Head to Tail MF=697 RMF=858



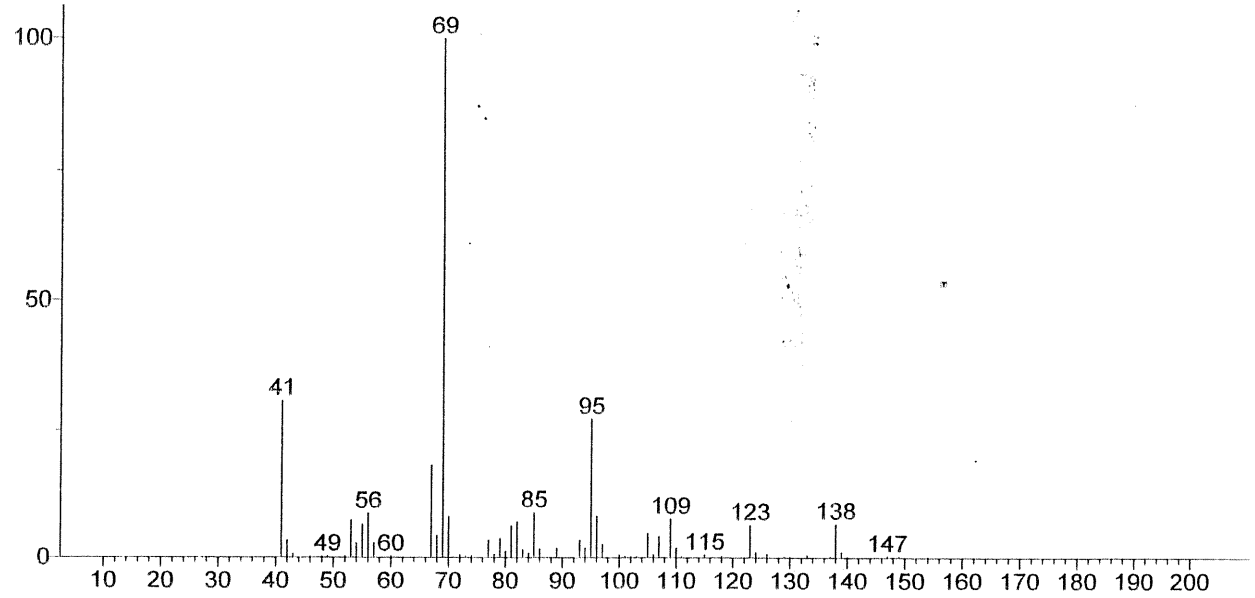

(replib) Benzeneacetaldehyde

Name: Benzeneacetaldehyde
Formula: $C_8H_8O$
MW: 120 CAS#: 122-78-1 NIST#: 53623 ID#: 11325 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS, IRDB
Contributor: FOOD RESEARCH REPORT 122, K.E. MURRAY & COLLEAGUES, DIV OF FOOD RESEARCH, CSIRO, AUSTRALIA
10 largest peaks:
91 999 | 65 320 | 92 320 | 39 280 | 120 280 | 51 130 | 63 120 | 50 70 | 41 60 | 89 60 |
Synonyms:
1.Acetaldehyde, phenyl-
2.α-Tolualdehyde
3.α-Toluic aldehyde
4.Hyacinthin
5.Phenylacetaldehyde
6.Phenylacetic aldehyde
7.Phenylethanal
8.2-Phenylethanal
9.PAA
10.Phenyl acetaldehyde

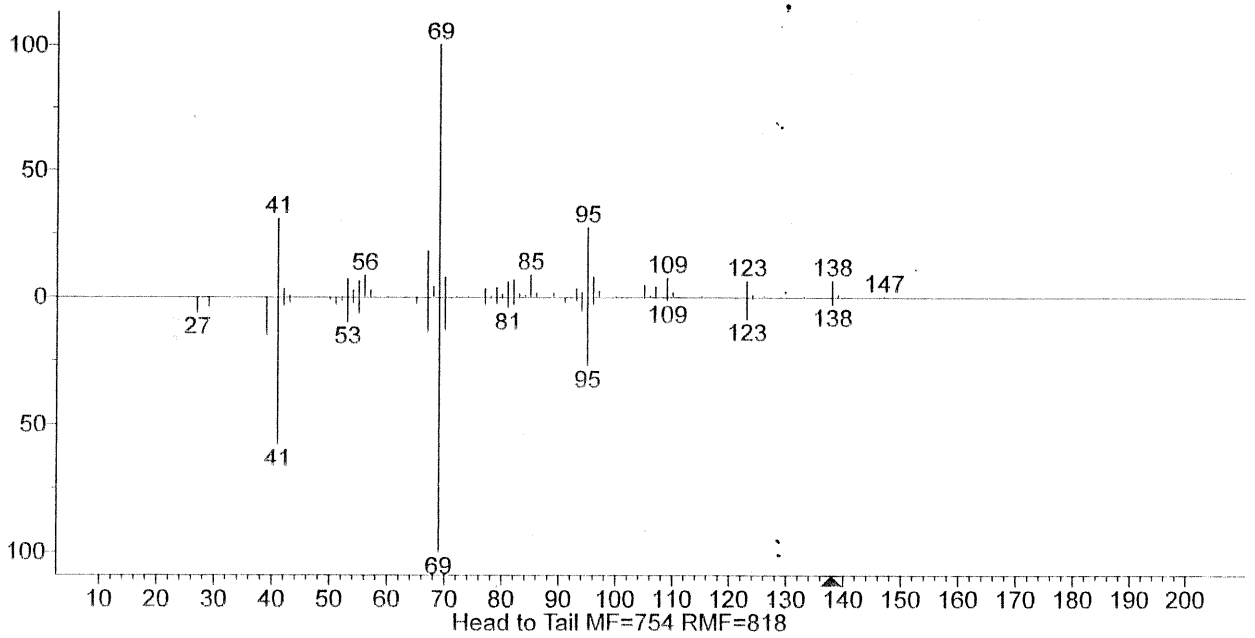
Estimated non-polar retention index (n-alkane scale):
Value: 1081 iu
Confidence interval (Aldehydes): 45(50%) 196(95%) iu

Retention index.
1. Value: 1048 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-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: 60 C
End T: 240 C
Heat Rate: 4 K/min
Source: Rezazadeh, S.; Hamedani, M.
P.; Dowlatabadi, R.; Yazdani, D.; Shafiee, A., Chemical composition of the essential oils of Stachys schtschegleevii Sosn. and Stachys balansae Boiss & Kotschy from Iran, Flavour Fragr. J., 21, 2006, 290-293.

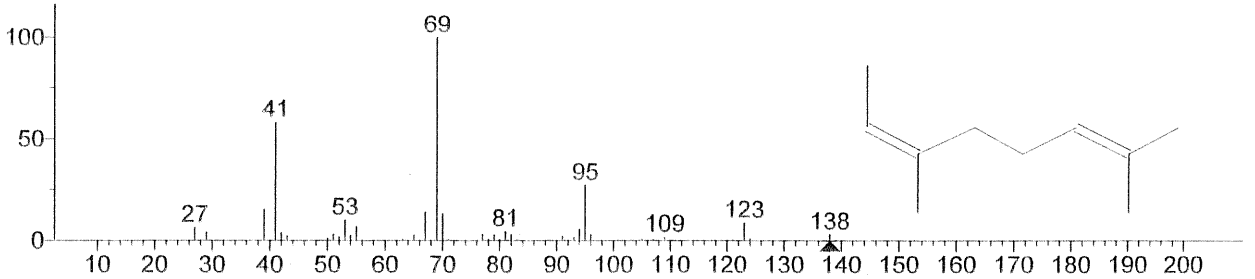
2. Value: 1012
iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column Length: 25
m
Carrier Gas: H2
Column Diameter: 0.25 mm
Data Type: Linear RI




(Text File) +EI Scan (16.877 min) ALI-OLE-H7-220421-.D Subtract



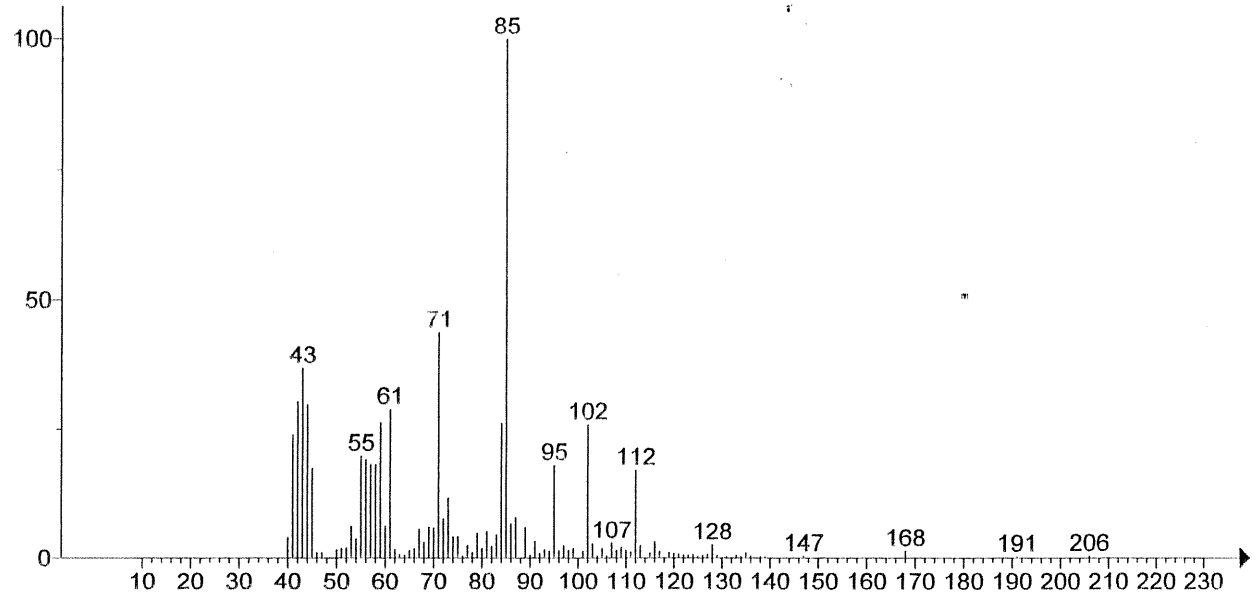

Head to Tail MF=754 RMF=818



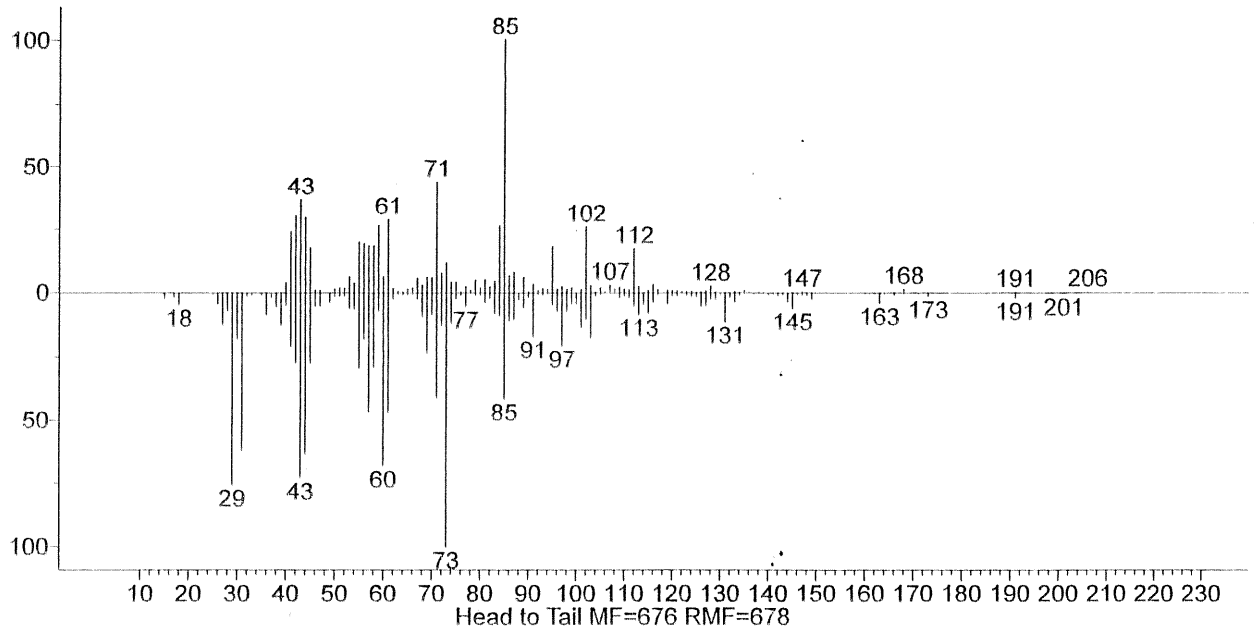

(mainlib) cis-2,6-Dimethyl-2,6-octadiene

Name: cis-2,6-Dimethyl-2,6-octadiene
Formula: $C_{10}H_{18}$
MW: 138 CAS#: 2492-22-0 NIST#: 114539 ID#: 30178 DB: mainlib
Other DBs: IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
69 999 | 41 578 | 95 270 | 39 150 | 67 138 | 70 129 | 53 97 | 123 84 | 55 65 | 27 61 |
Synonyms:
1.(6Z)-2,6-Dimethyl-2,6-octadiene #

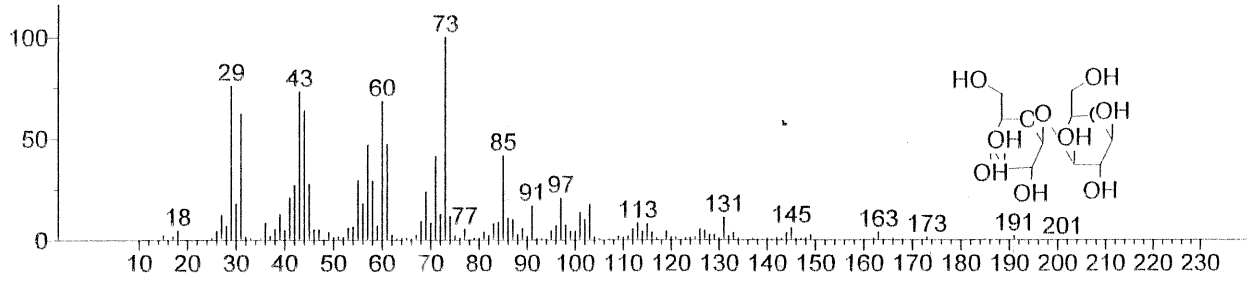
Estimated non-polar retention index (n-alkane scale):
Value: 985 iu
Confidence interval (Hydrocarbons): 39(50%) 167(95%) iu




(Text File) +EI Scan (17.547 min) ALI-OLE-H7-220421-.D



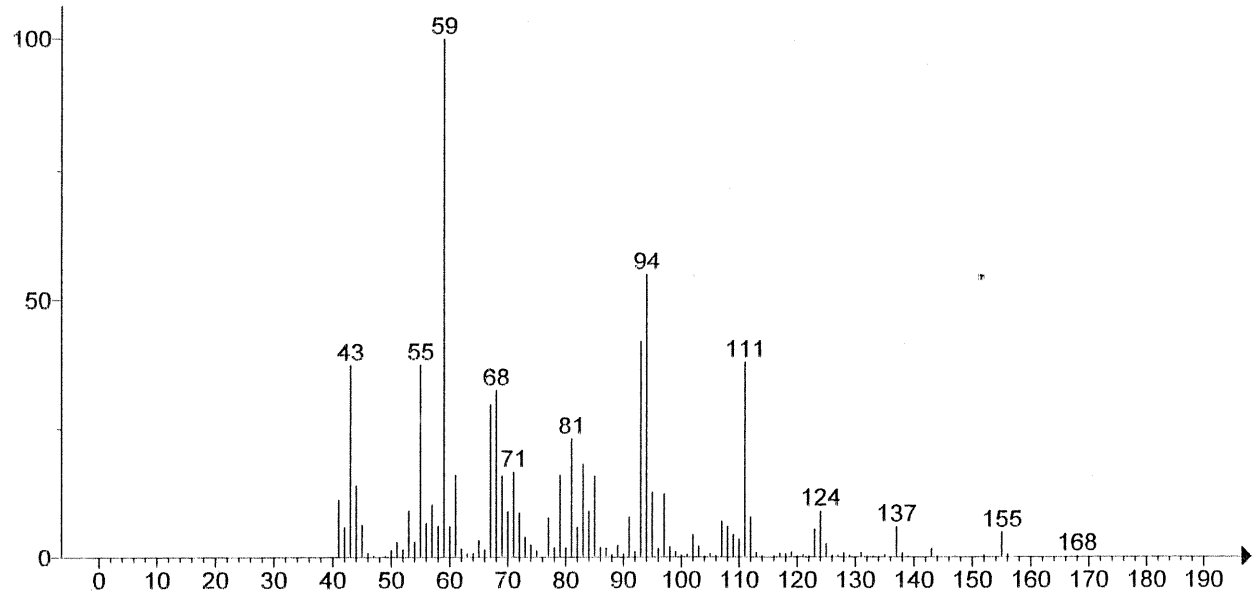

Head to Tail MF=676 RMF=678



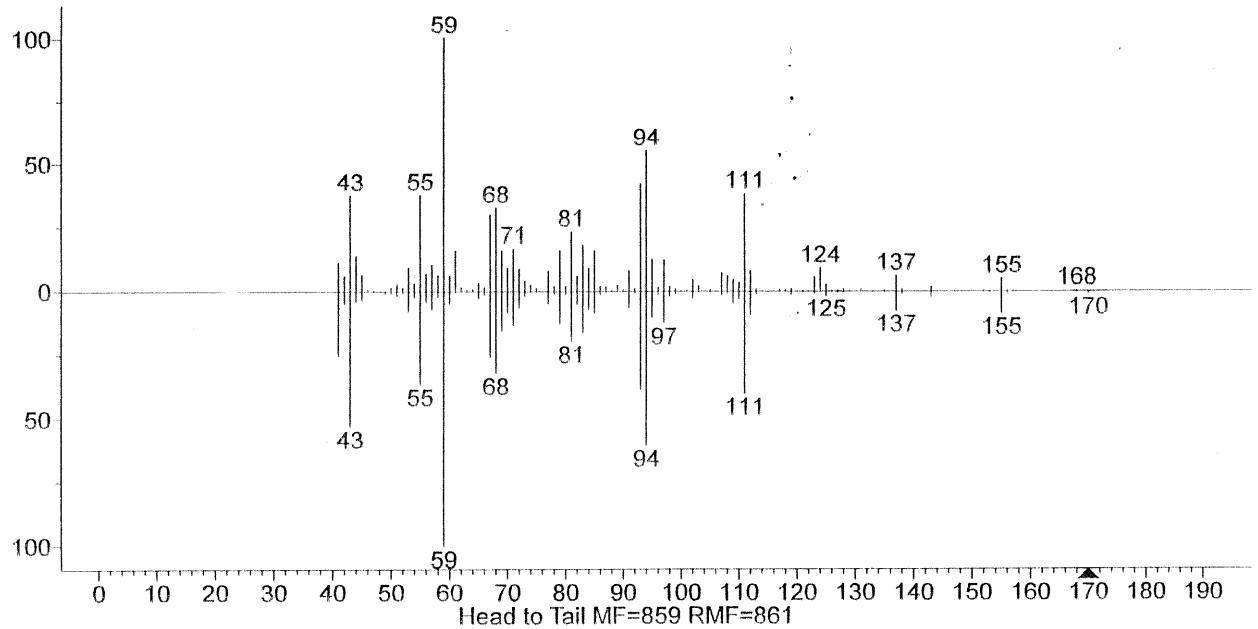

(replib) β-D-Glucopyranose, 4-O-β-D-galactopyranosyl-

Name: β-D-Glucopyranose, 4-O-β-D-galactopyranosyl-
Formula: $C_{12}H_{22}O_{11}$
MW: 342 CAS#: 5965-66-2 NIST#: 76424 ID#: 8344 DB: replib
Other DBs: TSCA, HODOC, EINECS
Contributor: RADIAN CORP
10 largest peaks:
73 999 | 29 757 | 43 729 | 60 681 | 44 636 | 31 620 | 61 470 | 57 468 | 85 416 | 71 412 |
Synonyms:
1.Lactose, β-
2.β-Lactose
3.4-O-Hexopyranosylhexopyranose #

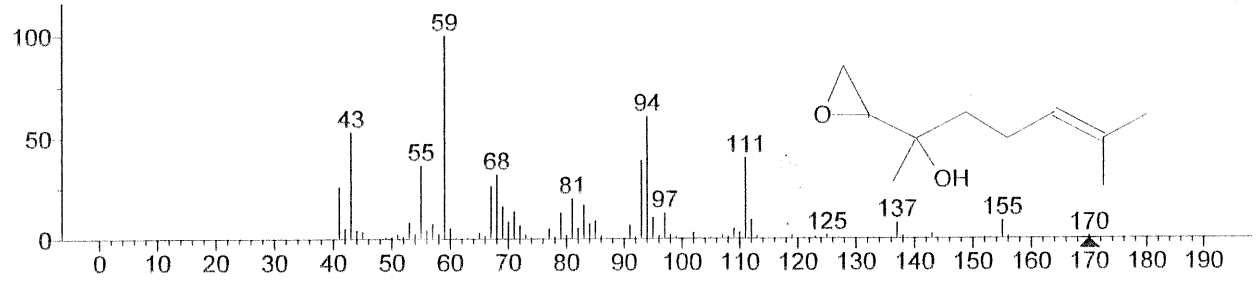
Estimated non-polar retention index (n-alkane scale):
Value: 3131 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu




(Text File) +EI Scan (17.767 min) ALI-OLE-H7-220421-.D



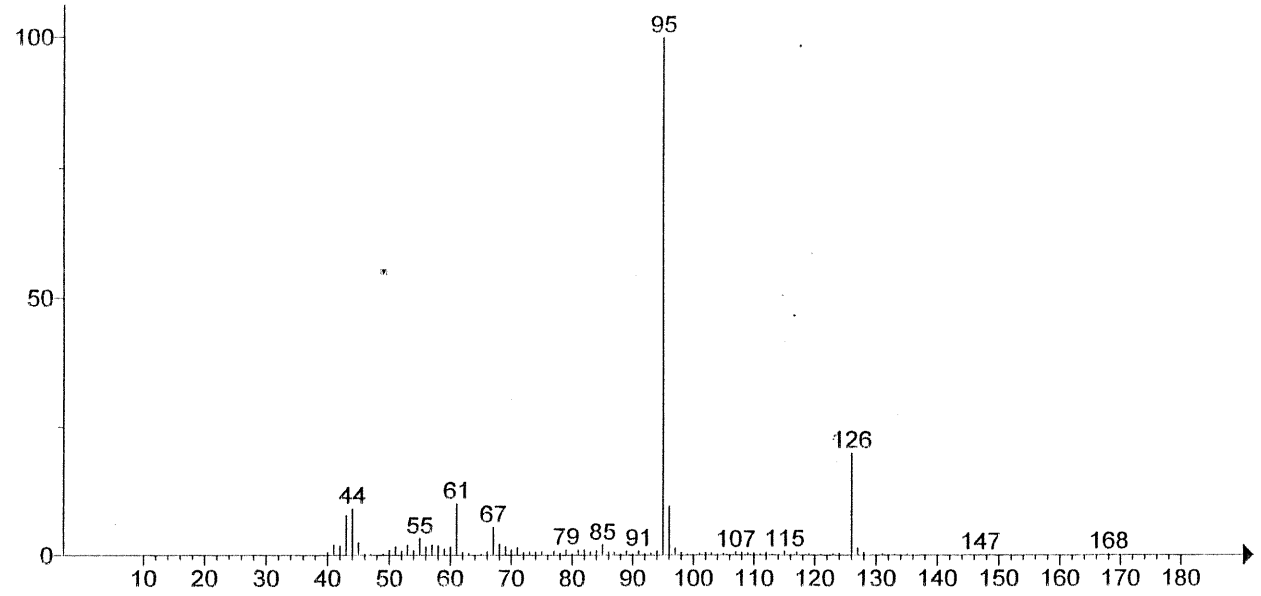

Head to Tail MF=859 RMF=861



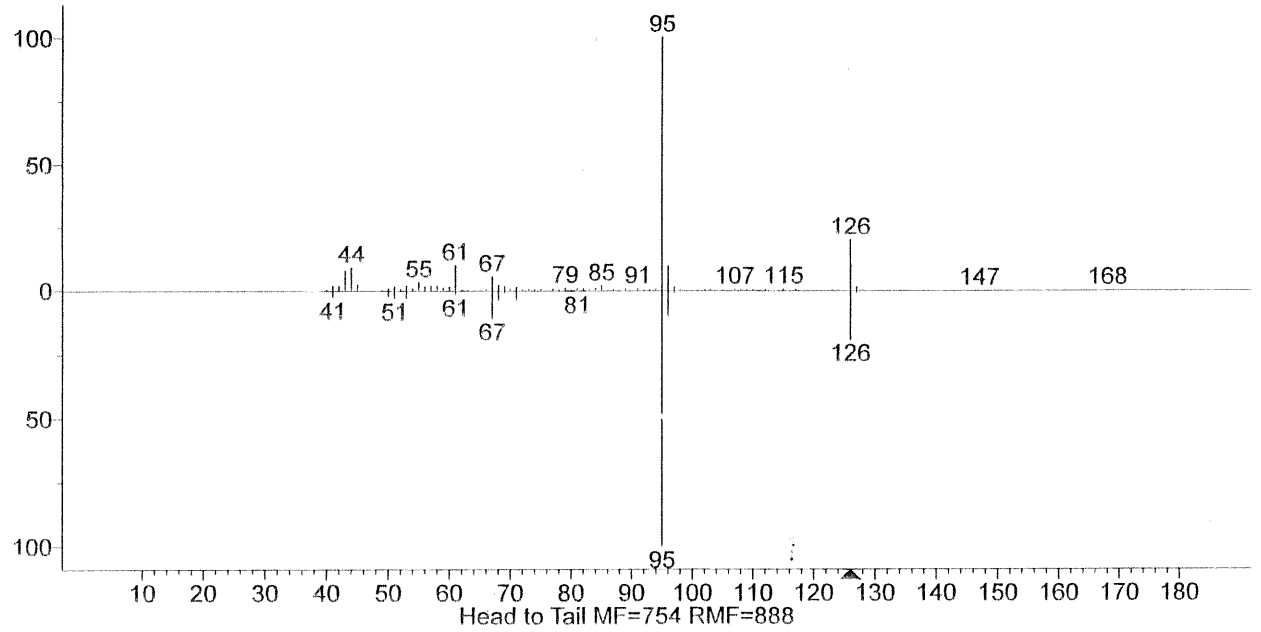

(mainlib) α-Methyl-α-[4-methyl-3-pentenyl]oxiranemethanol

Name: α-Methyl-α-[4-methyl-3-pentenyl]oxiranemethanol
Formula: $C_{10}H_{18}O_2$
MW: 170 NIST#: 132130 ID#: 26674 DB: mainlib
Contributor: Insect Chem. Ecol. Lab., USDA, Beltsville, MD 20705
10 largest peaks:
59 999 | 94 603 | 43 527 | 111 398 | 93 385 | 55 362 | 68 318 | 67 258 | 41 256 | 81 196 |
Synonyms:
no synonyms.

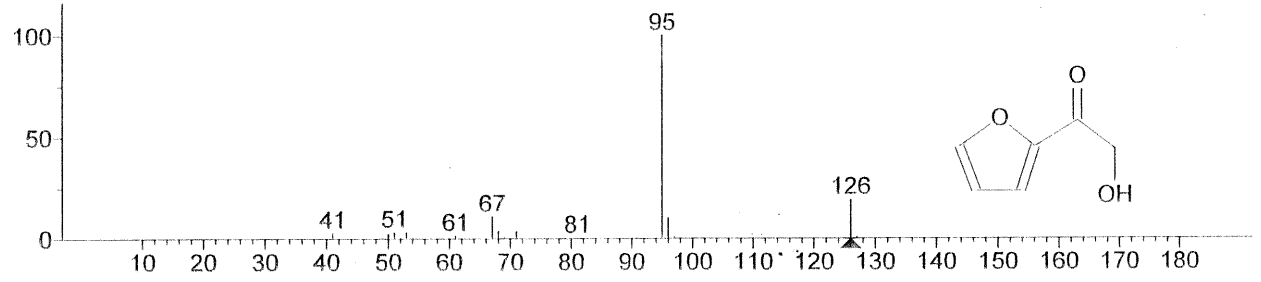
Estimated non-polar retention index (n-alkane scale):
Value: 1182 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu




(Text File) +EI Scan (18.099 min) ALI-OLE-H7-220421-.D




Head to Tail MF=754 RMF=888



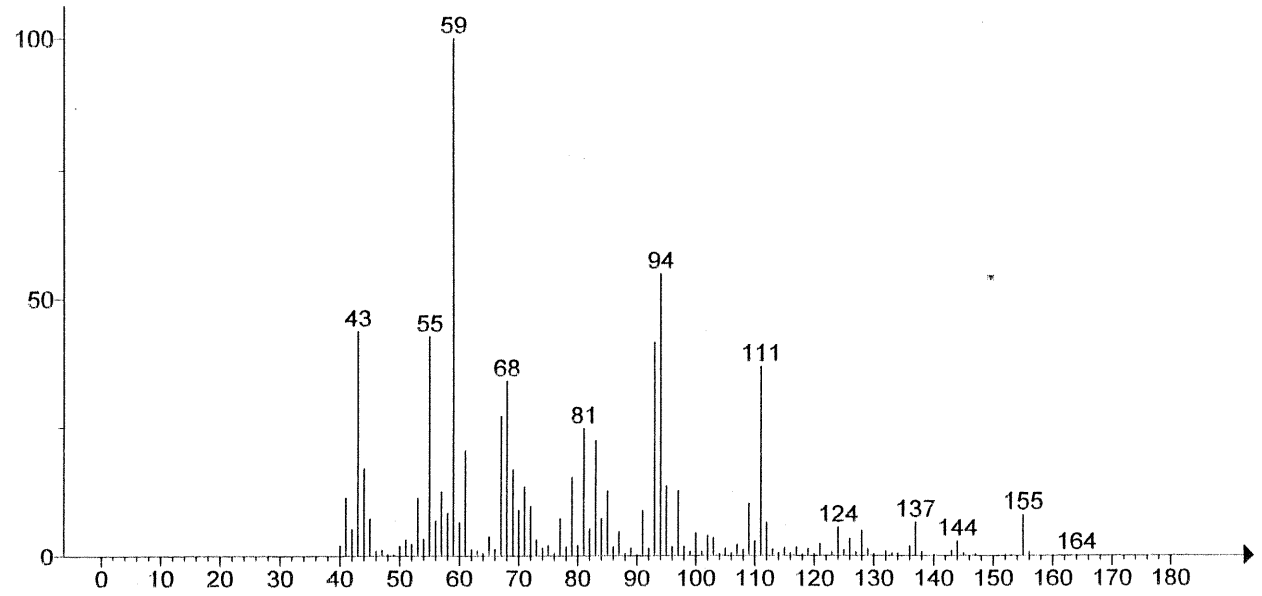

(mainlib) Furyl hydroxymethyl ketone

Name: Furyl hydroxymethyl ketone
Formula: $C_6H_6O_3$
MW: 126 CAS#: 17678-19-2 NIST#: 281423 ID#: 58741 DB: mainlib
Other DBs: None
Contributor: I.Cutzach ET AL.J.Agric.Food Chem.,47,1663(1999)
10 largest peaks:
95 999 | 126 190 | 67 107 | 96 100 | 68 36 | 71 36 | 51 29 | 53 29 | 41 26 | 50 21 |
Synonyms:
1.Ethanone, 1-(2-furanyl)-2-hydroxy-
2.Ketone, 2-furyl hydroxymethyl
3.2-(Hydroxyacetyl)furan
4.2-Furyl hydroxymethyl ketone
5.2-(2'-Hydroxyacetyl)furan
6.2-(1-Oxo-2-hydroxyethyl)furan
7.1-(2-Furyl)-2-hydroxyethanone #

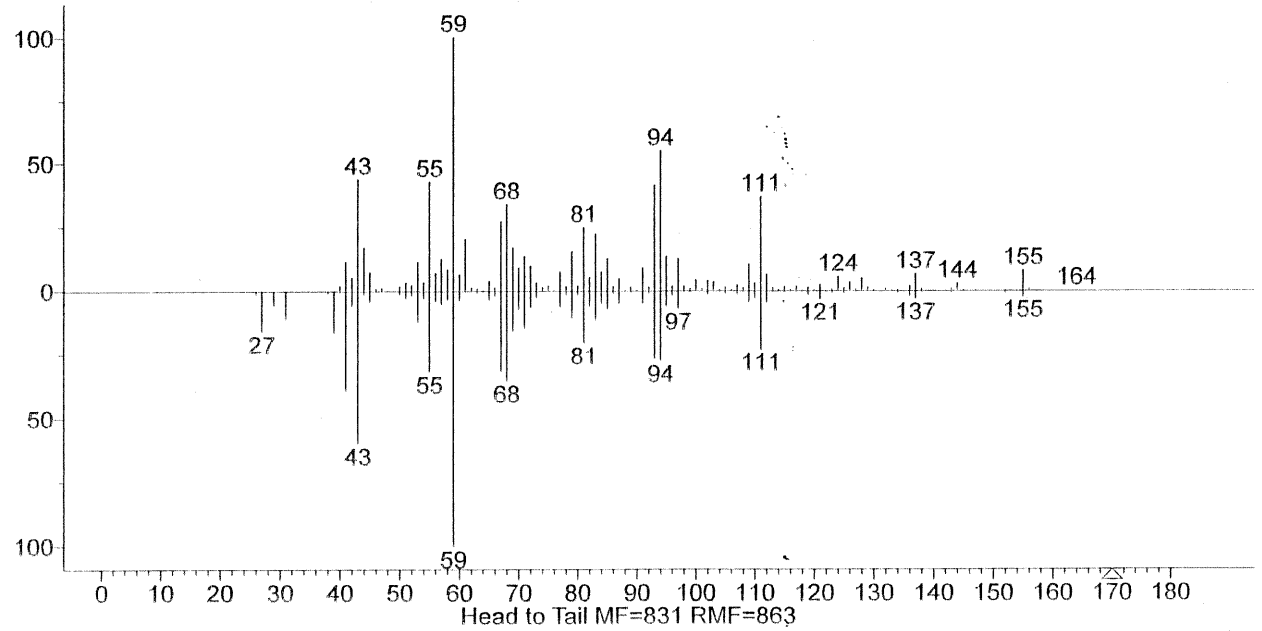
Estimated non-polar retention index (n-alkane scale):
Value: 1121 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1070 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.32 mm
Phase Thickness: 1 um
Data Type: Normal alkane
RI
Program Type: Ramp
Start T: 40 C
End T: 260 C
Heat Rate: 2 K/min
Source: Chen, J.; Ho, C.-T.,
Comparison of volatile generation in serine/threonine/glutamine-ribose/glucose/fructose model systems, J. Agric. Food Chem., 47, 1999, 643-647.

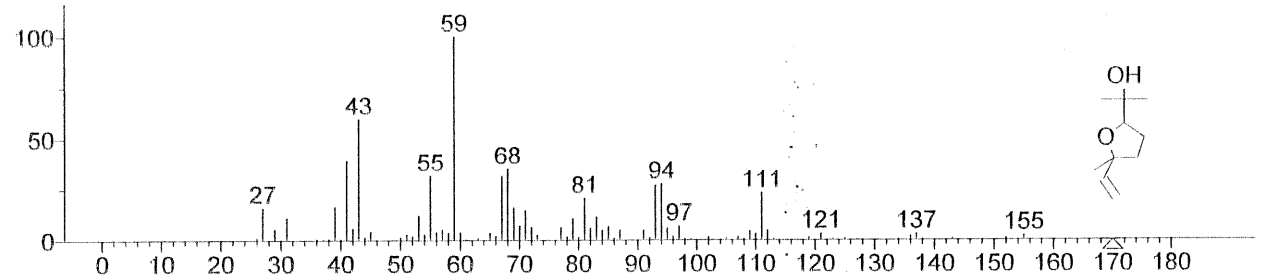
2. Value: 1056 iu
Column Type: Capillary
Column Class: Standard non
-polar
Active Phase: DB-1
Column Length: 60 m
Carrier Gas: He
Column Diameter: 0.32 mm
Phase Thickness:
1.0 um
Data Type: Normal alkane RI
Program Type: Ramp
Start T: 40 C
End T: 280 C




(Text File) +EI Scan (18.398 min) ALI-OLE-H7-220421-.D




Head to Tail MF=831 RMF=863



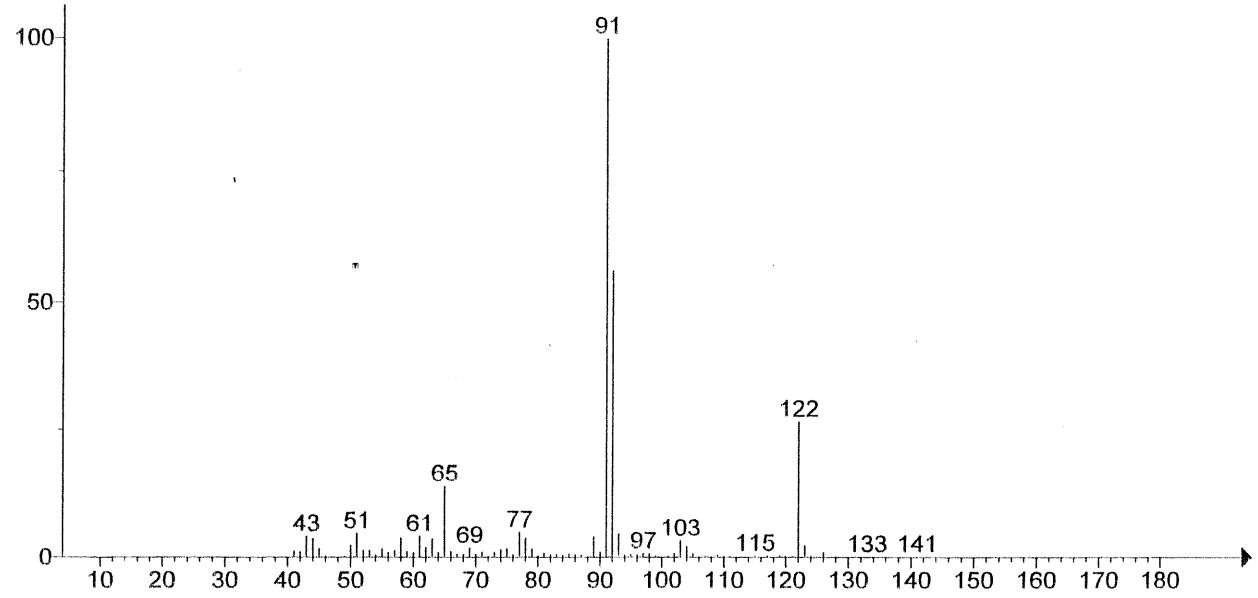

(mainlib) 2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, cis-

Name: 2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, cis-
Formula: $C_{10}H_{18}O_2$
MW: 170 CAS#: 5989-33-3 NIST#: 155746 ID#: 26148 DB: mainlib
Other DBs: TSCA, EINECS
Contributor: Chemical Concepts
10 largest peaks:
59 999 | 43 595 | 41 391 | 68 351 | 55 316 | 67 314 | 94 274 | 93 266 | 111 228 | 81 204 |
Synonyms:
1.Furfuryl alcohol, tetrahydro-α,α,5-trimethyl-5-vinyl-
2.cis-Linalool Oxide
3.cis-Linalyl Oxide
4.cis-5-Ethenyltetrahydro-α,α,5-Trimethyl-2-furanmethanol
5.Linalool oxide
6.Linalool oxide B
7.Linalyl oxide
8.Furfuryl alcohol, tetrahydro-α,α,5-trimethyl-5-vinyl- cis-5-Ethenyltetrahydro-α,α,5-trimethyl-2-furanmethanol
9.Linalool oxide cis
10.Linalool oxide, (Z)-
11.2-(5-Methyl-5-vinyltetrahydro-2-furanyl)-2-propanol #

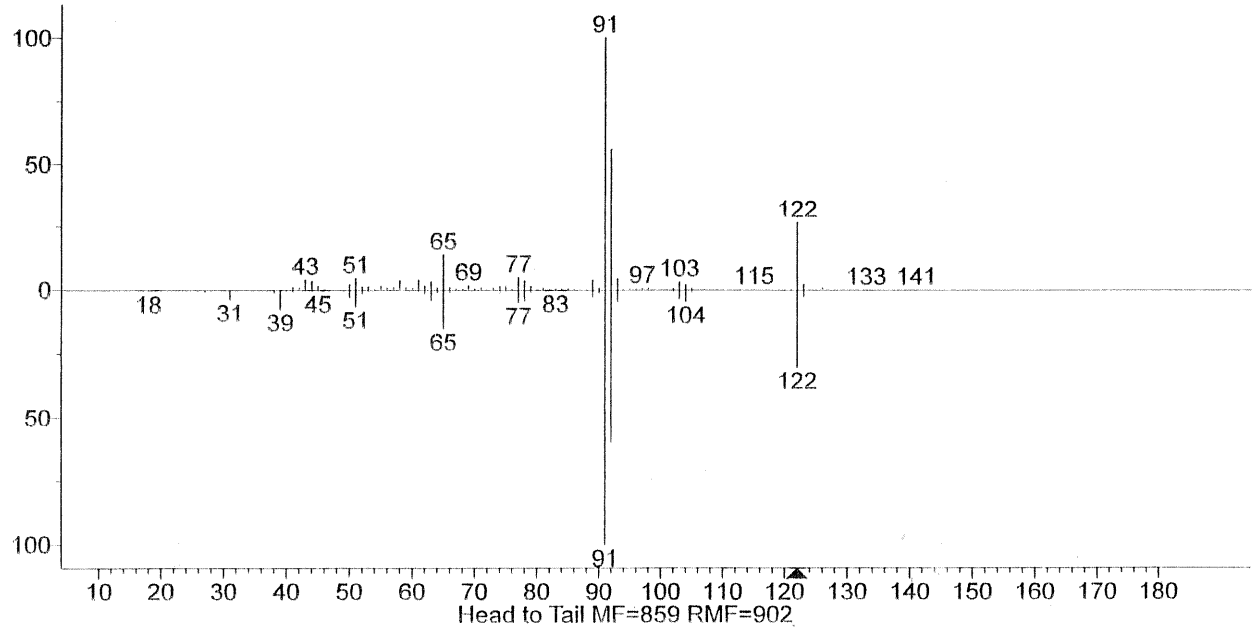
Estimated non-polar retention index (n-alkane scale):
Value: 1164 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1064 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP-Sil PONA
GB
Column Length: 100 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type:
Linear RI
Program Type: Ramp
Start T: 140 C
End T: 230 C
Heat Rate: 5 K/min
Start Time: 10 min
End Time:
25 min
Source: Cunicao, M.M.; Lopes, A.R.; Côcco, L.C.; Yamamoto, C.I.; Plocharski, R.C.B.; Miguel, M.D.; Junior, A.G.; Auer, C.G.; Miguel, O.G., Phytochemical and antibacterial evaluation of essential oils from Ottonia Martiana Miq. (Piperaceae), J. Braz. Chem. Soc., 18(1), 2007, 184-188.

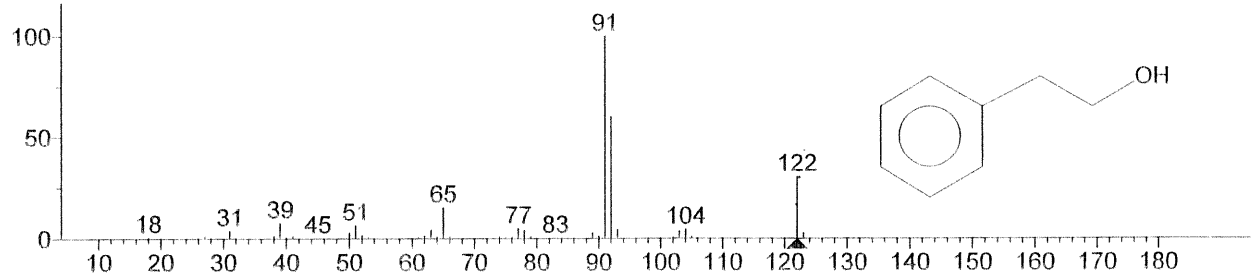
2. Value: 1089 iu
Column Type:
Capillary
Column Class: Standard non-polar
Active Phase: SPB-1
Column Length: 30 m
Carrier Gas:




(Text File) +EI Scan (19.382 min) ALI-OLE-H7-220421-.D




Head to Tail MF=859 RMF=902

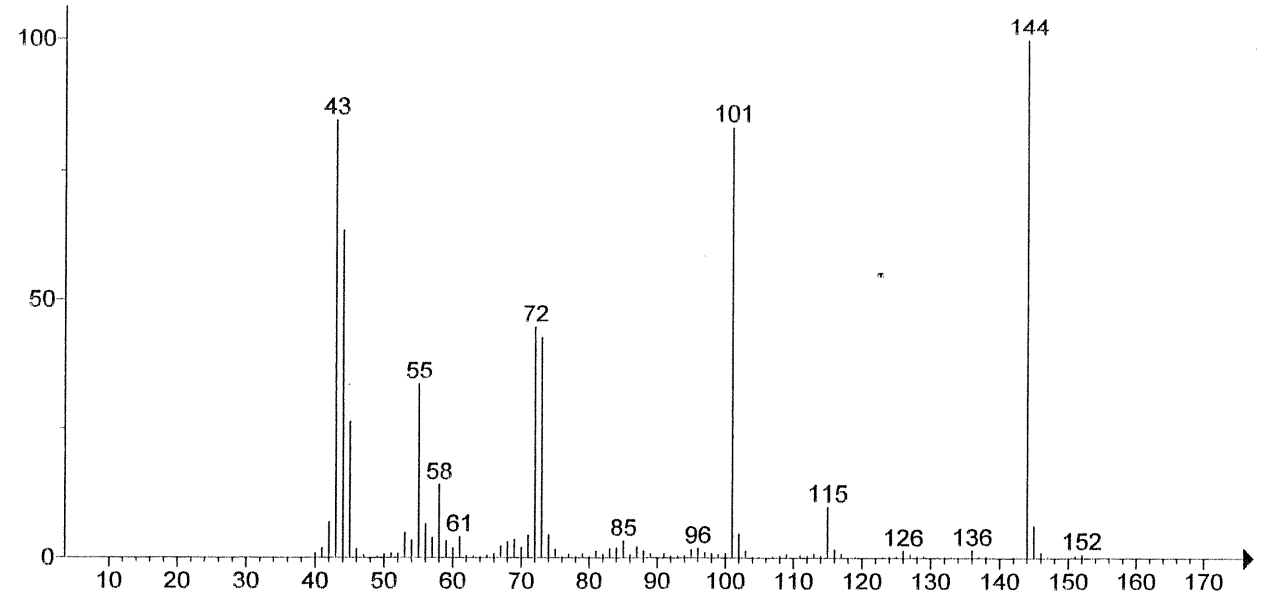



(replib) Phenylethyl Alcohol

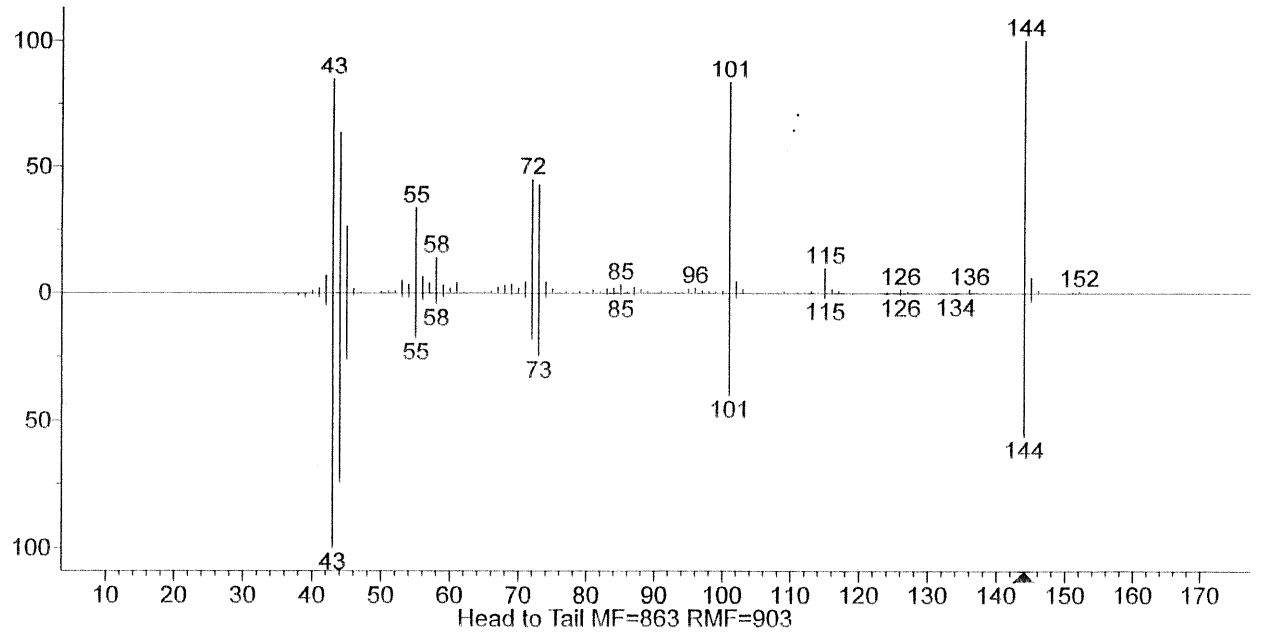
Name: Phenylethyl Alcohol
Formula: $C_8H_{10}O$
MW: 122 CAS#: 60-12-8 NIST#: 229405 ID#: 11425 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW- 710
10 largest peaks:
91 999 | 92 597 | 122 301 | 65 151 | 39 75 | 51 64 | 77 48 | 93 44 | 104 44 | 63 42 |
Synonyms:
1.Benzeneethanol
2.Phenethyl alcohol
3.β-Hydroxyethylbenzene
4.β-Phenethyl alcohol
5.β-Phenylethanol
6.β-Phenylethyl alcohol
7.β-PEA
8.Benzyl Carbinol
9.Ethanol, 2-phenyl-
10.Phenethanol
11.PEA
12.2-Phenethyl Alcohol
13.2-Phenylethanol
14.2-Phenylethyl alcohol
15.Methanol, benzyl-
16.Phenylethanol
17.Phenylethyl, b- alcohol
18.2-PEA
19.β-Fenethylalkohol
20.β-Fenylethanol
21.Orange oil
22.Rose oil
23.β-Phenethanol
24.2-Phenethanol
25.β-P.E.A.
26.1-Phenyl-2-ethanol
27.Hydroxyethylbenzene
28.Mellol
29.Beta-phenylethyl alcohol

Estimated non-polar retention index (n-alkane scale):
Value: 1136 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

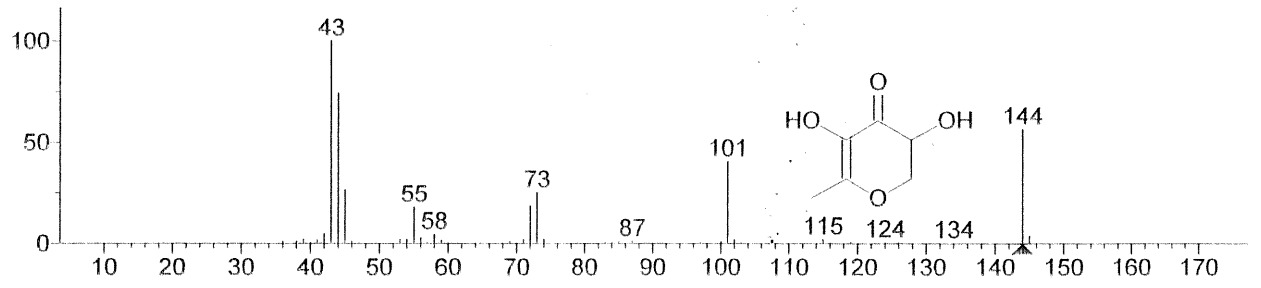
Retention index.
1. Value: 1082.4 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-Petro
Column
Length: 50 m
Column Diameter: 0.2 mm
Phase Thickness: 0.5 um
Data Type: Linear RI
Program Type:
Ramp




(Text File) +EI Scan (20.572 min) ALI-OLE-H7-220421-.D




Head to Tail MF=863 RMF=903




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

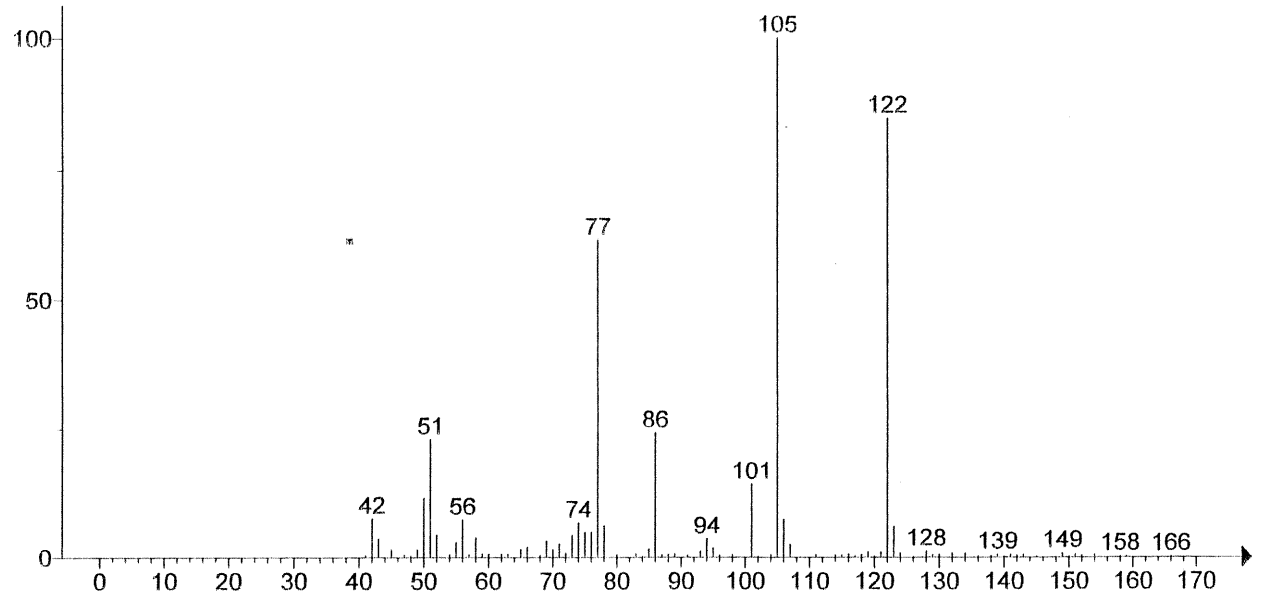
Name: 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
Formula: $C_6H_8O_4$
MW: 144 CAS#: 28564-83-2 NIST#: 108691 ID#: 1857 DB: replib
Other DBs: RTECS
Contributor: Philip Morris R&D
10 largest peaks:
43 999 | 44 742 | 144 563 | 101 402 | 45 264 | 73 249 | 72 182 | 55 177 | 42 48 | 58 43 |
Synonyms: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

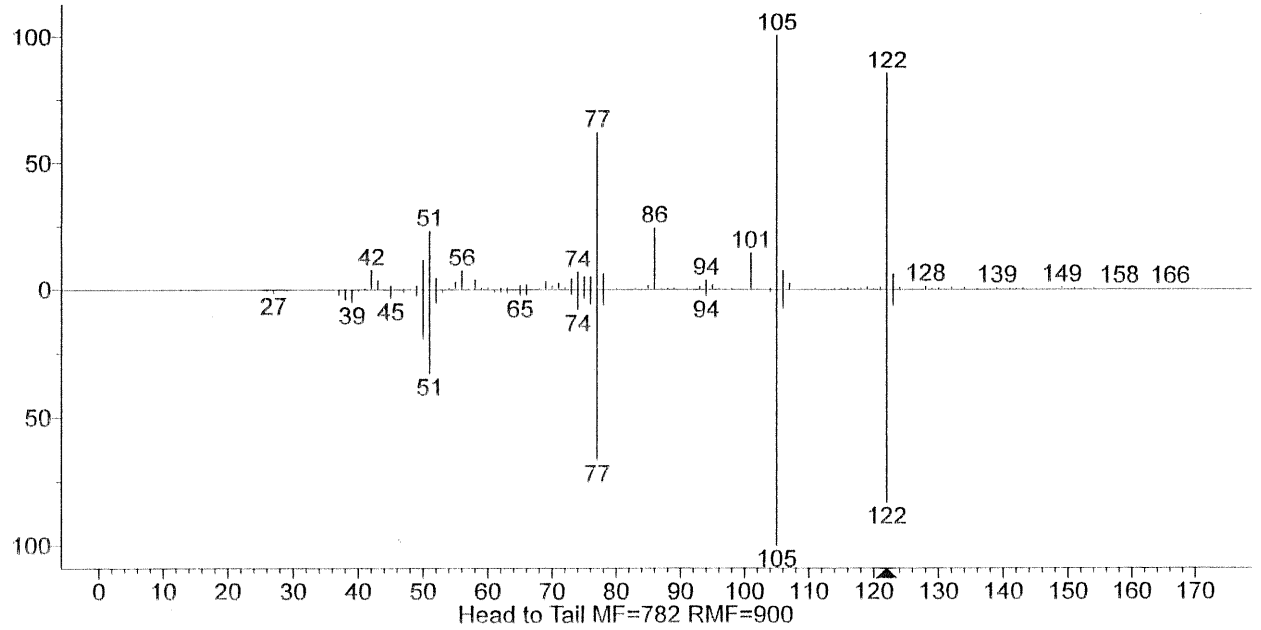
Retention index.
1. Value: 1119 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Complex
Description: -20C (5min) => 10C/min => 100C => 4C/min =>200C => 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.

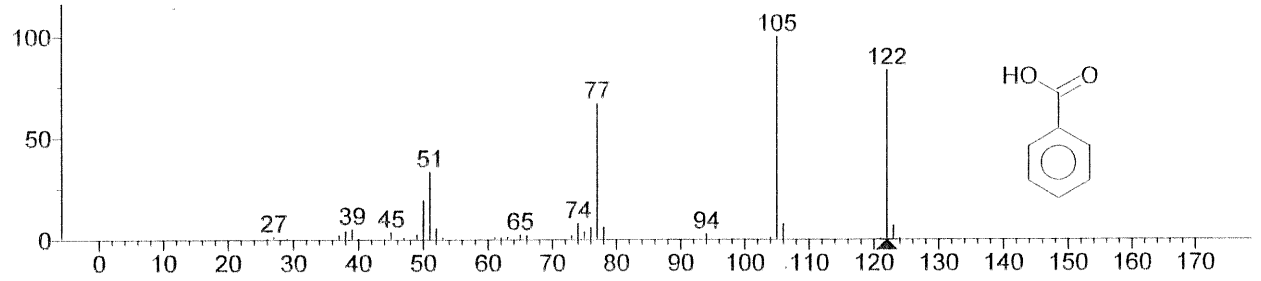
<...>




(Text File) +EI Scan (21.467 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=782 RMF=900

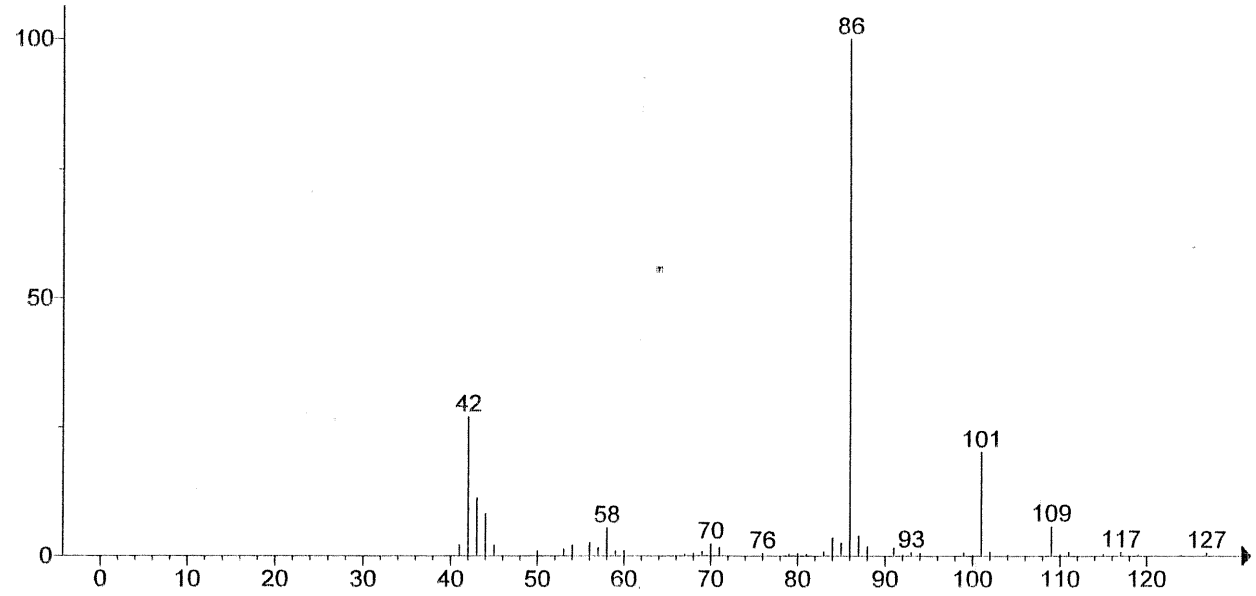



(mainlib) Benzoic acid

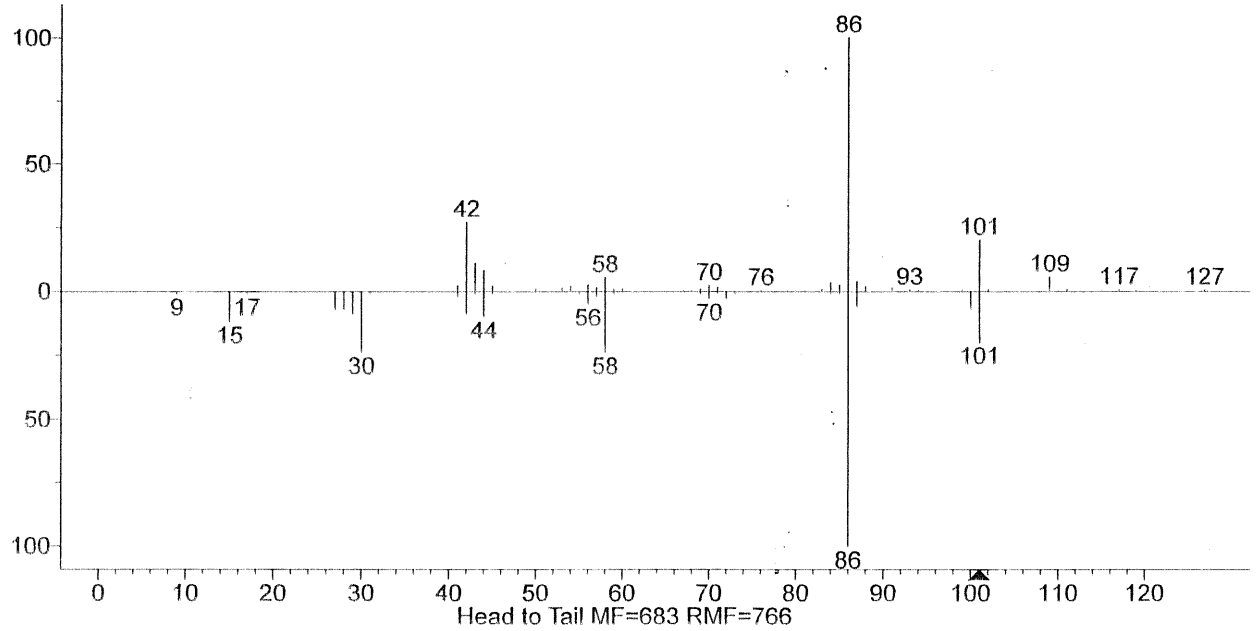
Name: Benzoic acid
Formula: $C_7H_6O_2$
MW: 122 CAS#: 65-85-0 NIST#: 290514 ID#: 68652 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1998.
10 largest peaks:
105 999 | 122 831 | 77 665 | 51 330 | 50 193 | 74 79 | 106 76 | 123 67 | 78 61 | 76 59 |
Synonyms:
1.Benzenecarboxylic acid
2.Benzeneformic acid
3.Benzenemethanoic acid
4.Benzoesaeure GK
5.Benzoesaeure GV
6.Carboxybenzene
7.Dracylic acid
8.Phenylcarboxylic acid
9.Phenylformic acid
10.Retarder BA
11.Retardex
12.Salvo, liquid
13.Solvo, powder
14.Tenn-Plas
15.Acide benzoique
16.Benzoic acid, tech.
17.Kyselina benzoova
18.Salvo
19.Benzoesaeure
20.Salvo powder
21.E 210
22.Ha 1
23.Ha 1 (acid)
24.Salvo liquid
25.Solvo powder
26.Phenylcarboxy
27.Benzenemethonic acid
28.Diacylic acid
29.Flowers of benjamin
30.Flowers of benzoin
31.Nipacide
32.Oracylic acid
33.Predominantly benzoic acid
34.Retarded BA
35.Retarder BA, BAX

Estimated non-polar retention index (n-alkane scale):
Value: 1150 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

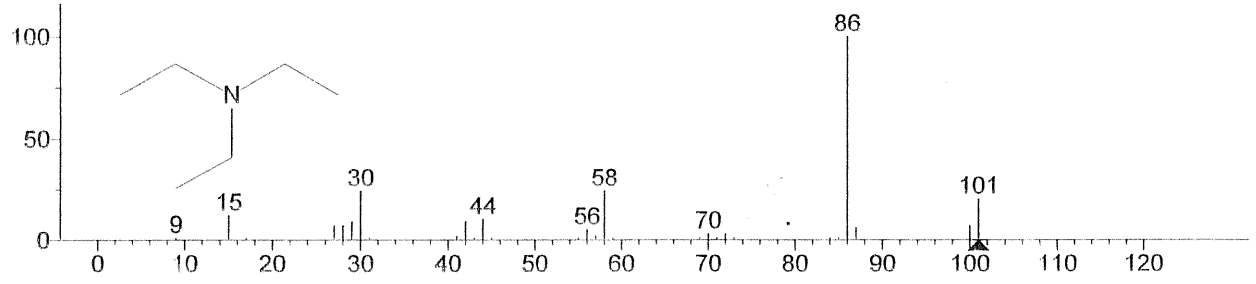
Retention index.
1. Value: 1160 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column




(Text File) +EI Scan (21.702 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=683 RMF=766



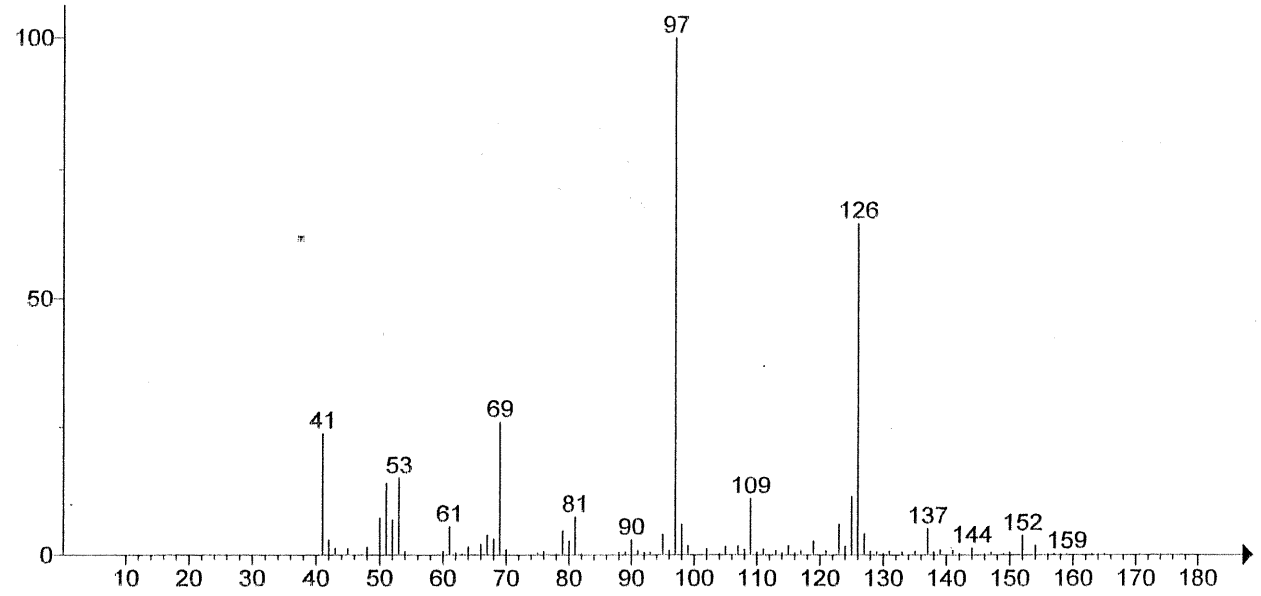

(replib) Triethylamine

Name: Triethylamine
Formula: $C_6H_{15}N$
MW: 101 CAS#: 121-44-8 NIST#: 51537 ID#: 10741 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, EINECS, IRDB
Contributor: CARL DJERASSI DEPT OF CHEM STANFORD UNIV STANFORD CALIF 94305
10 largest peaks:
86 999 | 30 240 | 58 240 | 101 200 | 15 120 | 44 100 | 29 90 | 42 90 | 27 70 | 28 70 |
Synonyms:
1.Ethanamine, N,N-diethyl-
2.(C2H5)3N
3.(Diethylamino)ethane
4.N,N-Diethylethanamine
5.TEN
6.Triaethylamin
7.Trietilamina
8.UN 1296
9.N,N,N-Triethylamine #

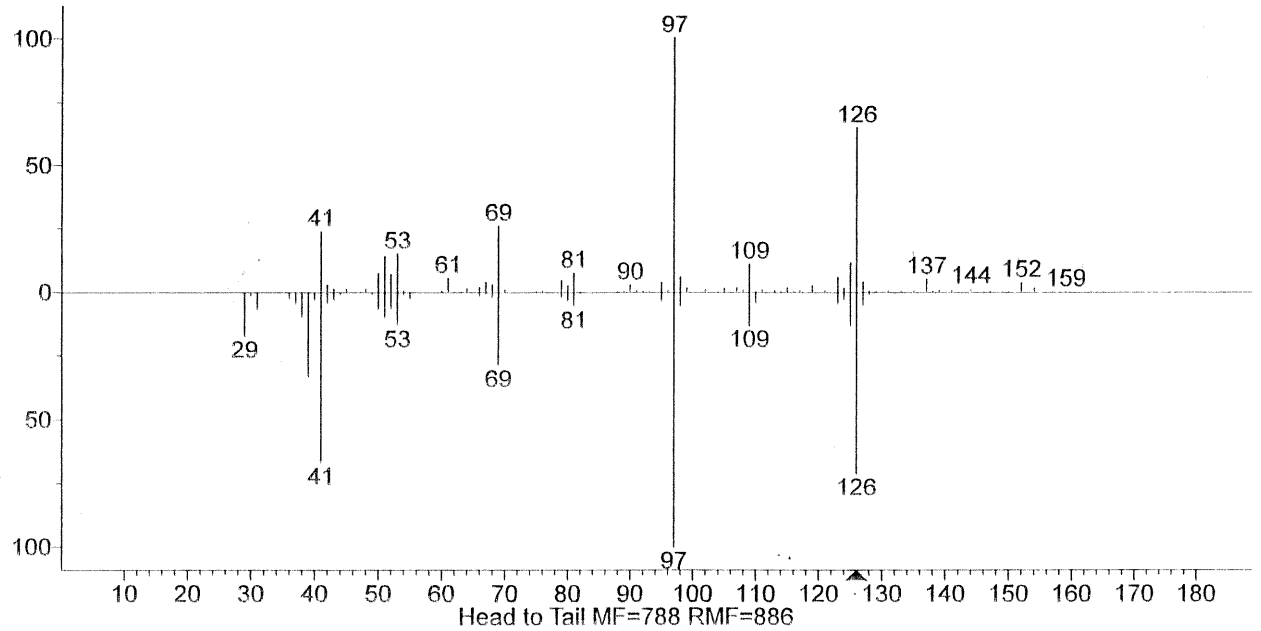
Estimated non-polar retention index (n-alkane scale):
Value: 667 iu
Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu

Retention index.
1. Value: 682 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column Length:
30 m
Carrier Gas: He
Column Diameter: 0.32 mm
Phase Thickness: 5 um
Data Type: Linear RI
Program Type:
Ramp
Start T: 35 C
End T: 270 C
Heat Rate: 10 K/min
Start Time: 1 min
Source: Bartelt, R.J., Calibration of a
commercial solid-phase microextraction device for measuring headspace concentrations of organic volatiles, Anal. Chem., 69, 1997, 364-372.

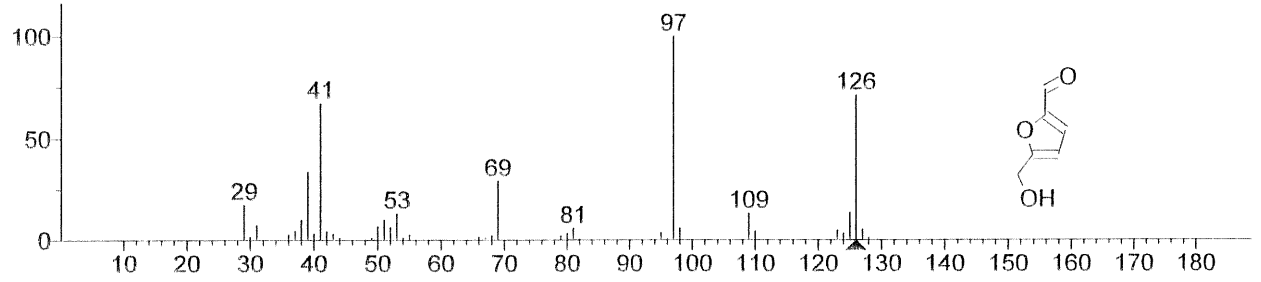
2. Value: 724 iu
Column Type: Packed
Column Class: Standard non-polar
Active
Phase: PMS-100
Column Length: 3 m
Carrier Gas: He
Substrate: Celite 545 (44-60 mesh)
Data Type: Kovats
RI
Program Type: Isothermal




(Text File) +EI Scan (23.623 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=788 RMF=886



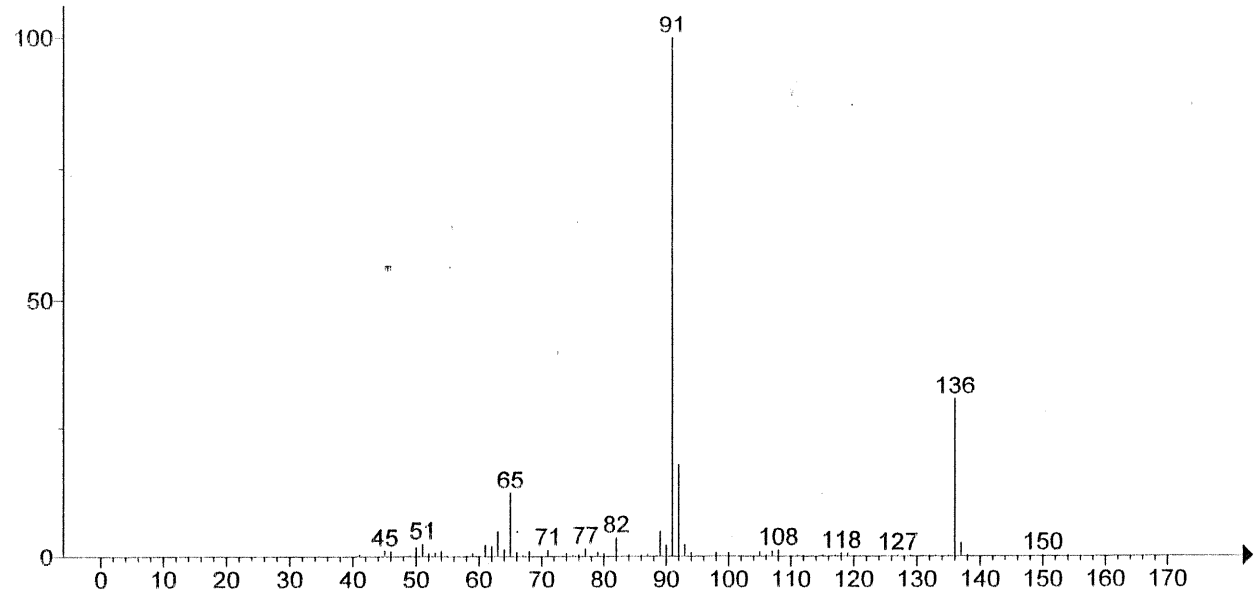

(replib) 2-Furancarboxaldehyde, 5-(hydroxymethyl)-

Name: 2-Furancarboxaldehyde, 5-(hydroxymethyl)-
Formula: $C_6H_6O_3$
MW: 126 CAS#: 67-47-0 NIST#: 60544 ID#: 12795 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS
Contributor: D.HENNEBERG, MAX-PLANCK INSTITUTE, MULHEIM, WEST GERMANY
10 largest peaks:
97 999 | 126 710 | 41 668 | 39 336 | 69 289 | 29 173 | 125 136 | 53 131 | 109 131 | 38 100 |
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

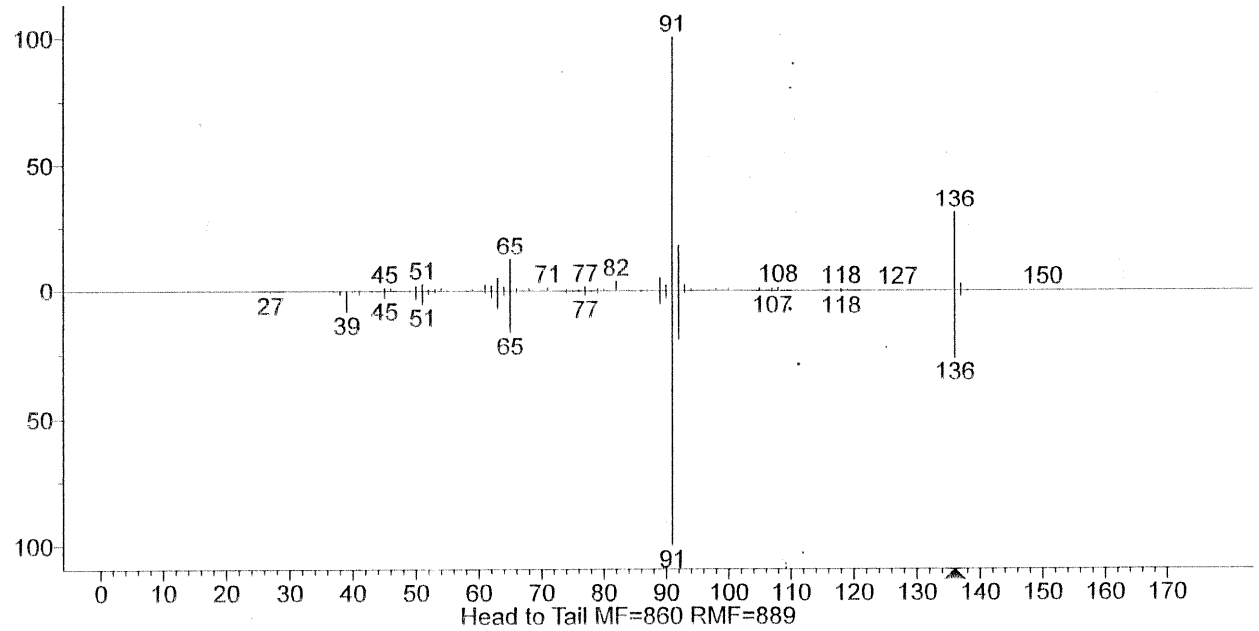
Estimated non-polar retention index (n-alkane scale):
Value: 1163 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

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.

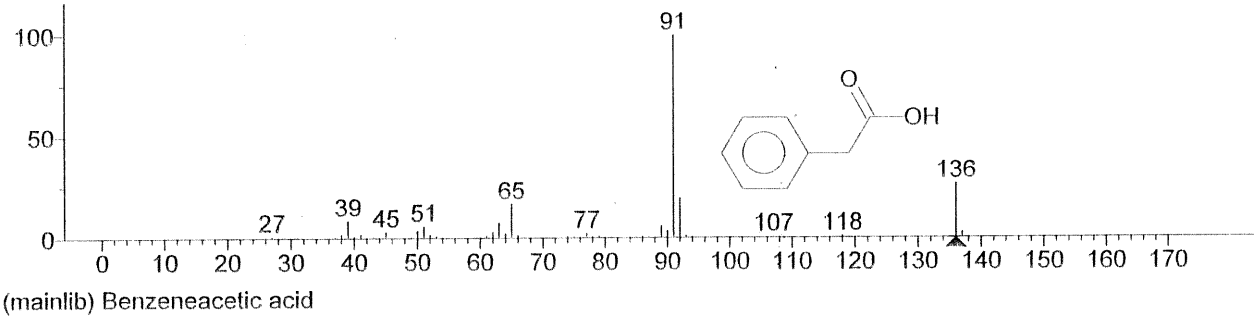
2. Value: 1208 iu




(Text File) +EI Scan (24.424 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=860 RMF=889



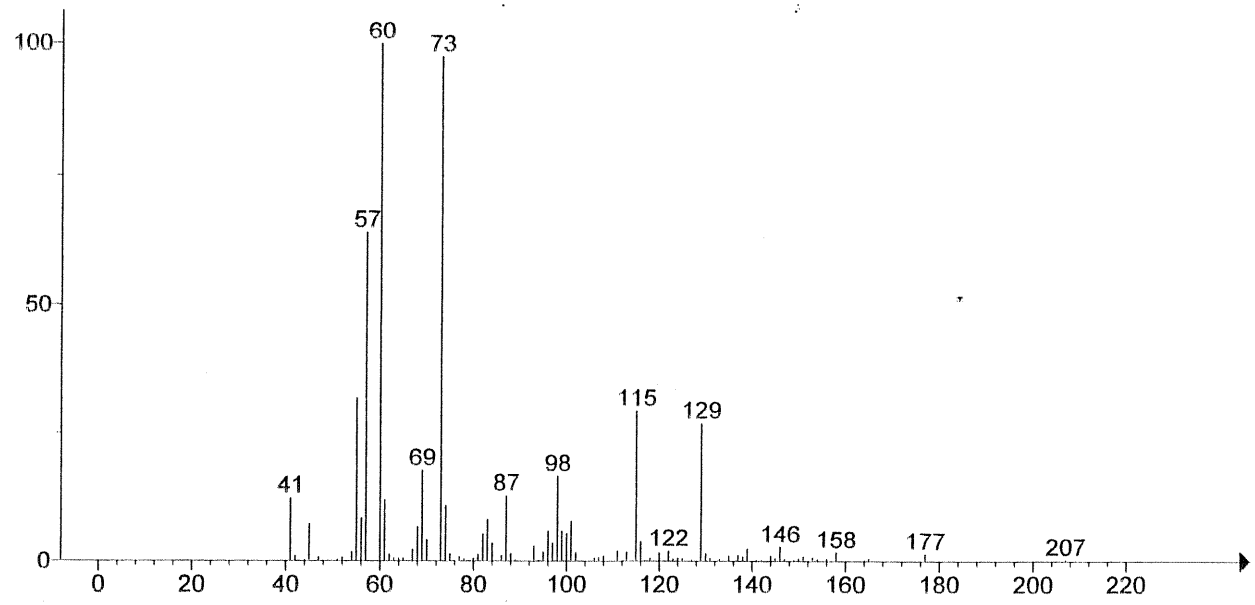

(mainlib) Benzeneacetic acid

Name: Benzeneacetic acid
Formula: $C_8H_8O_2$
MW: 136 CAS#: 103-82-2 NIST#: 352514 ID#: 53145 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
91 999 | 136 264 | 92 191 | 65 163 | 39 83 | 63 72 | 89 56 | 51 55 | 50 34 | 90 33 |
Synonyms:
1.Acetic acid, phenyl-
2.α-Toluic acid
3.Benzenacetic acid
4.Phenylacetic acid
5.ω-Phenylacetic acid
6.Phenylethanoic acid
7.Kyselina fenyloctova
8.2-Phenylacetic acid

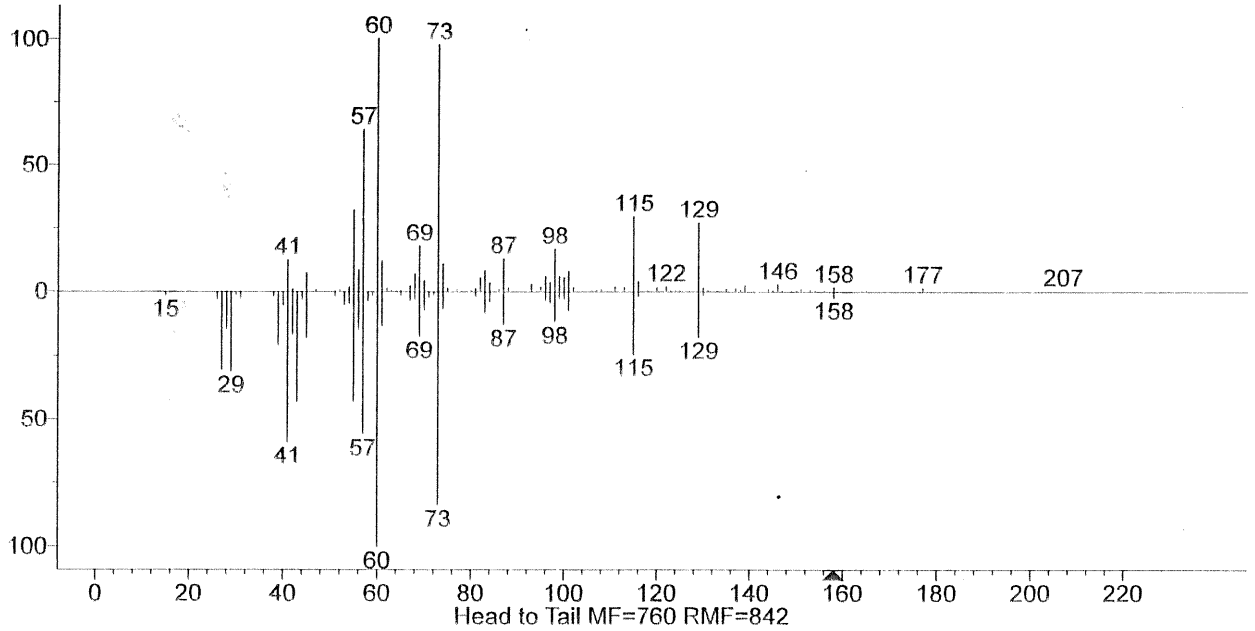
Estimated non-polar retention index (n-alkane scale):
Value: 1249 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.
1. Value: 1251 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 25 m
Column Diameter: 0.2 mm
Phase Thickness: 0.33 um
Data Type: Linear RI
Program Type:
Ramp
Start T: 50 C
End T: 300 C
Heat Rate: 4 K/min
Source: Osorio, C.; Alarcon, M.; Moreno, C.; Bonilla, A.;
Barrios, J.; Garzon, C.; Duque, C., Characterization of Odor-Active Volatiles in Champa ( Campomanesia lineatifolia R. & P.), J. Agric. Food Chem., 54, 2006, 509-516.

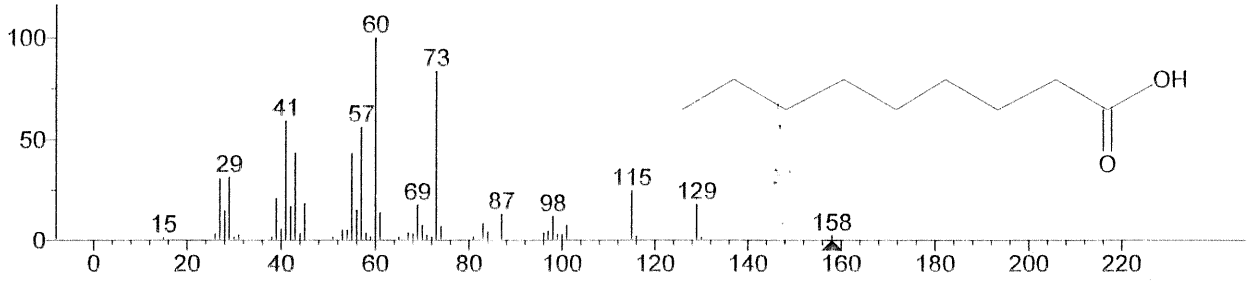
2. Value: 1240 iu
Column Type: Packed
Column Class:
Standard non-polar
Active Phase: SE-30
Column Length: 3.05 m
Carrier Gas: He
Substrate: Supelcoport and
Chromosorb
Data Type: Linear RI
Program Type: Ramp
Start T: 40 C
End T: 250 C
Heat Rate: 10 K/min




(Text File) +EI Scan (25.027 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=760 RMF=842



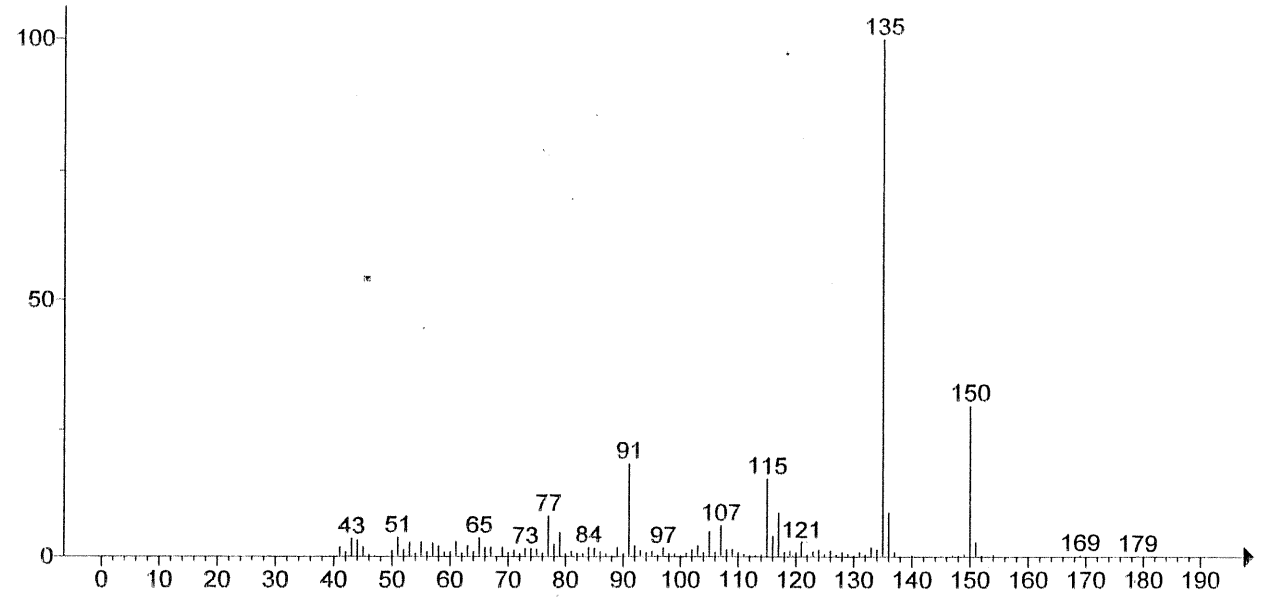

(replib) Nonanoic acid

Name: Nonanoic acid
Formula: $C_9H_{18}O_2$
MW: 158 CAS#: 112-05-0 NIST#: 114735 ID#: 6709 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
60 999 | 73 836 | 41 590 | 57 559 | 43 433 | 55 431 | 29 311 | 27 304 | 115 244 | 39 207 |
Synonyms:
1.n-Nonanoic acid
2.n-Nonoic acid
3.n-Nonylic acid
4.Nonoic acid
5.Nonylic acid
6.Pelargic acid
7.Pelargonic acid
8.1-Octanecarboxylic acid
9.Cirrasol 185a
10.Emfac 1202
11.Hexacid C-9
12.Pelargon
13.Emery's L-114
14.Emery 1202

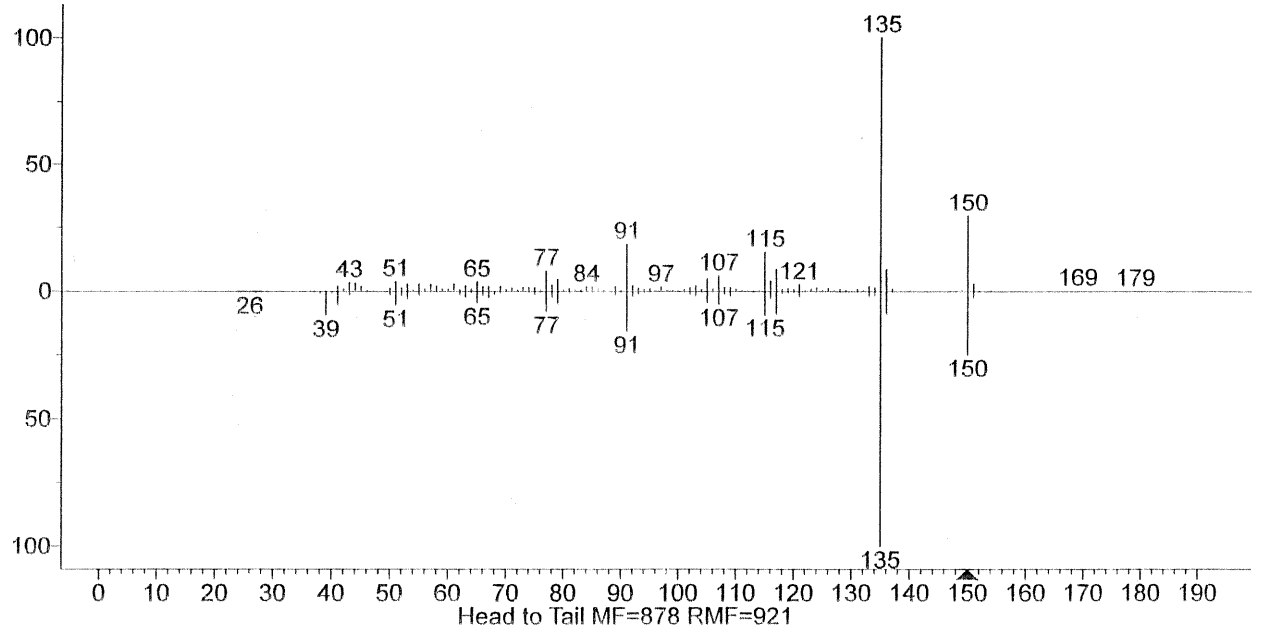
Estimated non-polar retention index (n-alkane scale):
Value: 1272 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.
1. Value: 1268 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 25 m
Column Diameter: 0.2 mm
Phase Thickness: 0.33 um
Data Type: Linear RI
Program Type:
Ramp
Start T: 50 C
End T: 300 C
Heat Rate: 4 K/min
Source: Osorio, C.; Alarcon, M.; Moreno, C.; Bonilla, A.;
Barrios, J.; Garzon, C.; Duque, C., Characterization of Odor-Active Volatiles in Champa ( Campomanesia lineatifolia R. & P.), J. Agric. Food Chem., 54, 2006, 509-516.

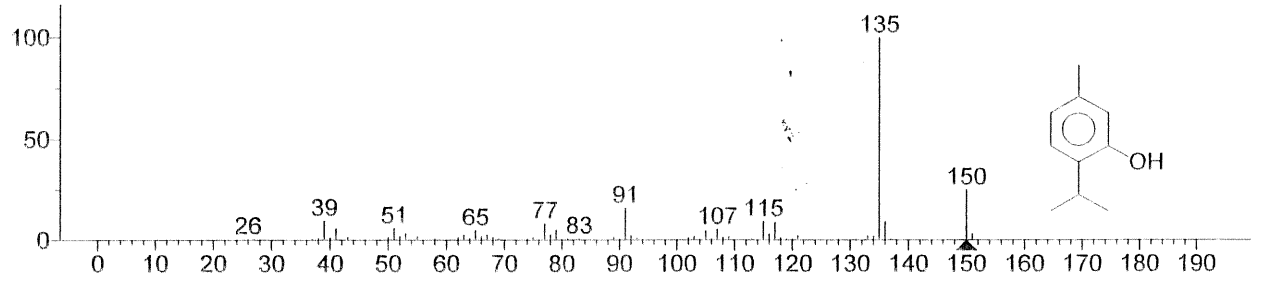
2. Value: 1263 iu
Column Type: Capillary
Column Class:
Standard non-polar
Active Phase: CP Sil 5 CB
Column Length: 25 m
Carrier Gas: H2
Column Diameter: 0.25




(Text File) +EI Scan (25.985 min) ALI-OLE-H7-220421-.D




Head to Tail MF=878 RMF=921

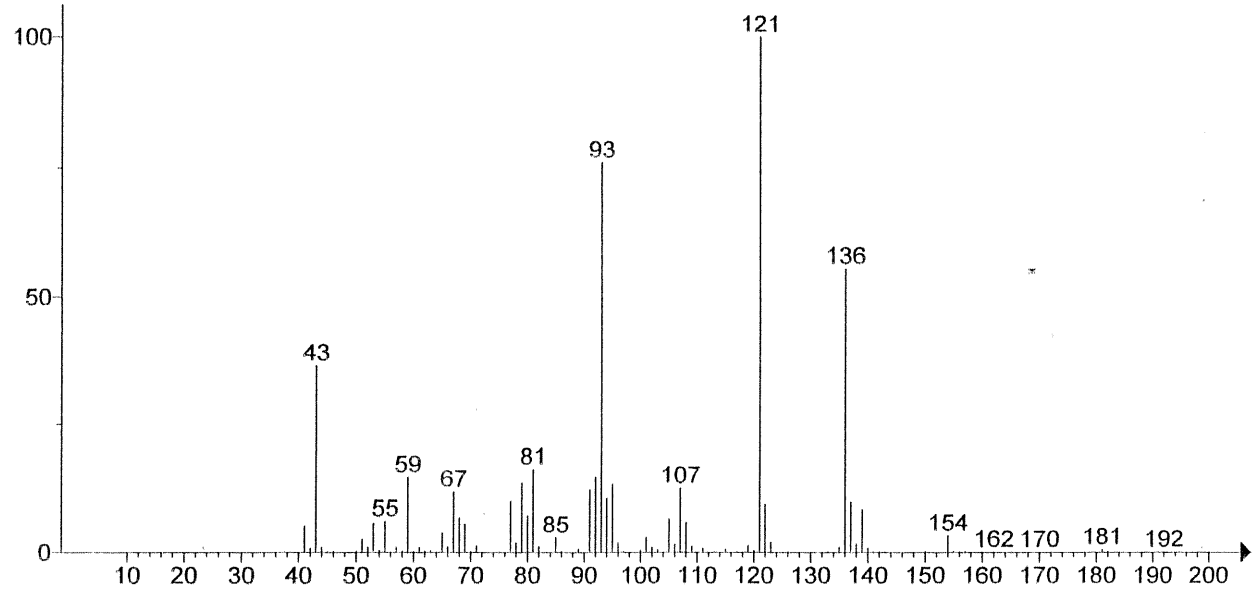



(mainlib) Thymol

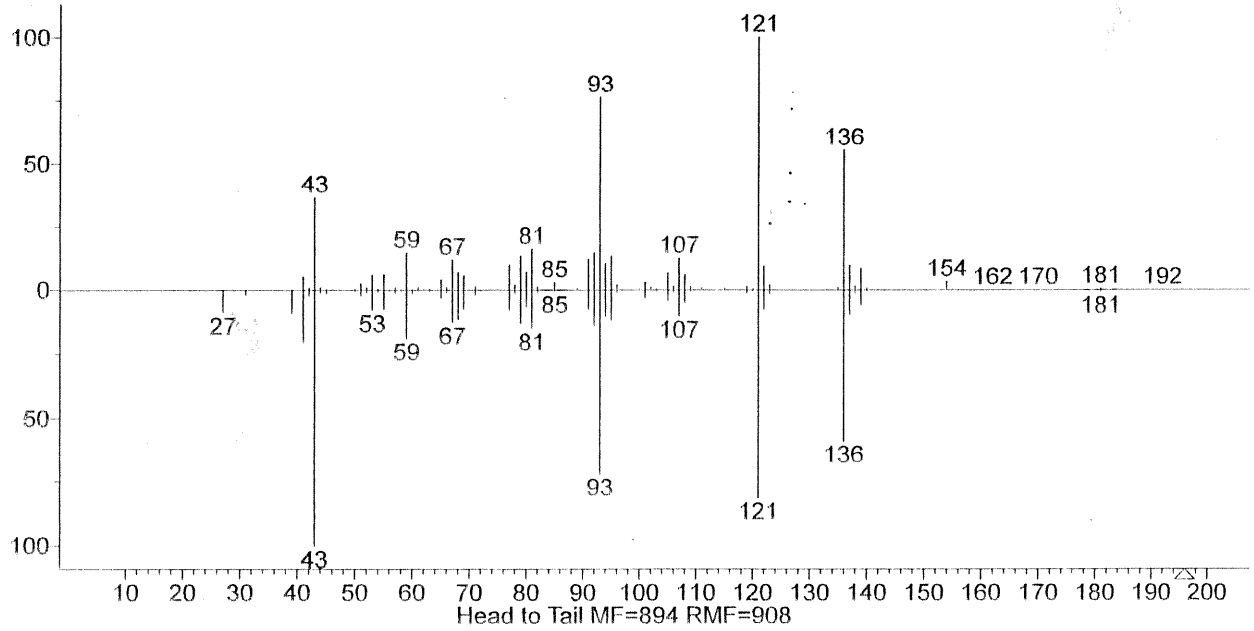
Name: Thymol
Formula: $C_{10}H_{14}O$
MW: 150 CAS#: 89-83-8 NIST#: 249386 ID#: 97695 DB: mainlib
Other DBs: Fine, TSCA, RTECS, USP, HODOC, NIH, EINECS
Contributor: TNO Volatile Compounds in Food - Chemical Concepts
10 largest peaks:
135 999 | 150 248 | 91 157 | 39 94 | 115 91 | 136 89 | 117 87 | 77 80 | 51 56 | 41 55 |
Synonyms:
1.Phenol, 5-methyl-2-(1-methylethyl)-
2.p-Cymen-3-ol
3.Thyme camphor
4.2-Isopropyl-5-methylphenol
5.3-Hydroxy-p-cymene
6.3-Methyl-6-isopropylphenol
7.5-Methyl-2-isopropylphenol
8.6-Isopropyl-m-cresol
9.6-Isopropyl-3-methylphenol
10.m-Cresol, 6-isopropyl-
11.p-Cymene, 3-hydroxy-
12.Isopropyl cresol
13.Phenol, 2-isopropyl-5-methyl-
14.Thymic acid
15.1-Hydroxy-5-methyl-2-isopropylbenzene
16.1-Methyl-3-hydroxy-4-isopropylbenzene
17.3-p-Cymenol
18.3-Hydroxy-1-methyl-4-isopropylbenzene
19.5-Methyl-2-isopropyl-1-phenol
20.5-Methyl-2-(1-methylethyl)phenol
21.Isopropyl-m-cresol
22.m-Thymol

Estimated non-polar retention index (n-alkane scale):
Value: 1262 iu
Confidence interval (Phenols): 70(50%) 301(95%) iu

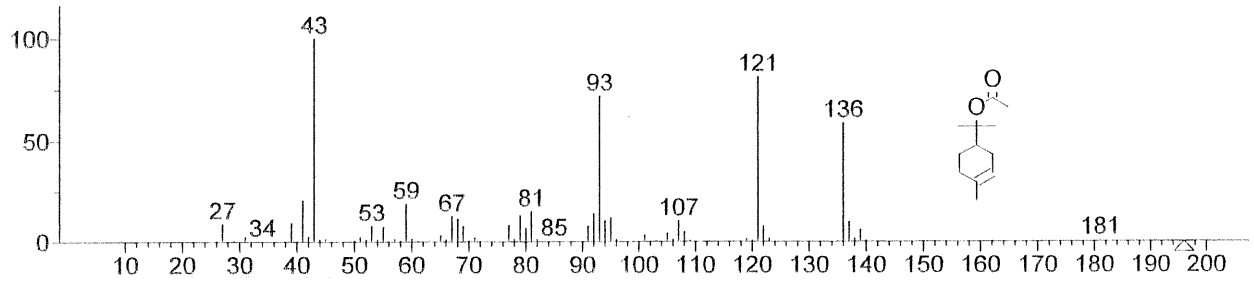
Retention index.
1. Value: 1266 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: RTX-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.22 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C
End T: 230 C
Heat Rate: 2 K/min
End Time: 30 min
Source: Bendahou,
M.; Muselli, A.; Grignon-Dubois, M.; Benyoucef, M.; Desjobert, J.-M.; Bernardini, A.-F.; Costa, J., Antimicrobial




(Text File) +EI Scan (28.102 min) ALI-OLE-H7-220421-.D Subtract



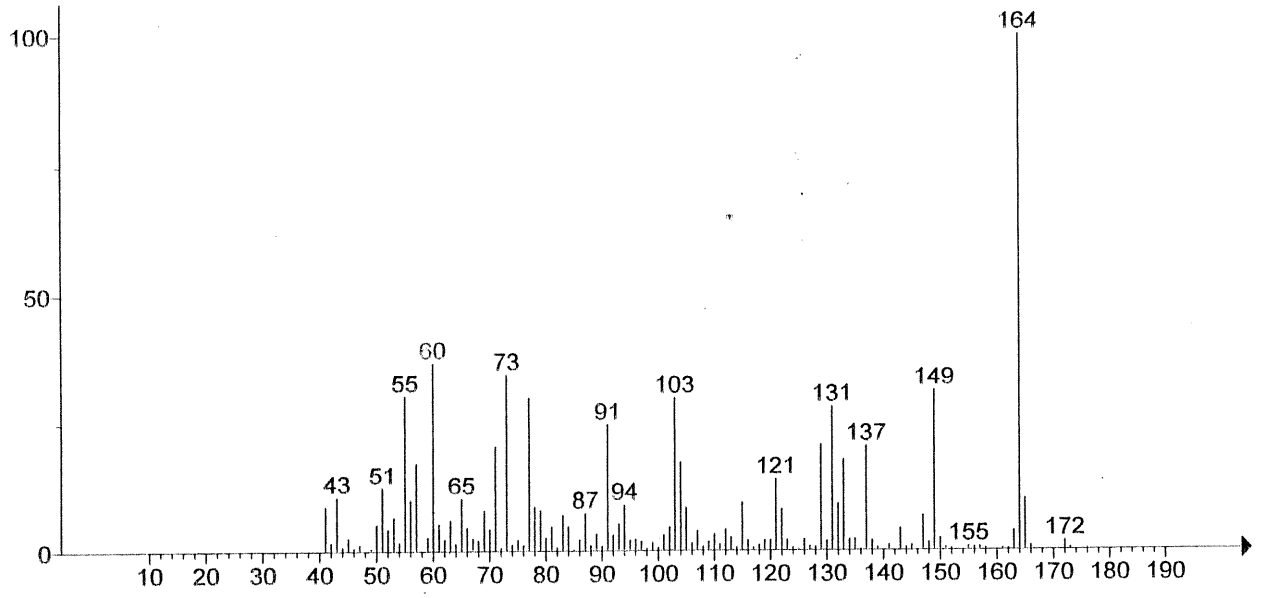

Head to Tail MF=894 RMF=908



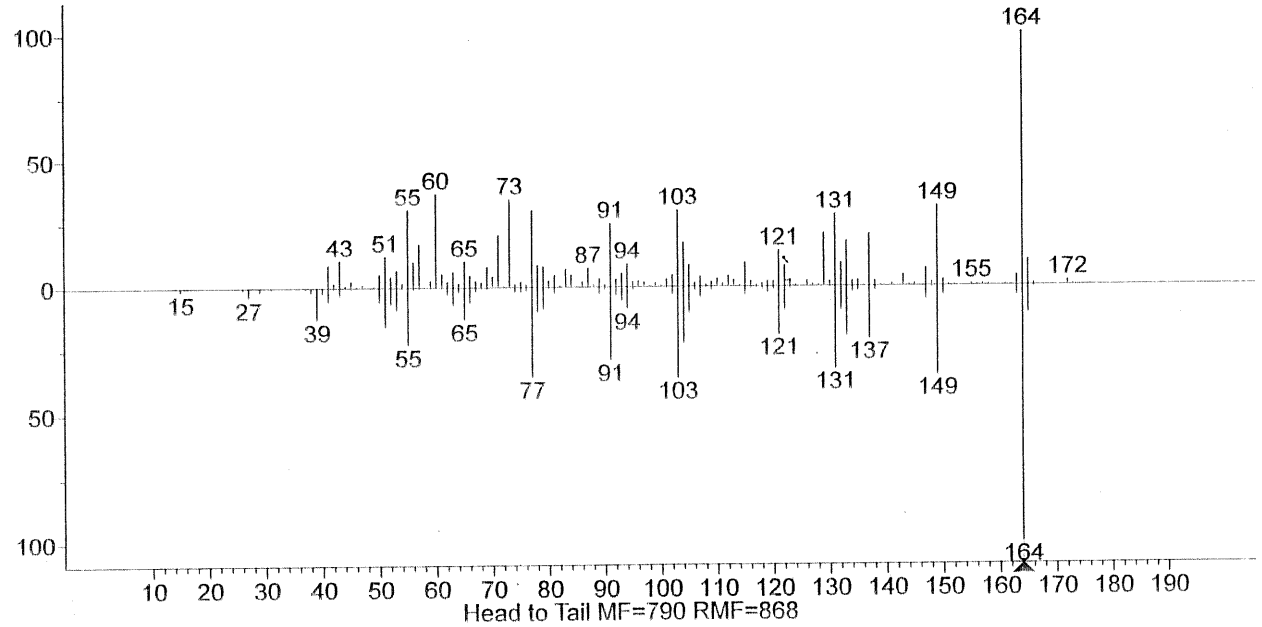

(replib) 3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate

Name: 3-Cyclohexene-1-methanol, α,α,4-trimethyl-, acetate
Formula: $C_{12}H_{20}O_2$
MW: 196 CAS#: 80-26-2 NIST#: 249543 ID#: 2926 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, EINECS
Contributor: TNO Volatile Compounds in Food - Chemical Concepts
10 largest peaks:
43 999 | 121 812 | 93 718 | 136 586 | 41 205 | 59 188 | 81 150 | 92 138 | 79 129 | 67 126 |
Synonyms:
1.p-Menth-1-en-8-ol, acetate
2.α-Terpineol acetate
3.α-Terpinyl acetate
4.Terpinyl acetate
5.1-Methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl acetate #

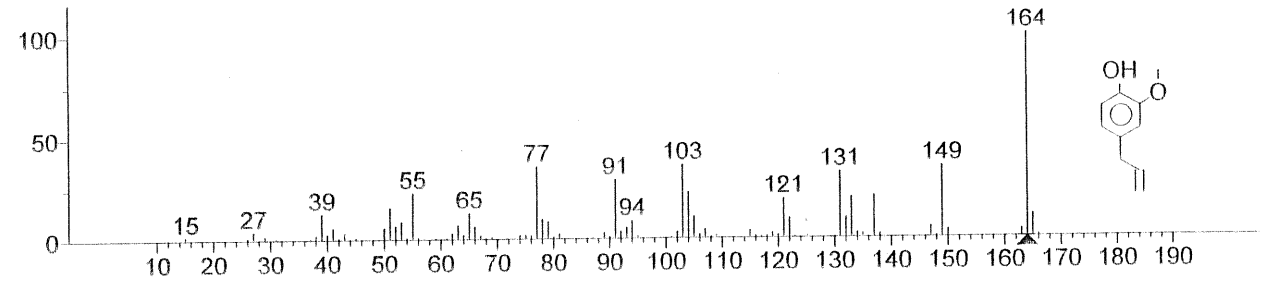
Estimated non-polar retention index (n-alkane scale):
Value: 1333 iu
Confidence interval (Esters): 47(50%) 201(95%) iu




(Text File) +EI Scan (28.366 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=790 RMF=868

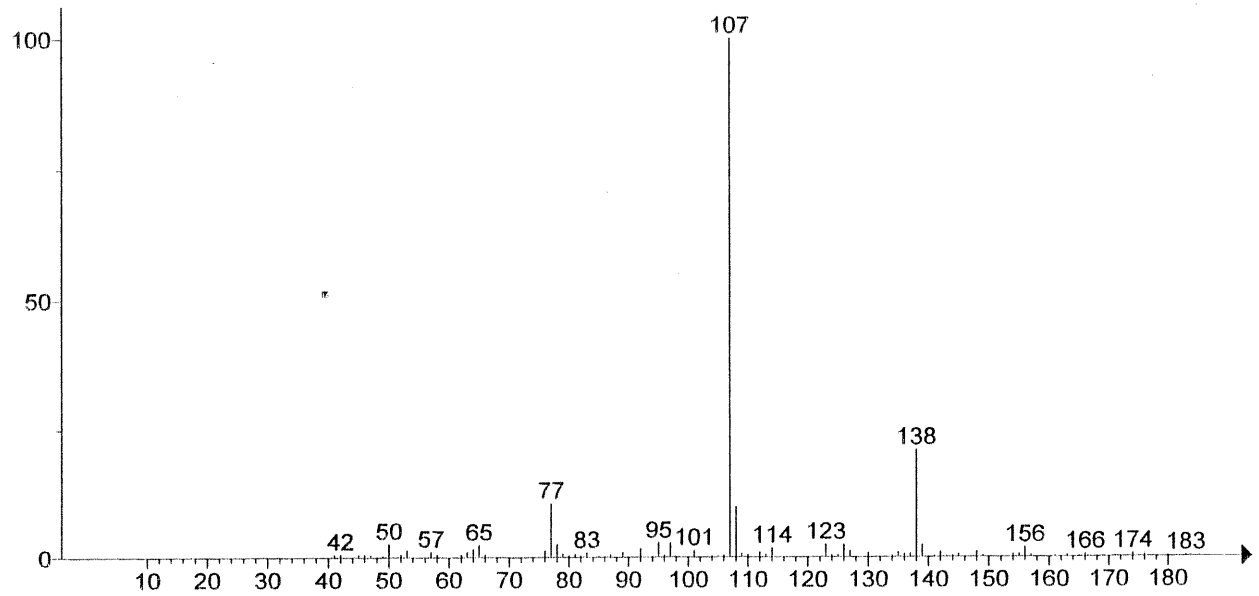



(mainlib) Eugenol

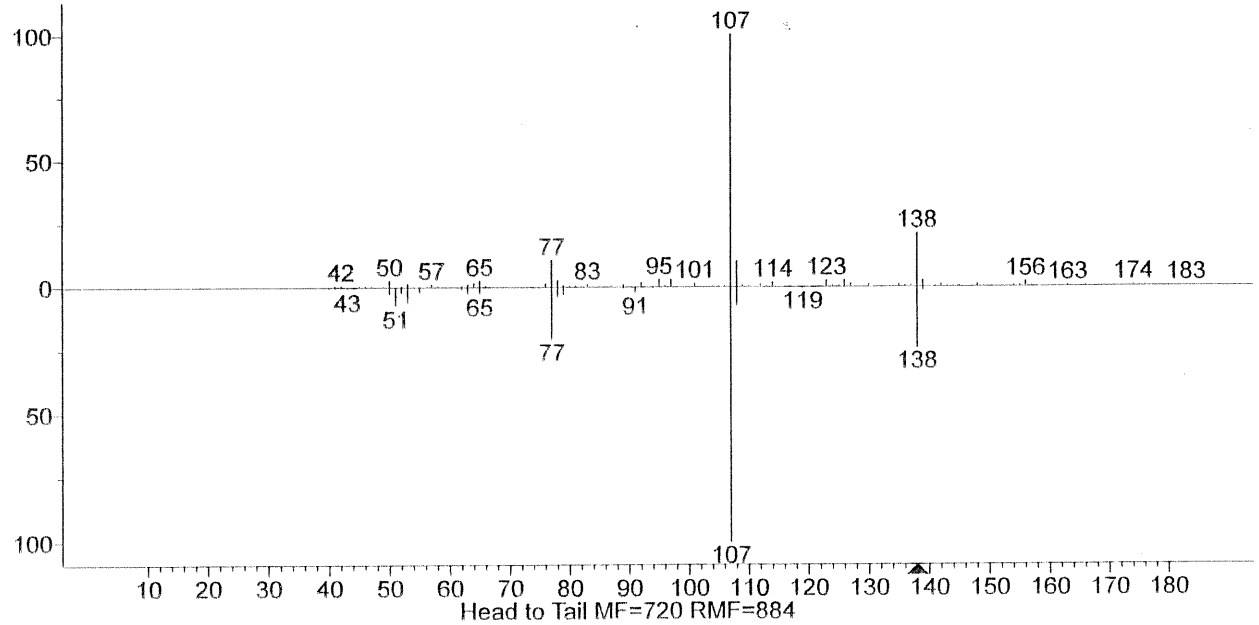
Name: Eugenol
Formula: $C_{10}H_{12}O_2$
MW: 164 CAS#: 97-53-0 NIST#: 291519 ID#: 121999 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1998.
10 largest peaks:
164 999 | 103 360 | 77 355 | 149 350 | 131 323 | 91 288 | 55 227 | 104 225 | 137 207 | 133 197 |
Synonyms:
1.Phenol, 2-methoxy-4-(2-propenyl)-
2.Phenol, 4-allyl-2-methoxy-
3.p-Allylguaiacol
4.p-Eugenol
5.Caryophyllic acid
6.Engenol
7.Eugenic acid
8.2-Methoxy-1-hydroxy-4-allylbenzene
9.2-Methoxy-4-allylphenol
10.4-Allyl-2-methoxyphenol
11.4-Allylguaiacol
12.4-Hydroxy-3-methoxyallylbenzene
13.NCI-C50453
14.1-Hydroxy-2-methoxy-4-allylbenzene
15.1-Hydroxy-2-methoxy-4-prop-2-enylbenzene
16.2-Methoxy-4-(2-propenyl)phenol
17.2-Methoxy-4-prop-2-enylphenol
18.4-Allyl-1-hydroxy-2-methoxybenzene
19.4-Allylcatechol-2-methyl ether
20.1,3,4-Eugenol
21.FA 100
22.Fema no. 2467
23.2-Metoksy-4-allilofenol
24.2-Hydroxy-5-allylanisole
25.2-Methoxy-4-(2-propenyl)phenyl
26.Allylguaiacol

Estimated non-polar retention index (n-alkane scale):
Value: 1392 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

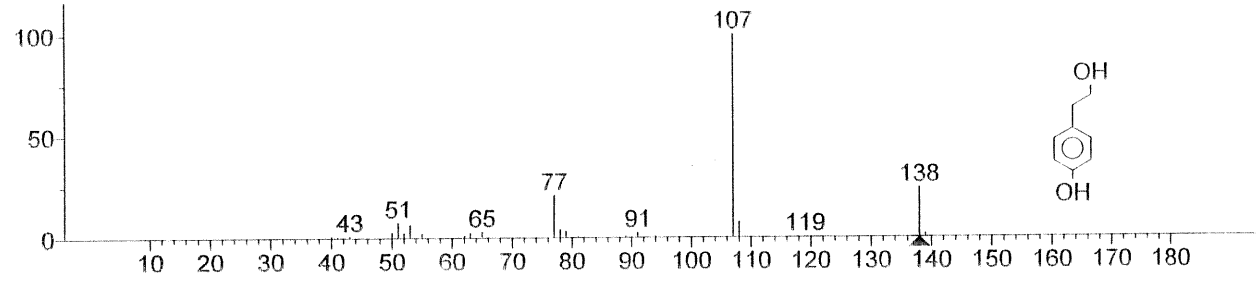
Retention index.
1. Value: 1337 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: BP-1
Column
Length: 50 m
Carrier Gas: He
Column Diameter: 0.22 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C
End T: 220 C




(Text File) +EI Scan (30.607 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=720 RMF=884




(replib) Benzeneethanol, 4-hydroxy-

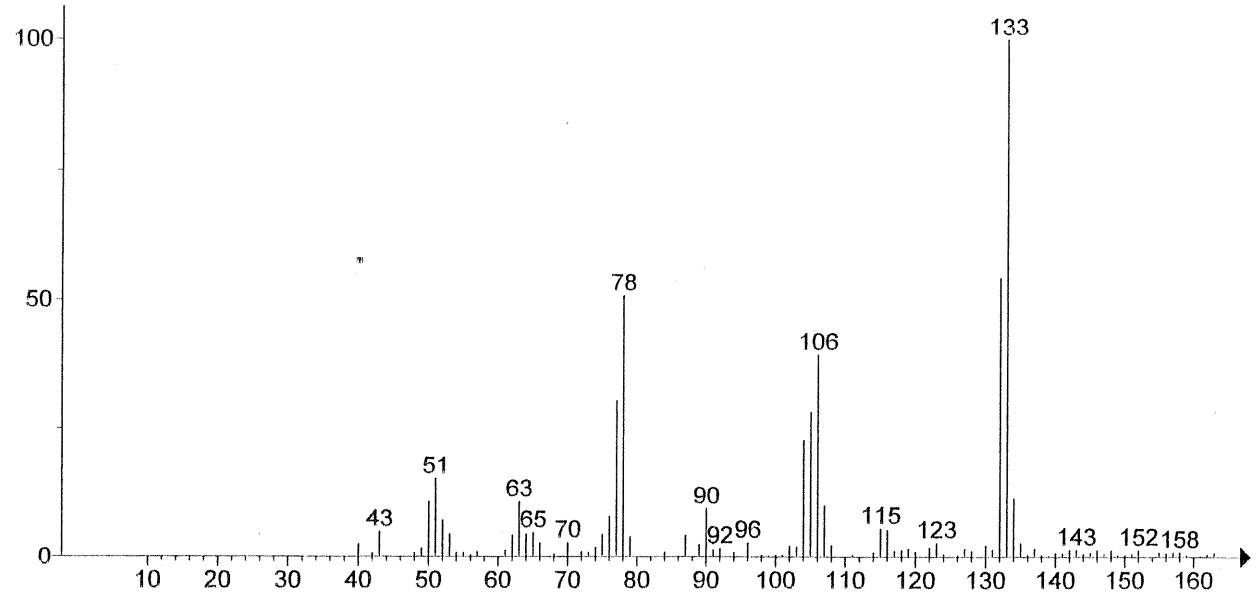
Name: Benzeneethanol, 4-hydroxy-
Formula: $C_8H_{10}O_2$
MW: 138 CAS#: 501-94-0 NIST#: 92403 ID#: 14558 DB: replib
Other DBs: Fine, TSCA, HODOC, NIH, EINECS
Contributor: J.E. WILKINSON S-CUBED, SAN DIEGO, CA.
10 largest peaks:
107 999 | 138 239 | 77 205 | 108 74 | 51 73 | 53 62 | 78 39 | 79 31 | 65 27 | 50 24 |
Synonyms:
1.4-(2-Hydroxyethyl)phenol
2.p-Hydroxyphenethyl alcohol
3.4-Hydroxyphenethyl alcohol
4.β-(p-Hydroxyphenyl)ethanol
5.β-(4-Hydroxyphenyl)ethanol
6.2-(p-Hydroxyphenyl)ethanol
7.2-(4-Hydroxyphenyl)ethanol
8.4-Hydroxyphenylethanol
9.Phenethyl alcohol, p-hydroxy-
10.p-Thyrosol
11.Tyrosol
12.p-Tyrosol
13.4-Hydroxyphenylethyl alcohol
14.p-Hydroxyphenylethyl alcohol

Estimated non-polar retention index (n-alkane scale):
Value: 1356 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

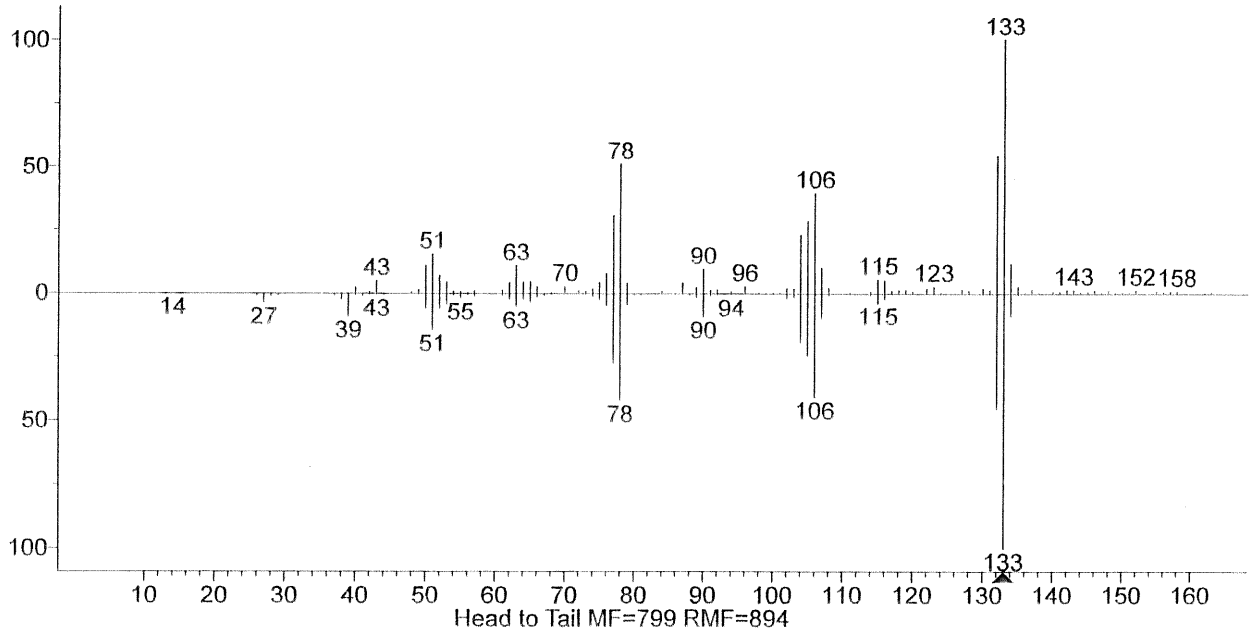
Retention index.
1. Value: 1451 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: HP
-5MS
Column Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type:
Normal alkane RI
Program Type: Complex
Description: 40C(3min)=> 2C/min=>180C=>10C/min=>250C(5min)

Source: Alissandrakis, E.; Kibaris, A.C.; Tarantilis, P.A.; Harizanis, P.C.; Polissiou, M., Flavour compounds of Greek cotton honey, J. Sci. Food Agric., 85, 2005, 1444-1452.

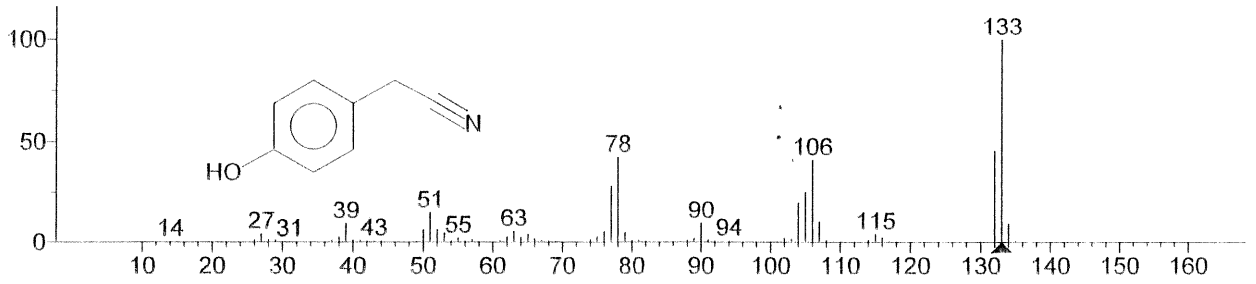
2. Value: 1478 iu
Column Type:
Capillary
Column Class: Semi-standard non-polar
Active Phase: SPB-5
Column Length: 30 m
Carrier Gas:
He
Column Diameter: 0.53 mm




(Text File) +EI Scan (32.172 min) ALI-OLE-H7-220421-.D Subtract



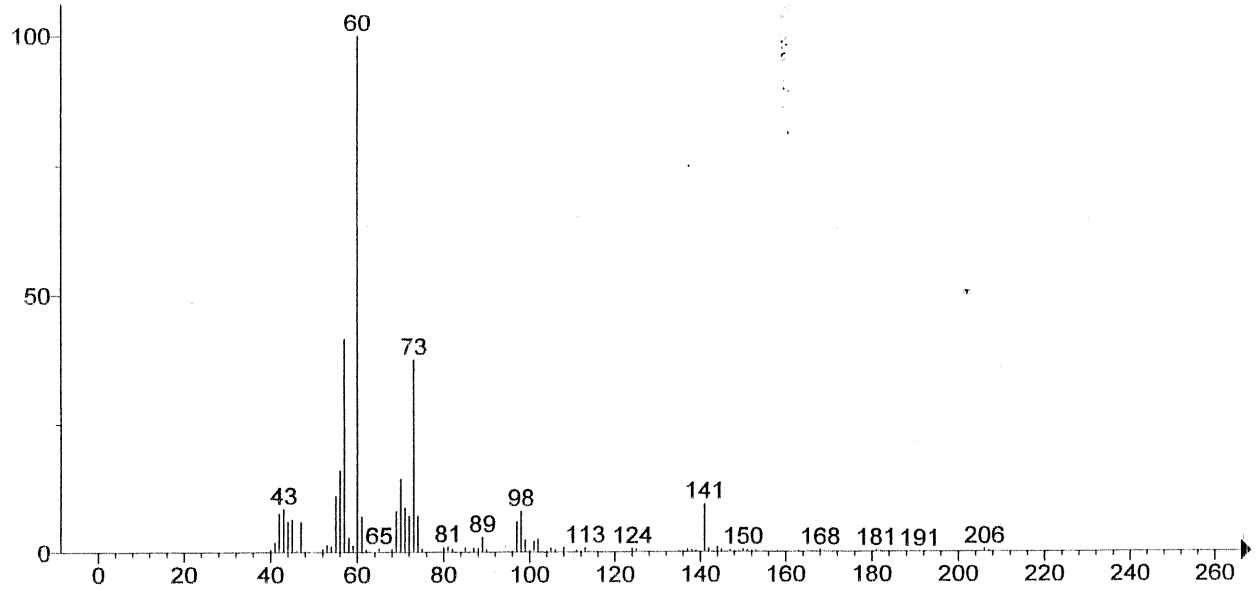

Head to Tail MF=799 RMF=894



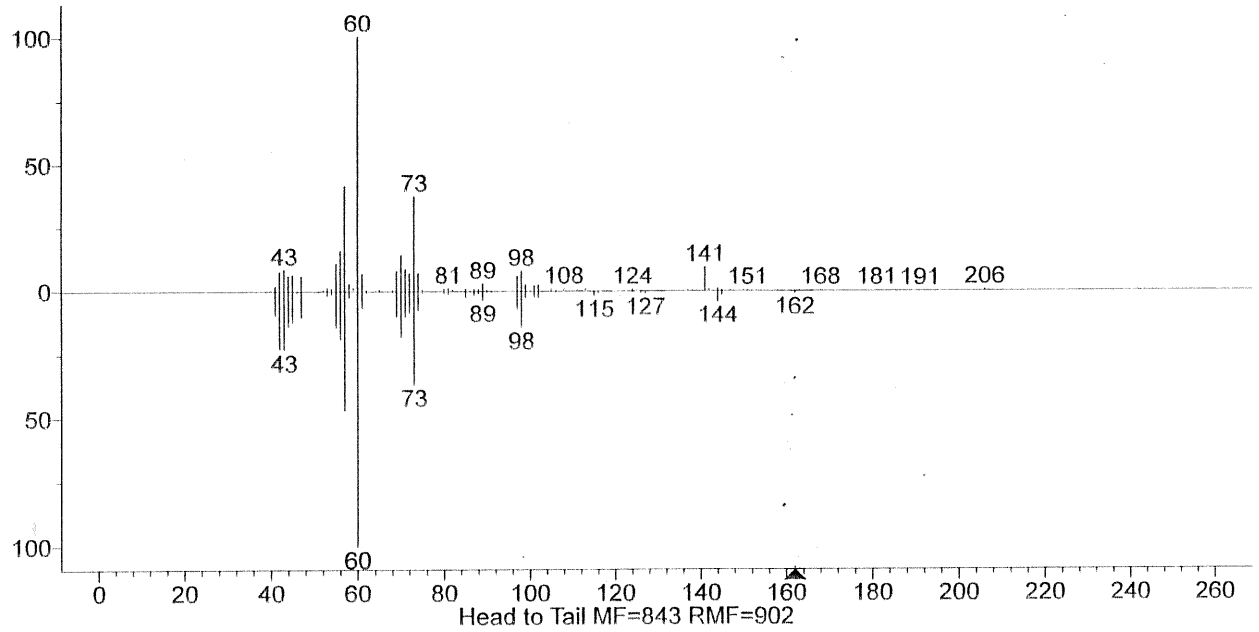

(mainlib) Benzeneacetonitrile, 4-hydroxy-

Name: Benzeneacetonitrile, 4-hydroxy-
Formula: $C_8H_7NO$
MW: 133 CAS#: 14191-95-8 NIST#: 236771 ID#: 94894 DB: mainlib
Other DBs: Fine, RTECS, HODOC, NIH, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-8839
10 largest peaks:
133 999 | 132 454 | 78 421 | 106 407 | 77 277 | 105 247 | 104 195 | 51 145 | 107 100 | 90 92 |
Synonyms:
1.Acetonitrile, (p-hydroxyphenyl)-
2.(4-Hydroxyphenyl)acetonitrile
3.p-Hydroxybenzyl cyanide
4.p-Hydroxyphenylacetonitrile
5.4-Hydroxybenzyl cyanide

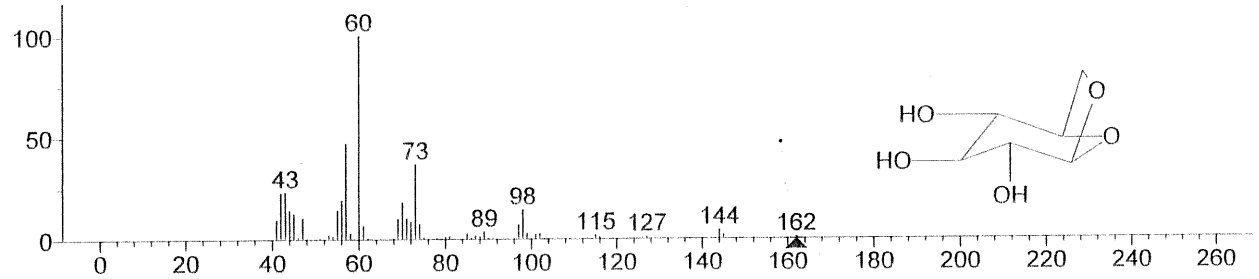
Estimated non-polar retention index (n-alkane scale):
Value: 1359 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu




(Text File) +EI Scan (32.956 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=843 RMF=902




(replib) β-D-Glucopyranose, 1,6-anhydro-

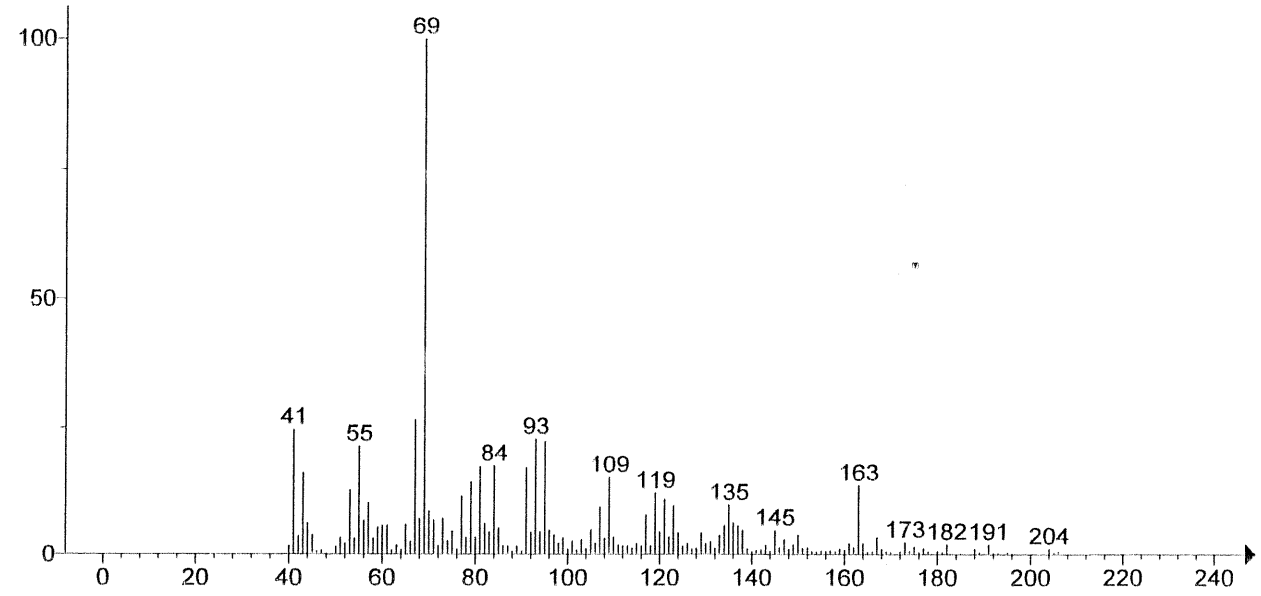
Name: β-D-Glucopyranose, 1,6-anhydro-
Formula: $C_6H_{10}O_5$
MW: 162 CAS#: 498-07-7 NIST#: 127044 ID#: 6692 DB: replib
Other DBs: NIH, EINECS
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892
10 largest peaks:
60 999 | 57 468 | 73 366 | 43 230 | 42 225 | 56 190 | 70 181 | 55 143 | 98 143 | 44 141 |
Synonyms:
1.Anhydro-d-mannosan
2.Levoglucosan
3.1,6-Anhydro-β-D-glucopyranose

Estimated non-polar retention index (n-alkane scale):
Value: 1404 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

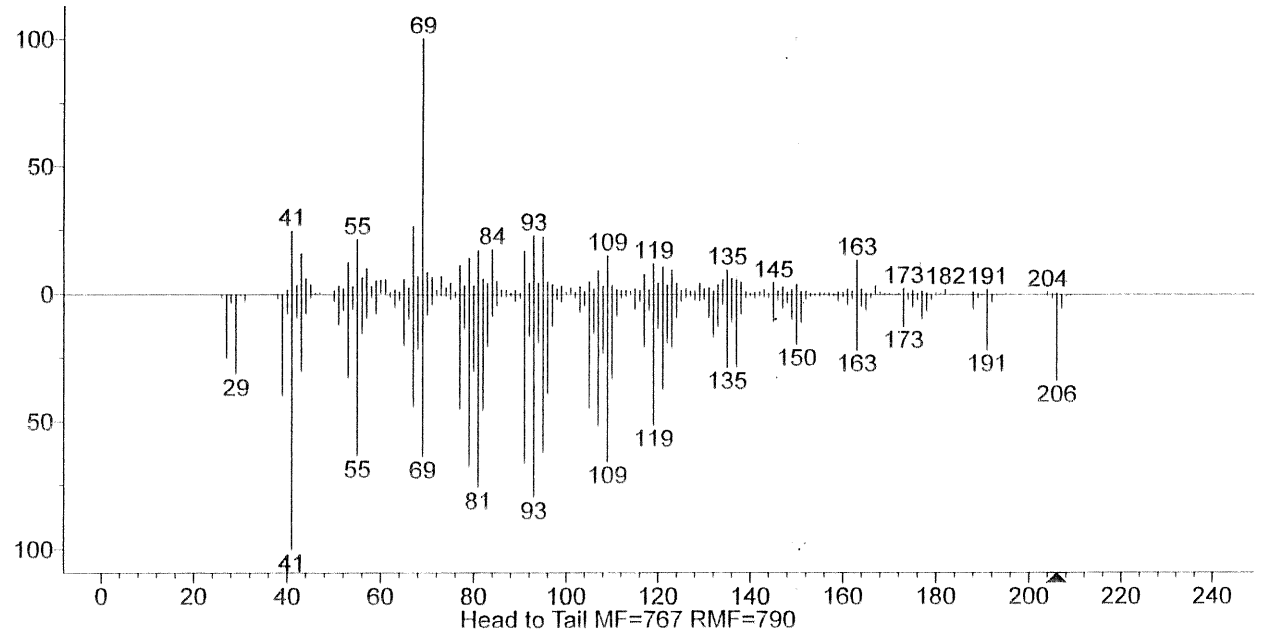
Retention index.
1. Value: 1426.2 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.25 mm
Data Type: Normal alkane RI
Program Type:
Ramp
Start T: 50 C
End T: 275 C
Heat Rate: 4 K/min
Start Time: 2 min
Source: Ralph, J.; Hatfield, R.D.,
Pyrolisys-GC-MS Characterization of Forage Materials, J. Agric. Food Chem., 39, 1991, 1426-1437.

2. Value:
1491.1 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: LM-5
Column Length:
30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program
Type: Complex
Description: 60C(2min) =>15C/min =>180C =>5C/min =>280C (10min)
Source: Ré-Poppi, N.;
Santiago-Silva, M., Polycyclic aromatic hydrocarbons and other selected organic compounds in ambient air of Campo Grande City, Brazil, Atmos. Environ., 39, 2005, 2839-2850.

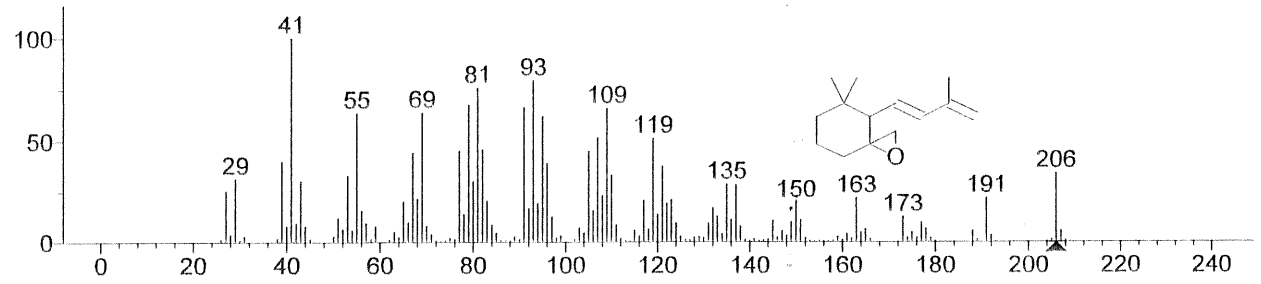
<...>




(Text File) +EI Scan (33.779 min) ALI-OLE-H7-220421-.D



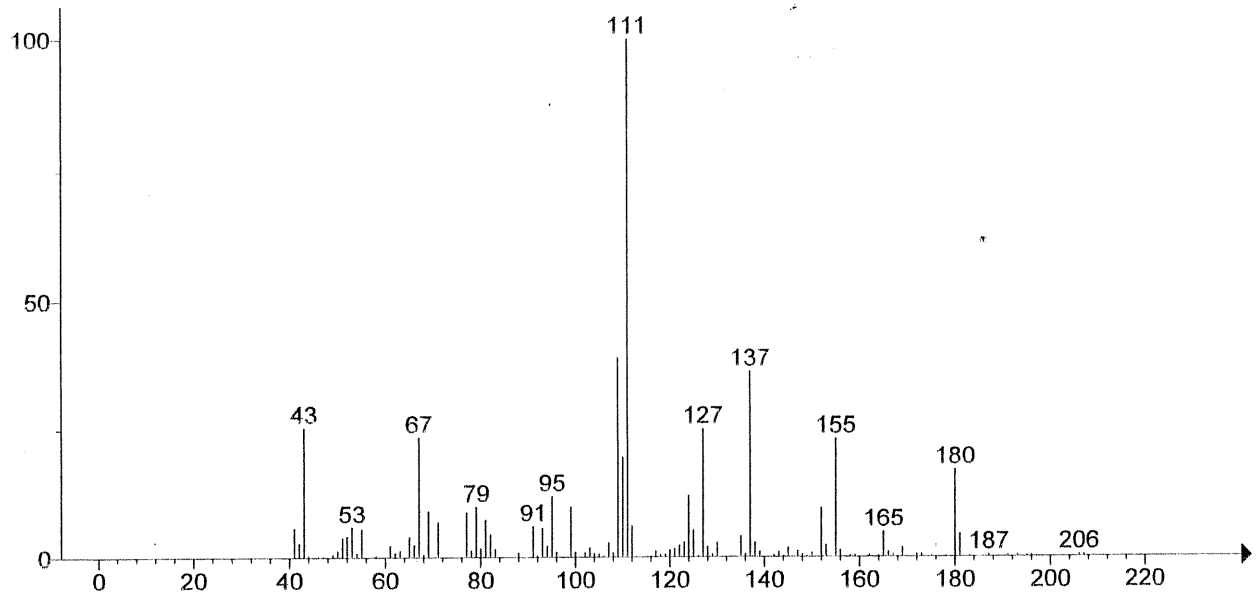

Head to Tail MF=767 RMF=790



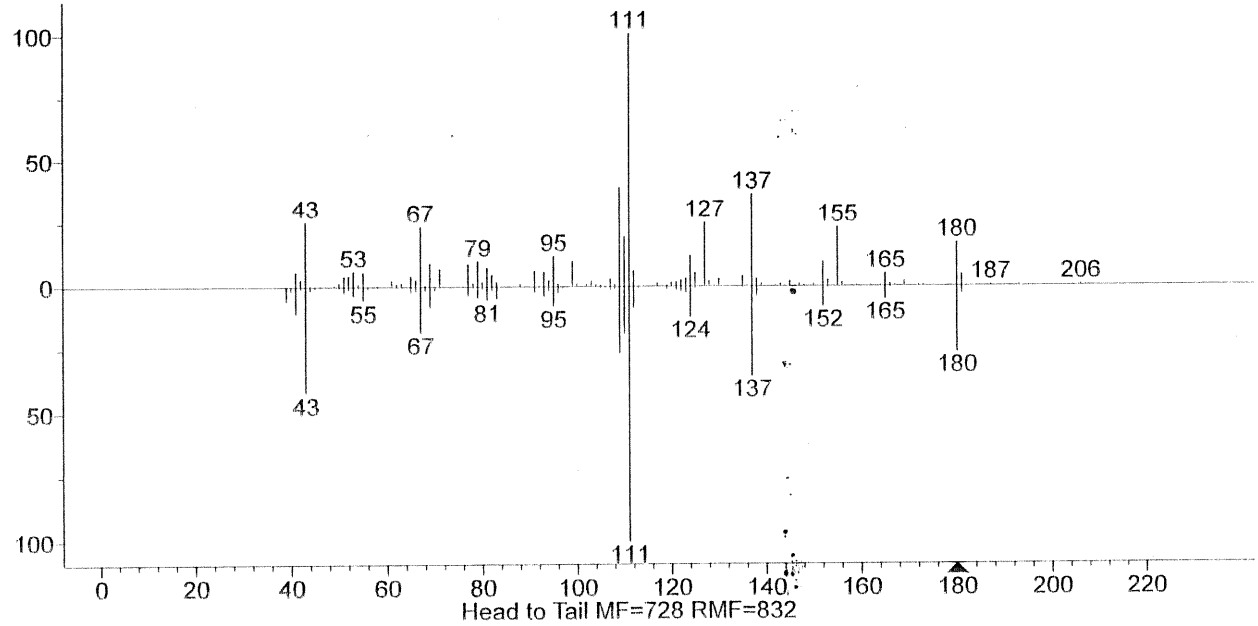

(mainlib) 1-Oxaspiro[2.5]octane, 5,5-dimethyl-4-(3-methyl-1,3-butadienyl)-

Name: 1-Oxaspiro[2.5]octane, 5,5-dimethyl-4-(3-methyl-1,3-butadienyl)-
Formula: $C_{14}H_{22}O$
MW: 206 NIST#: 195921 ID#: 3527 DB: mainlib
Contributor: Chemical Concepts
10 largest peaks:
41 999 | 93 794 | 81 757 | 79 675 | 91 664 | 109 657 | 69 637 | 55 633 | 95 619 | 107 517 |
Synonyms:
no synonyms.

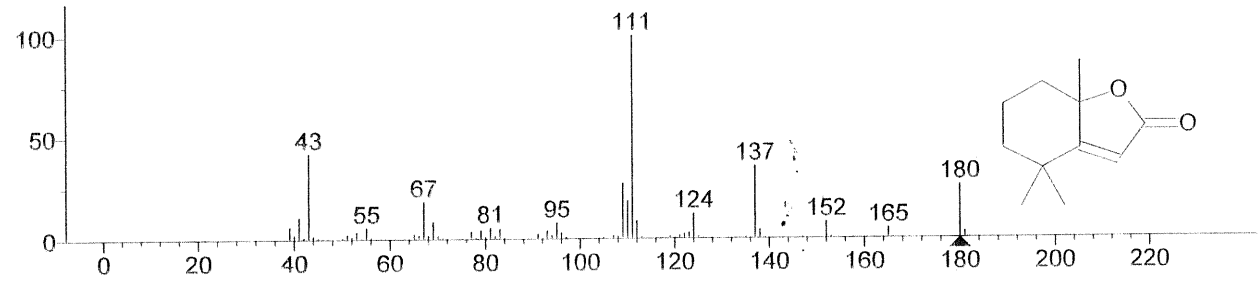
Estimated non-polar retention index (n-alkane scale):
Value: 1431 iu
Confidence interval (Ethers): 68(50%) 293(95%) iu




(Text File) +EI Scan (34.275 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=728 RMF=832



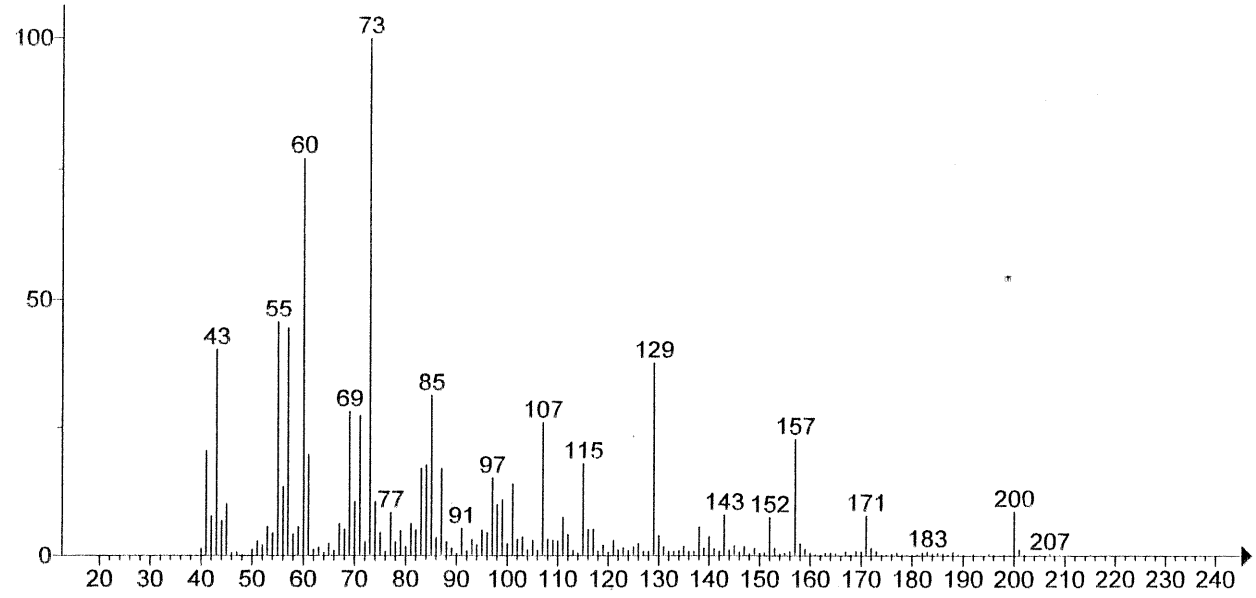

(mainlib) 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-

Name: 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-
Formula: $C_{11}H_{16}O_2$
MW: 180 CAS#: 17092-92-1 NIST#: 108912 ID#: 74534 DB: mainlib
Other DBs: NIH
Contributor: Philip Morris R&D
10 largest peaks:
111 999 | 43 418 | 137 353 | 109 268 | 180 259 | 110 184 | 67 181 | 124 119 | 41 106 | 112 85 |
Synonyms:
1.2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-
2.Actinidiolide, dihydro-
3.2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (S)-
4.Dihydroactinidiolide
5.4,4,7a-Trimethyl-5,6,7,7a-tetrahydro-1-benzofuran-2(4H)-one #

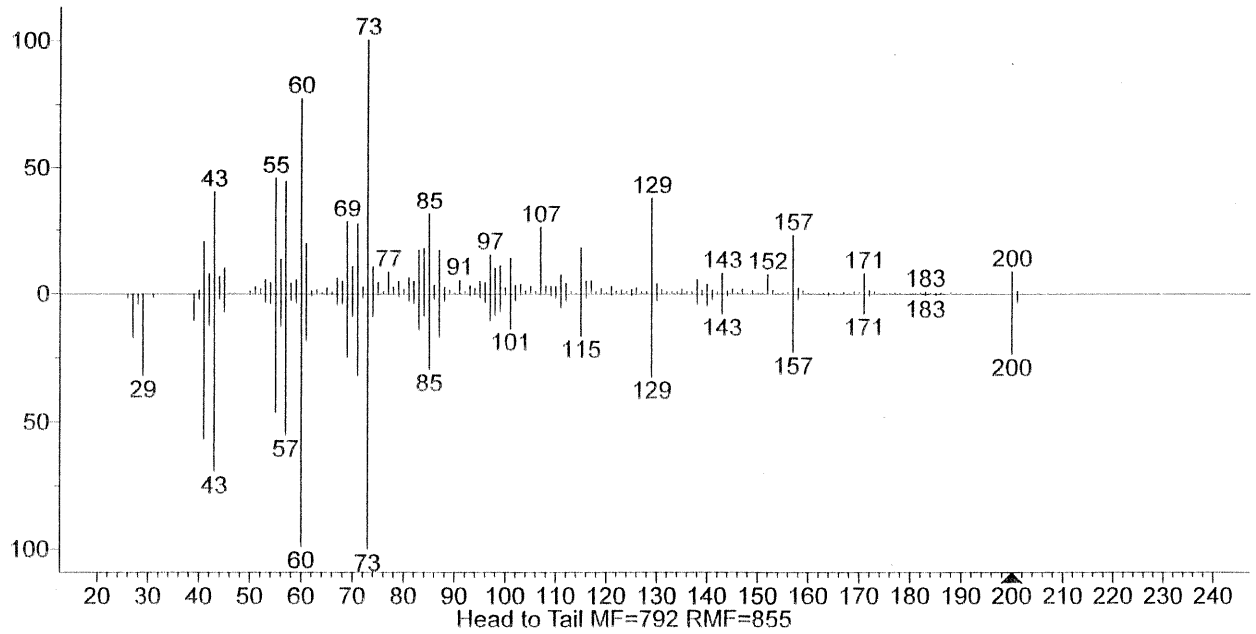
Estimated non-polar retention index (n-alkane scale):
Value: 1426 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 1532 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-1
Column
Length: 50 m
Carrier Gas: He
Column Diameter: 0.32 mm
Phase Thickness: 1.05 um
Data Type: Linear
RI
Program Type: Complex
Description: 20C(0.5min) =>60C=>4C/min=>250C
Source: Sing, A.S.C.; Smadja, J.;
Brevard, H.; Maignial, L.; Chaintreau, A.; Marion, J.-P., Volatile constituents of faham (Jumellea fragrans (Thou.) Schltr.), J. Agric. Food Chem., 40, 1992, 642-646.

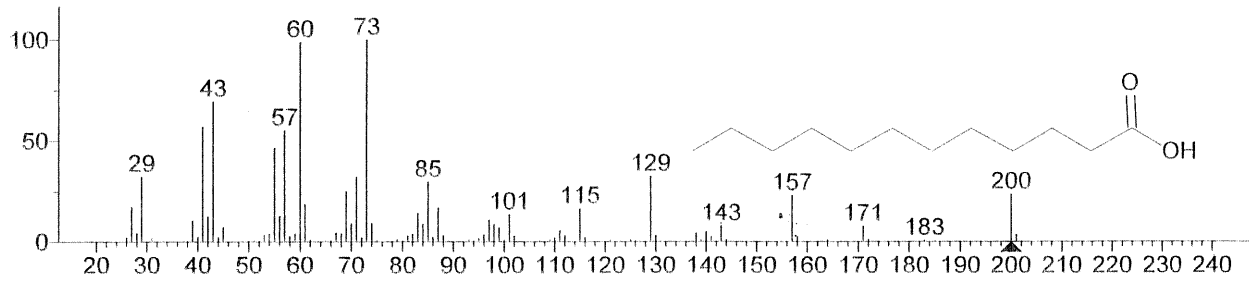
2. Value: 1471 iu
Column Type: Capillary
Column Class:
Standard non-polar
Active Phase: SPB-1
Column Length: 30 m
Carrier Gas: He
Column Diameter: 0.32
mm
Phase Thickness: 0.25 um
Data Type: Kovats RI
Program Type: Complex
Description: 40C(3min)
=>2C/min =>100C=>4C/min =>220C (7min)
Source: Borse, B.B.; Jagan Mohan Rao, L.; Nagalakshmi, S.;
Krishnamurthy, N., Fingerprint of black teas from India: identification of the regio-specific characteristics, Food Chem., 79, 2002, 419-424.




(Text File) +EI Scan (34.635 min) ALI-OLE-H7-220421-.D




Head to Tail MF=792 RMF=855

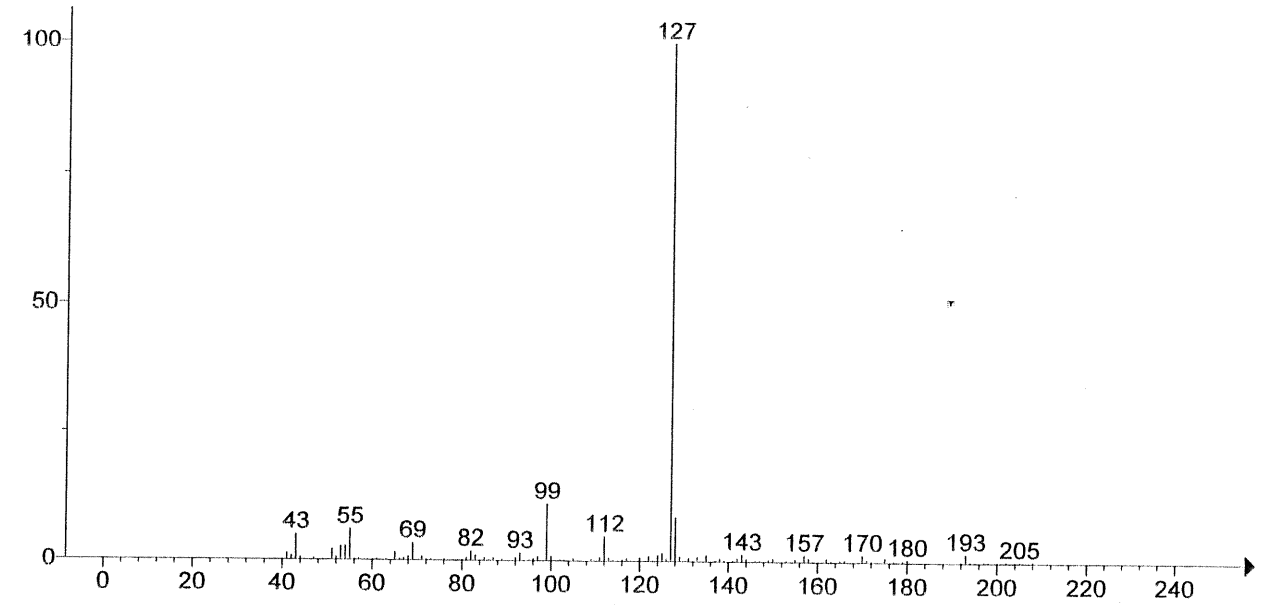



(mainlib) Dodecanoic acid

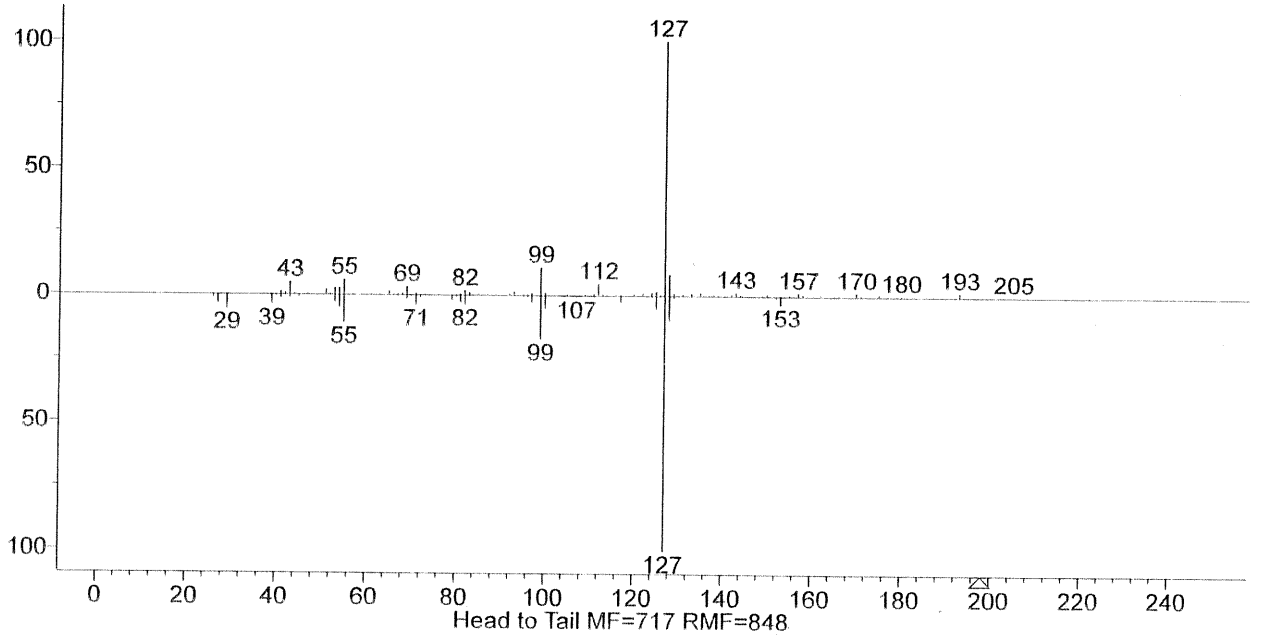
Name: Dodecanoic acid
Formula: $C_{12}H_{24}O_2$
MW: 200 CAS#: 143-07-7 NIST#: 221043 ID#: 35324 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Chemical Concepts
10 largest peaks:
73 999 | 60 987 | 43 693 | 41 567 | 57 550 | 55 463 | 129 323 | 29 320 | 71 320 | 85 295 |
Synonyms:
1.n-Dodecanoic acid
2.Neo-fat 12
3.Aliphat no. 4
4.Abl
5.Dodecylic acid
6.Lauric acid
7.Laurostearic acid
8.Neo-fat 12-43
9.Ninol aa62 extra
10.Univol u-314
11.Vulvic acid
12.1-Undecanecarboxylic acid
13.Duodecylic acid
14.C-1297
15.Coconut oil fatty acids
16.Hydrofol acid 1255
17.Hydrofol acid 1295
18.Wecoline 1295
19.Dodecoic acid
20.Hystrene 9512
21.Lunac L 70
22.Duodecyclic acid
23.Emery 650
24.n-Dodecanoate
25.Philacid 1200
26.Prifrac 2920
27.Undecane-1-carboxylic acid

Estimated non-polar retention index (n-alkane scale):
Value: 1570 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

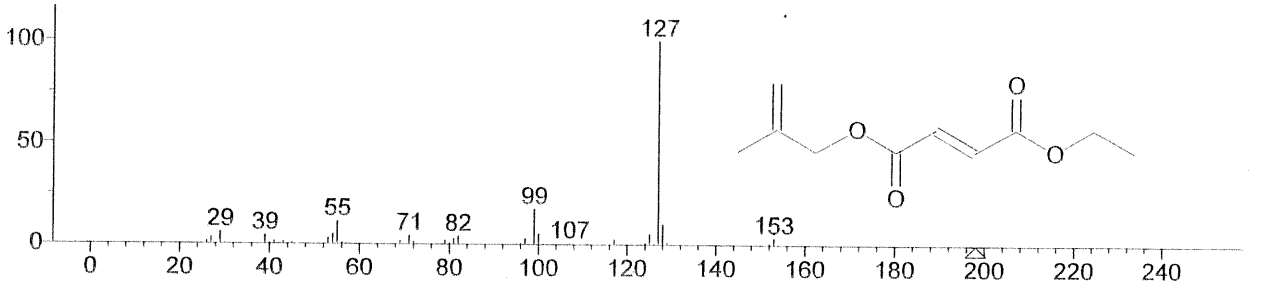
Retention index.
1. Value: 1556 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: RTX-1
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.22 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C




(Text File) +EI Scan (35.123 min) ALI-OLE-H7-220421-.D Subtract



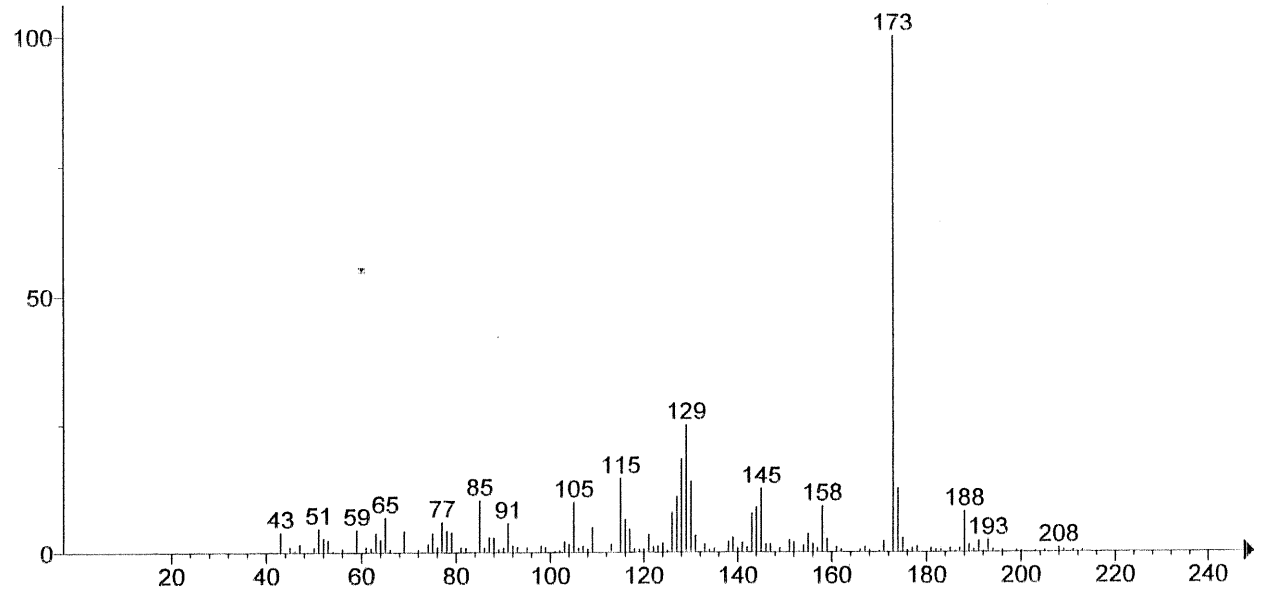

Head to Tail MF=717 RMF=848



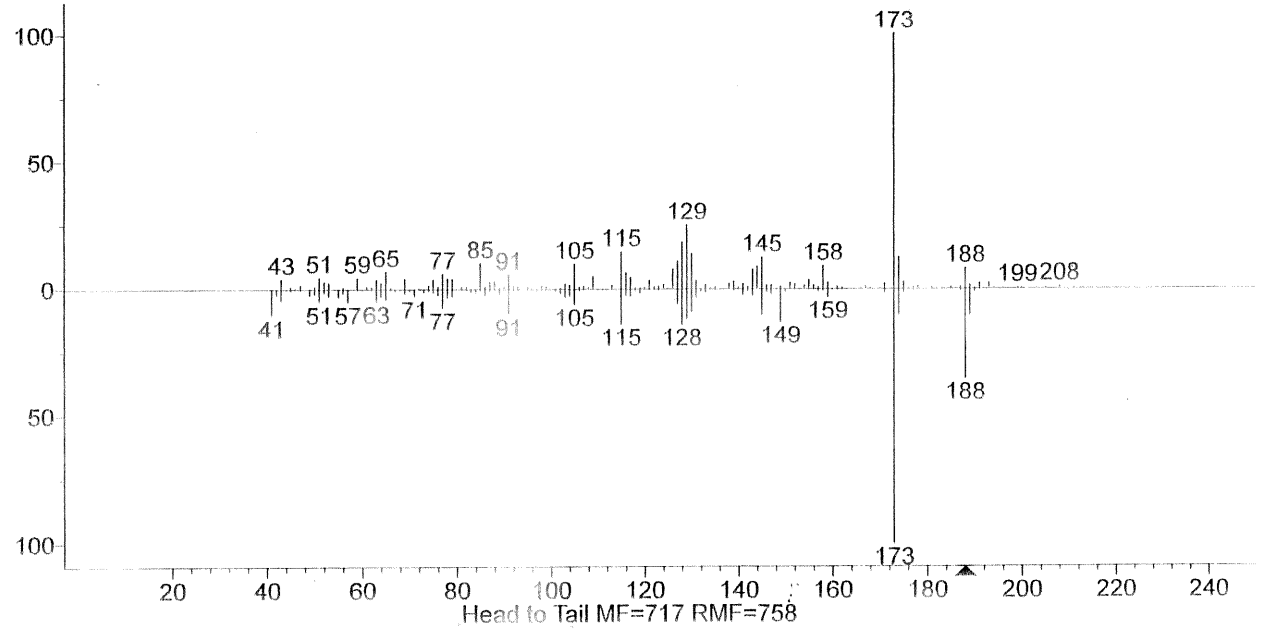

(mainlib) Fumaric acid, ethyl 2-methylallyl ester

Name: Fumaric acid, ethyl 2-methylallyl ester
Formula: $C_{10}H_{14}O_4$
MW: 198 NIST#: 330541 ID#: 89984 DB: mainlib
Contributor: Zaikin V.G., Borisov R.S., TIPS RAS, Moscow, Russia
10 largest peaks:
127 999 | 99 172 | 55 110 | 128 99 | 29 56 | 125 52 | 100 51 | 54 49 | 39 40 | 71 40 |
Synonyms:
no synonyms.

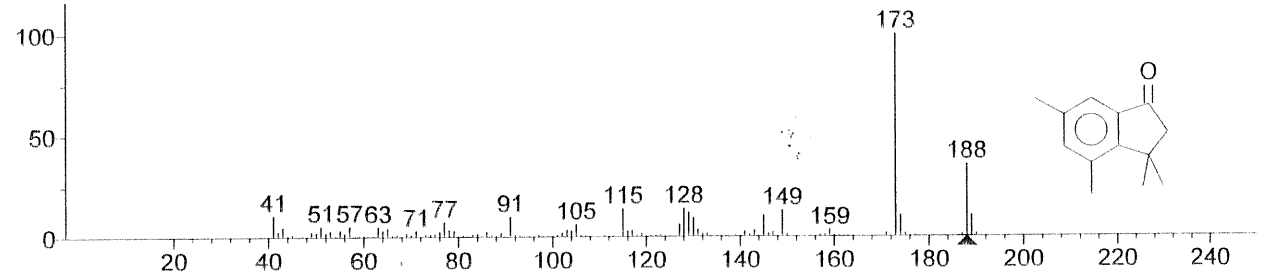
Estimated non-polar retention index (n-alkane scale):
Value: 1325 iu
Confidence interval (Esters): 47(50%) 201(95%) iu




(Text File) +EI Scan (36.531 min) ALI-OLE-H7-220421-.D Subtract



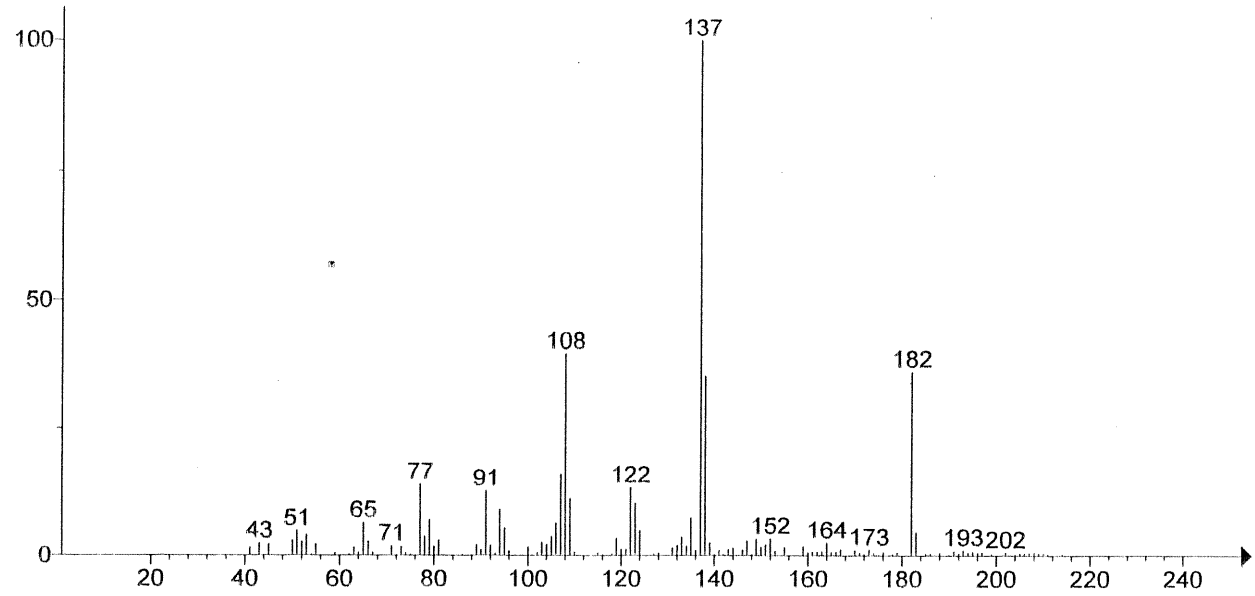

Head to Tail MF=717 RMF=758



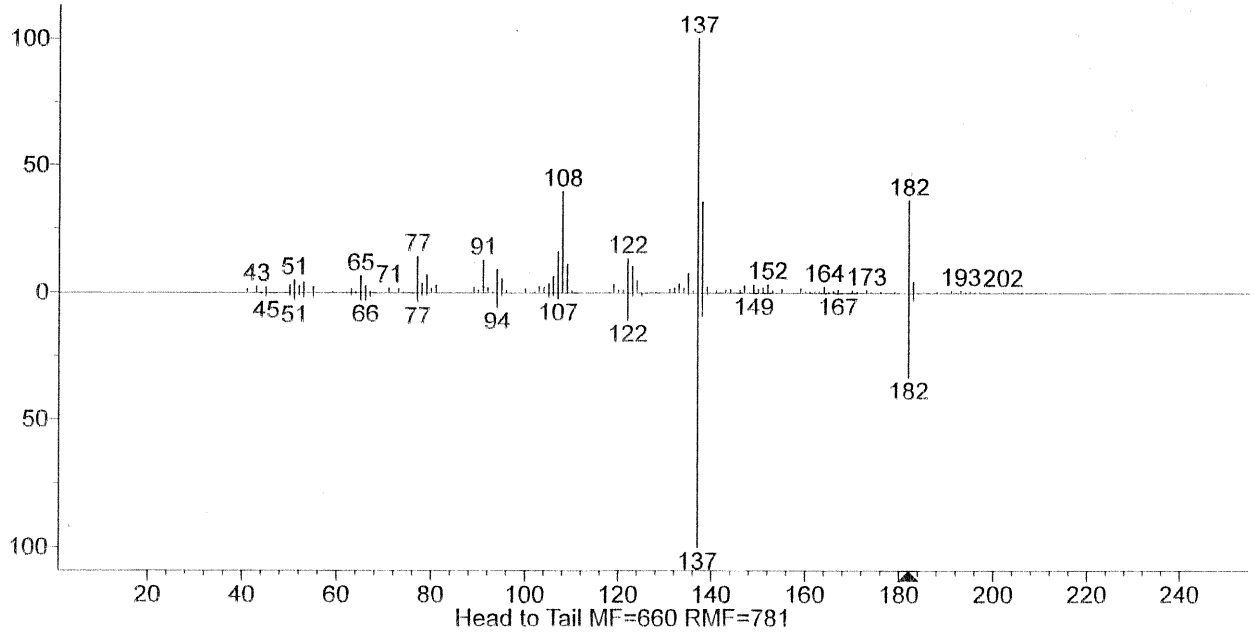

(mainlib) 1H-Inden-1-one, 2,3-dihydro-3,3,4,6-tetramethyl-

Name: 1H-Inden-1-one, 2,3-dihydro-3,3,4,6-tetramethyl-
Formula: $C_{13}H_{16}O$
MW: 188 CAS#: 55255-42-0 NIST#: 129192 ID#: 129096 DB: mainlib
Other DBs: None
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892
10 largest peaks:
173 999 | 188 353 | 128 139 | 115 138 | 149 129 | 129 119 | 41 105 | 145 105 | 174 105 | 189 105 |
Synonyms:
1.Benzo[b]dihydrofuran, 3,3,4,6-tetramethyl-
2.3,3,4,6-Tetramethyl-1-indanone #

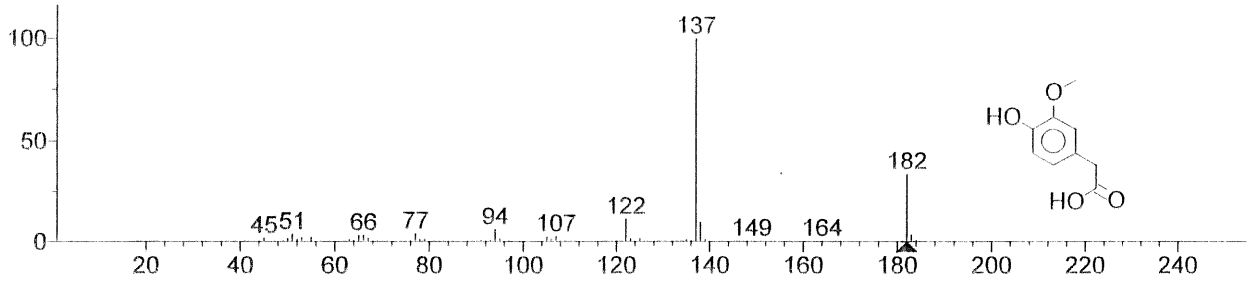
Estimated non-polar retention index (n-alkane scale):
Value: 1579 iu
Confidence interval (Ketones): 57(50%) 246(95%) iu




(Text File) +EI Scan (37.454 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=660 RMF=781



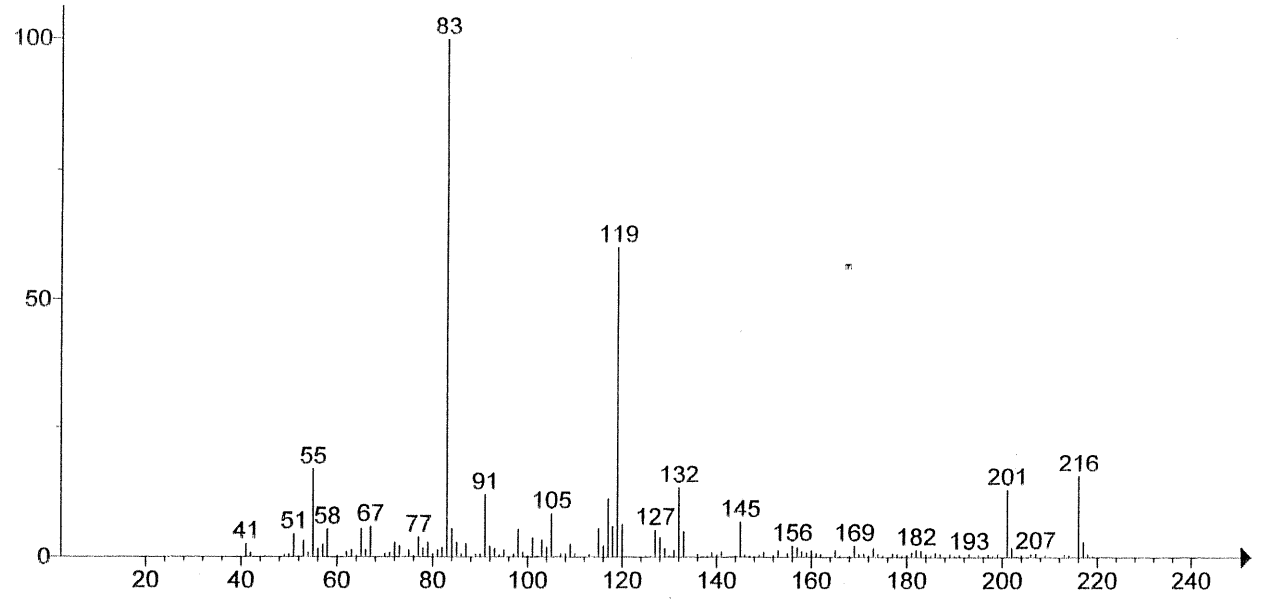

(replib) Benzeneacetic acid, 4-hydroxy-3-methoxy-

Name: Benzeneacetic acid, 4-hydroxy-3-methoxy-
Formula: $C_9H_{10}O_4$
MW: 182 CAS#: 306-08-1 NIST#: 248367 ID#: 18756 DB: replib
Other DBs: Fine, TSCA, EPA, HODOC, NIH, EINECS
Contributor: Patti Price, Georgia Bureau of Investigation, Decatur, Georgia
10 largest peaks:
137 999 | 182 334 | 122 110 | 138 95 | 94 59 | 77 39 | 51 35 | 183 32 | 66 31 | 65 29 |
Synonyms:
1.Acetic acid, (4-hydroxy-3-methoxyphenyl)-
2.(4-Hydroxy-3-methoxyphenyl)acetic acid
3.Homovanillic acid
4.HMPA
5.HVA
6.Vanillacetic Acid
7.3-Methoxy-4-hydroxyphenylacetic acid
8.4-Hydroxy-3-methoxybenzeneacetic acid
9.Homovanillinic acid
10.Homovanilic acid
11.Vanilacetic acid

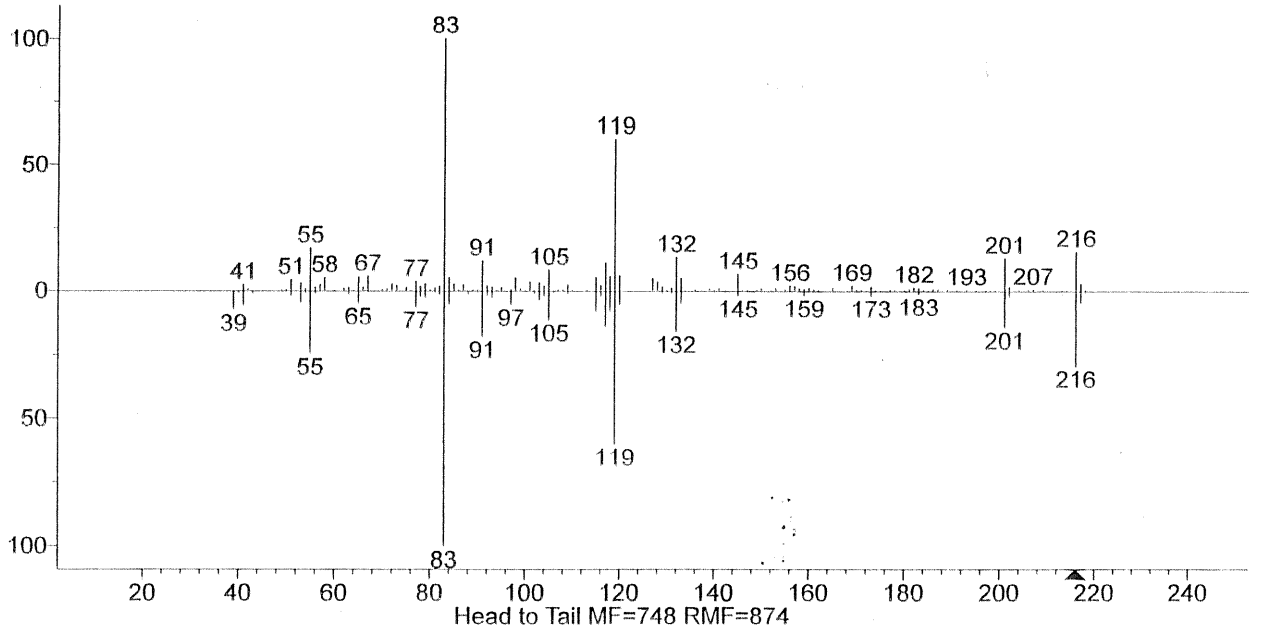
Estimated non-polar retention index (n-alkane scale):
Value: 1659 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index.
1. Value: 1603 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-1
Column
Length: 50 m
Carrier Gas: He
Column Diameter: 0.2 mm
Phase Thickness: 0.5 um
Data Type: Normal alkane
RI
Program Type: Ramp
Start T: 60 C
End T: 250 C
Heat Rate: 2 K/min
End Time: 120 min
Source: Castel,
C.; Fernandez, X.; Lizzani-Cuvelier, L.; Perichet, C.; Lavoine, S., Characterization of the Chemical Composition of a Byproduct from Siam Benzoin Gum, J. Agric. Food Chem., 54, 2006, 8848-8854.

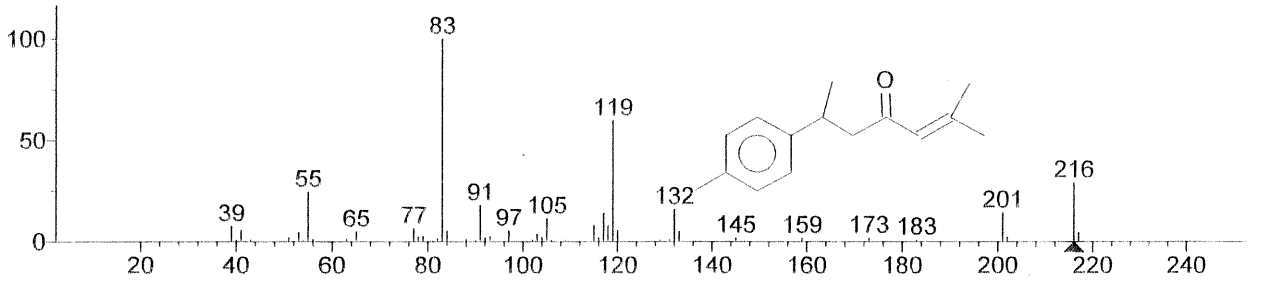
2. Value: 1633 iu
Column
Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: DB-5MS
Column Length: 30 m
Carrier
Gas: H2/N2
Column Diameter: 0.25 mm




(Text File) +EI Scan (37.963 min) ALI-OLE-H7-220421-.D Subtract



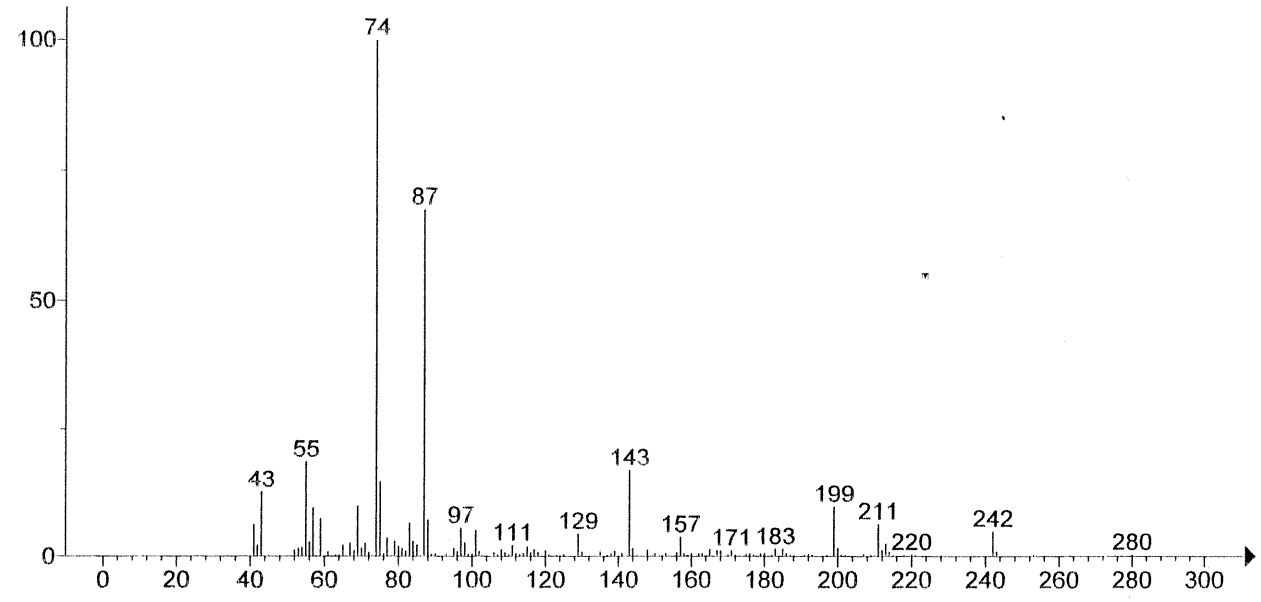

Head to Tail MF=748 RMF=874



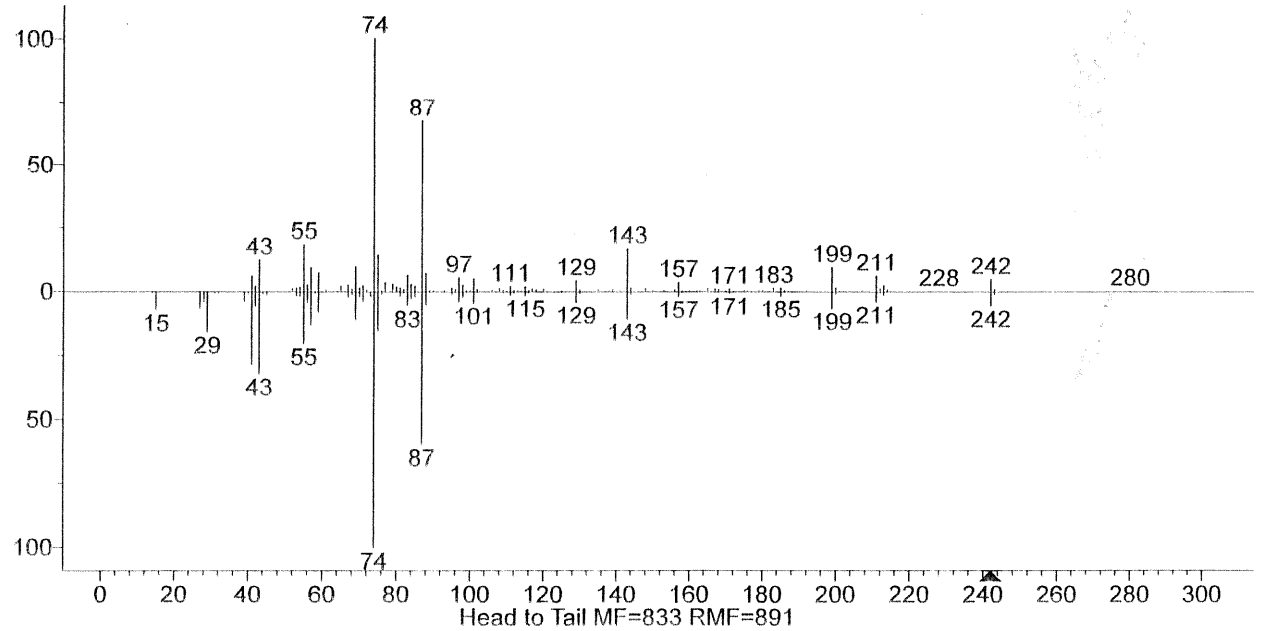

(mainlib) Ar-tumerone

Name: Ar-tumerone
Formula: $C_{15}H_{20}O$
MW: 216 NIST#: 292710 ID#: 45357 DB: mainlib
Contributor: R.Hiserodt ET AL. J.Chrom. 740,51(1996)
10 largest peaks:
83 999 | 119 597 | 216 290 | 55 243 | 91 177 | 132 157 | 201 141 | 117 140 | 105 112 | 118 79 |
Synonyms:
no synonyms.

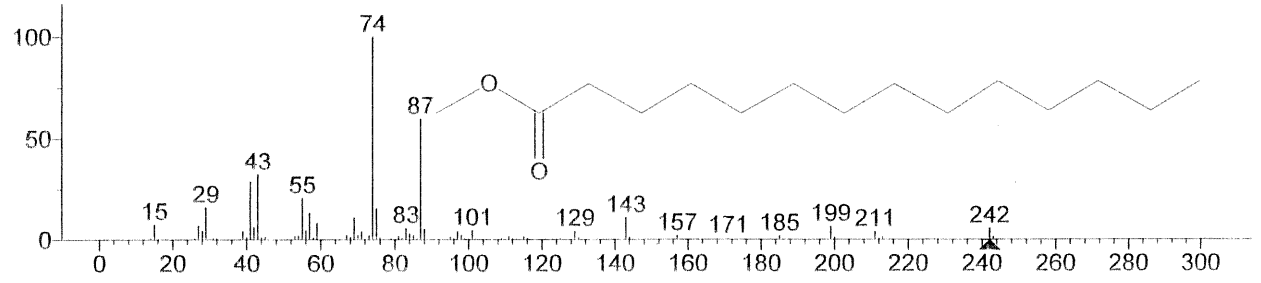
Estimated non-polar retention index (n-alkane scale):
Value: 1660 iu
Confidence interval (Ketones): 57(50%) 246(95%) iu




(Text File) +EI Scan (39.346 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=833 RMF=891




(replib) Methyl tetradecanoate

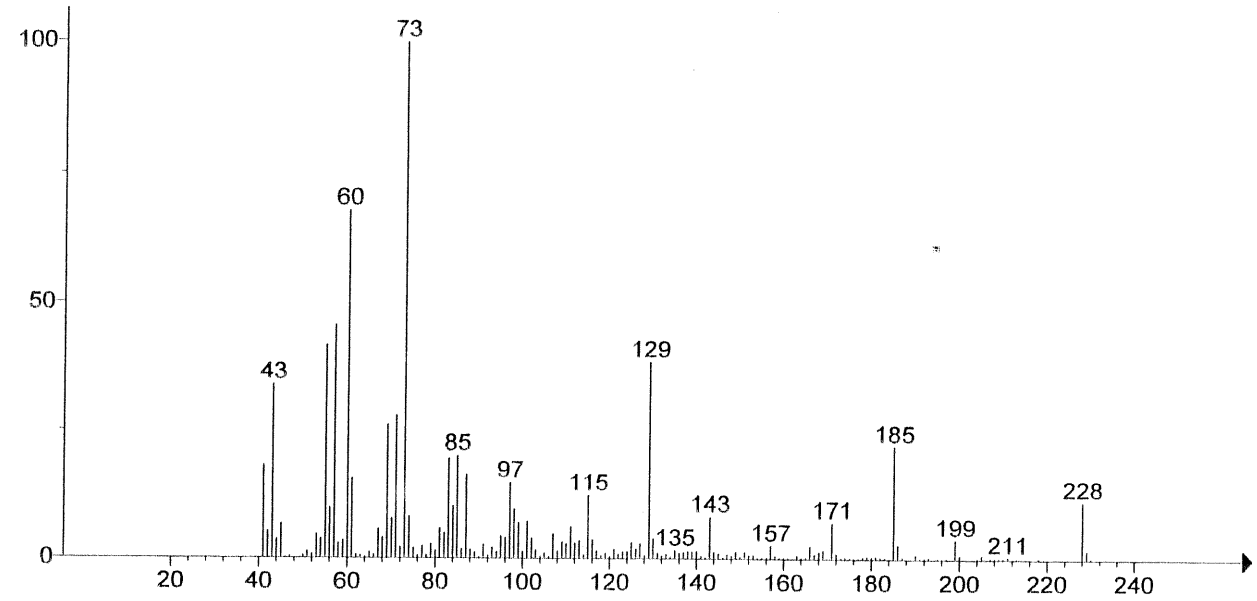
15

Name: Methyl tetradecanoate
Formula: $C_{15}H_{30}O_2$
MW: 242 CAS#: 124-10-7 NIST#: 79125 ID#: 9077 DB: replib
Other DBs: Fine, TSCA, EPA, HODOC, NIH, EINECS, IRDB
Contributor: O A MAMER, MCGILL UNIVERSITY, MONTREAL, HEM. P
10 largest peaks:
74 999 | 87 595 | 43 321 | 41 286 | 55 204 | 29 158 | 75 153 | 57 131 | 69 109 | 143 107 |
Synonyms:
1.Tetradecanoic acid, methyl ester
2.Myristic acid, methyl ester
3.Metholeneat 2495
4.Methyl myristate
5.Methyl n-tetradecanoate
6.Uniphat A50
7.Emery 2214

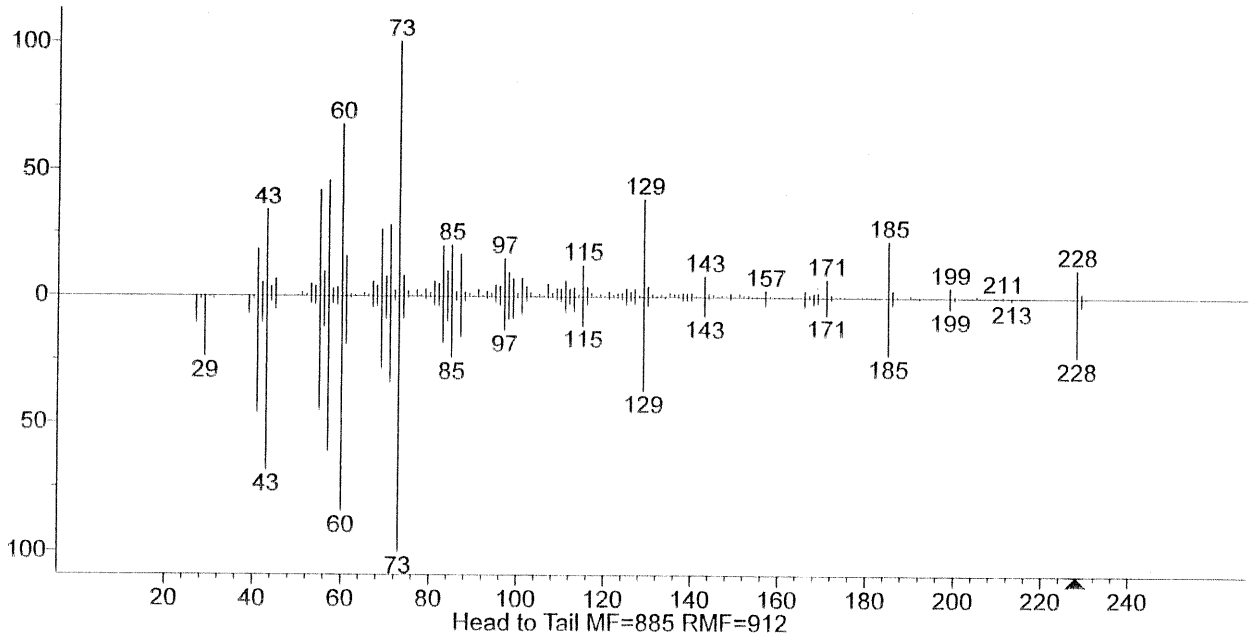
Estimated non-polar retention index (n-alkane scale):
Value: 1680 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 1713 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column
Length: 60 m
Carrier Gas: He
Column Diameter: 0.32 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C
End T: 280 C
Heat Rate: 3 K/min
Start Time: 10 min
End Time: 60
min
Source: Pino, J.; Almora, K.; Marbot, R., Volatile components of papaya (Carica papaya L., maradol variety) fruit, Flavour Fragr. J., 18, 2003, 492-496.

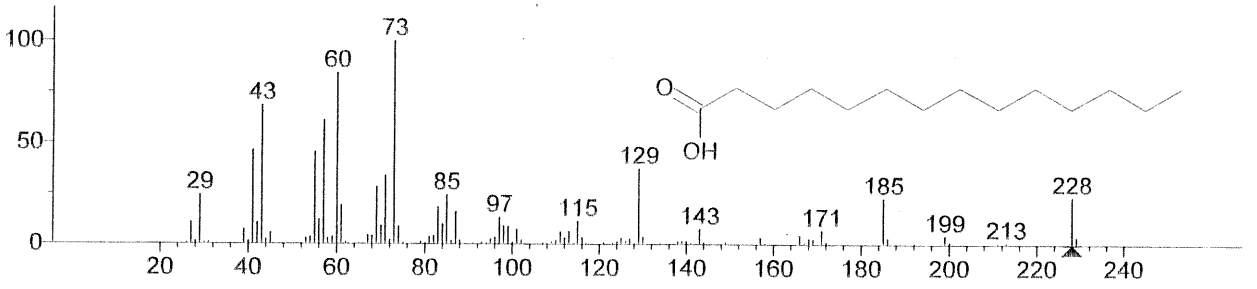
2. Value: 1714 iu
Column Type: Capillary
Column Class: Standard
non-polar
Active Phase: HP-1
Column Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase
Thickness: 0.33 um
Data Type: Linear RI
Program Type: Ramp




(Text File) +EI Scan (40.312 min) ALI-OLE-H7-220421-.D




Head to Tail MF=885 RMF=912



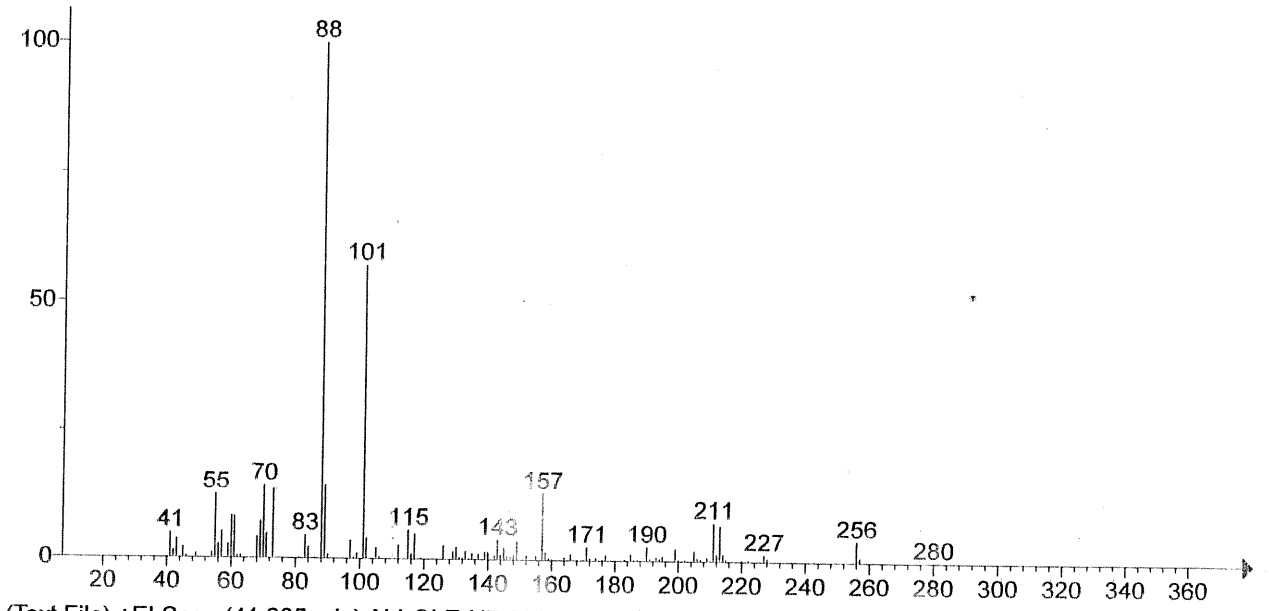

(replib) Tetradecanoic acid

Name: Tetradecanoic acid
Formula: $C_{14}H_{28}O_2$
MW: 228 CAS#: 544-63-8 NIST#: 189107 ID#: 8471 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Chemical Concepts
10 largest peaks:
73 999 | 60 841 | 43 681 | 57 609 | 41 461 | 55 451 | 129 371 | 71 338 | 69 282 | 85 241 |
Synonyms:
1.Myristic acid
2.n-Tetradecanoic acid
3.n-Tetradecoic acid
4.Neo-Fat 14
5.Univol U 316S
6.1-Tridecanecarboxylic acid
7.Coconut oil fatty acids
8.Crodacid
9.Emery 655
10.Hydrofol acid 1495
11.Hystrene 9014
12.n-Tetradecan-1-oic acid
13.Emery 654
14.Hystrene 9514
15.Philacid 1400
16.Prifac 2940
17.Prifrac 2940
18.Univol U 3165
19.Univol U320

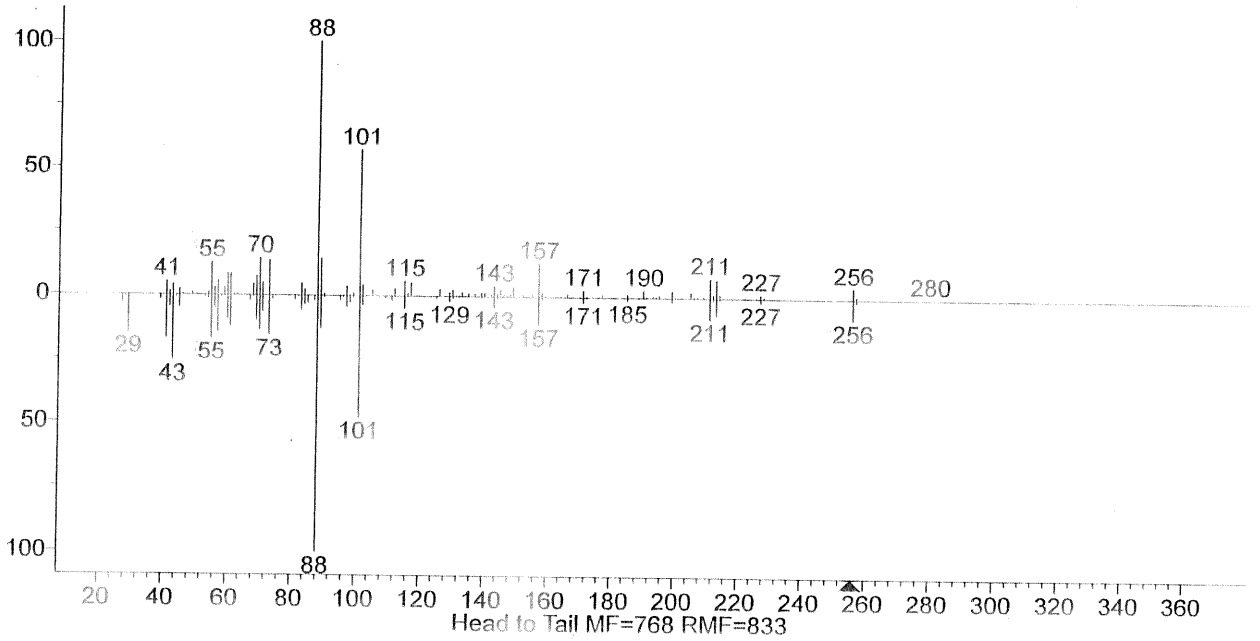
Estimated non-polar retention index (n-alkane scale):
Value: 1769 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.
1. Value: 1748 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.

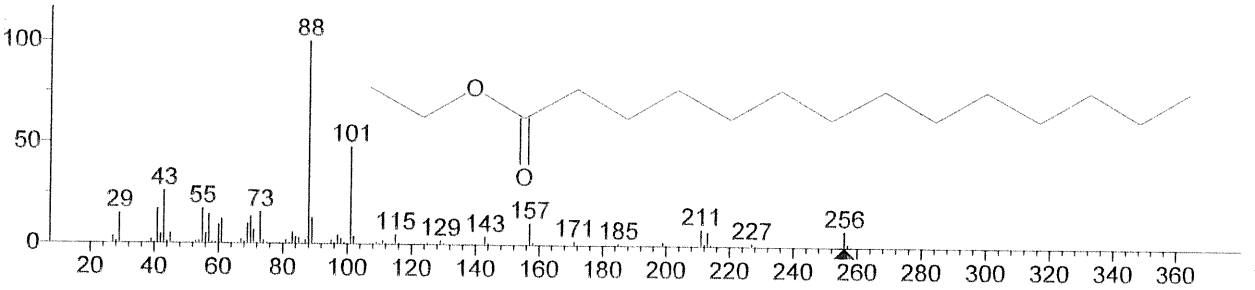
2. Value: 1772 iu




(Text File) +EI Scan (41.285 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=768 RMF=833



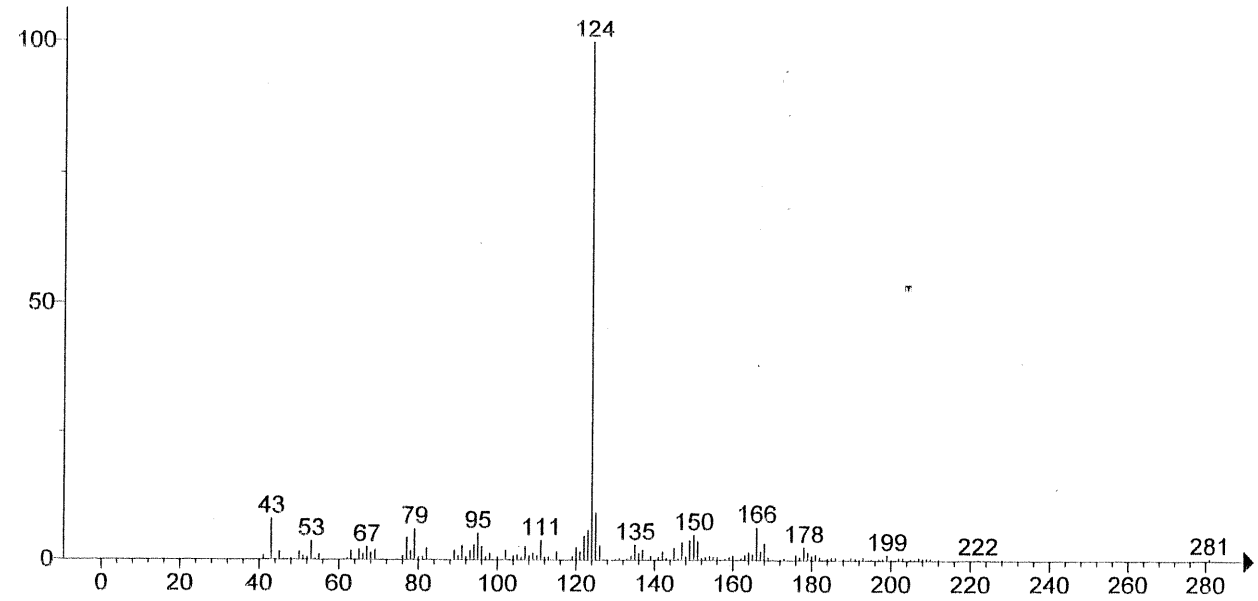

(replib) Tetradecanoic acid, ethyl ester

Name: Tetradecanoic acid, ethyl ester
Formula: $C_{16}H_{32}O_2$
MW: 256 CAS#: 124-06-1 NIST#: 156923 ID#: 11112 DB: replib
Other DBs: Fine, TSCA, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Chemical Concepts
10 largest peaks:
88 999 | 101 477 | 43 257 | 55 170 | 41 168 | 73 154 | 29 147 | 57 143 | 70 134 | 89 128 |
Synonyms:
1.Myristic acid, ethyl ester
2.Ethyl myristate
3.Ethyl tetradecanoate
4.Ethyl ester of tetradecanoic acid
5.Ethyl N-tetradecanoate

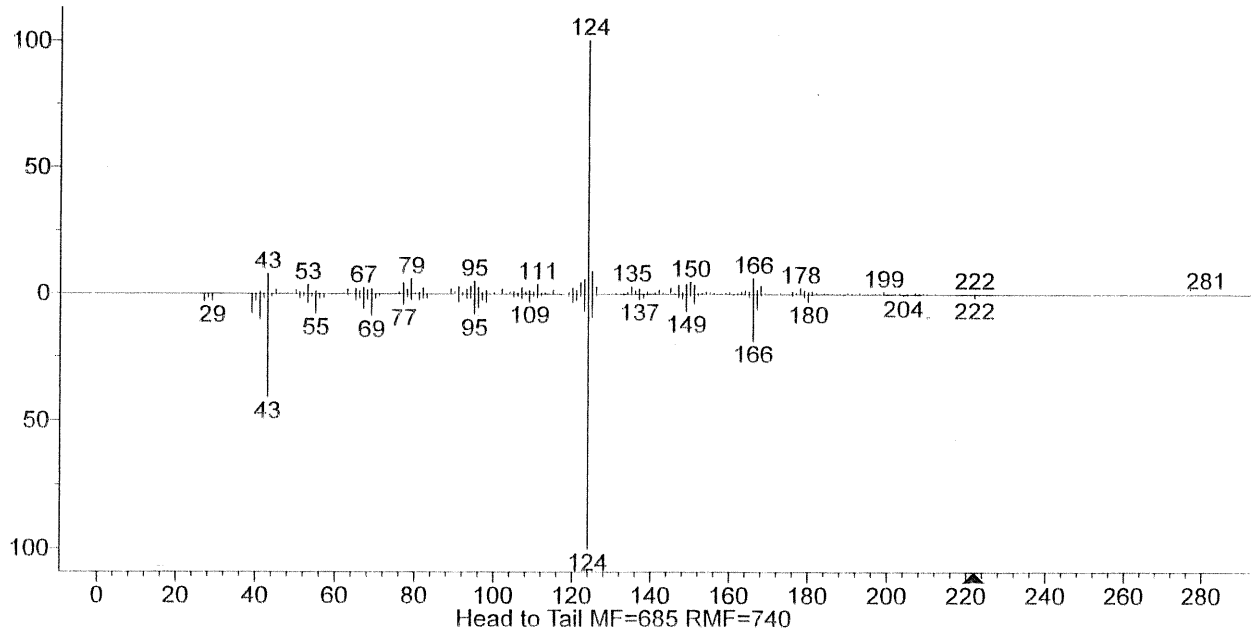
Estimated non-polar retention index (n-alkane scale):
Value: 1779 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 1778 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: BP-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: 60 C
End T: 220 C
Heat Rate: 5 K/min
End Time: 13 min
Source: Raina, V.
K.; Kumar, A.; Srivastava, S.K.; Syamsundar, K.V.; Kahol, A.P., Essential oil composition of 'kewda' (Pandanus odoratissimus) from India, Flavour Fragr. J., 19, 2004, 434-436.

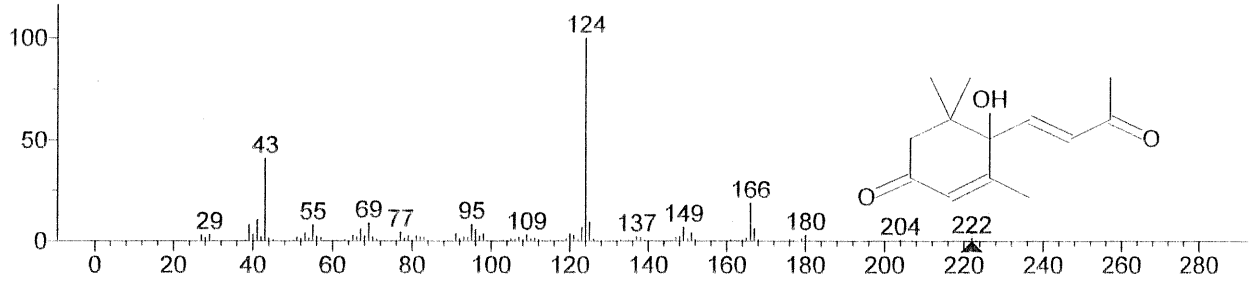
2. Value: 1782 iu
Column Type:
Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column Length: 60 m
Carrier Gas:
He
Column Diameter: 0.32 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program Type: Ramp
Start T:
60 C
End T: 280 C




(Text File) +EI Scan (41.588 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=685 RMF=740




(replib) 2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-4-(3-oxo-1-butenyl)-

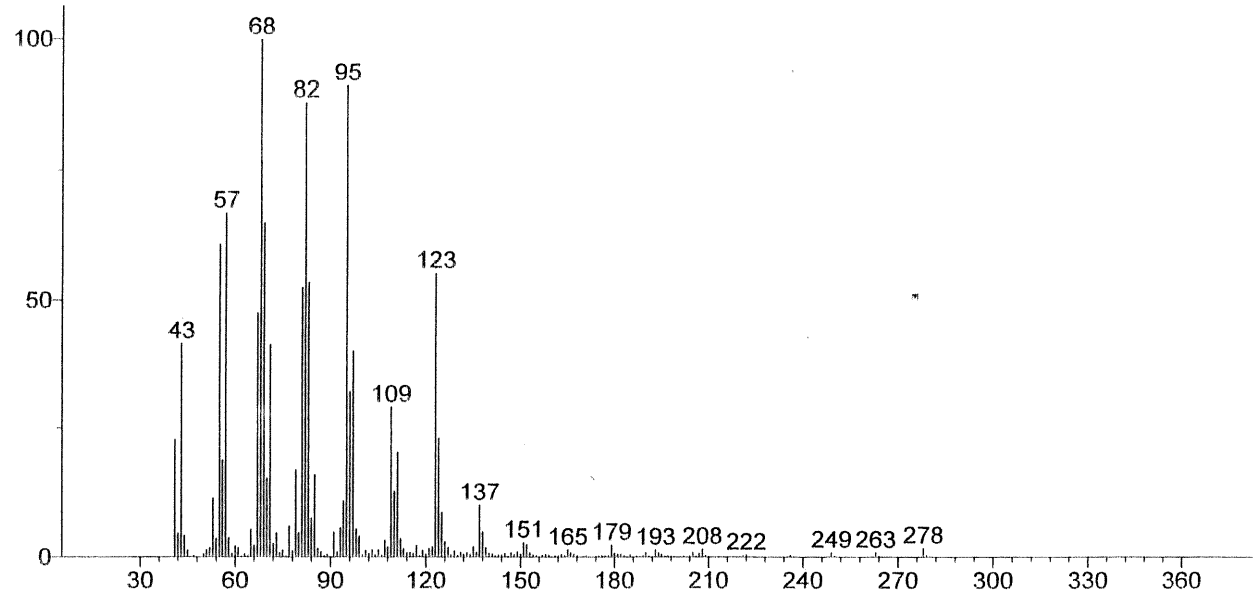
Name: 2-Cyclohexen-1-one, 4-hydroxy-3,5,5-trimethyl-4-(3-oxo-1-butenyl)-
Formula: $C_{13}H_{18}O_3$
MW: 222 CAS#: 7070-24-8 NIST#: 188889 ID#: 17031 DB: replib
Other DBs: None
Contributor: Chemical Concepts
10 largest peaks:
124 999 | 43 408 | 166 186 | 41 105 | 125 93 | 69 88 | 95 82 | 39 80 | 55 79 | 123 68 |
Synonyms:
1.4-Hydroxy-3,5,5-trimethyl-4-[(1E)-3-oxo-1-butenyl]-2-cyclohexen-1-one #

Estimated non-polar retention index (n-alkane scale):
Value: 1751 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

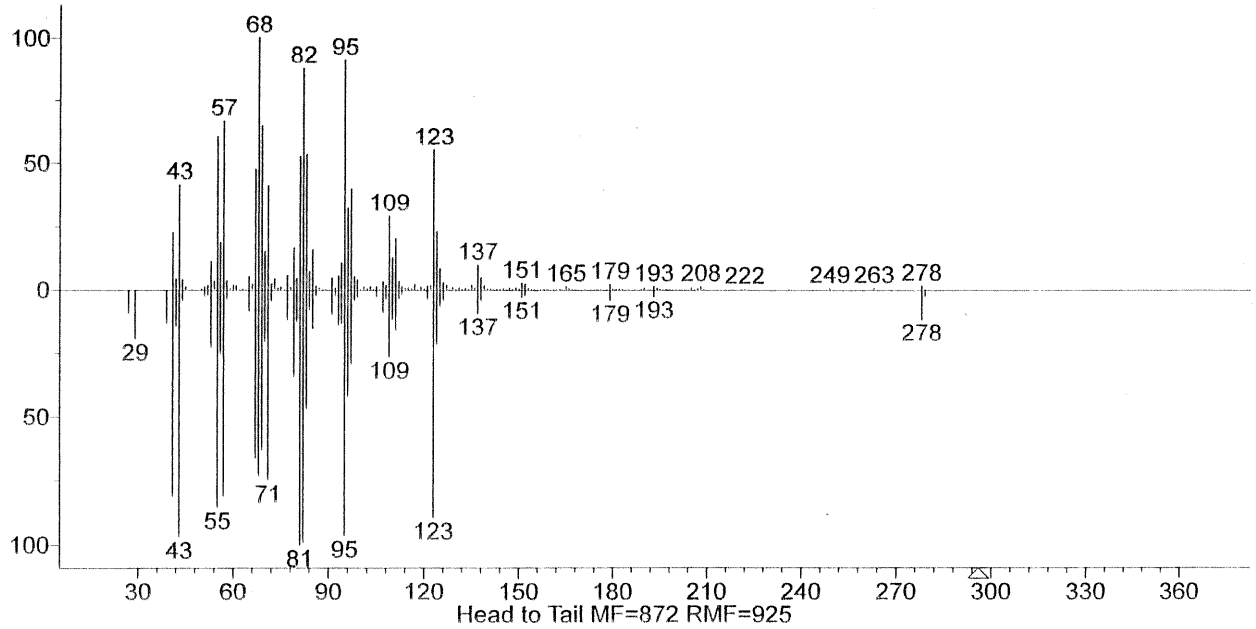
Retention index.
1. Value: 1729 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: BP-1
Column
Length: 12 m
Carrier Gas: H2
Data Type: Linear RI
Program Type: Ramp
Start T: 40 C
End T: 240 C
Heat
Rate: 4 K/min
Start Time: 2 min
End Time: 75 min
Source: Tan, S.T.; Wilkins, A.L.; Holland, P.T.; McGhie, T.K.,
Extractives from New Zealand unifloral honeys. 2. Degraded carotenoids and other substances from heather honey,
J. Agric. Food Chem., 37, 1989, 1217-1221.

2. Value: 1760 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: 36 0C ^ 20 K/min -> 85 0C
^ 1 K/min -> 145 oC ^ 3 K/min -> 250 0C
Source: Guyot-Declerck, C.; Chevance, F.; Lermusieau, G.; Collin, S.,
Optimized extraction procedure for quantifying norisoprenoids in honey and honey food products, J. Agric. Food
Chem., 48, 2000, 5850-5855.

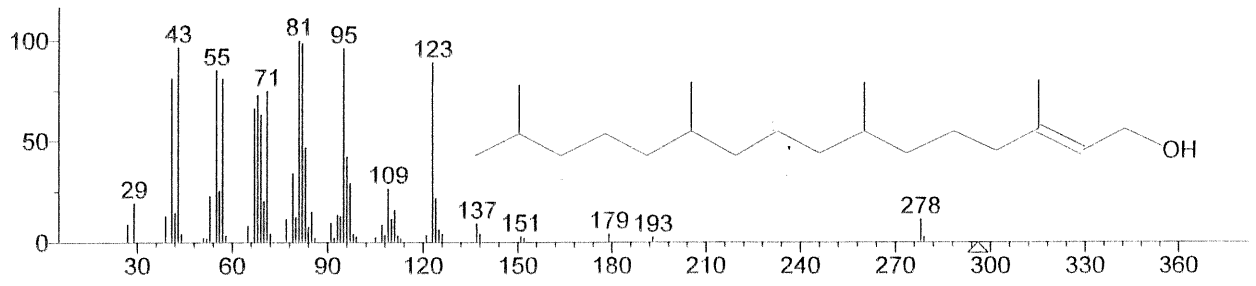
<...>




(Text File) +EI Scan (42.800 min) ALI-OLE-H7-220421-.D




Head to Tail MF=872 RMF=925



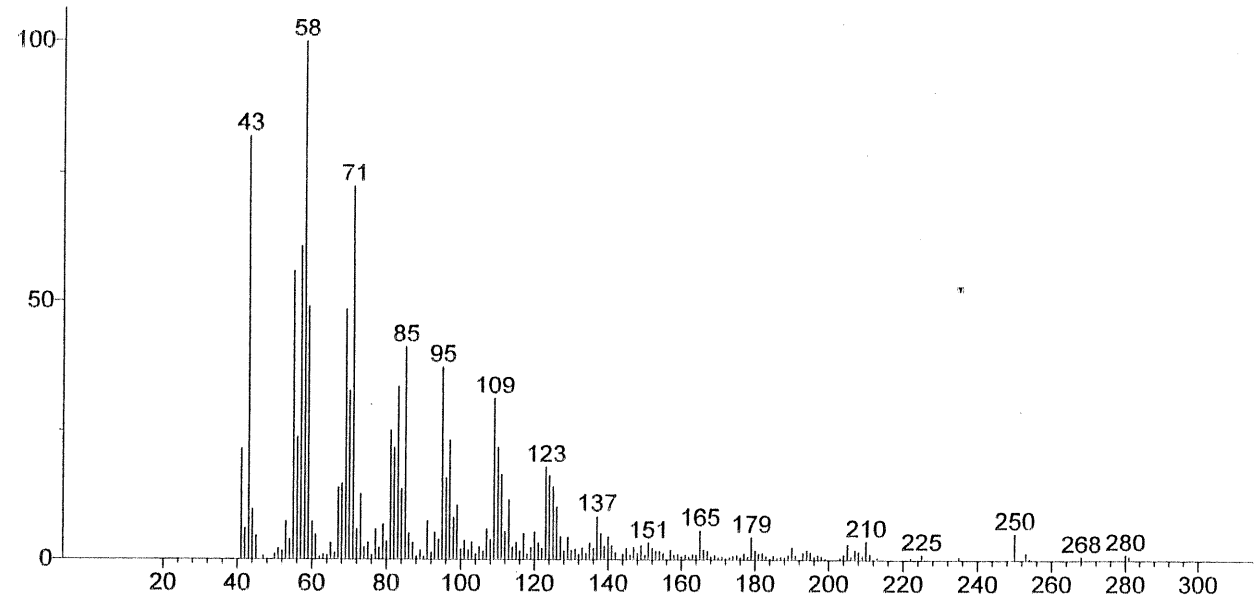

(mainlib) 3,7,11,15-Tetramethyl-2-hexadecen-1-ol

85

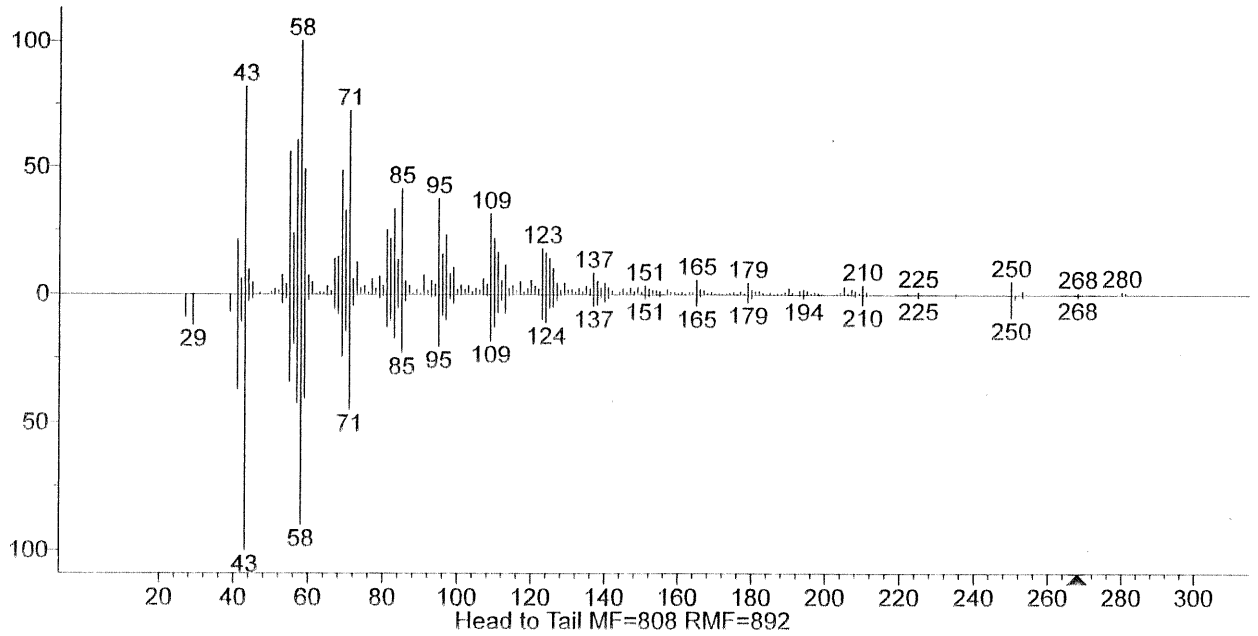
Name: 3,7,11,15-Tetramethyl-2-hexadecen-1-ol
Formula: $C_{20}H_{40}O$
MW: 296 CAS#: 102608-53-7 NIST#: 114703 ID#: 43206 DB: mainlib
Other DBs: IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
81 999 | 82 986 | 43 965 | 95 962 | 123 892 | 55 852 | 41 811 | 57 811 | 71 748 | 68 728 |
Synonyms:
1.(2E)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol #

Estimated non-polar retention index (n-alkane scale):
Value: 2045 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

Retention index.
1. Value: 2119.33 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: SE
-54
Column Length: 25 m
Column Diameter: 0.31 mm
Data Type: Linear RI
Program Type: Ramp
Start T: 35
C
End T: 230 C
Heat Rate: 4 K/min
Start Time: 3 min
End Time: 10 min
Source: Yin, W.; Xiu, Z.; Aijin, H.,
Analysis of the volatile components in trogopterorum feces by capillary gas chromatography and gas chromatography/mass spectrometry, Fenxi Huaxue, 29(2), 2001, 195-198.




(Text File) +EI Scan (43.028 min) ALI-OLE-H7-220421-.D




Head to Tail MF=808 RMF=892


(mainlib) 2-Pentadecanone, 6,10,14-trimethyl-

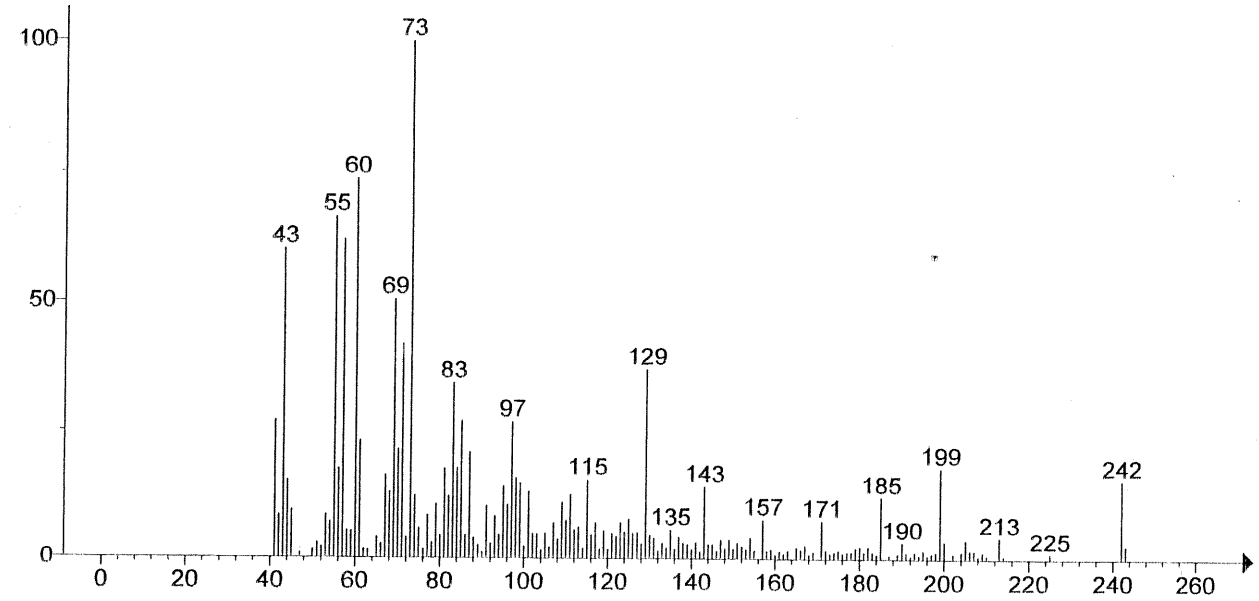
65

Name: 2-Pentadecanone, 6,10,14-trimethyl-
Formula: $C_{18}H_{36}O$
MW: 268 CAS#: 502-69-2 NIST#: 12976 ID#: 7533 DB: mainlib
Other DBs: TSCA, EINECS
Contributor: STC 0011
10 largest peaks:
43 999 | 58 898 | 71 450 | 57 426 | 59 407 | 41 373 | 55 345 | 69 245 | 85 229 | 95 203 |
Synonyms:
1.Hexahydrofarnesyl acetone
2.6,10,14-Trimethyl-2-pentadecanone

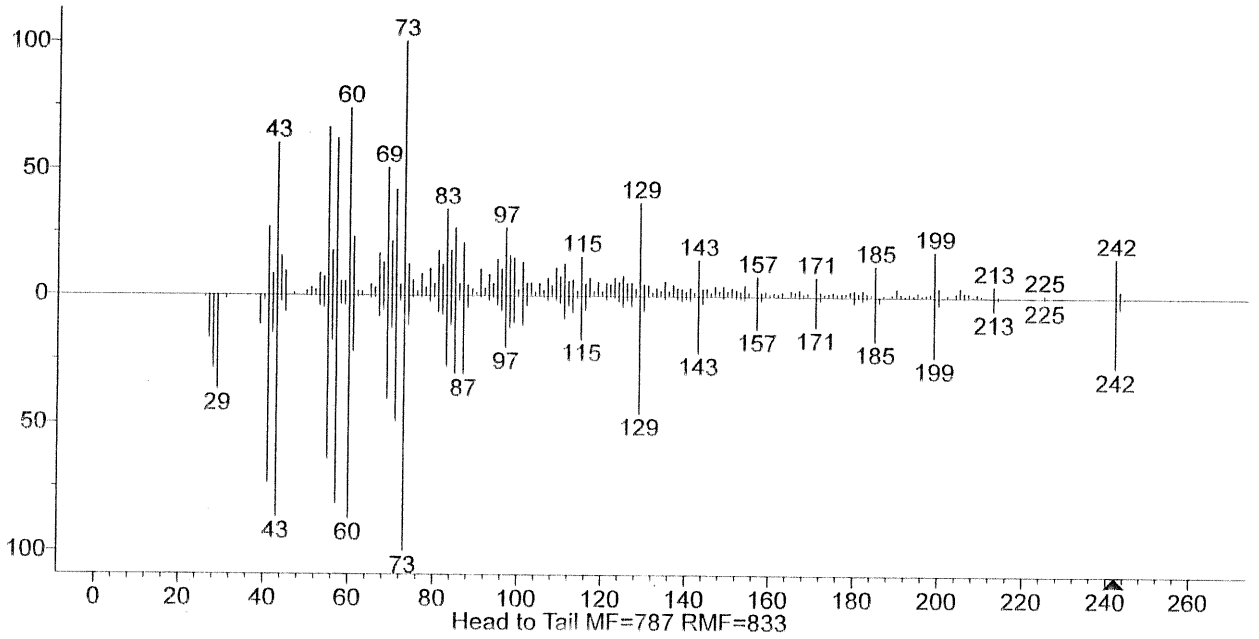
Estimated non-polar retention index (n-alkane scale):
Value: 1754 iu
Confidence interval (Ketones): 57(50%) 246(95%) iu

Retention index.
1. Value: 1838 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: 50 C
End T: 250 C
Heat Rate: 5 K/min
Start Time: 3 min
End Time: 15
min
Source: Blagojevic, P.; Radulovic, N.; Palic, R.; Stojanovic, G., Chemical composition of the essential oils of Serbian wild-growing Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-4789.

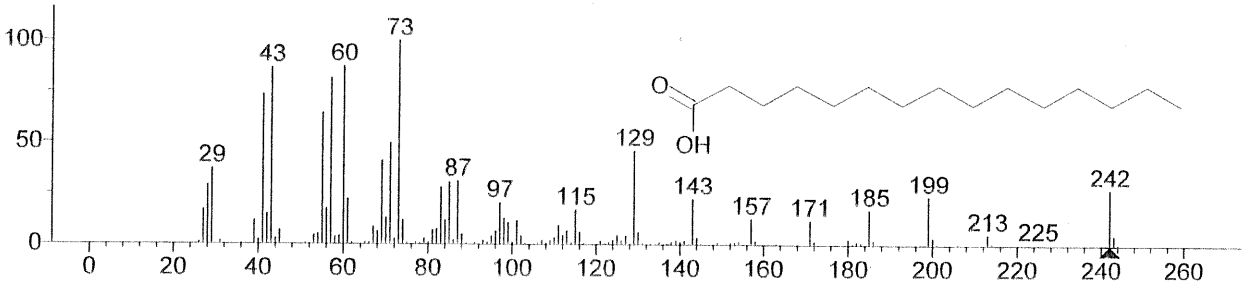
2.
Value: 1858 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column Length:
30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program
Type: Ramp
Start T: 60 C
End T: 240 C
Heat Rate: 4 K/min
Source: Rezazadeh, S.; Hamedani, M.P.;




(Text File) +EI Scan (43.441 min) ALI-OLE-H7-220421-.D




Head to Tail MF=787 RMF=833



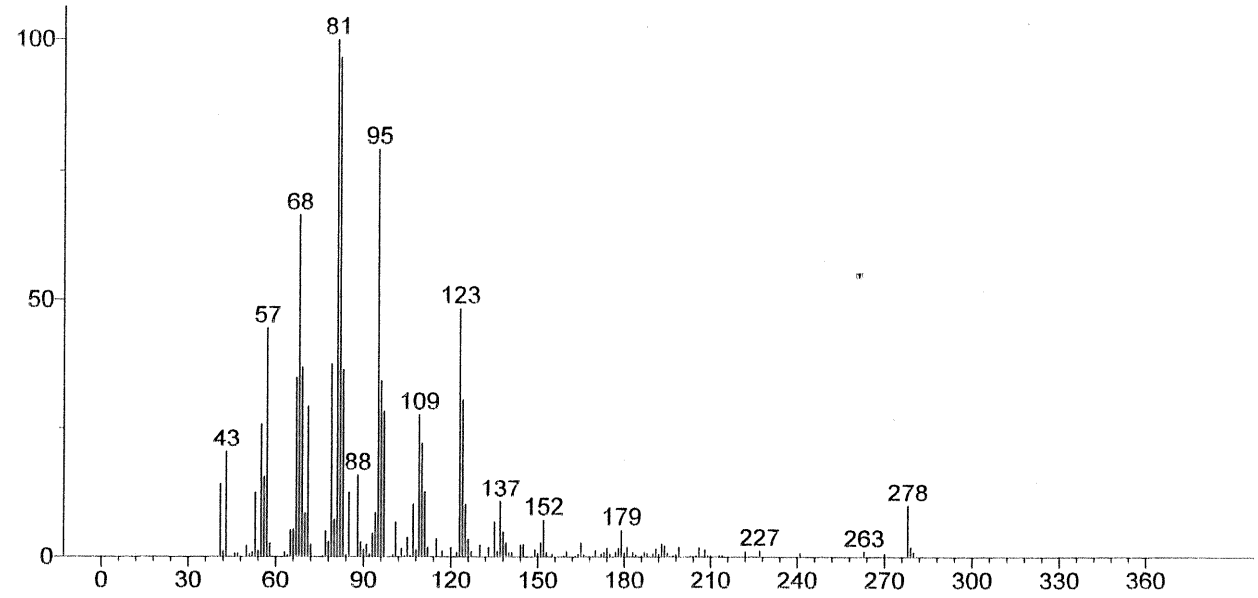

(replib) Pentadecanoic acid

Name: Pentadecanoic acid
Formula: $C_{15}H_{30}O_2$
MW: 242 CAS#: 1002-84-2 NIST#: 221146 ID#: 8469 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS, IRDB
Contributor: Chemical Concepts
10 largest peaks:
73 999 | 60 871 | 43 865 | 57 814 | 41 734 | 55 641 | 71 493 | 129 457 | 69 405 | 29 367 |
Synonyms:
1.Pentadecylic acid
2.n-Pentadecanoic acid
3.n-Pentadecylic acid

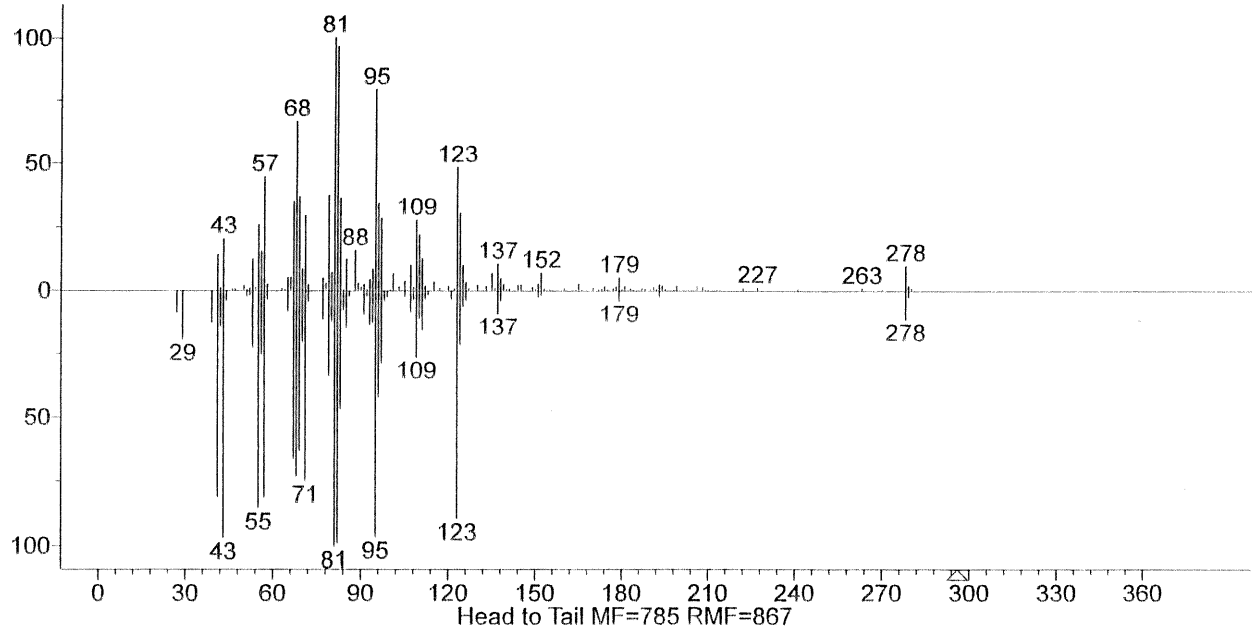
Estimated non-polar retention index (n-alkane scale):
Value: 1869 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.
1. Value: 1823 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.

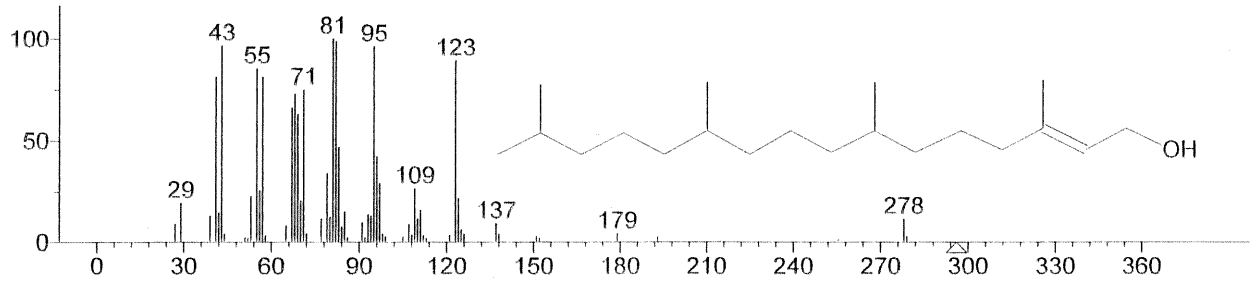
2.
Value: 1823 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column
Length: 25 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.4 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 80 C
End T: 270 C
Heat Rate: 10 K/min
Source: Ziegenbein, F.C.; Hanssen,
H.-P.; König, W.A., Chemical constituents of the essential oils of three wood-rotting fungi, Flavour Fragr. J., 21,
2006, 813-816.




(Text File) +EI Scan (43.680 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=785 RMF=867

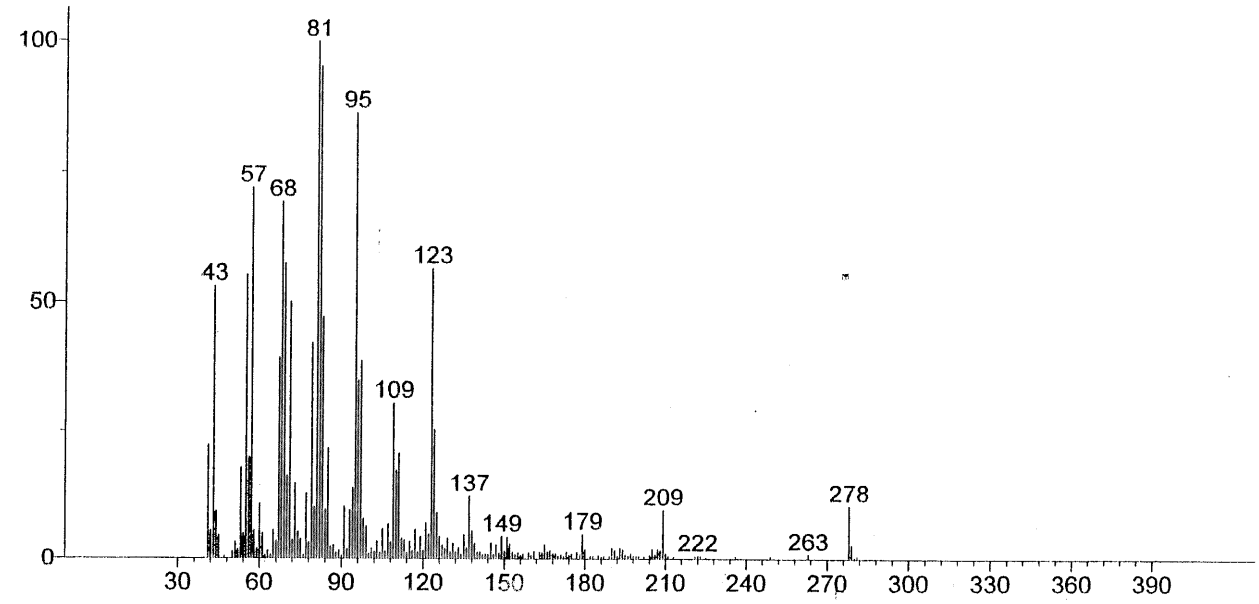



(mainlib) 3,7,11,15-Tetramethyl-2-hexadecen-1-ol

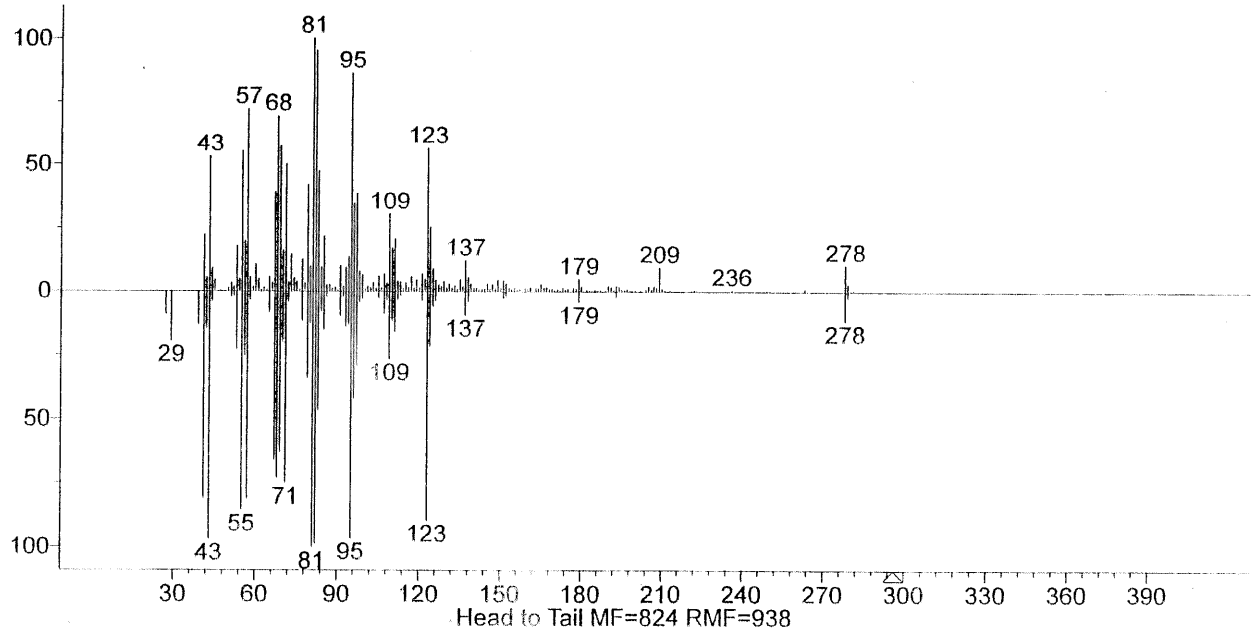
Name: 3,7,11,15-Tetramethyl-2-hexadecen-1-ol
Formula: $C_{20}H_{40}O$
MW: 296 CAS#: 102608-53-7 NIST#: 114703 ID#: 43206 DB: mainlib
Other DBs: IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
81 999 | 82 986 | 43 965 | 95 962 | 123 892 | 55 852 | 41 811 | 57 811 | 71 748 | 68 728 |
Synonyms:
1.(2E)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol #

Estimated non-polar retention index (n-alkane scale):
Value: 2045 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

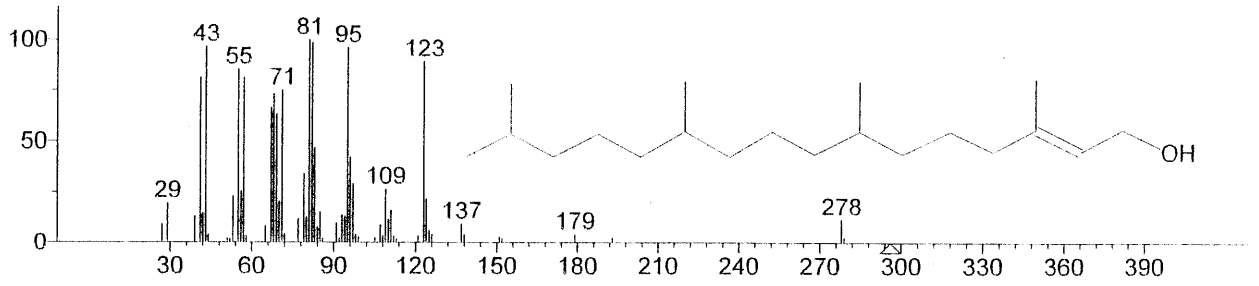
Retention index.
1. Value: 2119.33 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: SE
-54
Column Length: 25 m
Column Diameter: 0.31 mm
Data Type: Linear RI
Program Type: Ramp
Start T: 35
C
End T: 230 C
Heat Rate: 4 K/min
Start Time: 3 min
End Time: 10 min
Source: Yin, W.; Xiu, Z.; Aijin, H.,
Analysis of the volatile components in trogopterorum feces by capillary gas chromatography and gas chromatography/mass spectrometry, Fenxi Huaxue, 29(2), 2001, 195-198.




(Text File) +EI Scan (44.382 min) ALI-OLE-H7-220421-.D




Head to Tail MF=824 RMF=938

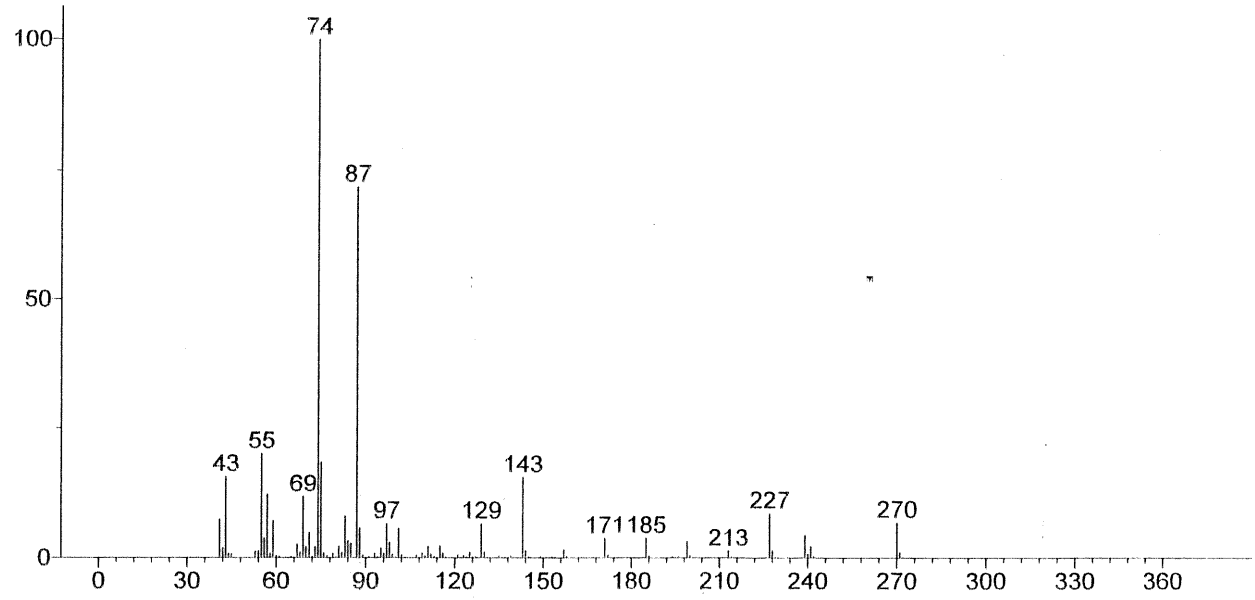



(mainlib) 3,7,11,15-Tetramethyl-2-hexadecen-1-ol

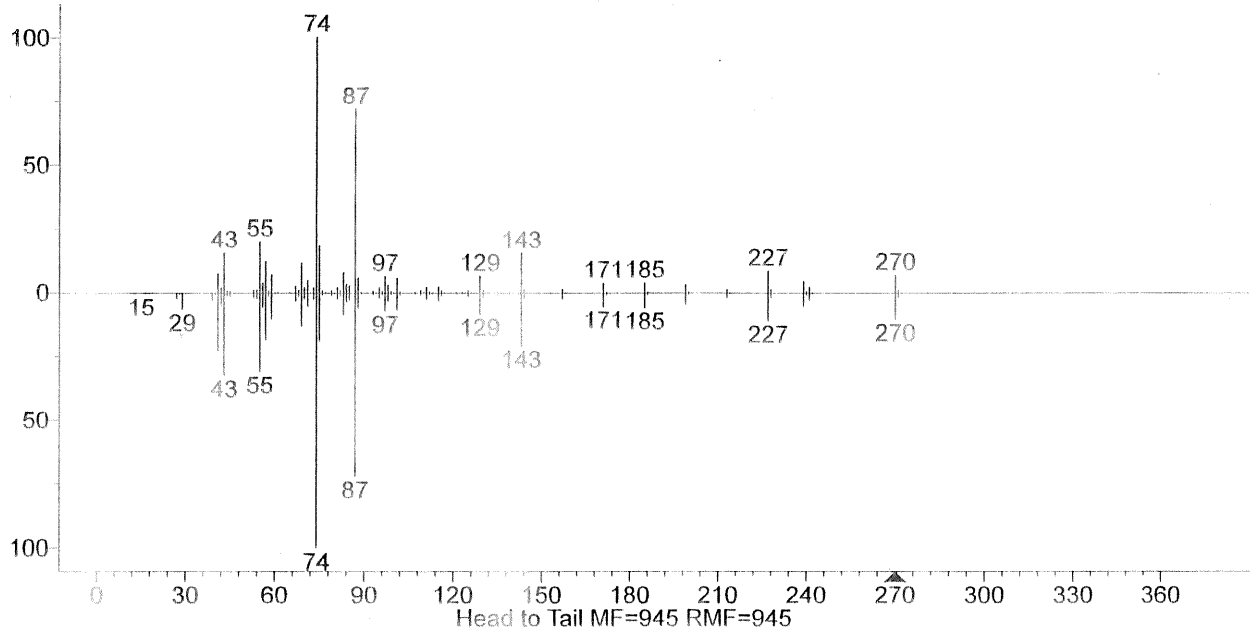
Name: 3,7,11,15-Tetramethyl-2-hexadecen-1-ol
Formula: $C_{20}H_{40}O$
MW: 296 CAS#: 102608-53-7 NIST#: 114703 ID#: 43206 DB: mainlib
Other DBs: IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:
81 999 | 82 986 | 43 965 | 95 962 | 123 892 | 55 852 | 41 811 | 57 811 | 71 748 | 68 728 |
Synonyms:
1.(2E)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol #

Estimated non-polar retention index (n-alkane scale):
Value: 2045 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

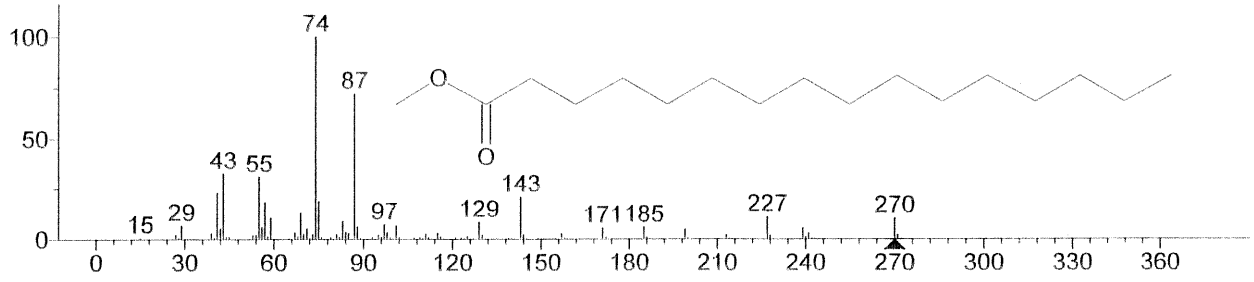
Retention index.
1. Value: 2119.33 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: SE
-54
Column Length: 25 m
Column Diameter: 0.31 mm
Data Type: Linear RI
Program Type: Ramp
Start T: 35
C
End T: 230 C
Heat Rate: 4 K/min
Start Time: 3 min
End Time: 10 min
Source: Yin, W.; Xiu, Z.; Aijin, H.,
Analysis of the volatile components in trogopterorum feces by capillary gas chromatography and gas chromatography/mass spectrometry, Fenxi Huaxue, 29(2), 2001, 195-198.




(Text File) +EI Scan (46.178 min) ALI-OLE-H7-220421-.D




Head to Tail MF=945 RMF=945



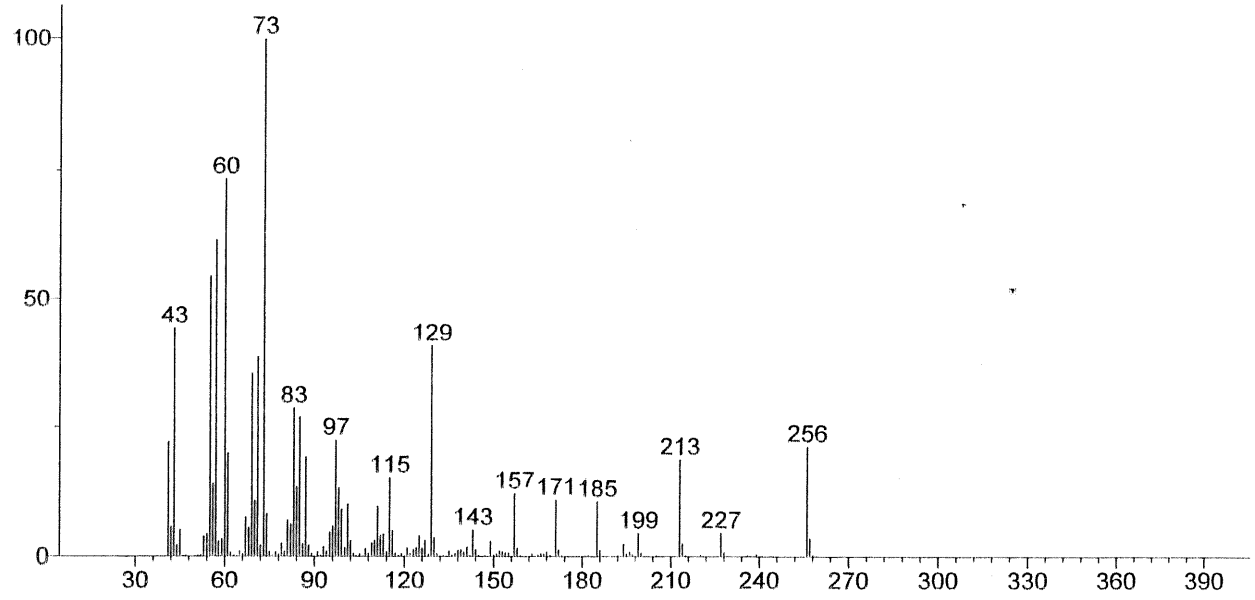

(mainlib) Hexadecanoic acid, methyl ester

Name: Hexadecanoic acid, methyl ester
Formula: $C_{17}H_{34}O_2$
MW: 270 CAS#: 112-39-0 NIST#: 333716 ID#: 38248 DB: mainlib
Other DBs: Fine, TSCA, EPA, HODOC, NIH, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
74 999 | 87 720 | 43 325 | 55 310 | 41 228 | 143 208 | 75 188 | 57 183 | 69 132 | 227 110 |
Synonyms:
1.Palmitic acid, methyl ester
2.n-Hexadecanoic acid methyl ester
3.Metholene 2216
4.Methyl hexadecanoate
5.Methyl n-hexadecanoate
6.Methyl palmitate
7.Uniphat A60
8.Emery 2216
9.Radia 7120

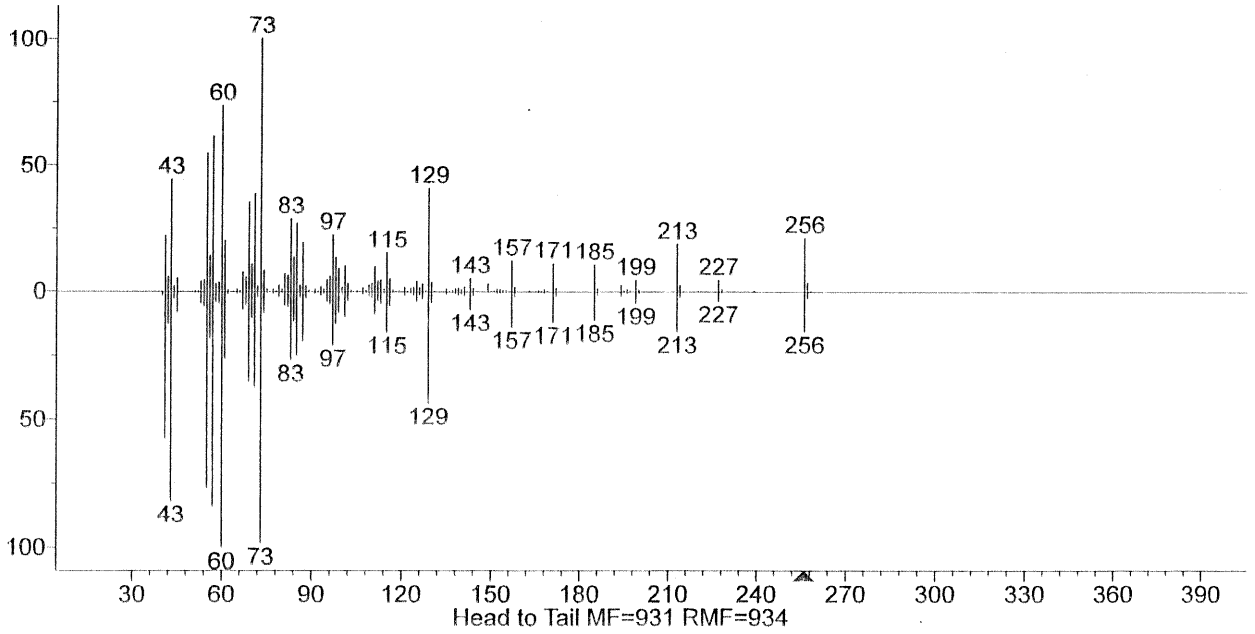
Estimated non-polar retention index (n-alkane scale):
Value: 1878 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 1908 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: 50 C
End T: 250 C
Heat Rate: 5 K/min
Start Time: 3 min
End Time: 15
min
Source: Blagojevic, P.; Radulovic, N.; Palic, R.; Stojanovic, G., Chemical composition of the essential oils of Serbian wild-growing Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-4789.

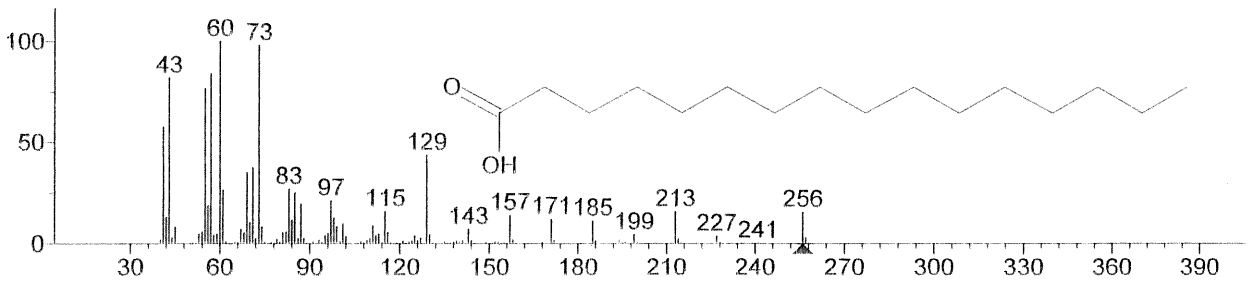
2.
Value: 1909 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: SPB-1
Column Length:
30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um




(Text File) +EI Scan (48.153 min) ALI-OLE-H7-220421-.D




Head to Tail MF=931 RMF=934



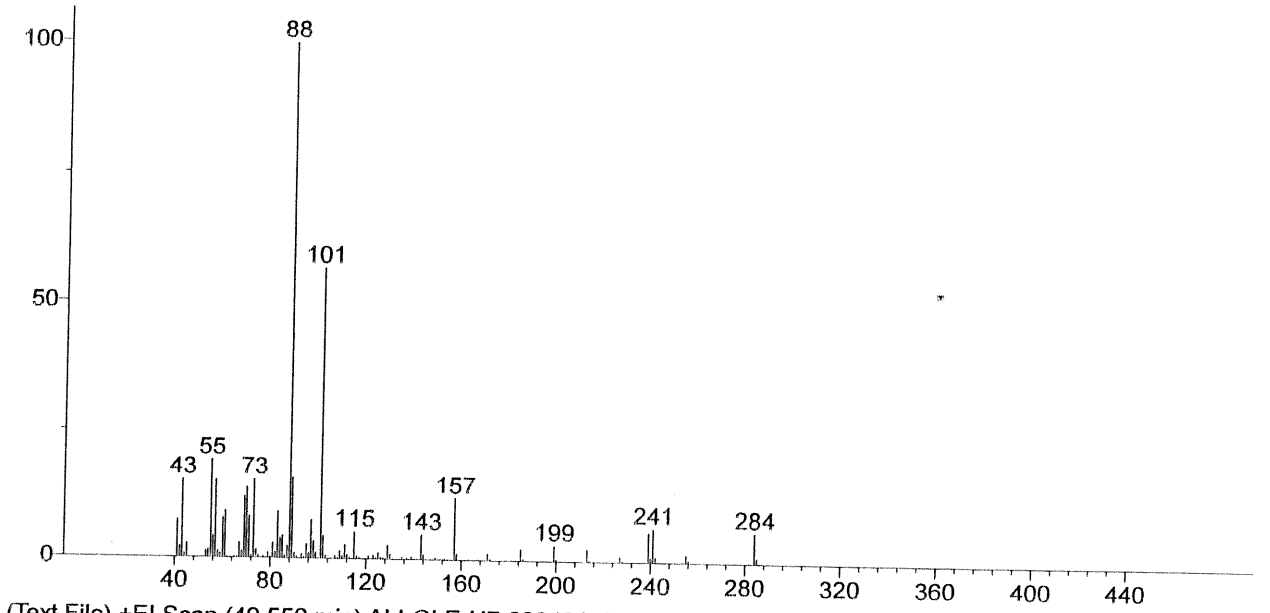

(replib) n-Hexadecanoic acid

Name: n-Hexadecanoic acid
Formula: $C_{16}H_{32}O_2$
MW: 256 CAS#: 57-10-3 NIST#: 335494 ID#: 6723 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Drug Lab
10 largest peaks:
60 999 | 73 980 | 57 840 | 43 817 | 55 767 | 41 574 | 129 435 | 71 373 | 69 351 | 83 267 |
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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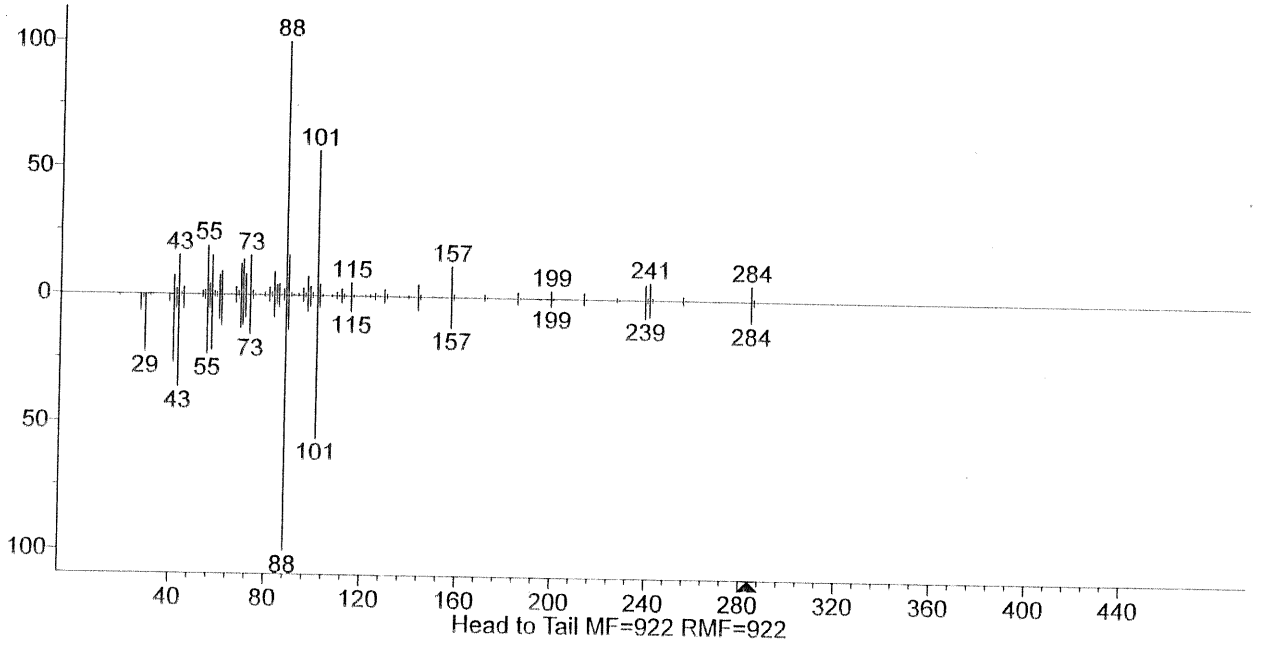
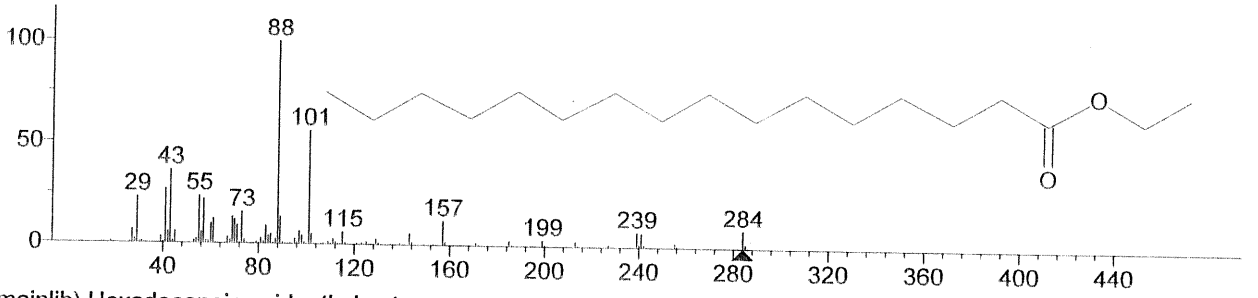



Head to Tail MF=922 RMF=922



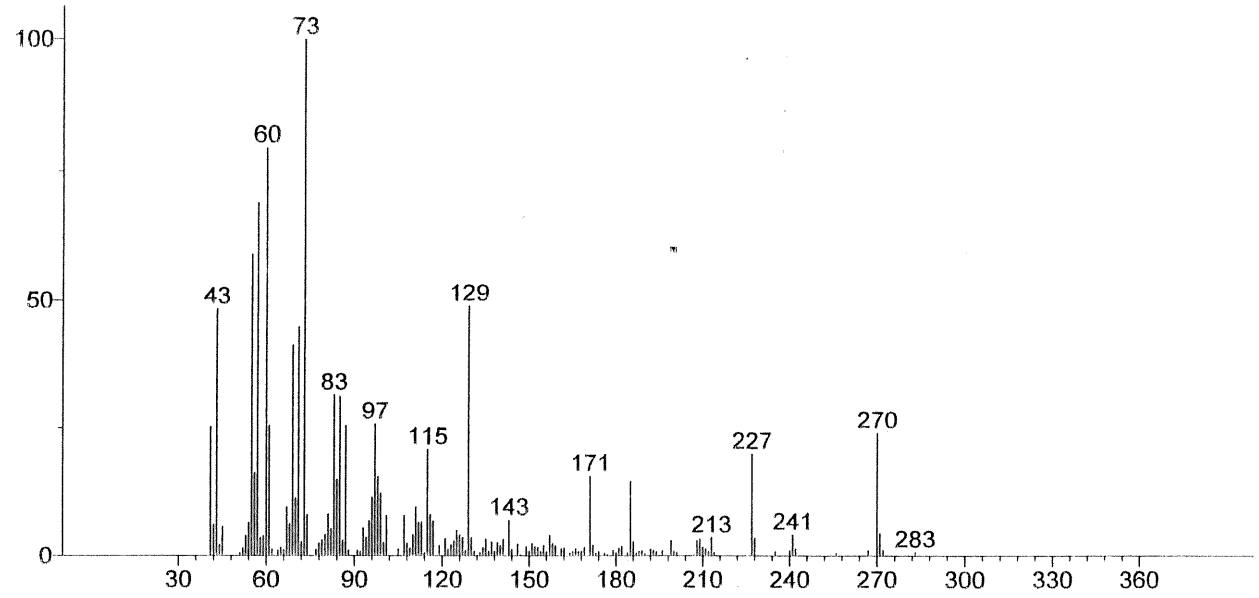

(mainlib) Hexadecanoic acid, ethyl ester

Name: Hexadecanoic acid, ethyl ester
Formula: $C_{18}H_{36}O_2$
MW: 284 CAS#: 628-97-7 NIST#: 233204 ID#: 49485 DB: mainlib
Other DBs: Fine, TSCA, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-5396
10 largest peaks:
88 999 | 101 559 | 43 362 | 41 268 | 55 233 | 29 227 | 57 217 | 73 156 | 89 136 | 69 132 |
Synonyms:
1.Palmitic acid, ethyl ester
2.Ethyl hexadecanoate
3.Ethyl palmitate

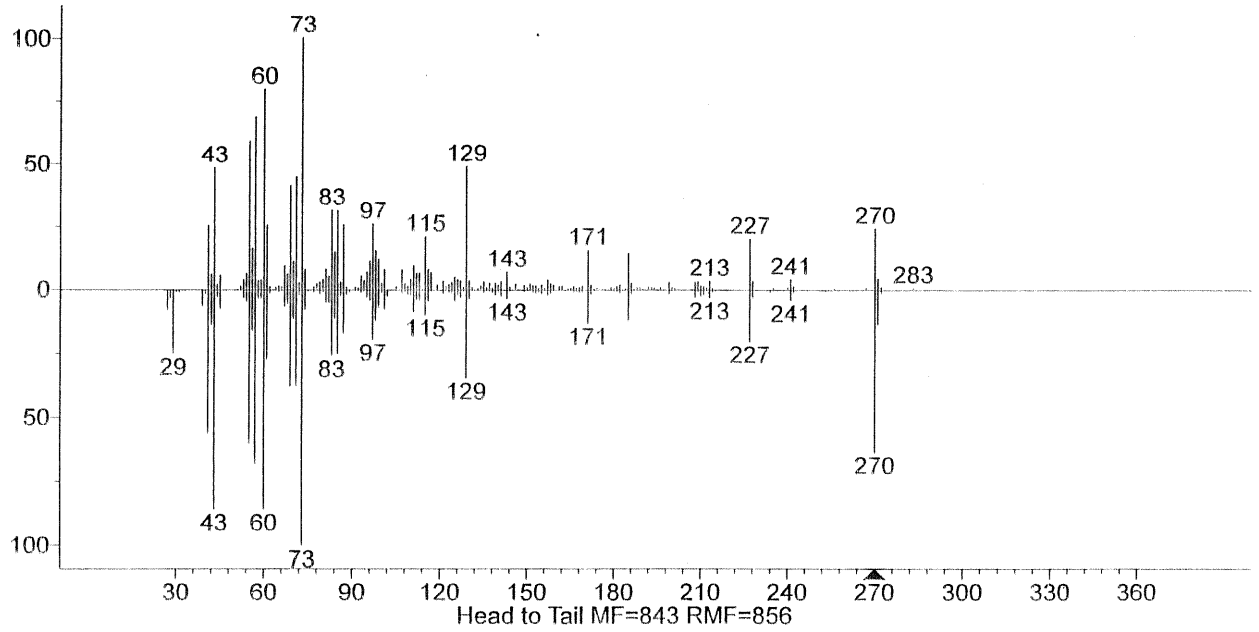
Estimated non-polar retention index (n-alkane scale):
Value: 1978 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 1968 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: 50 C
End T: 250 C
Heat Rate: 5 K/min
Start Time: 3 min
End Time: 15
min
Source: Blagojevic, P.; Radulovic, N.; Palic, R.; Stojanovic, G., Chemical composition of the essential oils of Serbian wild-growing Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-4789.

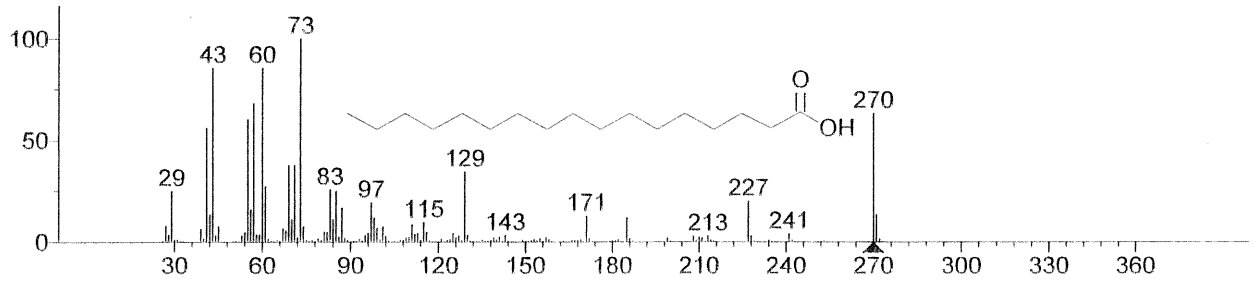
2.
Value: 1966 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-1
Column Length:
50 m
Carrier Gas: He
Column Diameter: 0.2 mm
Phase Thickness: 0.33 um
Data Type: Linear RI
Program
Type: Ramp
Start T: 60 C
End T: 250 C
Heat Rate: 2 K/min




(Text File) +EI Scan (53.616 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=843 RMF=856



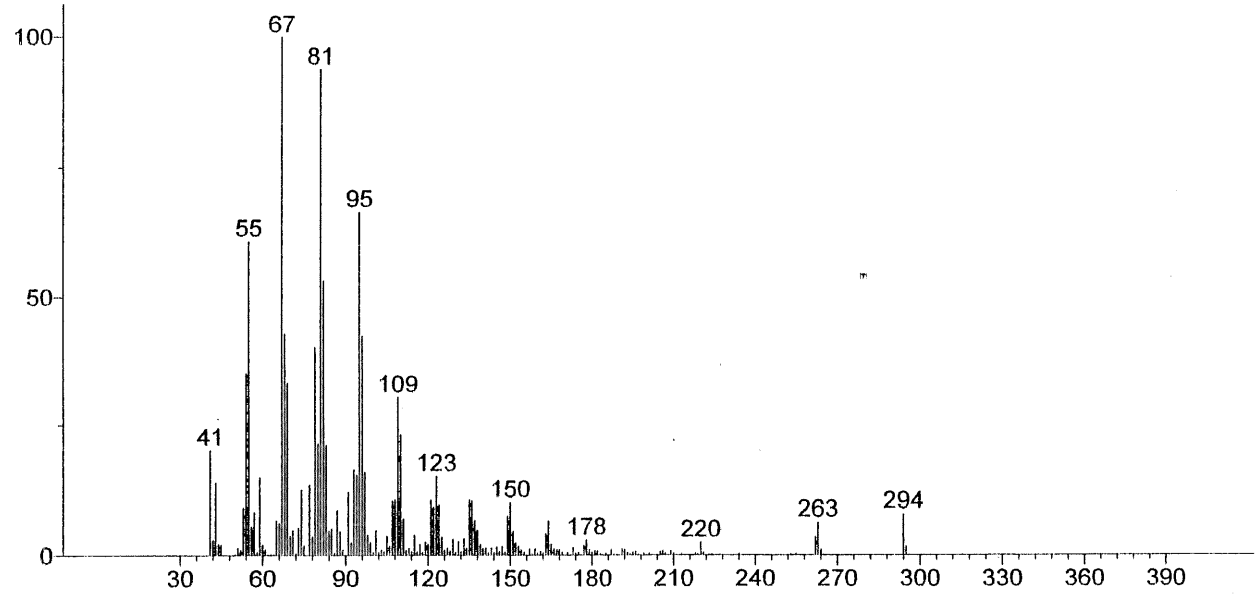

(replib) Heptadecanoic acid

Name: Heptadecanoic acid
Formula: $C_{17}H_{34}O_2$
MW: 270 CAS#: 506-12-7 NIST#: 36447 ID#: 8383 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS, IRDB
Contributor: R.T.HOLMAN,UNIVERSITY OF MINNESOTA
10 largest peaks:
73 999 | 43 856 | 60 856 | 57 680 | 270 632 | 55 600 | 41 560 | 69 376 | 71 376 | 129 344 |
Synonyms:
1.n-Heptadecanoic acid
2.n-Heptadecoic acid
3.n-Heptadecylic acid
4.Margaric acid
5.Margarinic acid
6.Normal-heptadecanoic acid

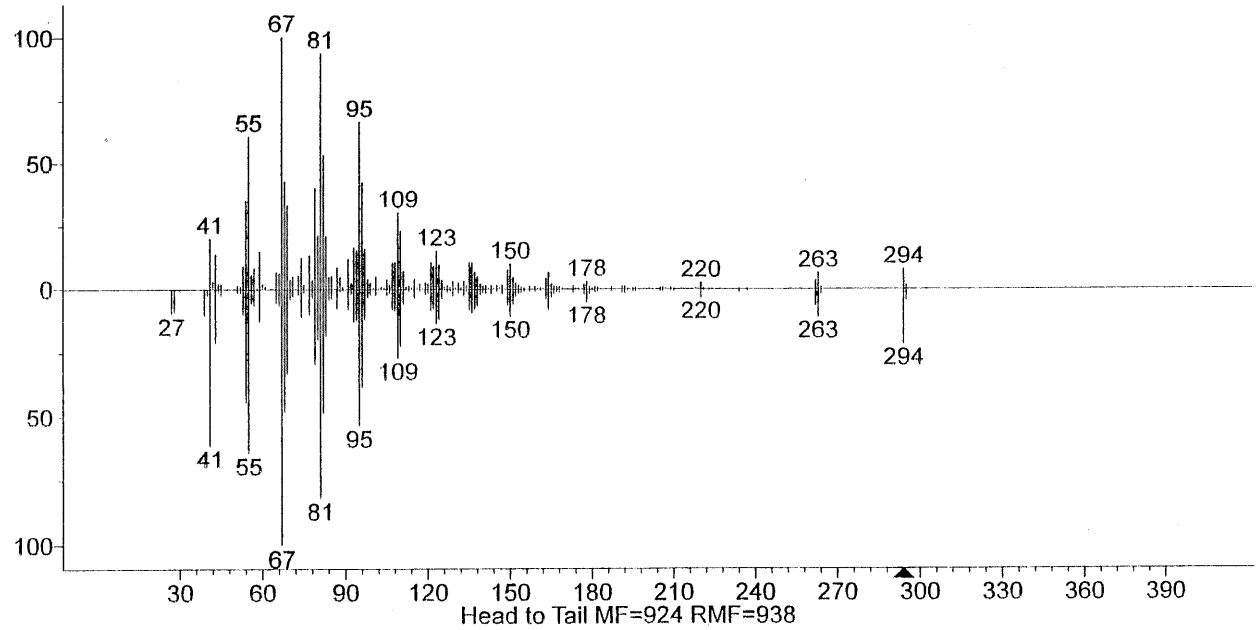
Estimated non-polar retention index (n-alkane scale):
Value: 2067 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

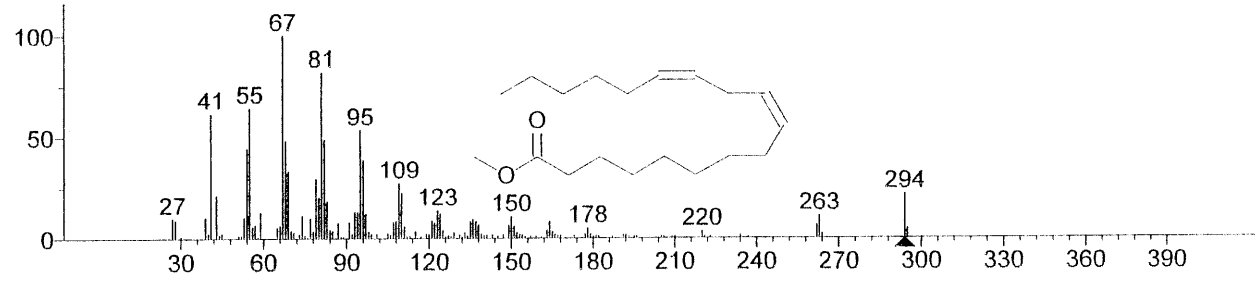
Retention index.
1. Value: 2038 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 30 m
Column Diameter: 0.2 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program Type:
Ramp
Start T: 50 C
End T: 300 C
Heat Rate: 5 K/min
Start Time: 2 min
End Time: 5 min
Source: Johnson, C.
I.; Urso, A.; Geleta, L., Broad spectrum analysis of municipal and industrial effluents discharged into the Peace, Athabasca and Slave river basins: characterization of effluent samples, 1994 - Volume 1 of 2, Northern River Basins Study Project Report No. 121, Norther River Basins Study, Edmonton, Alberta, 1997, 27.

2. Value: 2039
iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column Length: 30
m
Column Diameter: 0.2 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program Type: Ramp
Start T: 50
C




(Text File) +EI Scan (56.186 min) ALI-OLE-H7-220421-.D



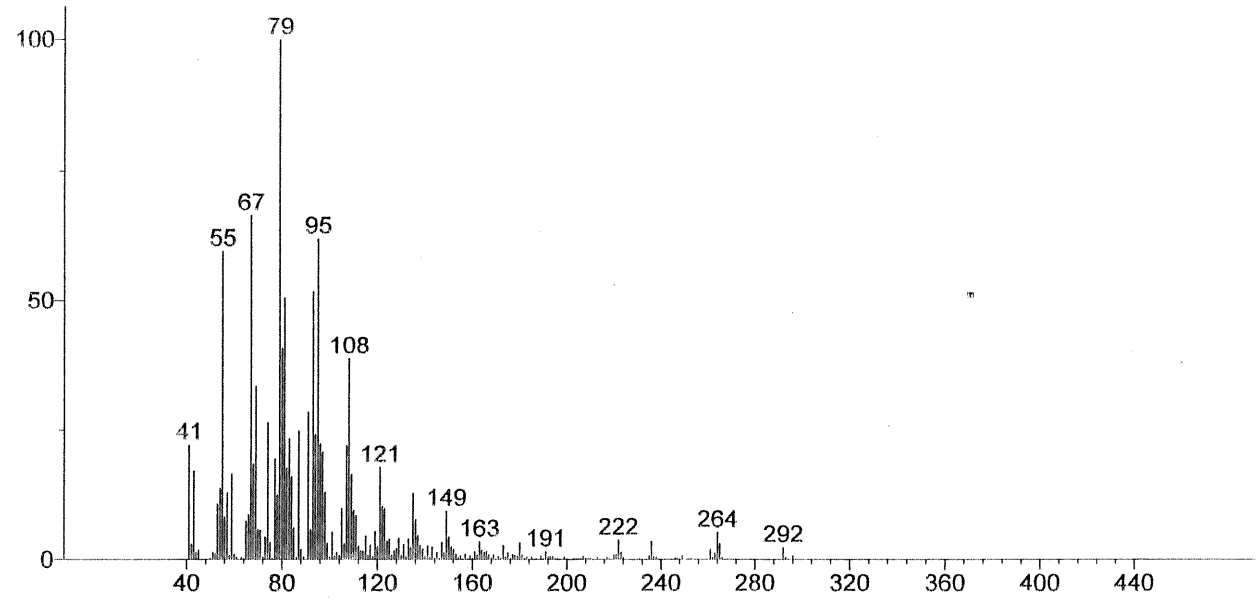

(replib) 9,12-Octadecadienoic acid (Z,Z)-, methyl ester

Name: 9,12-Octadecadienoic acid (Z,Z)-, methyl ester
Formula: $C_{19}H_{34}O_2$
MW: 294 CAS#: 112-63-0 NIST#: 79485 ID#: 7214 DB: replib
Other DBs: Fine, TSCA, EPA, HODOC, NIH, EINECS
Contributor: O A MAMER, MCGILL UNIVERSITY, MONTREAL, CANADA
10 largest peaks:
67 999 | 81 817 | 55 641 | 41 613 | 95 534 | 82 486 | 68 480 | 54 442 | 96 385 | 69 330 |
Synonyms:
1.Linoleic acid, methyl ester
2.Methyl cis,cis-9,12-octadecadienoate
3.Methyl linoleate
4.Methyl octadecadienoate
5.Methyl 9-cis,12-cis-octadecadienoate
6.Methyl (9Z,12Z)-9,12-octadecadienoate #

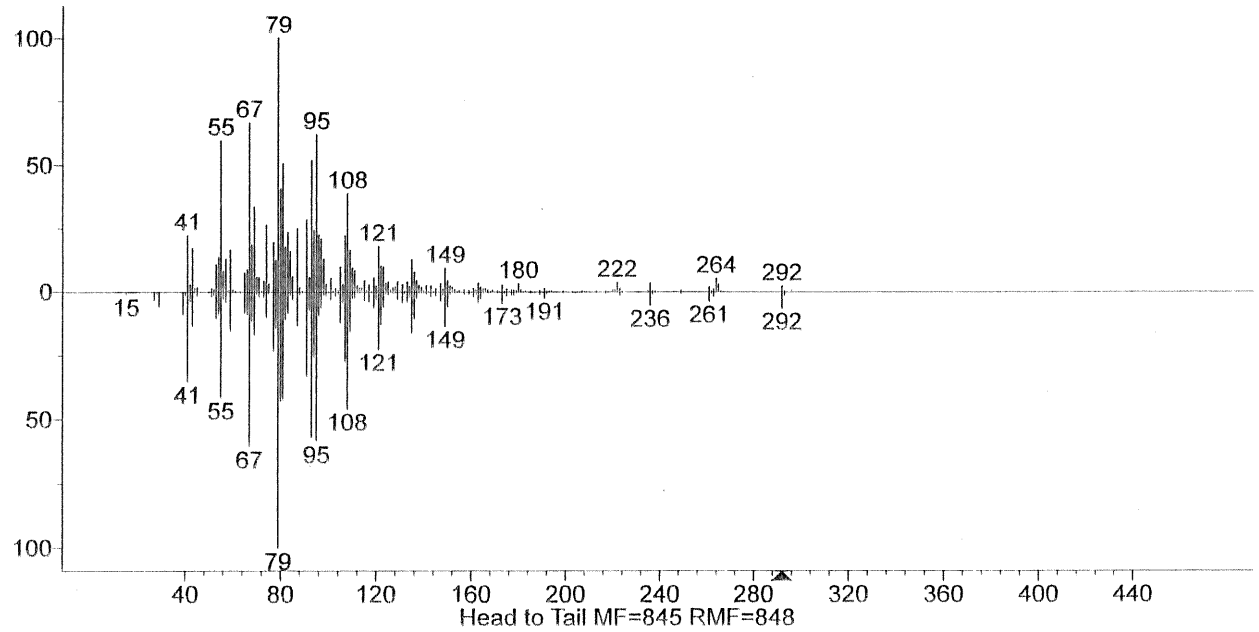
Estimated non-polar retention index (n-alkane scale):
Value: 2093 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

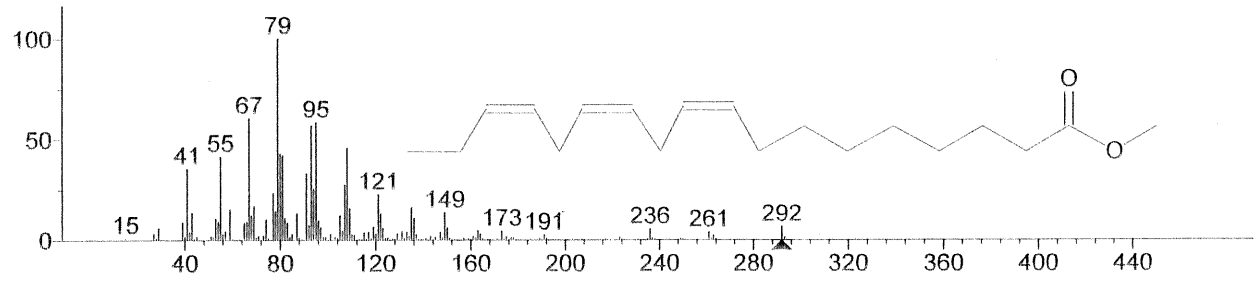
Retention index.
1. Value: 2071 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: SPB-1
Column
Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 50 C
End T: 250 C
Heat Rate: 5 K/min
Start Time: 3 min
End Time: 15
min
Source: Blagojevic, P.; Radulovic, N.; Palic, R.; Stojanovic, G., Chemical composition of the essential oils of Serbian wild-growing Srtemisia absinthium and Artemisia vulgaris, J. Agric. Food Chem., 54, 2006, 4780-4789.

2.
Value: 2087 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: BP-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




(Text File) +EI Scan (56.774 min) ALI-OLE-H7-220421-.D



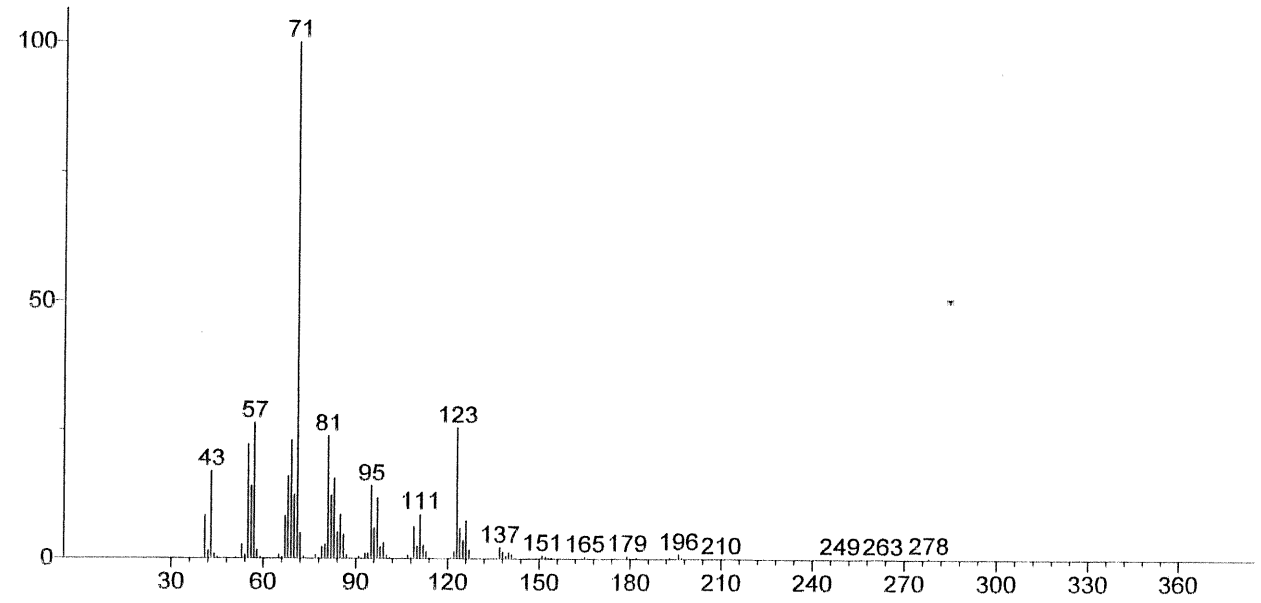

(mainlib) 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-

Name: 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-
Formula: $C_{19}H_{32}O_2$
MW: 292 CAS#: 301-00-8 NIST#: 333199 ID#: 41712 DB: mainlib
Other DBs: Fine, TSCA, HODOC, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
79 999 | 67 603 | 95 583 | 93 567 | 108 457 | 80 430 | 81 422 | 55 414 | 41 354 | 91 332 |
Synonyms:
1.Linolenic acid, methyl ester
2.Methyl all-cis-9,12,15-octadecatrienoate
3.Methyl linolenate
4.Methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate #

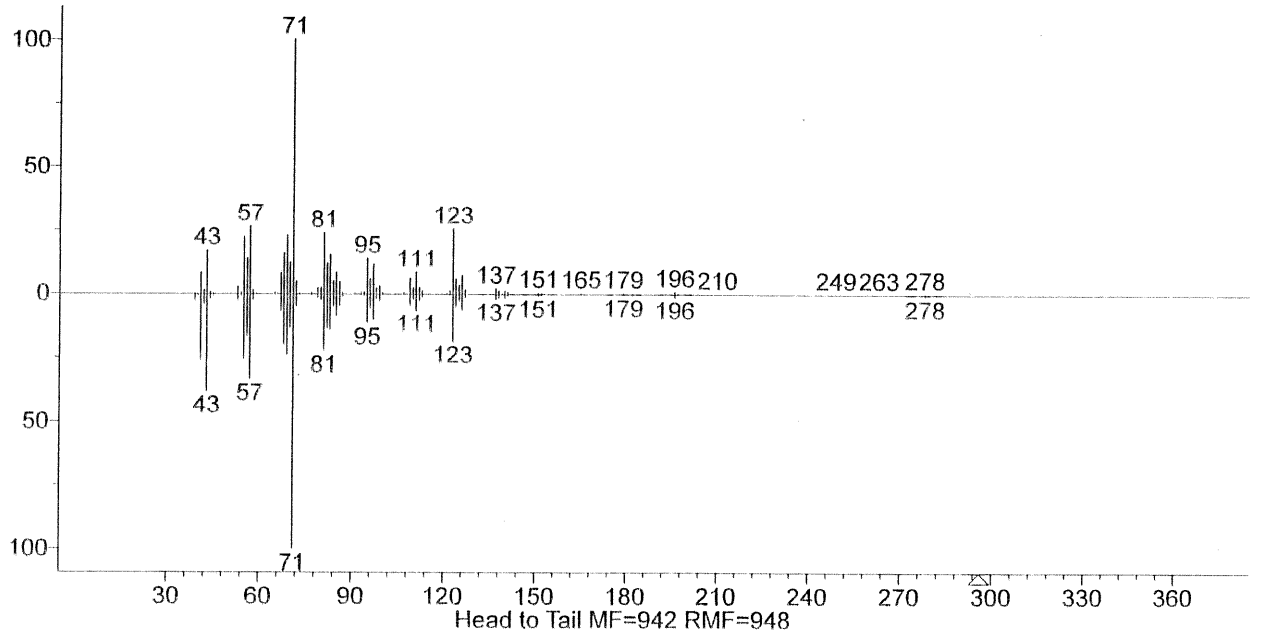
Estimated non-polar retention index (n-alkane scale):
Value: 2101 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 2077 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: 50 C
End T: 250 C
Heat Rate: 5 K/min
Start Time: 3 min
End Time: 15
min
Source: Radulovic, N.; Lazarevic, J.; Stojanovic, G.; Palic, R., Chemotaxonomically significant 2-ethyl substituted fatty acids from Stachys milanii Petrovic (Lamiaceae), Biochem. Syst. Ecol., 34, 2006, 341-344.

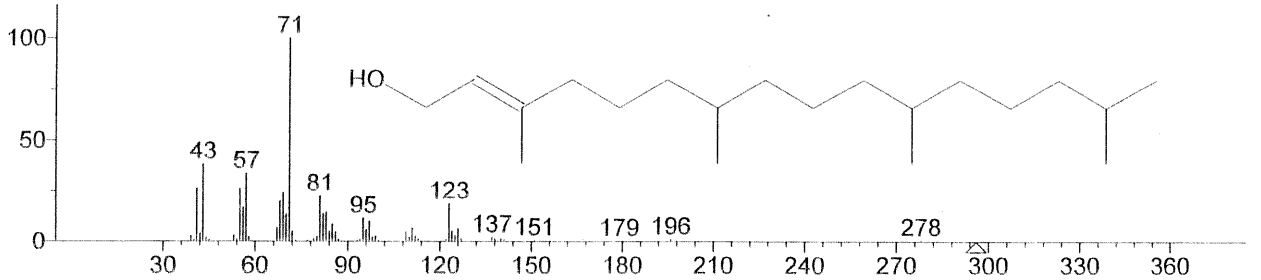
2.
Value: 2098 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-1
Column Length:
30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.33 um
Data Type: Linear RI
Program
Type: Ramp
Start T: 40 C
End T: 260 C




(Text File) +EI Scan (57.725 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=942 RMF=948




(replib) Phytol

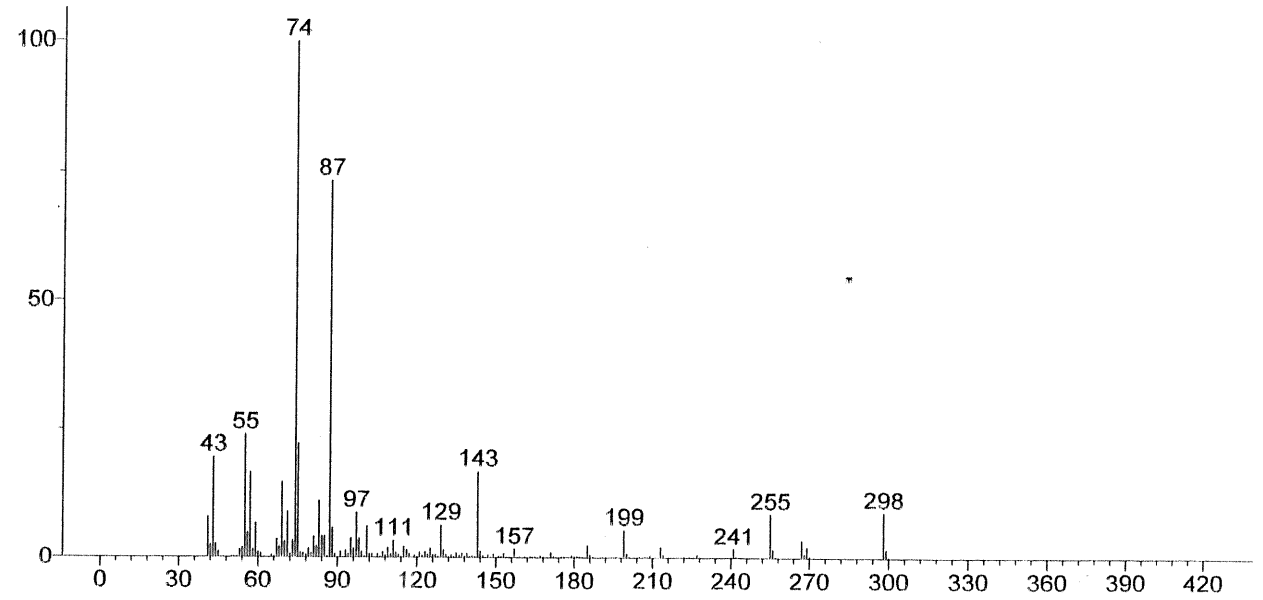
105

Name: Phytol
Formula: $C_{20}H_{40}O$
MW: 296 CAS#: 150-86-7 NIST#: 108727 ID#: 8051 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, EINECS
Contributor: Philip Morris R&D
10 largest peaks:
71 999 | 43 381 | 57 334 | 41 260 | 55 259 | 69 239 | 81 223 | 68 199 | 123 184 | 56 169 |
Synonyms:
1.2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-
2.trans-Phytol
3.3,7,11,15-Tetramethyl-2-hexadecen-1-ol
4.(2E)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol #

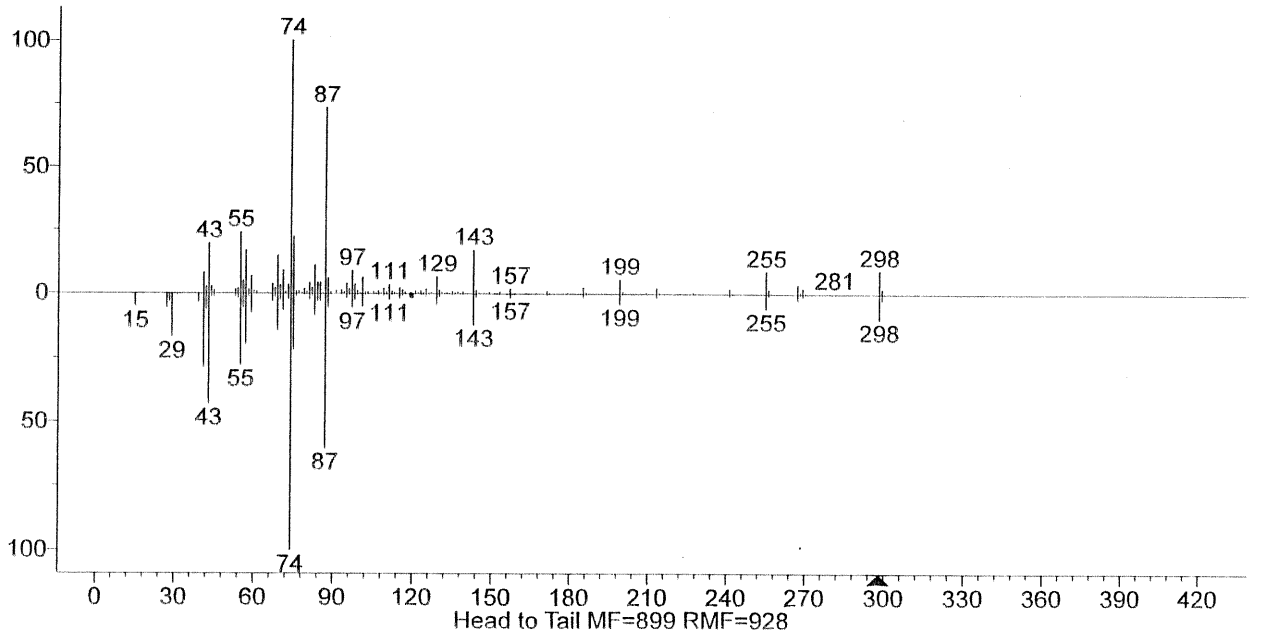
Estimated non-polar retention index (n-alkane scale):
Value: 2045 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu

Retention index.
1. Value: 2104 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: 50 C
End T: 250 C
Heat Rate: 5 K/min
Start Time: 3 min
End Time: 15
min
Source: Radulovic, N.; Lazarevic, J.; Stojanovic, G.; Palic, R., Chemotaxonomically significant 2-ethyl substituted fatty acids from Stachys milanii Petrovic (Lamiaceae), Biochem. Syst. Ecol., 34, 2006, 341-344.

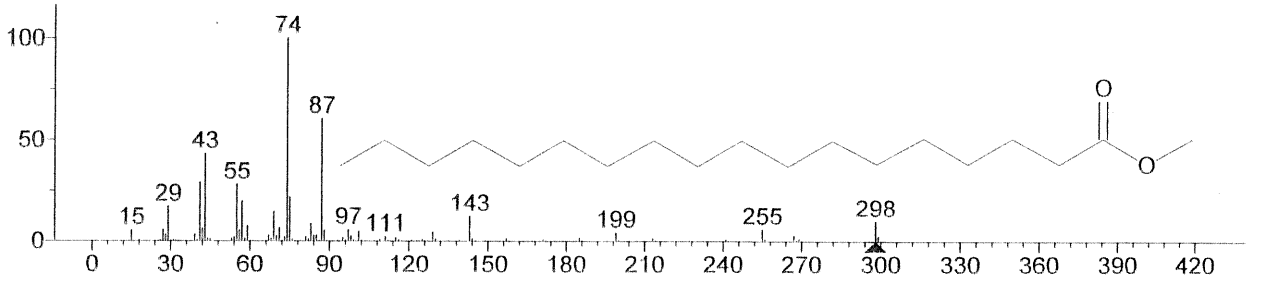
2.
Value: 2099 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: RTX-1
Column Length:
60 m
Carrier Gas: He
Column Diameter: 0.22 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program
Type: Ramp
Start T: 60 C
End T: 230 C




(Text File) +EI Scan (58.716 min) ALI-OLE-H7-220421-.D




Head to Tail MF=899 RMF=928




(replib) Octadecanoic acid, methyl ester

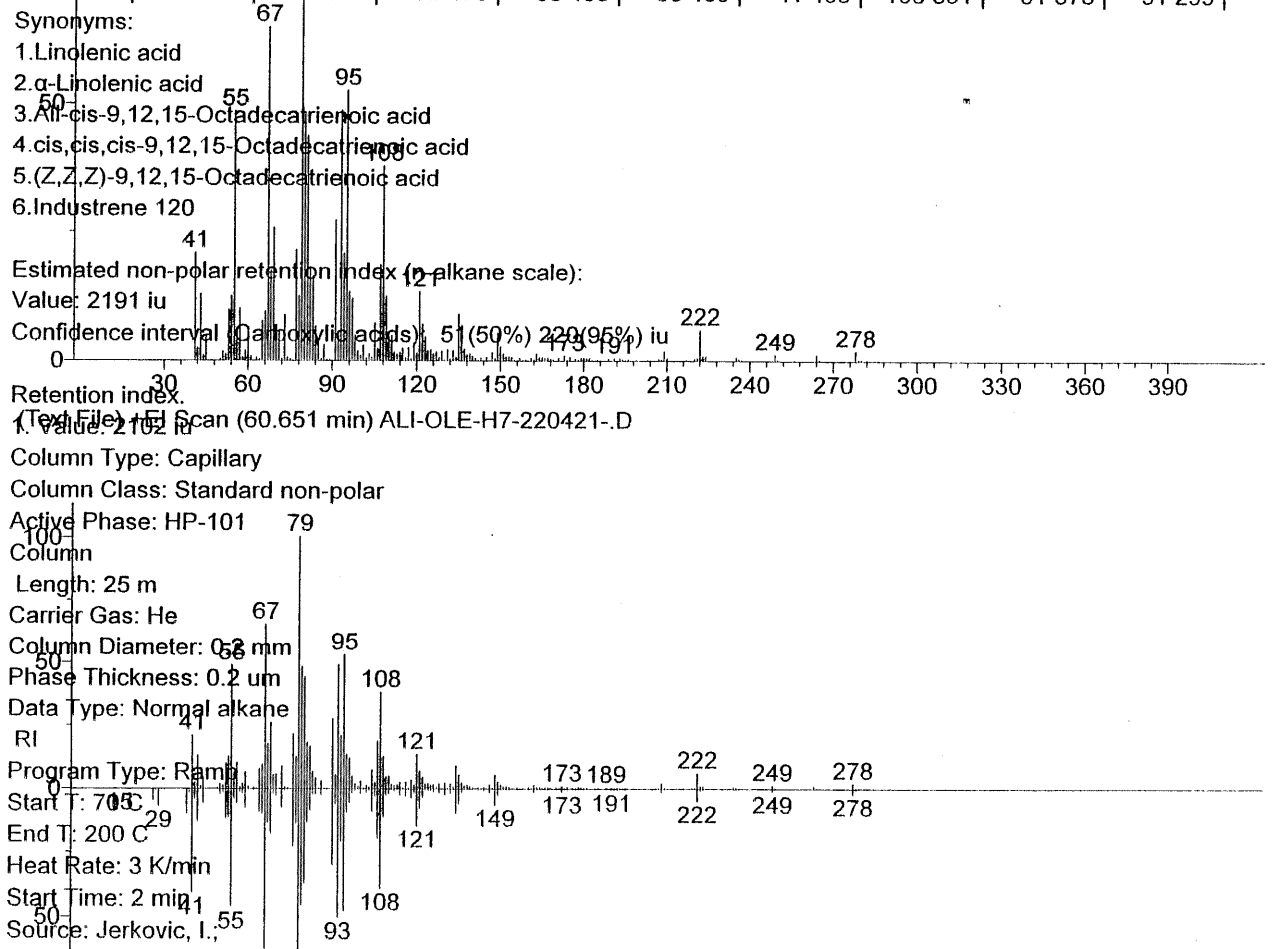
Name: Octadecanoic acid, methyl ester
Formula: $C_{19}H_{38}O_2$
MW: 298 CAS#: 112-61-8 NIST#: 79123 ID#: 9086 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: O A MAMER, MCGILL UNIVERSITY, MONTREAL,
10 largest peaks:
74 999 | 87 604 | 43 430 | 41 289 | 55 278 | 75 218 | 57 197 | 29 169 | 69 143 | 143 121 |
Synonyms:
1.Stearic acid, methyl ester
2.n-Octadecanoic acid, methyl ester
3.Kemester 9718
4.Methyl n-octadecanoate
5.Methyl octadecanoate
6.Methyl stearate
7.Metholene 2218
8.Emery 2218
9.Kemester 9018
10.Methyl ester of octadecanoic acid
11.Kemester 4516
12.Methyl (Z)-9-octadecenoate

Estimated non-polar retention index (n-alkane scale):
Value: 2077 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

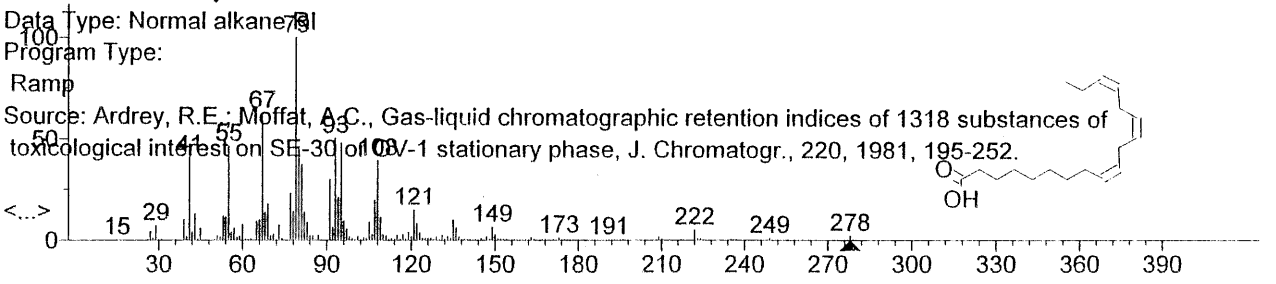
Retention index.
1. Value: 2133 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-1
Column
Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.33 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 40 C
End T: 260 C
Heat Rate: 2 K/min
Start Time: 5 min
End Time: 20
min
Source: Senatore, F.; Rigano, D.; de Fusco, R.; Bruno, M., Volatile components of Centaurea cineraria L. subsp. umbrosa (lacaita) Pign. and Centaurea napifolia L. (Asteraceae), two species growing wild in Sicily, Flavour Fragr. J., 18, 2003, 248-251.

2. Value: 2111 iu
Column Type: Capillary
Column Class: Standard non
-polar
Active Phase: DB-1
Column Length: 15 m

Name: 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
Formula: $C_{18}H_{30}O_2$
MW: 278 CAS#: 463-40-1 NIST#: 333201 ID#: 41695 DB: mainlib
Other DBs: Fine, TSCA, HODOC, NIH, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
79 999 | 67 624 | 93 503 | 95 478 | 55 463 | 80 460 | 41 408 | 108 391 | 81 373 | 91 299 |
Synonyms:
1.Linolenic acid
2.α-Linolenic acid
3.All-cis-9,12,15-Octadecatrienoic acid
4.cis,cis,cis-9,12,15-Octadecatrienoic acid
5.(Z,Z,Z)-9,12,15-Octadecatrienoic acid
6.Industrene 120
Estimated non-polar retention index (n-alkane scale):
Value: 2191 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu
Retention index.
1. Value: 2192 iu
(Text File) +EI Scan (60.651 min) ALI-OLE-H7-220421-.D
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: HP-101
Column
Length: 25 m
Carrier Gas: He
Column Diameter: 0.2 mm
Phase Thickness: 0.2 um
Data Type: Normal alkane
RI
Program Type: Ramp
Start T: 70 C
End T: 200 C
Heat Rate: 3 K/min
Start Time: 2 min
Source: Jerkovic, I.; Mastelic, J.; Marijanovic, Z., Bound volatile compounds and essential oil from the fruit of Maclura pomifera (Raf.) Schneid. (osage orange), Flavour Fragr. J., 22, 2007, 84-88.



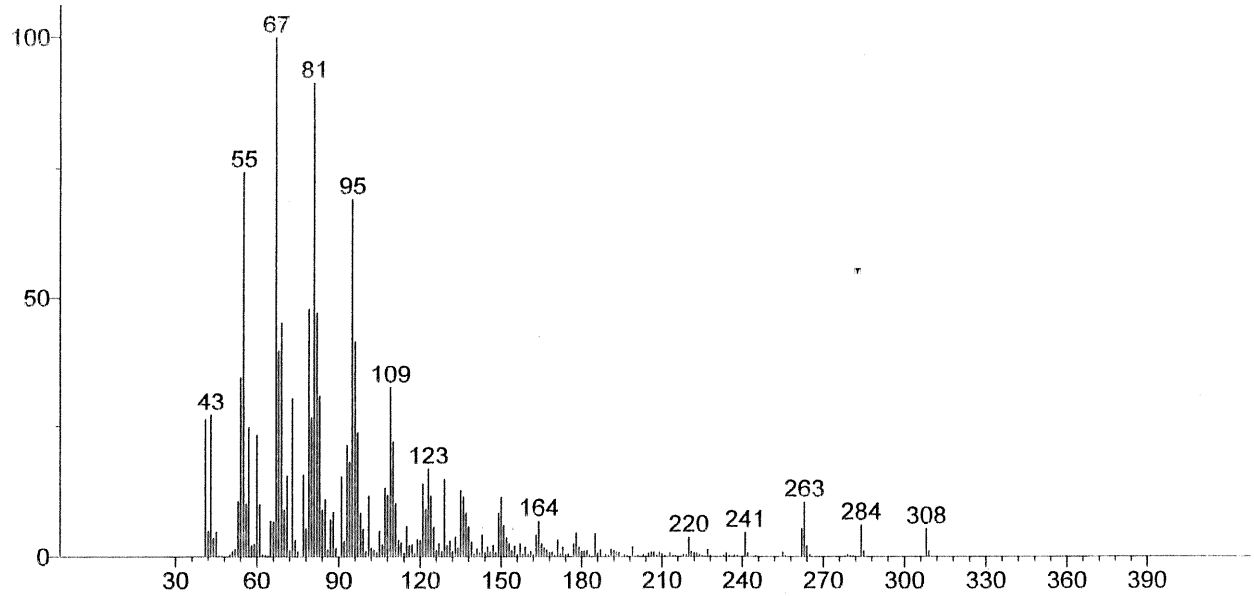

2. Value: 2178 iu
Column Type: Other
Column
Class: Standard non-polar
Active Phase: Methyl Silicone
Data Type: Normal alkane RI
Program Type:
Ramp
Source: Ardrey, R.E.; Moffat, A.C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 and OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.



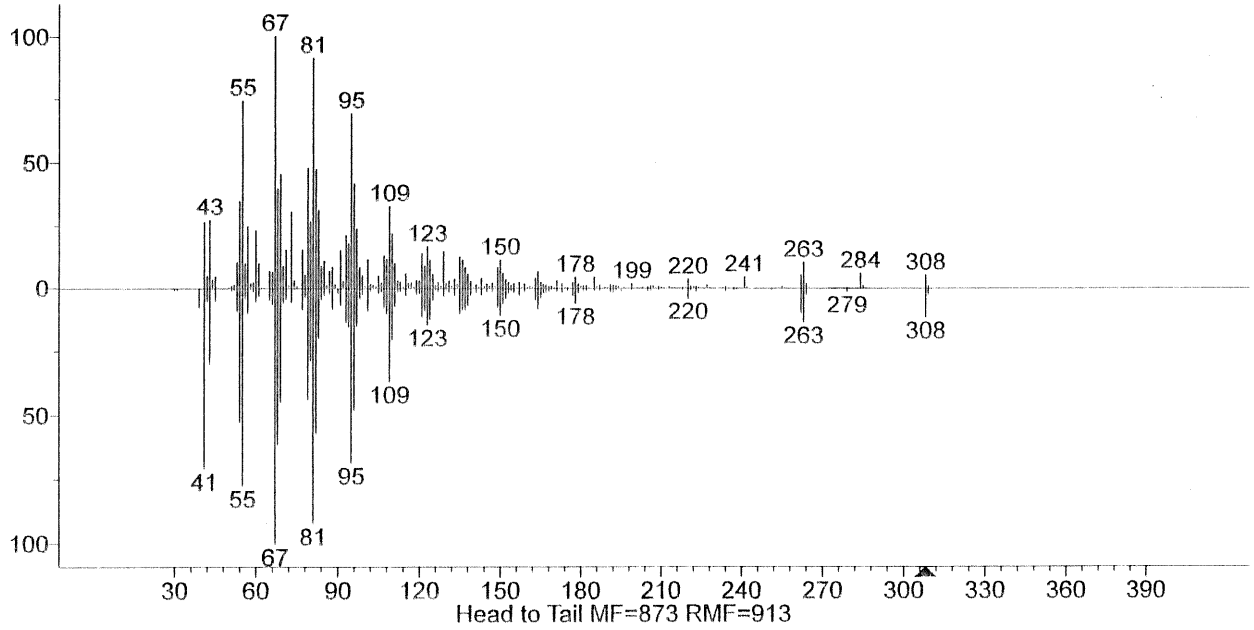




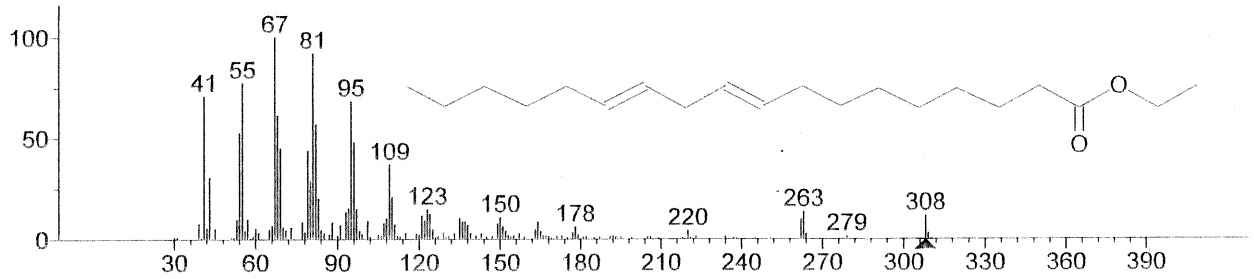
(mainlib) 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-




(Text File) +EI Scan (61.999 min) ALI-OLE-H7-220421-.D




Head to Tail MF=873 RMF=913




(mainlib) 9,12-Octadecadienoic acid, ethyl ester

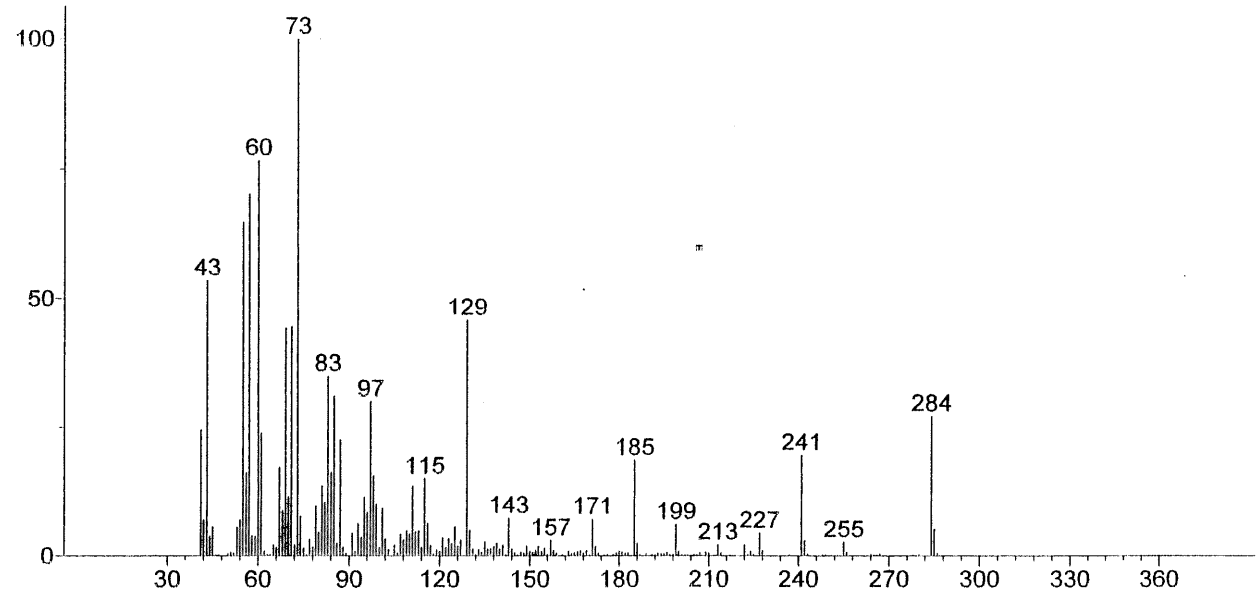
Name: 9,12-Octadecadienoic acid, ethyl ester
Formula: $C_{20}H_{36}O_2$
MW: 308 CAS#: 7619-08-1 NIST#: 249157 ID#: 28827 DB: mainlib
Other DBs: HODOC
Contributor: TNO Volatile Compounds in Food - Chemical Concepts
10 largest peaks:
67 999 | 81 919 | 55 772 | 41 707 | 95 683 | 68 613 | 82 569 | 54 525 | 96 478 | 69 448 |
Synonyms:
1.Ethyl (9E,12E)-9,12-octadecadienoate #

Estimated non-polar retention index (n-alkane scale):
Value: 2193 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

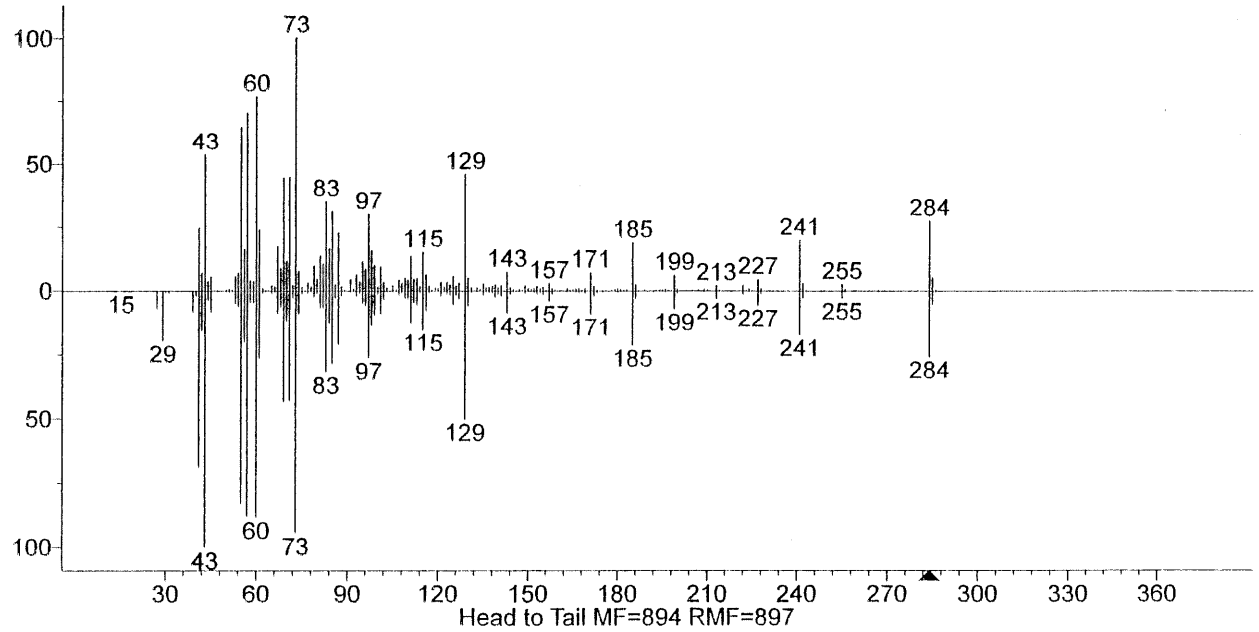
Retention index.
1. Value: 2171 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: HP
-5MS
Column Length: 30 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type:
Normal alkane RI
Program Type: Complex
Description: 40C (10min) => 3C/min =>120C =>10C/min =>250C
(5min)
Source: Ansorena, D.; Gimeno, O.; Astiasarán, I.; Bello, J., Analysis of volatile compounds by GC-MS of a dry fermented sausage: chorizo de Pamplona, Food Res. Int., 34, 2001, 67-75.

2. Value: 2527 iu
Column Type:
Capillary
Column Class: Standard polar
Active Phase: CP-Wax 52CB
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: 45C(5min) =>10C/min =>80C =>2C/min =>240C
Source: Romeo, V.; Ziino, M.; Giuffrrida,
D.; Condurso, C.; Verzera, A., Flavour profile of capers (Capparis spinosa L.) from the Eolian Archipelago by HS -SPME/GC?MS, Food Chem., 101, 2007, 1272-1278.

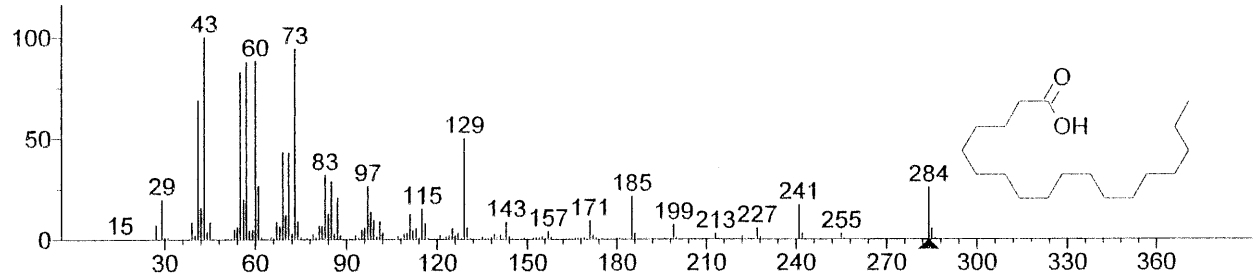
<...>




(Text File) +EI Scan (62.252 min) ALI-OLE-H7-220421-.D

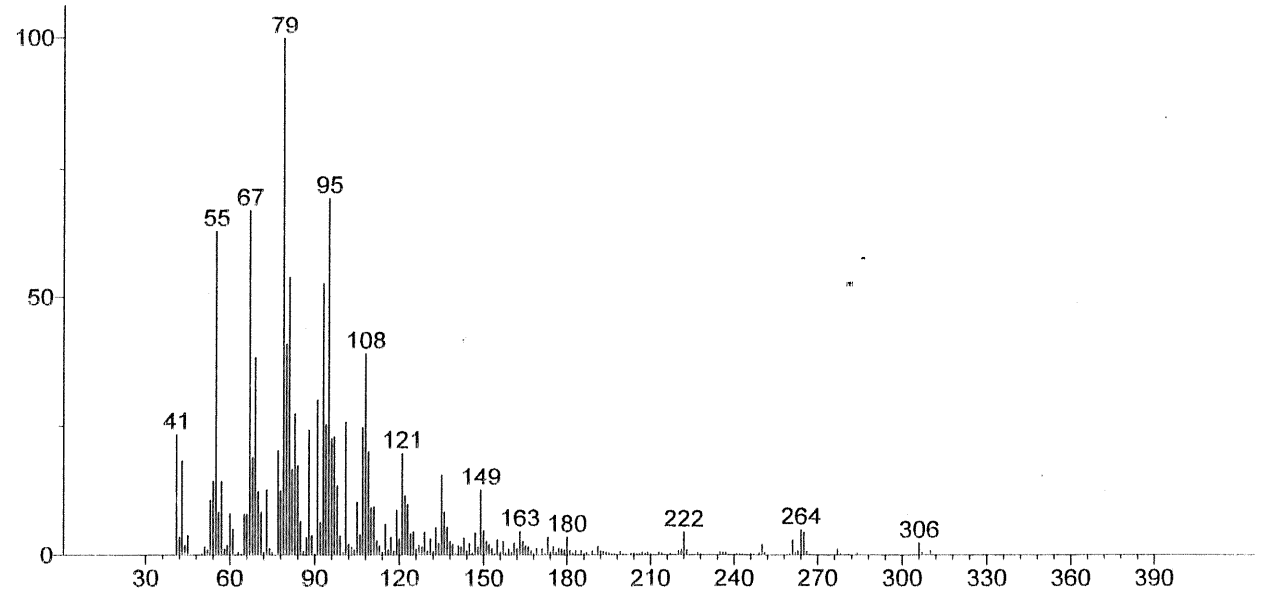



Head to Tail MF=894 RMF=897

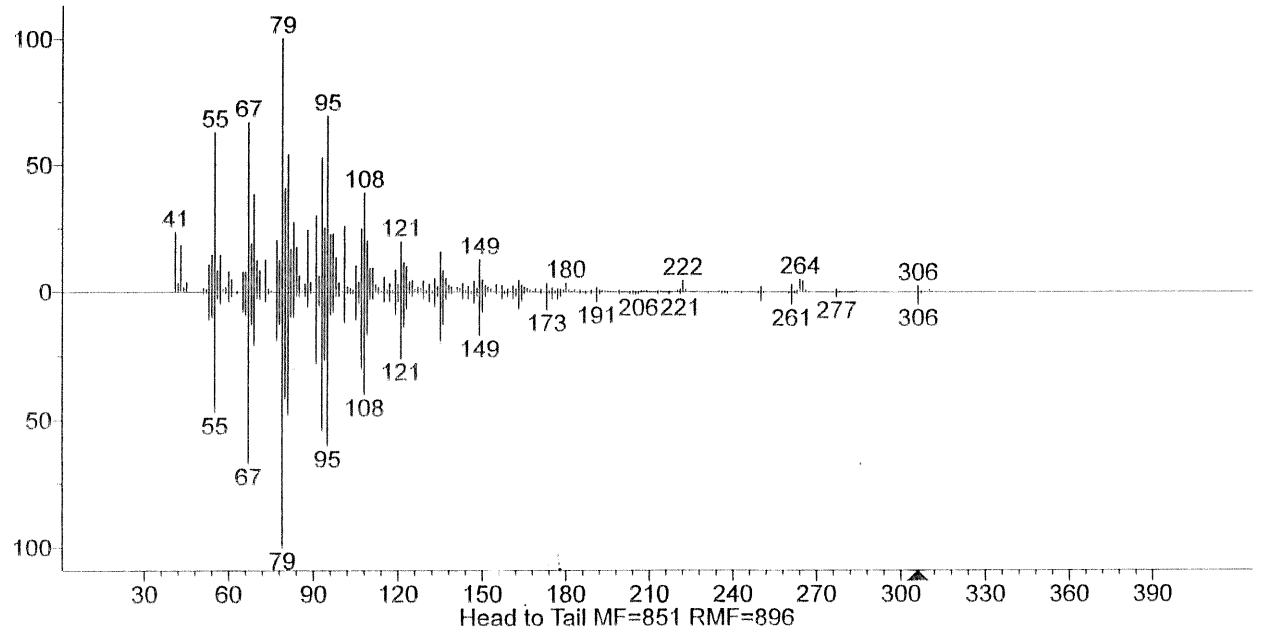



(mainlib) Octadecanoic acid

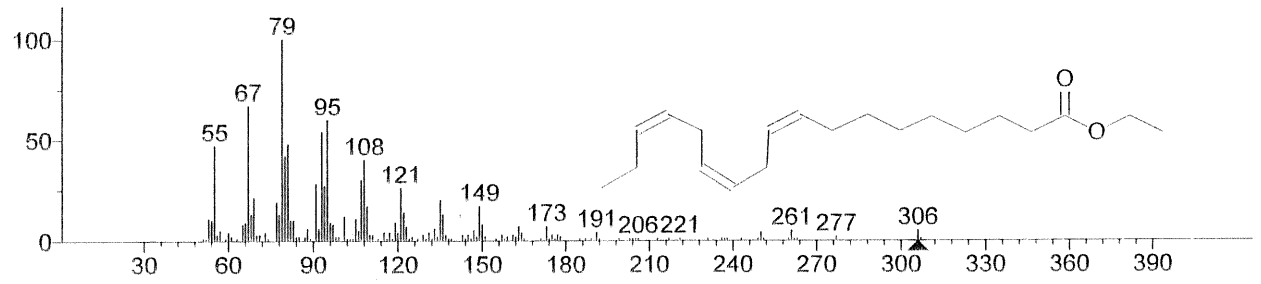
Name: Octadecanoic acid
Formula: $C_{18}H_{36}O_2$
MW: 284 CAS#: 57-11-4 NIST#: 290961 ID#: 8481 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1998.
10 largest peaks:
43 999 | 73 942 | 60 881 | 57 875 | 55 827 | 41 688 | 129 500 | 69 432 | 71 429 | 83 317 |
Synonyms:
1.Stearic acid
2.n-Octadecanoic acid
3.Humko Industrene R
4.Hydrofol Acid 150
5.Hystrene S-97
6.Hystrene T-70
7.Hystrene 80
8.Industrene R
9.Kam 1000
10.Kam 2000
11.Kam 3000
12.Neo-Fat 18
13.Neo-Fat 18-53
14.Neo-Fat 18-54
15.Neo-Fat 18-55
16.Neo-Fat 18-59
17.NAA 173
18.PD 185
19.Stearex Beads
20.Stearophanic acid
21.Steric acid
22.Vanicol
23.1-Heptadecanecarboxylic acid
24.Heptadecanecarboxylic acid
25.Neo-fat 18-61
26.Pearl stearic
27.Century 1240
28.Dar-chem 14
29.Emersol 120
30.Emersol 132
31.Emersol 150
32.Formula 300
33.Glycon dp
34.Glycon tp
35.Glycon S-70
36.Glycon S-80
37.Glycon S-90
38.Groco 54
39.Groco 55
40.Groco 55l
41.Groco 58
42.Groco 59
43.Hy-phi 1199
44.Hy-phi 1205
45.Hy-phi 1303
46.Hy-phi 1401




(Text File) +EI Scan (62.722 min) ALI-OLE-H7-220421-.D



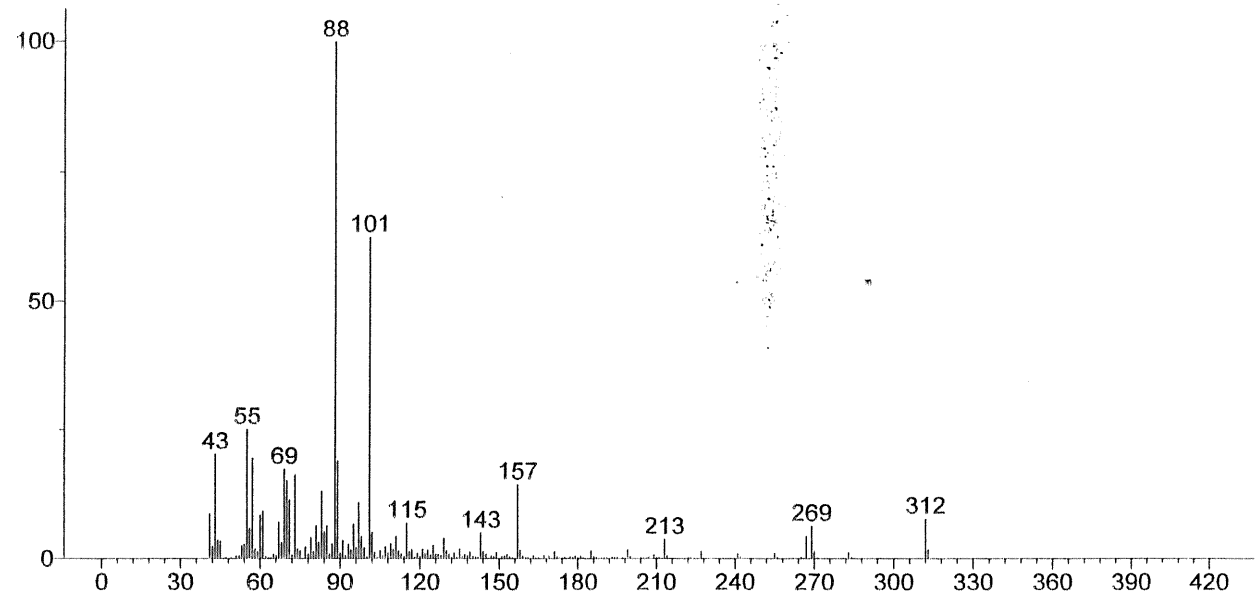

Head to Tail MF=851 RMF=896



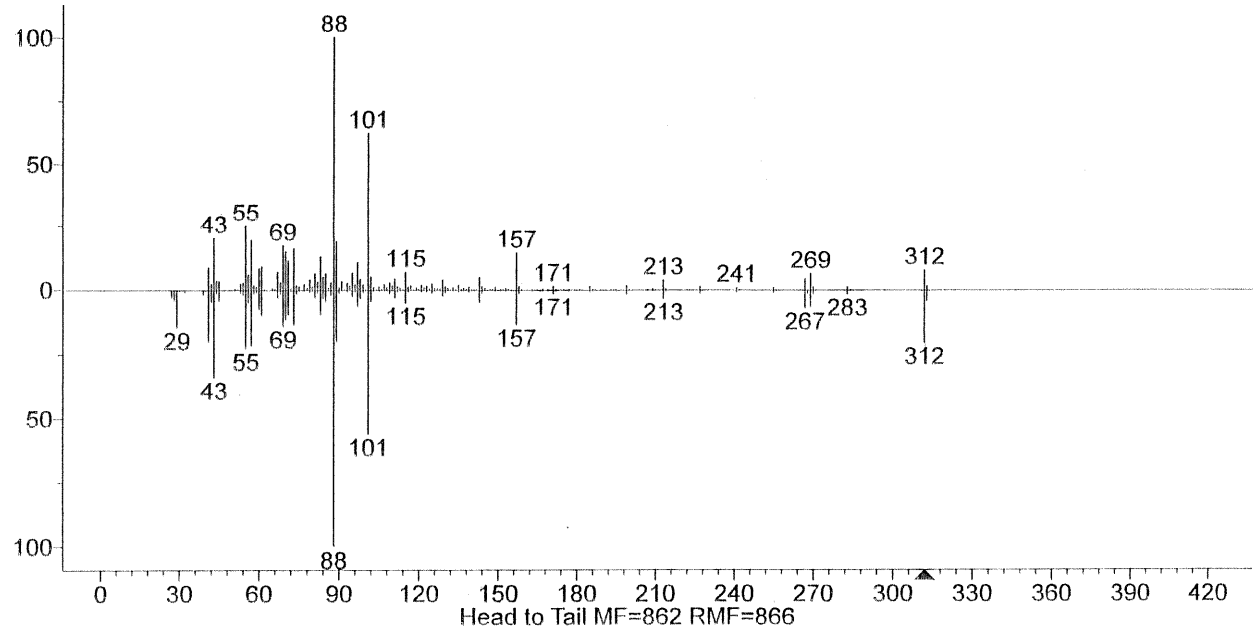

(mainlib) Ethyl 9,12,15-octadecatrienoate

Name: Ethyl 9,12,15-octadecatrienoate
Formula: $C_{20}H_{34}O_2$
MW: 306 NIST#: 336774 ID#: 41709 DB: mainlib
Contributor: William W. Christie, Mylnefield Lipid Analysis, Invergowrie, Dundee, Scotland, UK
10 largest peaks:
79 999 | 67 669 | 95 599 | 93 539 | 81 479 | 55 469 | 80 419 | 108 399 | 107 299 | 91 279 |
Synonyms:
no synonyms.

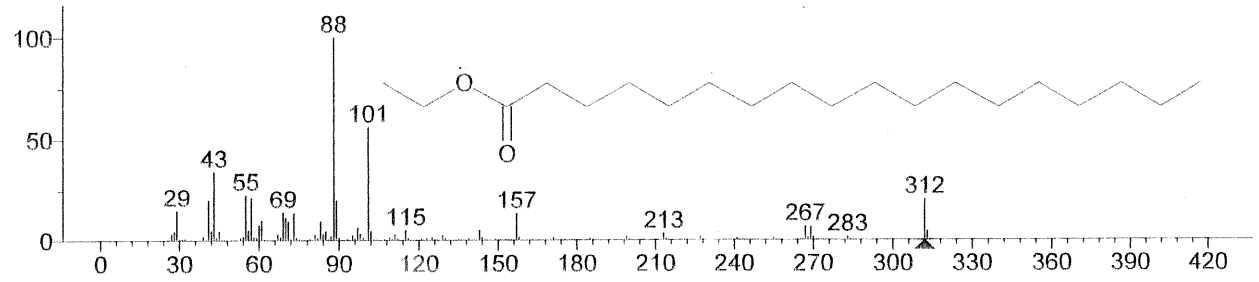
Estimated non-polar retention index (n-alkane scale):
Value: 2201 iu
Confidence interval (Esters): 47(50%) 201(95%) iu




(Text File) +EI Scan (65.260 min) ALI-OLE-H7-220421-.D




Head to Tail MF=862 RMF=866



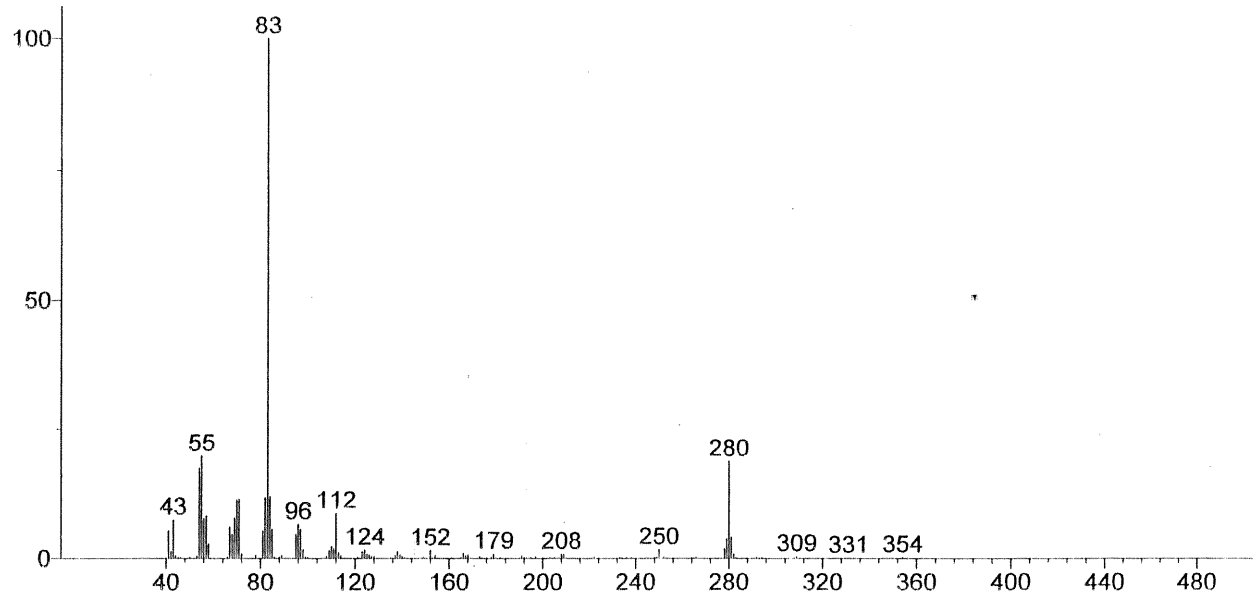

(replib) Octadecanoic acid, ethyl ester

Name: Octadecanoic acid, ethyl ester
Formula: $C_{20}H_{40}O_2$
MW: 312 CAS#: 111-61-5 NIST#: 36393 ID#: 11117 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS, IRDB
Contributor: R.T.HOLMAN,UNIVERSITY OF MINNESOTA
10 largest peaks:
88 999 | 101 559 | 43 339 | 55 226 | 57 213 | 312 203 | 41 200 | 89 200 | 29 146 | 69 139 |
Synonyms:
1.Stearic acid, ethyl ester
2.Ethyl n-octadecanoate
3.Ethyl octadecanoate
4.Ethyl stearate
5.Radia 7185

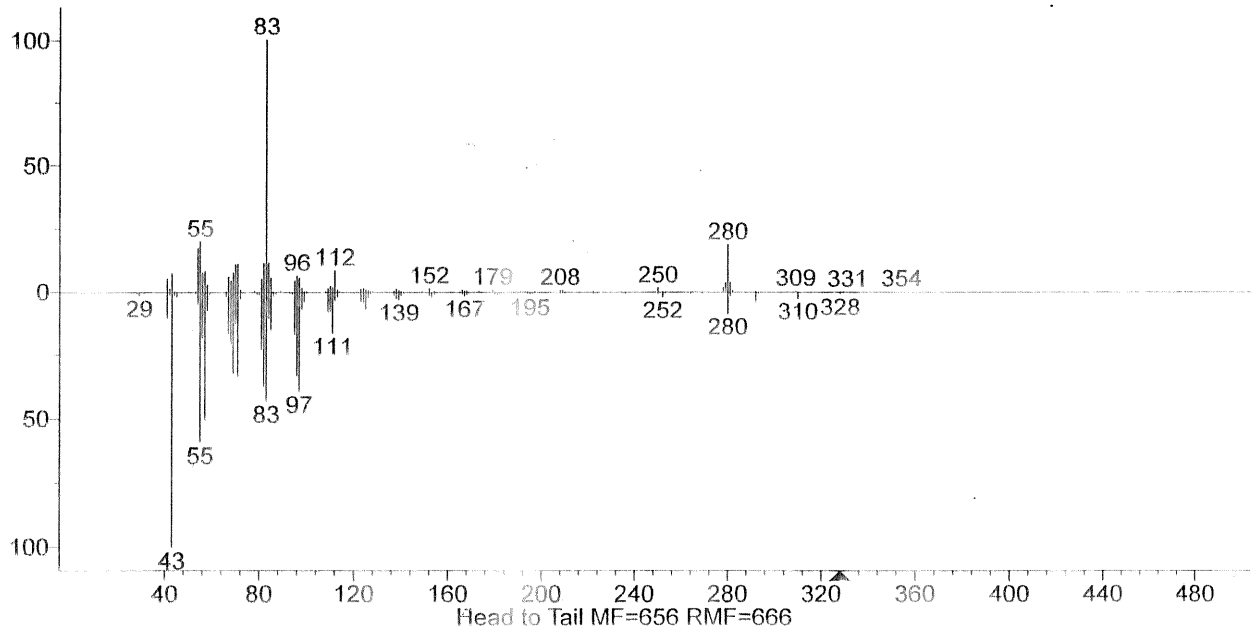
Estimated non-polar retention index (n-alkane scale):
Value: 2177 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 2181 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: 0.4 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 60 C
End T: 280 C
Heat Rate: 3 K/min
Start Time: 10 min
End Time: 60
min
Source: Pino, J.A.; Marbot, R.; Vázquez, C., Characterization of volatiles in strawberry guava (Psidium cattleianum Sabine) fruit, J. Agric. Food Chem., 49, 2001, 5883-5887.

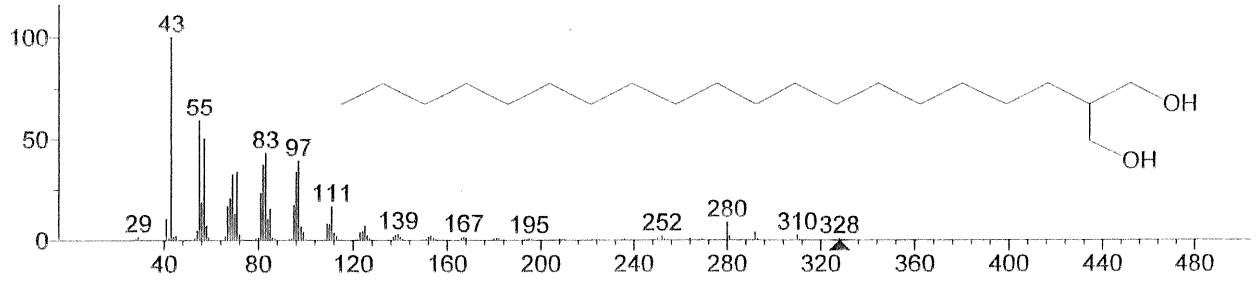
2. Value: 2202 iu
Column Type:
Capillary
Column Class: Standard non-polar
Active Phase: OV-1
Column Length: 25 m
Carrier Gas:
He
Column Diameter: 0.32 mm
Data Type: Linear RI
Program Type: Ramp
Start T: 40 C
End T: 280 C
Heat




(Text File) +EI Scan (72.088 min) ALI-OLE-H7-220421-.D Subtract



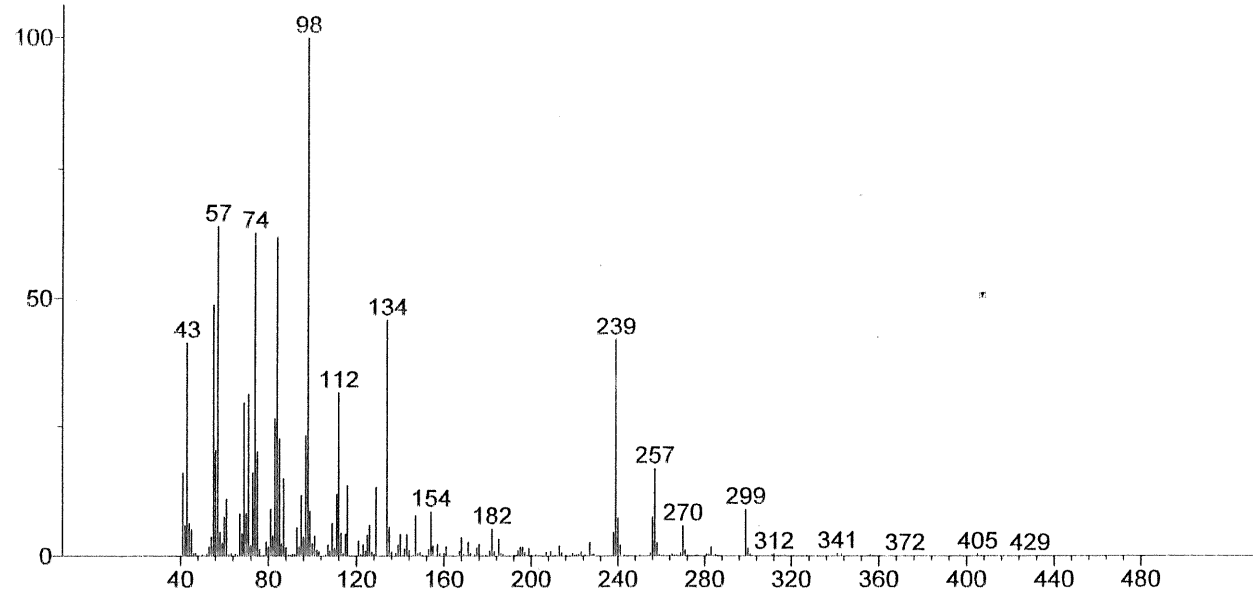

Head to Tail MF=656 RMF=666



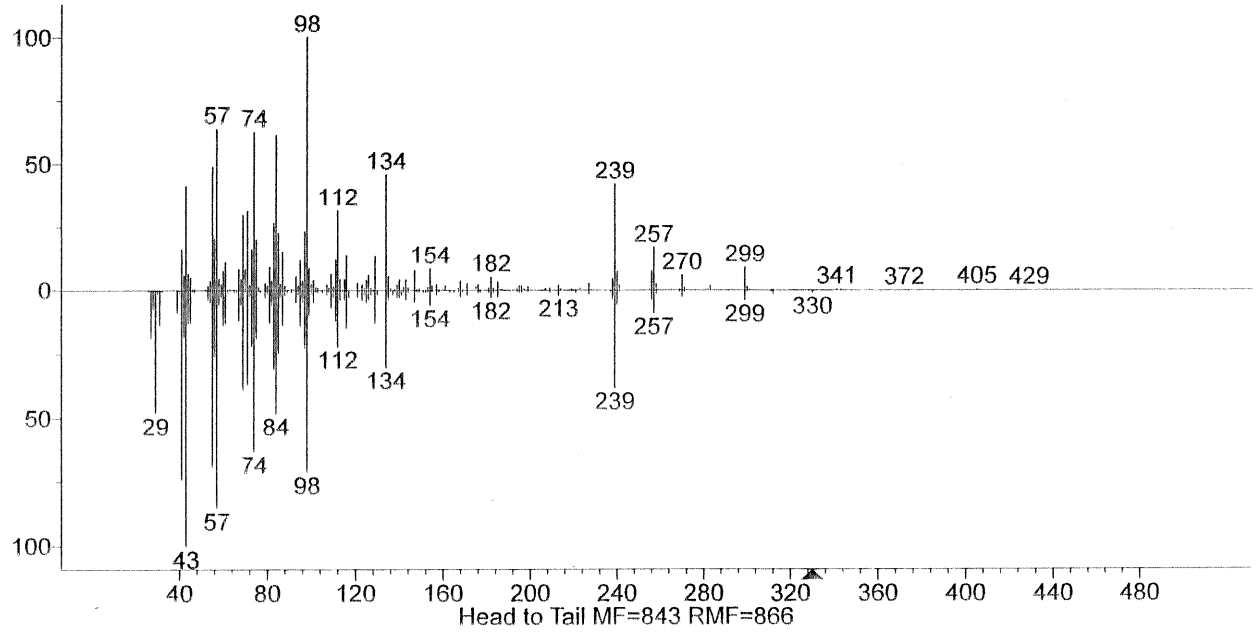

(mainlib) 2-Octadecyl-propane-1,3-diol

Name: 2-Octadecyl-propane-1,3-diol
Formula: $C_{21}H_{44}O_2$
MW: 328 CAS#: 5337-61-1 NIST#: 193417 ID#: 6741 DB: mainlib
Other DBs: None
Contributor: Chemical Concepts
10 largest peaks:
43 999 | 55 589 | 57 503 | 83 429 | 97 391 | 82 372 | 71 337 | 96 337 | 69 323 | 81 232 |
Synonyms:
1.2-Octadecyl-1,3-propanediol #

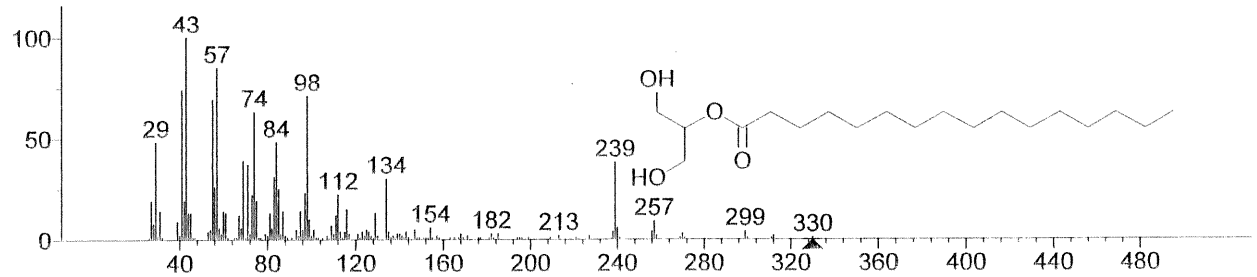
Estimated non-polar retention index (n-alkane scale):
Value: 2530 iu
Confidence interval (Alcohols): 41(50%) 176(95%) iu




(Text File) +EI Scan (75.951 min) ALI-OLE-H7-220421-.D Subtract



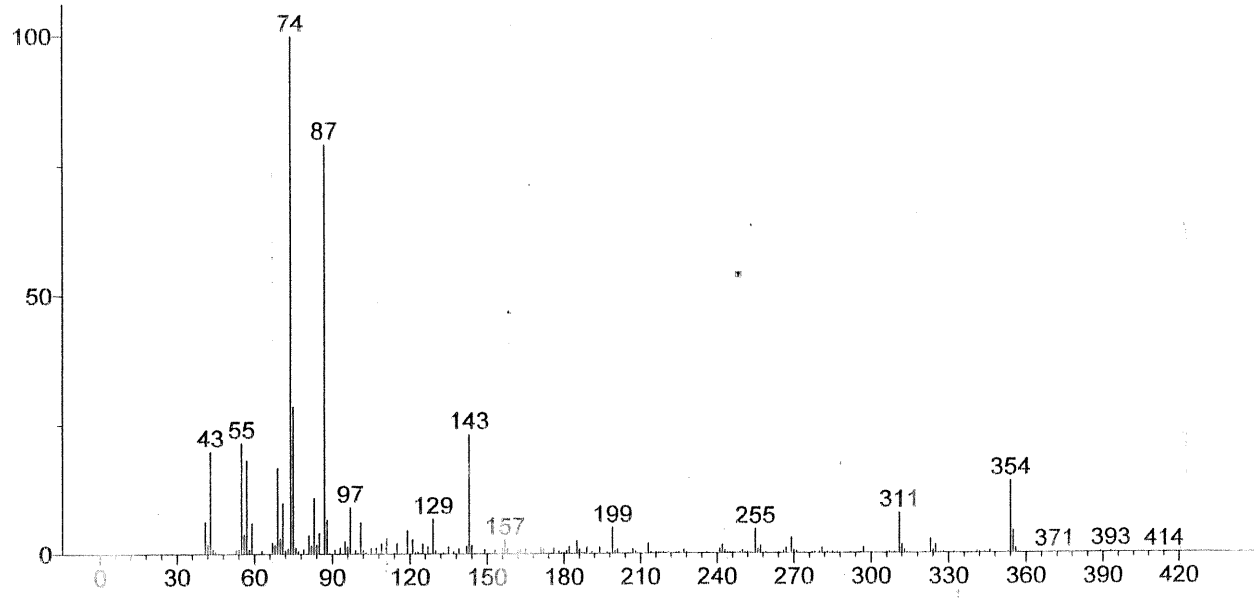

Head to Tail MF=843 RMF=866



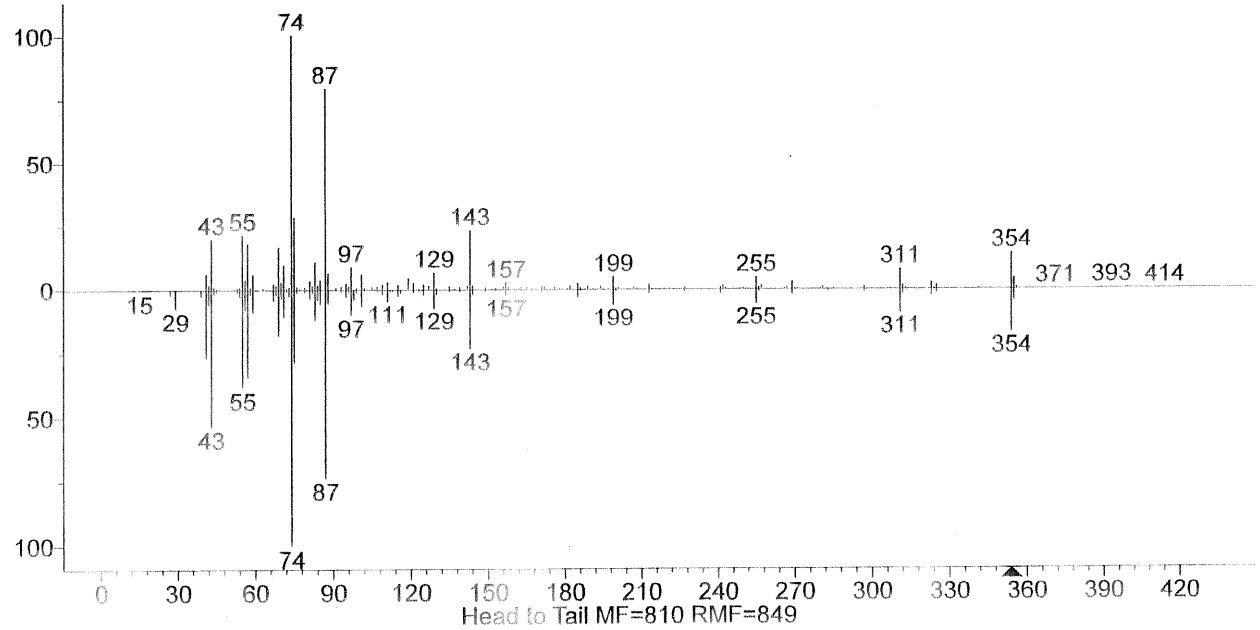

(mainlib) Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Name: Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester
Formula: $C_{19}H_{38}O_4$
MW: 330 CAS#: 23470-00-0 NIST#: 15400 ID#: 7156 DB: mainlib
Other DBs: None
10 largest peaks:
43 999 | 57 850 | 41 740 | 98 710 | 55 690 | 74 630 | 29 480 | 84 480 | 69 390 | 239 380 |
Synonyms:
1.Palmitin, 2-mono-
2.Palmitic acid β-monoglyceride
3.2-Hexadecanoyl glycerol
4.2-Monopalmitin
5.2-Monopalmitoyl-sn-glycerol
6.1,2,3-Propanetriol 2-hexandecanoyl ester
7.Glycerol β-palmitate
8.2-Hydroxy-1-(hydroxymethyl)ethyl palmitate #

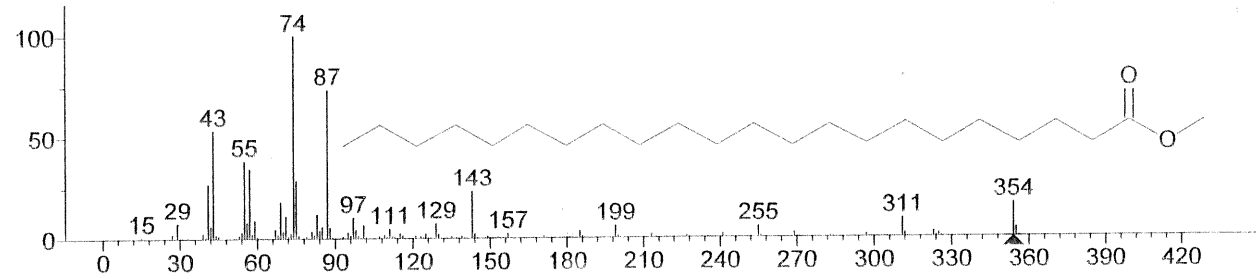
Estimated non-polar retention index (n-alkane scale):
Value: 2498 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu




(Text File) +EI Scan (76.286 min) ALI-OLE-H7-220421-.D Subtract




Head to Tail MF=810 RMF=849



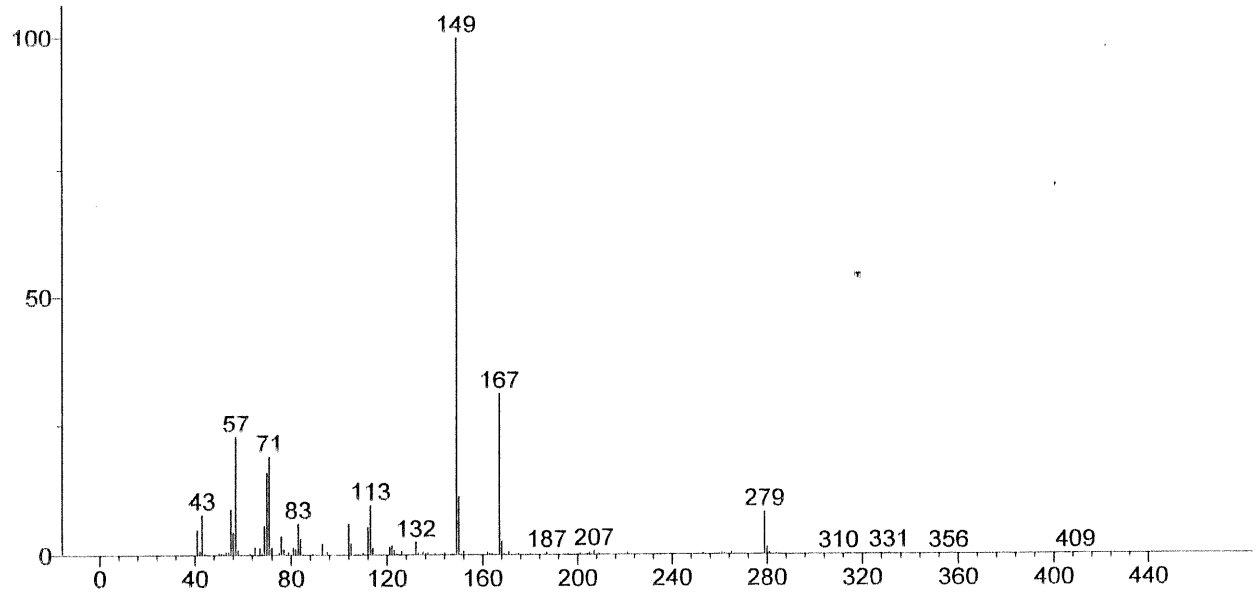

(mainlib) Docosanoic acid, methyl ester

Name: Docosanoic acid, methyl ester
Formula: $C_{23}H_{46}O_2$
MW: 354 CAS#: 929-77-1 NIST#: 333108 ID#: 38271 DB: mainlib
Other DBs: Fine, TSCA, HODOC, NIH, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
74 999 | 87 734 | 43 534 | 55 383 | 57 344 | 75 284 | 41 266 | 143 230 | 69 180 | 354 167 |
Synonyms:
1.Behenic acid, methyl ester
2.Methyl behenate
3.Methyl docosanoate
4.n-Docosanoic acid methyl ester
5.Kemester 9022

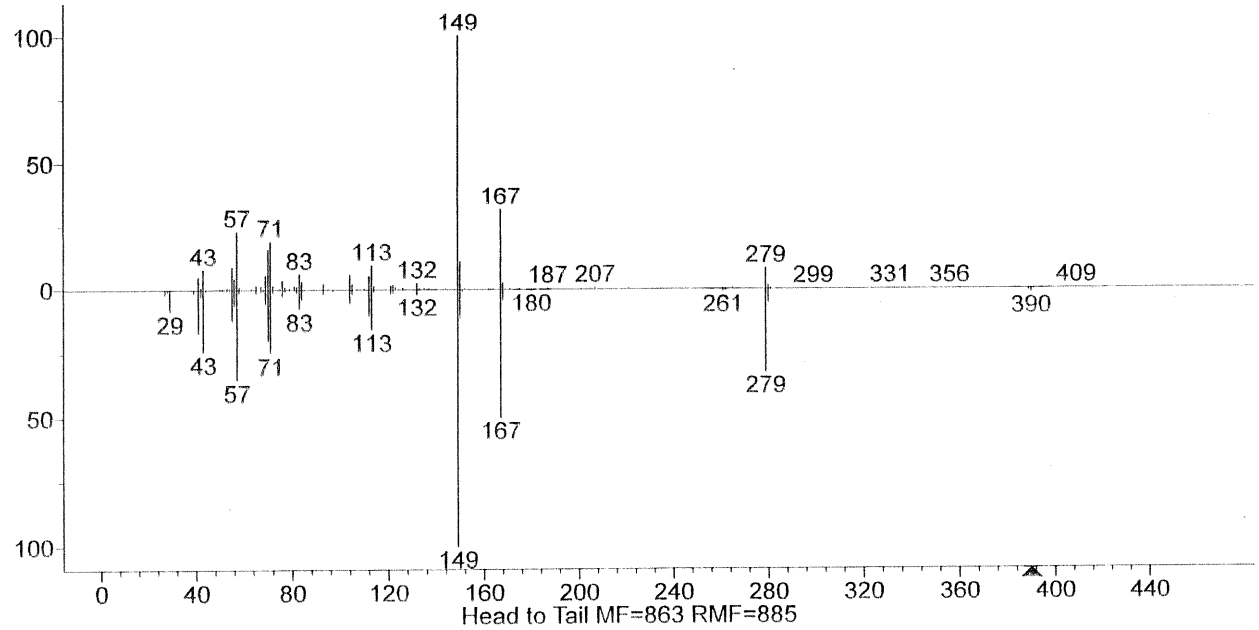
Estimated non-polar retention index (n-alkane scale):
Value: 2475 iu
Confidence interval (Esters): 47(50%) 201(95%) iu

Retention index.
1. Value: 2531 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: CP Sil 5 CB
Column
Length: 50 m
Carrier Gas: H2
Column Diameter: 0.25 mm
Phase Thickness: 0.15 um
Data Type: Linear
RI
Program Type: Ramp
Start T: 40 C
End T: 300 C
Heat Rate: 4 K/min
Start Time: 3 min
Source: Heinrich,
G.; Pfeifhofer, H.W.; Stabentheiner, E.; Sawidis, T., Glandular hairs of Sigesbeckia jorullensis Kunth (Asteraceae): morphology, histochemistry and composition of essential oil, Ann. Bot. Rome, 89, 2002, 459-469.

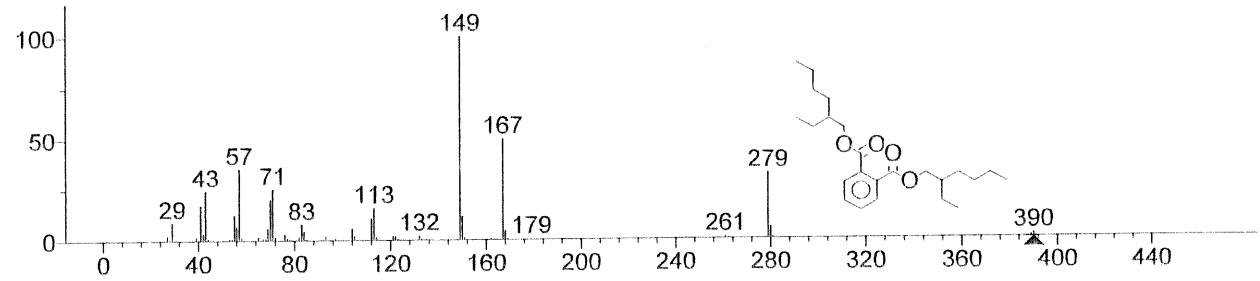
2. Value: 2502
iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column Length: 30
m
Column Diameter: 0.2 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program Type: Ramp
Start T: 50
C
End T: 300 C
Heat Rate: 5 K/min




(Text File) +EI Scan (76.668 min) ALI-OLE-H7-220421-.D Subtract

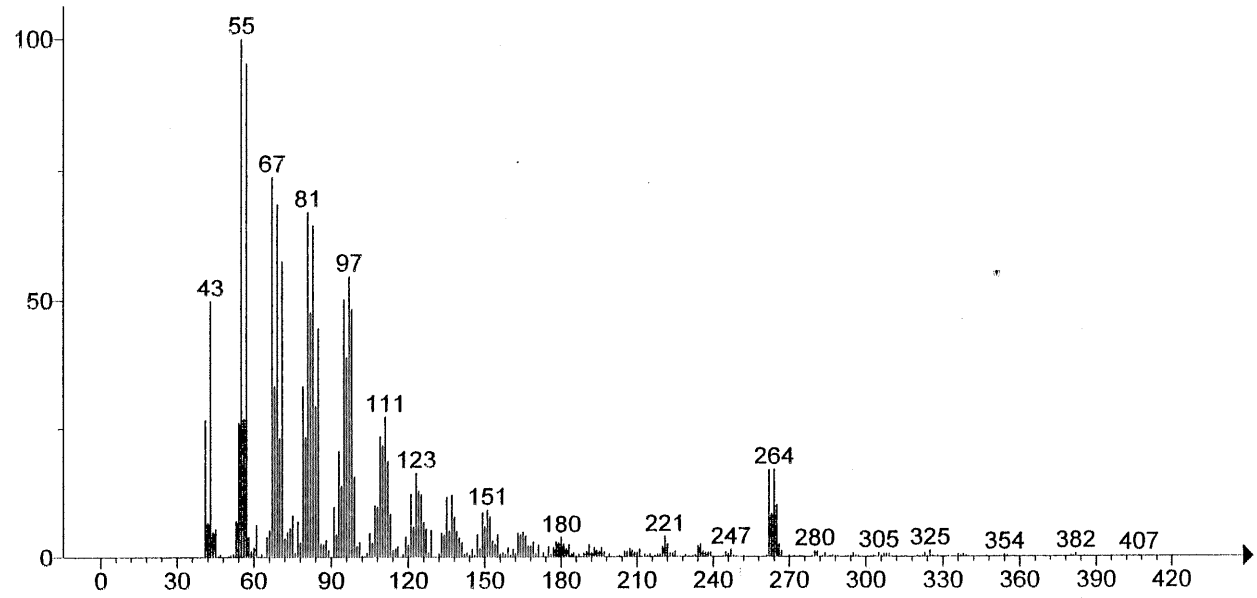



Head to Tail MF=863 RMF=885

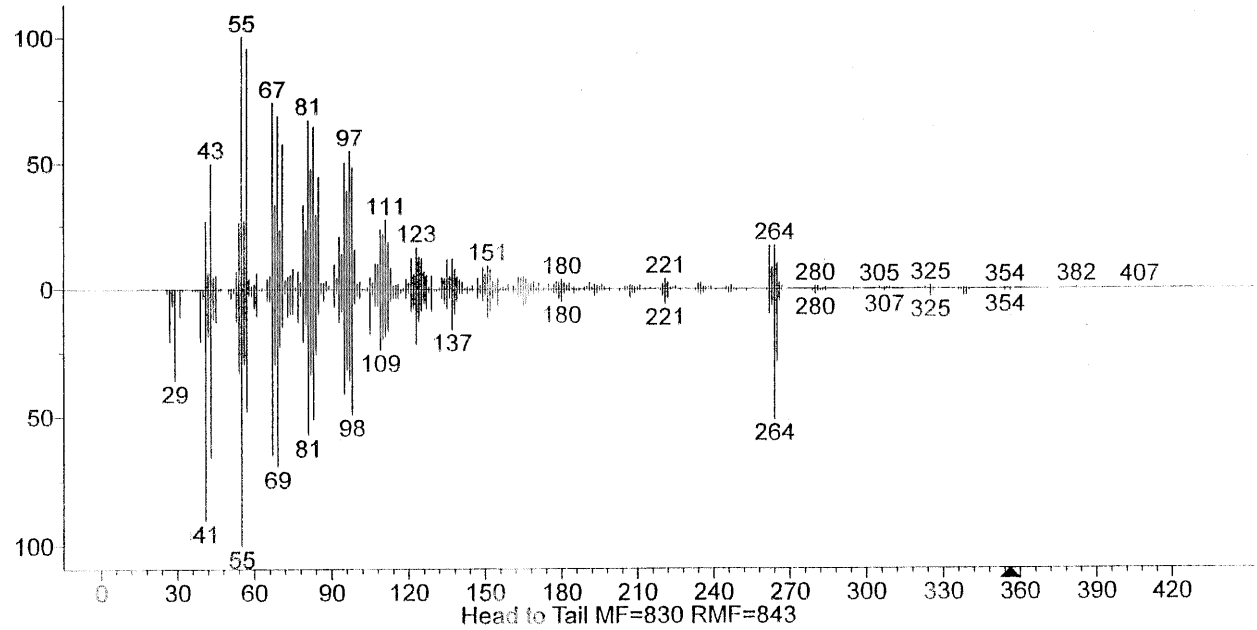



(mainlib) Bis(2-ethylhexyl) phthalate

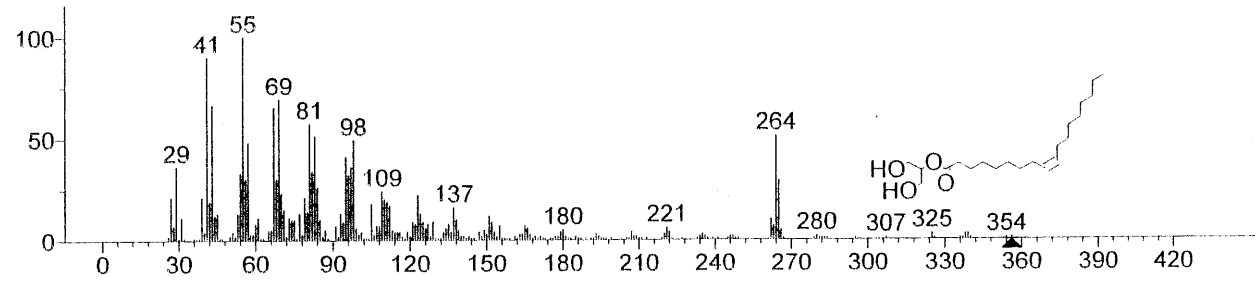
Name: Bis(2-ethylhexyl) phthalate
Formula: $C_{24}H_{38}O_4$
MW: 390 CAS#: 117-81-7 NIST#: 229113 ID#: 110646 DB: mainlib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-8633
10 largest peaks:
149 999 | 167 497 | 57 351 | 279 322 | 71 249 | 43 242 | 70 200 | 41 170 | 113 156 | 55 125 |
Synonyms:
1.1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
2.Phthalic acid, bis(2-ethylhexyl) ester
3.Bis(2-ethylhexyl) 1,2-benzenedicarboxylate
4.Bisoflex 81
5.Compound 889
6.Di(ethylhexyl) phthalate
7.Di(2-ethylhexyl) phthalate
8.Dioctyl phthalate
9.DEHP
10.DOP
11.Ethylhexyl Phthalate
12.Eviplast 80
13.Eviplast 81
14.Fleximel
15.Flexol DOP
16.Kodaflex DOP
17.Octoil
18.Octyl phthalate
19.Palatinol AH
20.Pittsburgh PX-138
21.Sicol 150
22.Staflex DOP
23.Truflex DOP
24.Vestinol AH
25.Vinicizer 80
26.Witcizer 312
27.1,2-Benzenedicarboxylic acid, bis(ethylhexyl) ester
28.2-Ethylhexyl phthalate
29.Dioctyl-o-benzenedicarboxylate
30.Phthalic acid di(2-ethylhexyl) ester
31.di-iso-Octyl phthalate
32.Bis(ethylhexyl) phthalate
33.Bisoflex DOP
34.Celluflex DOP
35.Di(2-ethylhexyl) o-phthalate
36.Di-sec-octyl phthalate
37.Flexol plasticizer DOP
38.Hercoflex 260
39.NCI-C52733
40.Polycizer 162
41.PX-138
42.RC plasticizer DOP
43.Behp
44.Bis-(2-ethylhexyl)ester kyseliny ftalove
45.DAF 68
46.Di(2-ethylhexyl)orthophthalate




(Text File) +EI Scan (78.821 min) ALI-OLE-H7-220421-.D Subtract



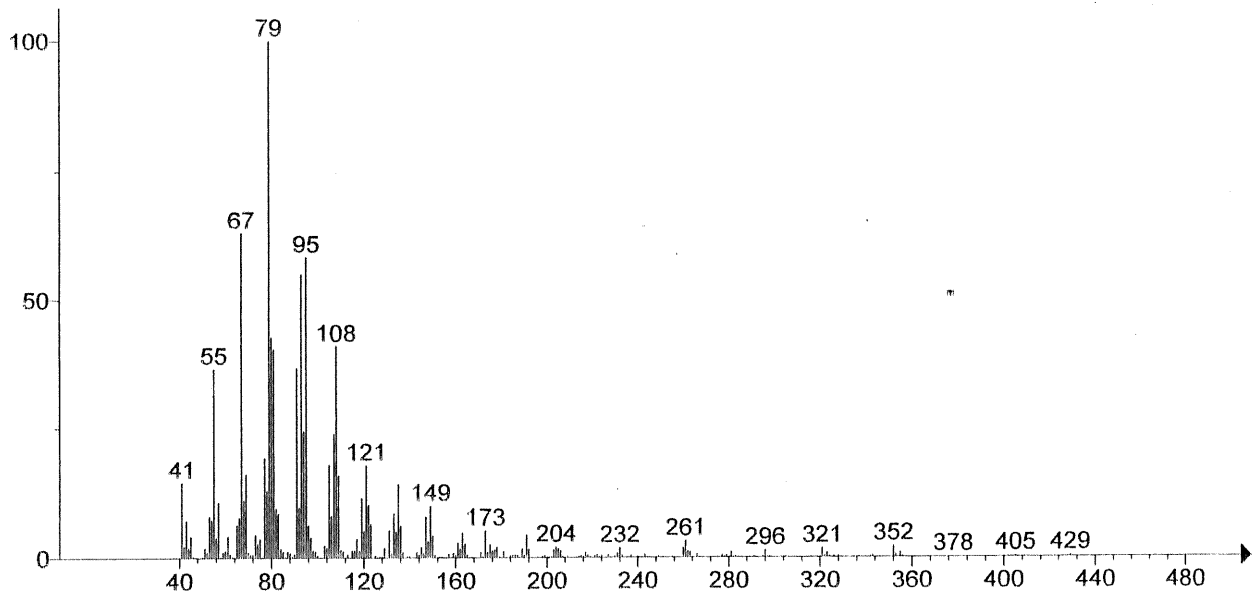

Head to Tail MF=830 RMF=843



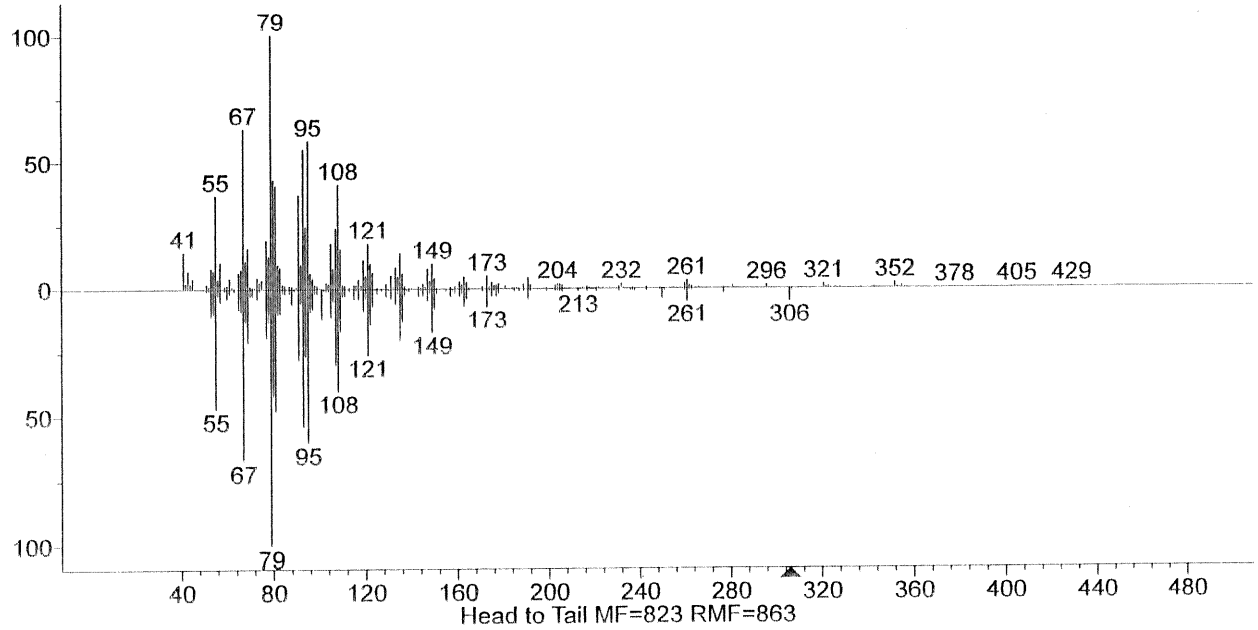

(mainlib) 9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Name: 9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester
Formula: $C_{21}H_{40}O_4$
MW: 356 CAS#: 3443-84-3 NIST#: 16061 ID#: 17482 DB: mainlib
Other DBs: None
10 largest peaks:
55 999 | 41 900 | 69 690 | 43 660 | 67 650 | 81 570 | 83 510 | 264 510 | 98 490 | 57 480 |
Synonyms:
1.Olein, 2-mono-
2.β-Monoolein
3.Glycerol 2-monooleate
4.2-Monoolein
5.2-Monooleoylglycerol
6.2-Oleoyl glycerol ether
7.2-Oleoylglycerol
8.2-Hydroxy-1-(hydroxymethyl)ethyl (9Z)-9-octadecenoate #

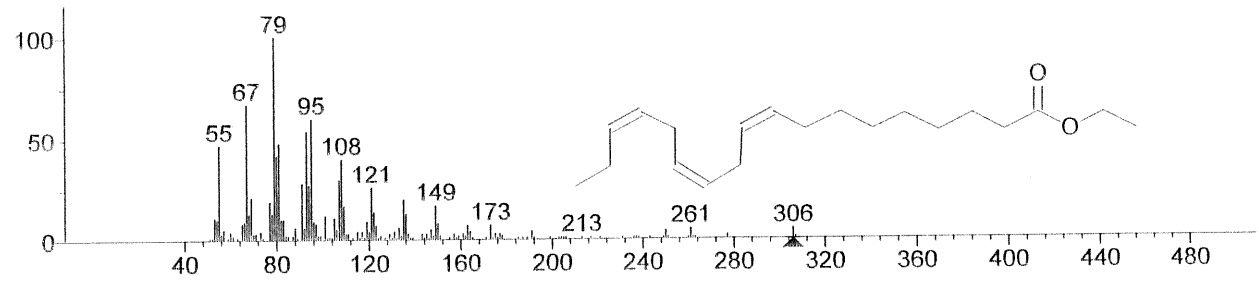
Estimated non-polar retention index (n-alkane scale):
Value: 2705 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu




(Text File) +EI Scan (78.931 min) ALI-OLE-H7-220421-.D Subtract



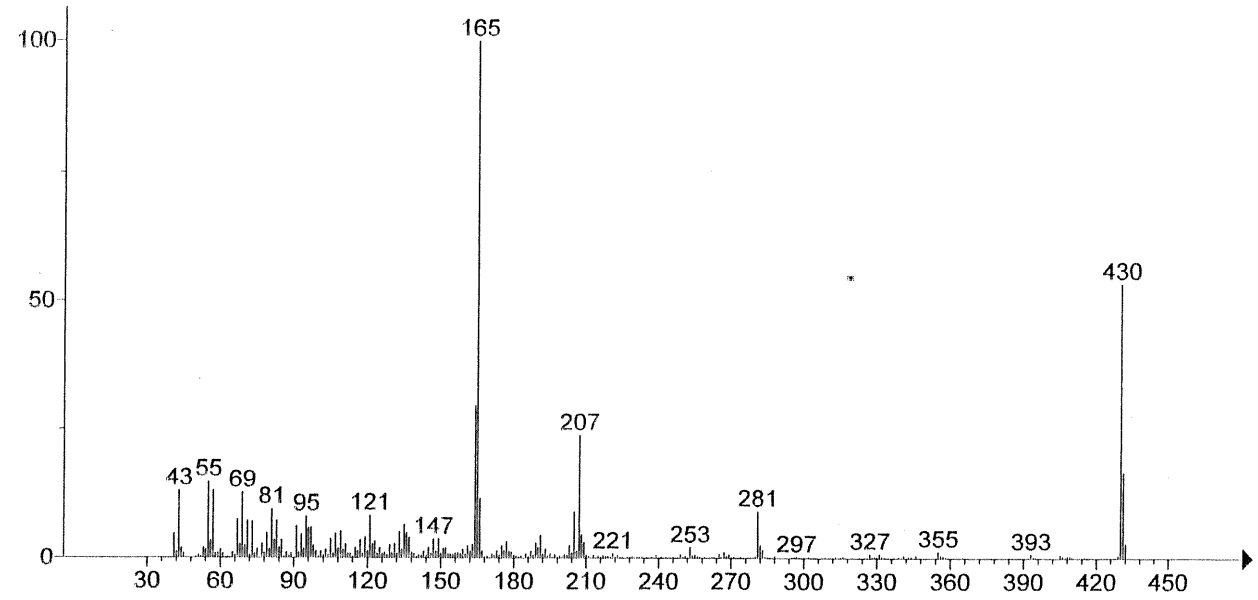

Head to Tail MF=823 RMF=863



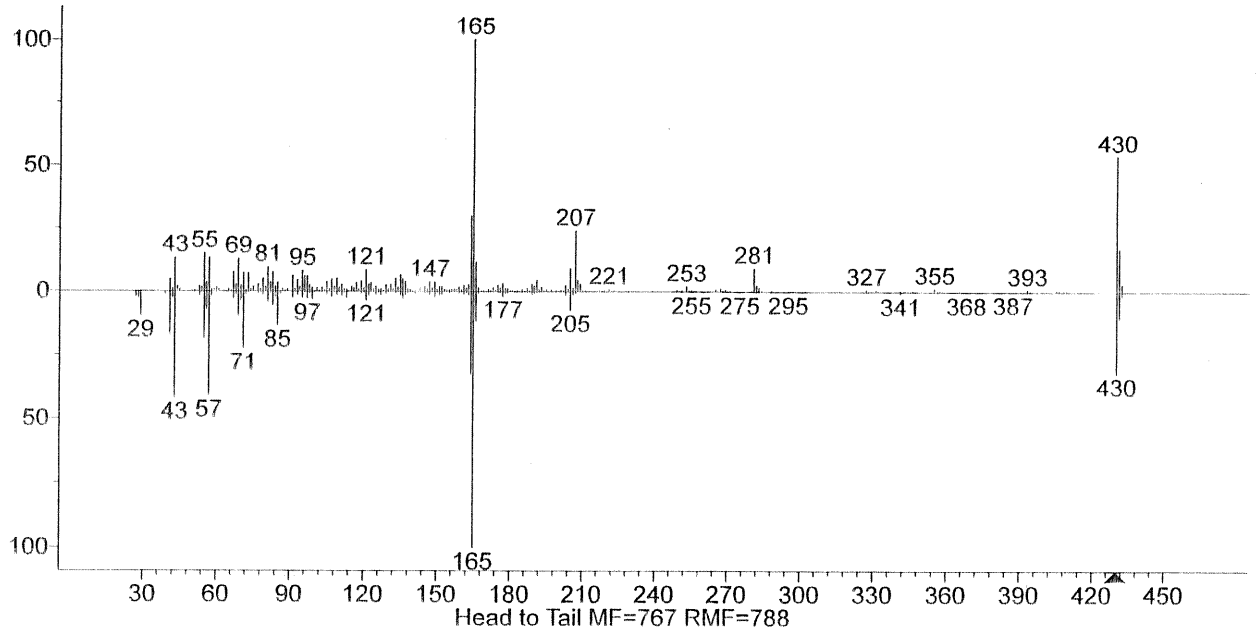

(mainlib) Ethyl 9,12,15-octadecatrienoate

Name: Ethyl 9,12,15-octadecatrienoate
Formula: $C_{20}H_{34}O_2$
MW: 306 NIST#: 336774 ID#: 41709 DB: mainlib
Contributor: William W. Christie, Mylnefield Lipid Analysis, Invergowrie, Dundee, Scotland, UK
10 largest peaks:
79 999 | 67 669 | 95 599 | 93 539 | 81 479 | 55 469 | 80 419 | 108 399 | 107 299 | 91 279 |
Synonyms:
no synonyms.

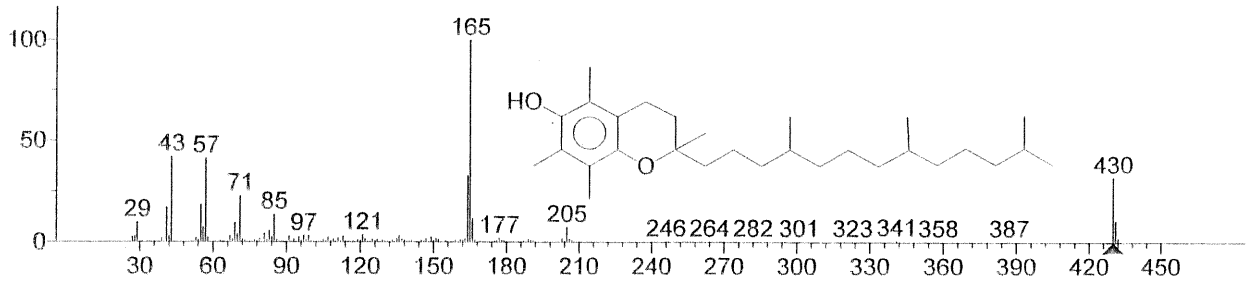
Estimated non-polar retention index (n-alkane scale):
Value: 2201 iu
Confidence interval (Esters): 47(50%) 201(95%) iu




(Text File) +EI Scan (86.513 min) ALI-OLE-H7-220421-.D

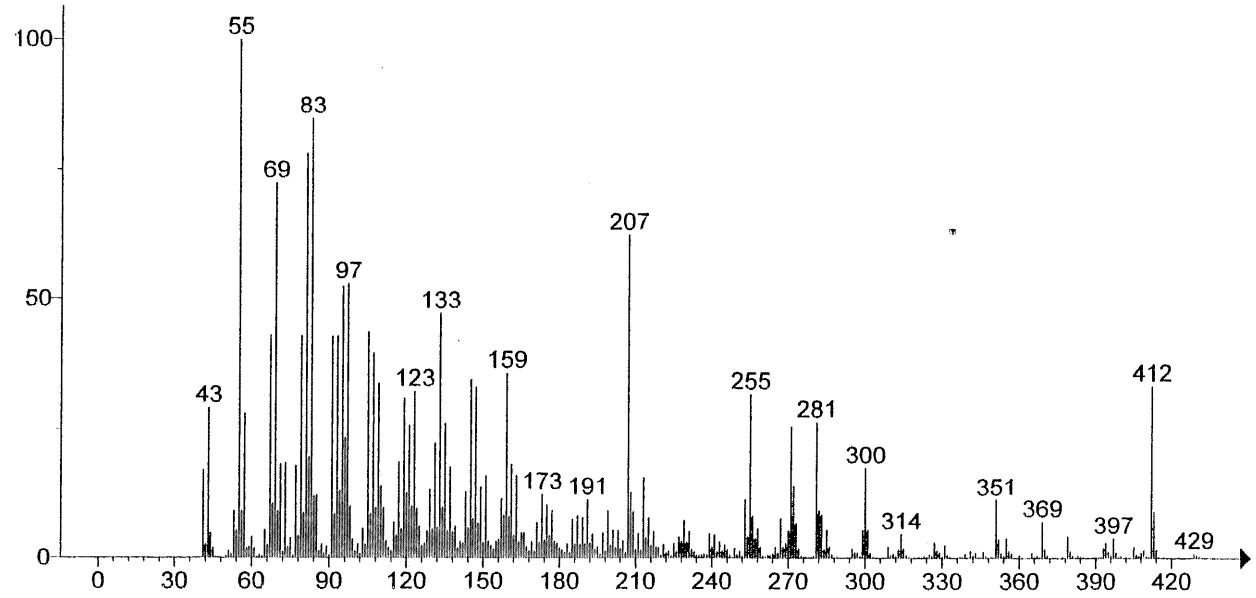



Head to Tail MF=767 RMF=788

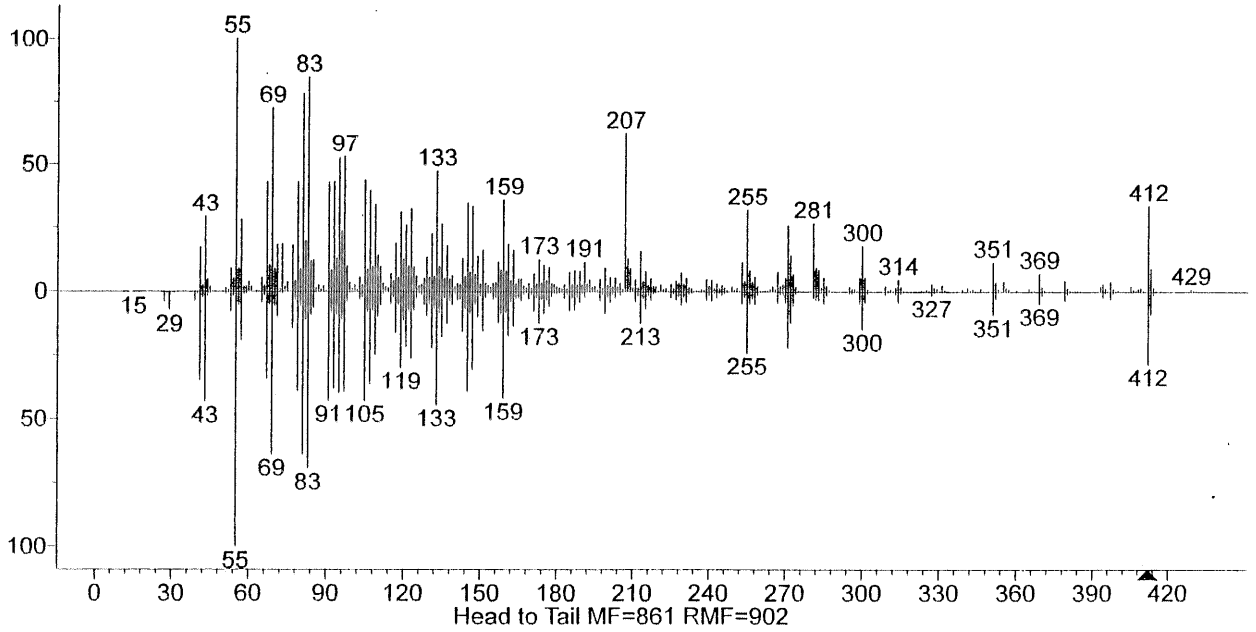



(mainlib) Vitamin E

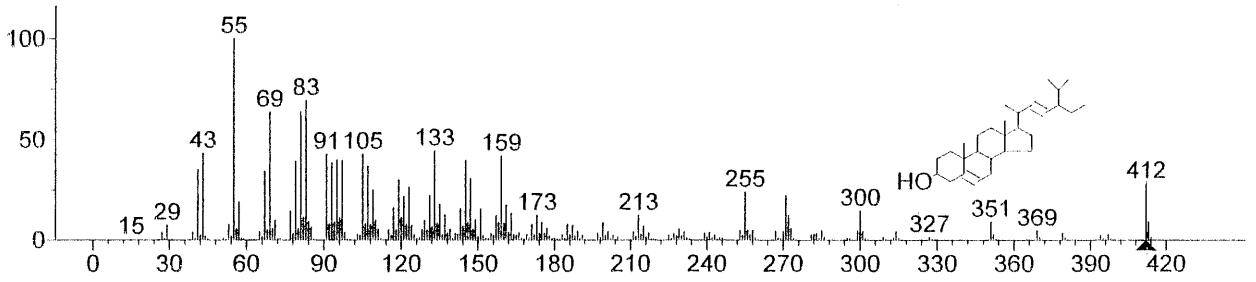
Name: Vitamin E
Formula: $C_{29}H_{50}O_2$
MW: 430 CAS#: 59-02-9 NIST#: 151382 ID#: 122577 DB: mainlib
Other DBs: TSCA, RTECS, HODOC, NIH, EINECS
Contributor: Chemical Concepts
10 largest peaks:
165 999 | 43 419 | 57 410 | 164 326 | 430 318 | 71 226 | 55 185 | 41 171 | 85 135 | 166 117 |
Synonyms:
1.2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, [2R-[2R*(4R*,8R*)]]-
2.α-Tocopherol
3.α-Tokoferol
4.(All-R)-α-Tocopherol
5.(2R,4'R,8'R)-α-Tocopherol
6.D-α-tocopherol
7.Almefrol
8.Antisterility vitamin
9.Denamone
10.Emipherol
11.Endo E
12.Ephynal
13.Eprolin
14.Eprolin S
15.Epsilan
16.Esorb
17.Etamican
18.Etavit
19.Evion
20.Evitaminum
21.Ilitia
22.Phytogermine
23.Profecundin
24.Spavit E
25.Syntopherol
26.Tokopharm
27.Vascuals
28.Verrol
29.Vi-E
30.Vitaplex E
31.Vitayonon
32.Viteolin
33.5,7,8-Trimethyltocol
34.component of E and C-Level
35.component of Estopherol
36.Aquasol E
37.Lan-E
38.Med-E
39.Vita E
40.Covi-ox
41.Spavit
42.(R,R,R)-α-Tocopherol
43.(+)-α-Tocopherol
44.(+)-α-Tocopherolα-tocopherolantisterility vitamin
45.[2R-2R*(4R*,8R*)]-3,4-Dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol
46.2,5,7,8-Tetramethyl-2-(4',8',12'-trimethyltridecyl)-6-chromanol




(Text File) +EI Scan (90.369 min) ALI-OLE-H7-220421-.D




Head to Tail MF=861 RMF=902



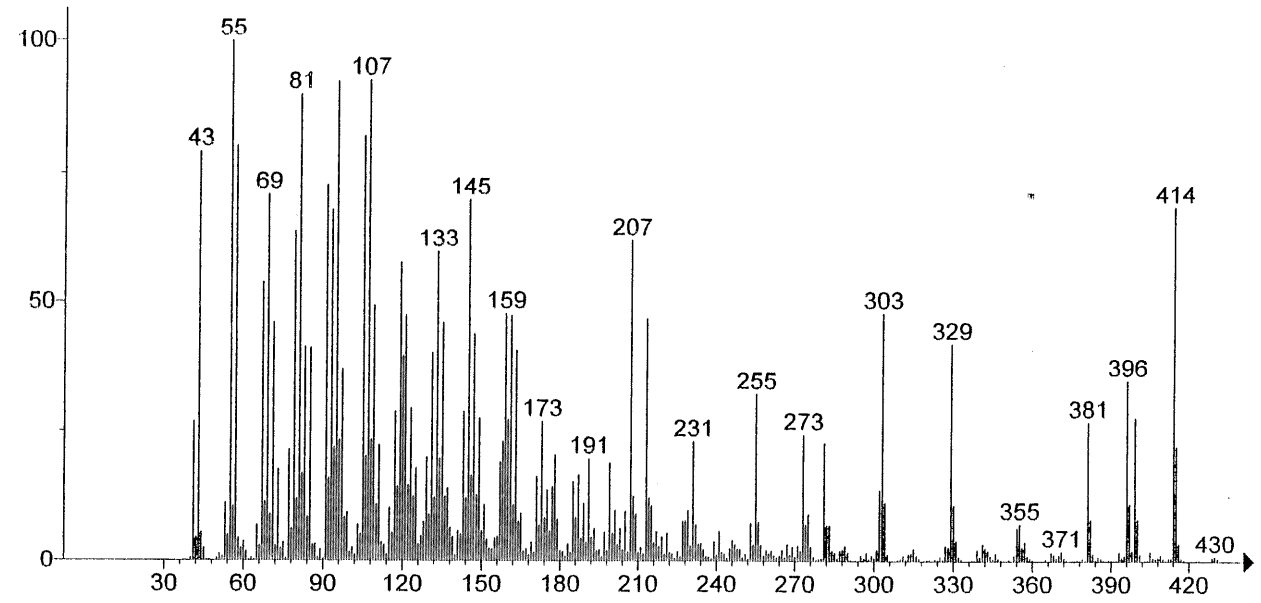

(mainlib) Stigmasterol

Name: Stigmasterol
Formula: $C_{29}H_{48}O$
MW: 412 CAS#: 83-48-7 NIST#: 352610 ID#: 18876 DB: mainlib
Other DBs: Fine, HODOC, NIH, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
55 999 | 83 692 | 81 638 | 69 636 | 133 444 | 43 431 | 91 427 | 105 427 | 159 418 | 95 398 |
Synonyms:
1.Stigmasta-5,22-dien-3-ol, (3β,22E)-
2.Stigmasta-5,22-dien-3β-ol
3.β-Stigmasterol
4.(24S)-5,22-Stigmastadien-3β-ol
5.Stigmasta-5,22-dien-3-ol, (3β)-
6.Stigmasterin
7.Phytosterol
8.5,22-Cholestadien-24-ethyl-3β-ol
9..DELTA.5,22-Stigmastadien-3β-ol
10.I-Stigmasterol
11.Stigmasta-5,22-dien-3-ol
12.(22E)-Stigmasta-5,22-dien-3-ol #

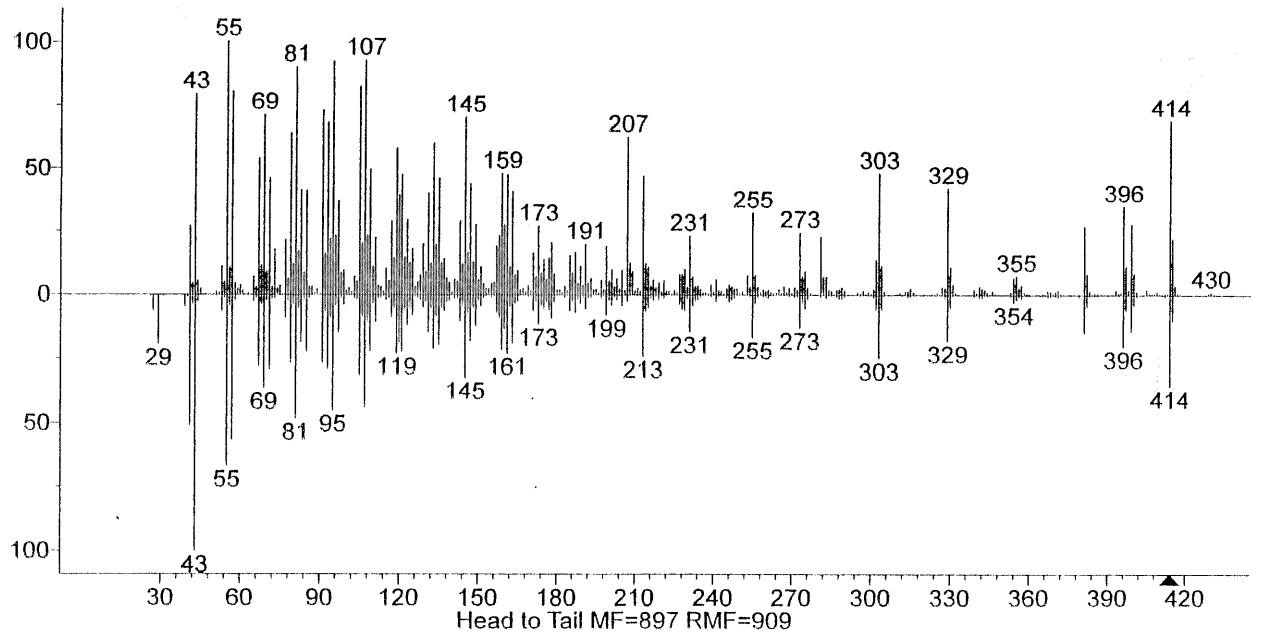
Estimated non-polar retention index (n-alkane scale):
Value: 2739 iu
Confidence interval (Low reliability): 174(50%) 752(95%) iu

Retention index.
1. Value: 3221.93 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column
Length: 30 m
Carrier Gas: H2
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Kovats
RI
Program Type: Isothermal
Start T: 270 C
Source: Stránský, K.; Valterová, I.; Fiedler, P., Nonsaponifiable lipid components of the pollen of elder (Sambucus nigra L.), J. Chromatogr. A, 936, 2001, 173-181.

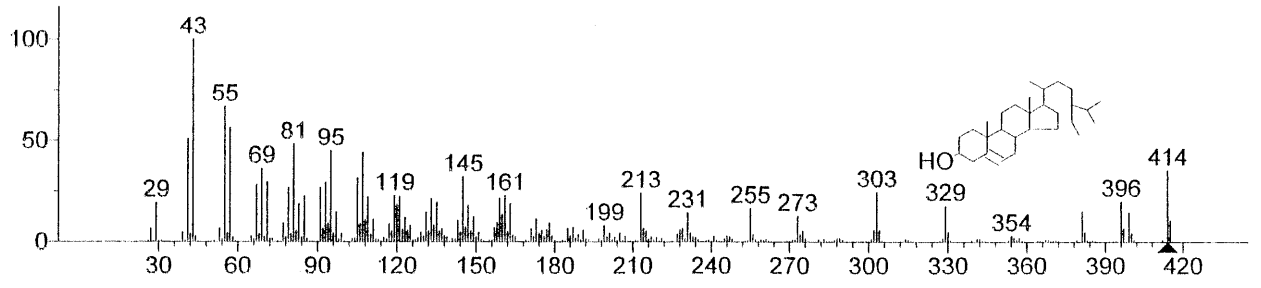
2. Value: 3222.15
iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Column Length: 30
m
Carrier Gas: H2
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Kovats RI
Program




(Text File) +EI Scan (92.251 min) ALI-OLE-H7-220421-.D




Head to Tail MF=897 RMF=909




(mainlib) γ-Sitosterol

Name: γ-Sitosterol
Formula: $C_{29}H_{50}O$
MW: 414 CAS#: 83-47-6 NIST#: 151558 ID#: 6743 DB: mainlib
Other DBs: HODOC, EINECS
Contributor: Chemical Concepts
10 largest peaks:
43 999 | 55 667 | 57 563 | 41 507 | 81 481 | 95 449 | 107 440 | 69 362 | 414 354 | 145 321 |
Synonyms:
1.Stigmast-5-en-3-ol, (3β,24S)-
2.Stigmast-5-en-3β-ol, (24S)-
3.Clionasterol
4.Fucosterol, β-dihydro-
5.24β-Ethyl-5-cholesten-3β-ol
6.β-Dihydrofucosterol
7.22,23-Dihydroporiferasterol
8.24S-Ethylcholest-5-en-3β-ol
9.24β-Ethylcholesterol
10.Stigmast-5-en-3-ol #

Estimated non-polar retention index (n-alkane scale):
Value: 2731 iu
Confidence interval (Low reliability): 174(50%) 752(95%) iu

Retention index.
1. Value: 3066 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.