

Additional file 2

AMB Express

Antimicrobial Potential of Toothpaste formulated from Extracts of *Syzygium aromaticum*, *Dennettia tripetala* and *Jatropha curcas* latex against some Oral Pathogenic Microorganisms

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³Biotechnology Unit, Department of Biological Sciences, Kings University, PMB 555, Odeomu, Nigeria

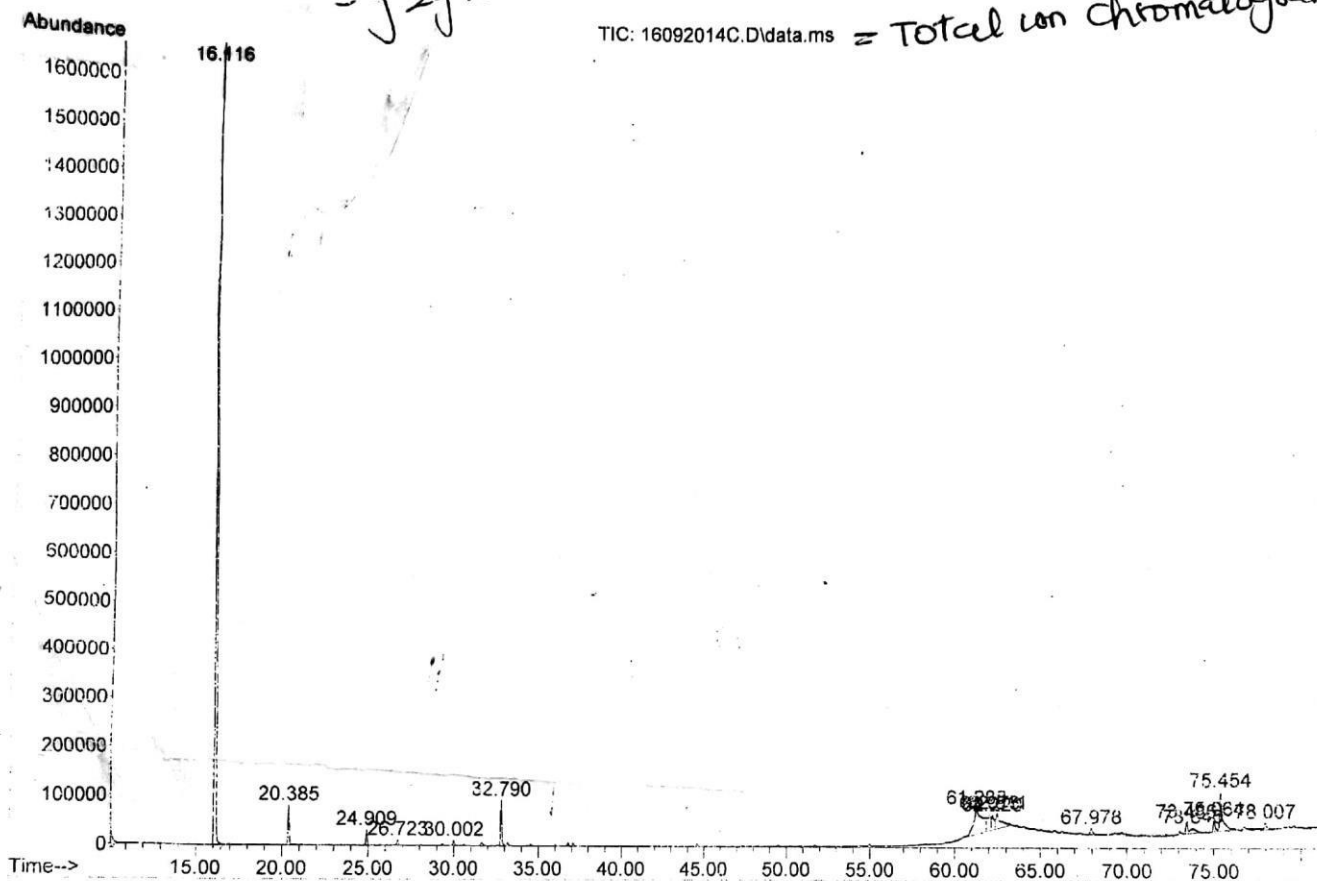
*Corresponding author: ooluwasina@futa.edu.ng, +2348107246660

Additional file 2: the chromatogram of *Syzygium aromaticum* extract. GCMS revealed the library ID of bioactive compounds in the extract with their peaks, area, retention time, molecular formulae and respective weight.

Sample Name: GBENGA CHEM. PEP
 Asc Info :
 al Number: 1

Syzygium

TIC: 16092014C.D\data.ms = Total ion chromatogram.



Sample : GBENGA CHEM. PEP
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\Database\NIST11.L

Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	16.118	57.57	C:\Database\NIST11.L			
			Formic acid, (2-methylphenyl)methyl ester	24532	1000368-93-3	64
			Benzenemethanol, 2-methyl-, acetate	33429	017373-93-2	64
			Glutaric acid, di(phenethyl) ester	176924	1000358-69-4	64
2	20.386	2.90	C:\Database\NIST11.L			
			Phenol, 2-methoxy-3-(2-propenyl)-	33399	001941-12-4	98
			Eugenol	33238	000097-53-0	98
			Eugenol	33241	000097-53-0	98
3	24.907	1.12	C:\Database\NIST11.L			
			Caryophyllene	64272	000087-44-5	99
			Caryophyllene	64275	000087-44-5	96
			Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-	64418	013877-93-5	93
4	26.721	0.52	C:\Database\NIST11.L			
			1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	81047	000078-36-4	53
			Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl-	15869	000488-97-1	47
			1,6-Octadien-3-ol, 3,7-dimethyl-, formate	47002	000115-99-1	47
5	30.005	0.38	C:\Database\NIST11.L			
			1-Methyltricyclo[2.2.1.0(2,6)]heptane	5508	004601-85-8	49
			Cyclohexane, ethenylidene-	5446	005664-20-0	43
			Tricyclo[2.2.2.0(1,4)]octane	5473	036120-88-4	38
6	32.792	3.36	C:\Database\NIST11.L			
			1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	79437	040716-66-3	91
			Nerolidol 2	79382	1000285-43-6	91
			1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-	79426	007212-44-4	90
7	61.287	11.80	C:\Database\NIST11.L			
			9,12-Octadecadienoic acid (Z,Z)-	127649	000060-33-3	95
			9,12-Octadecadienoic acid (Z,Z)-	127647	000060-33-3	89
			Cyclopropaneoctanal, 2-octyl-	127746	056196-06-6	68
8	62.071	3.30	C:\Database\NIST11.L			
			2-Methyl-Z,Z-3,13-octadecadienol	127747	1000130-90-5	94
			9,12-Octadecadienoic acid (Z,Z)-	127647	000060-33-3	93
			9,12-Octadecadienoic acid (Z,Z)-	127649	000060-33-3	90
9	62.220	2.20	C:\Database\NIST11.L			
			2-Methyl-Z,Z-3,13-octadecadienol	127747	1000130-90-5	93
			Octadec-9-enoic acid	129341	1000190-13-7	90
			9,12-Octadecadienoic acid (Z,Z)-	127647	000060-33-3	70
10	62.512	4.39	C:\Database\NIST11.L			
			Cyclopropaneoctanal, 2-octyl-	127746	056196-06-6	82
			9-Octadecenoic acid (Z)-, 2,3-dihydro-	188140	000060-33-3	82

droxypropyl ester
Cycloeicosane

127768 000296-56-0 81

11 67.976 0.80 C:\Database\NIST11.L
✓Cyclododecane✓
1,19-Eicosadiene✓
Cyclododecane

36738 000294-62-2 53
126193 014811-95-1 46
36737 000294-62-2 41

12 73.486 1.21 C:\Database\NIST11.L

✓9-Octadecenal, (Z)-
✓9-Octadecenoic acid (Z)-, 2-hydrox
yethyl ester
9-Octadecenoic acid (Z)-, 2-hydrox
y-1-(hydroxymethyl)ethyl ester

115866 002423-10-1 93
166116 004500-01-0 62

13 73.841 1.49 C:\Database\NIST11.L

cis-9-Hexadecenal
9-Octadecenal, (Z)-
✓Trichloroacetic acid, undec-2-enyl
ester

92517 056219-04-6 30
115866 002423-10-1 15
155835 1000299-26-1 15

14 75.066 1.18 C:\Database\NIST11.L

2(1H)-Naphthalenone, octahydro-4a-
methyl-7-(1-methylethyl)-, (4a.alp
ha., 7.beta., 8a.beta.)-
✓1,3,12-Nonadecatriene
cis,cis-7,10,-Hexadecadienal

67892 054594-42-2 92
112661 1000131-11-1 87
90904 056829-23-3 62

15 75.455 6.69 C:\Database\NIST11.L

9-Octadecenal, (Z)-
✓2-Methyl-Z,Z-3,13-octadecadienol
9,12-Octadecadienoic acid (Z,Z)-

115866 002423-10-1 90
127747 1000130-90-5 83
127647 000060-33-3 70

16 78.007 1.10 C:\Database\NIST11.L

Phthalic acid, cylclohexylmethyl p
entyl ester
Di(Z)-hex-3-enyl phthalate
Di(E)-hex-3-enyl phthalate

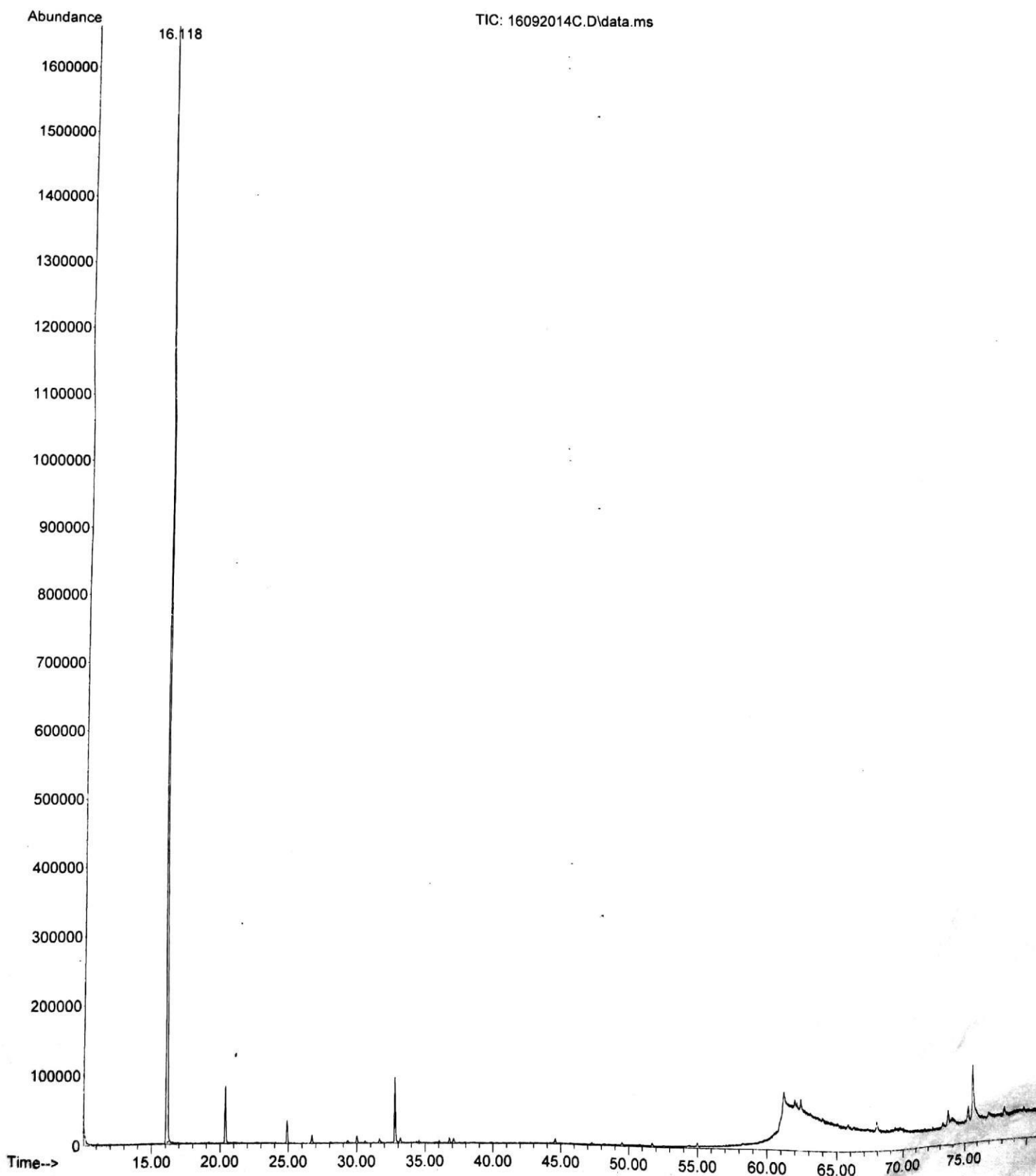
170888 1000309-07-5 43
169298 1000373-65-0 38
169297 1000373-64-8 38

Path :
File :
Cq On
Operator
Sample

Sample : GBENGA CHEM. PEP
Misc :
ALS Vial : 1 Sample Multiplier: 1

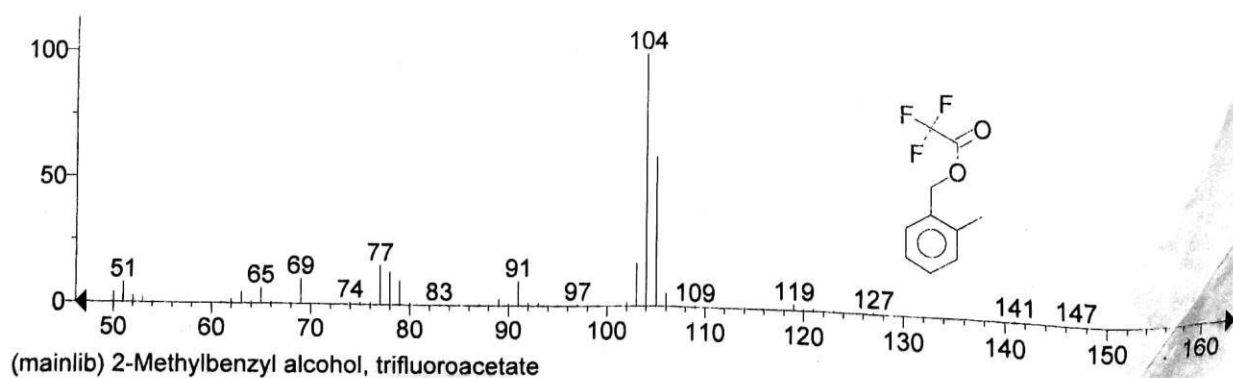
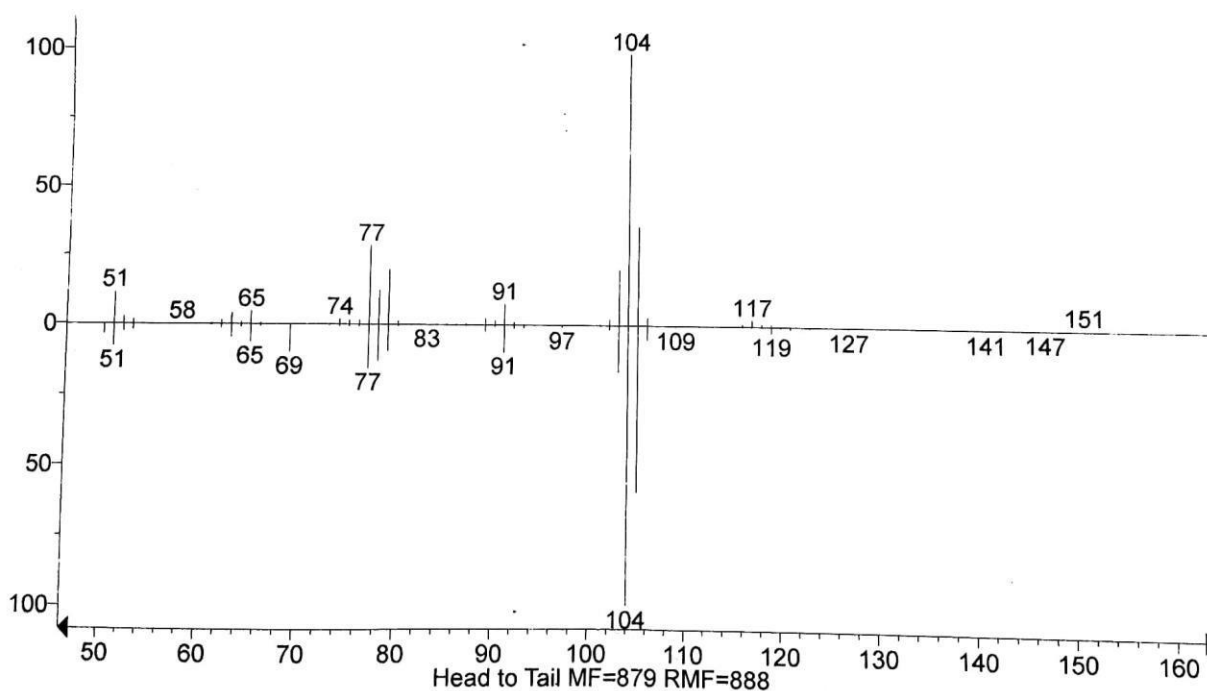
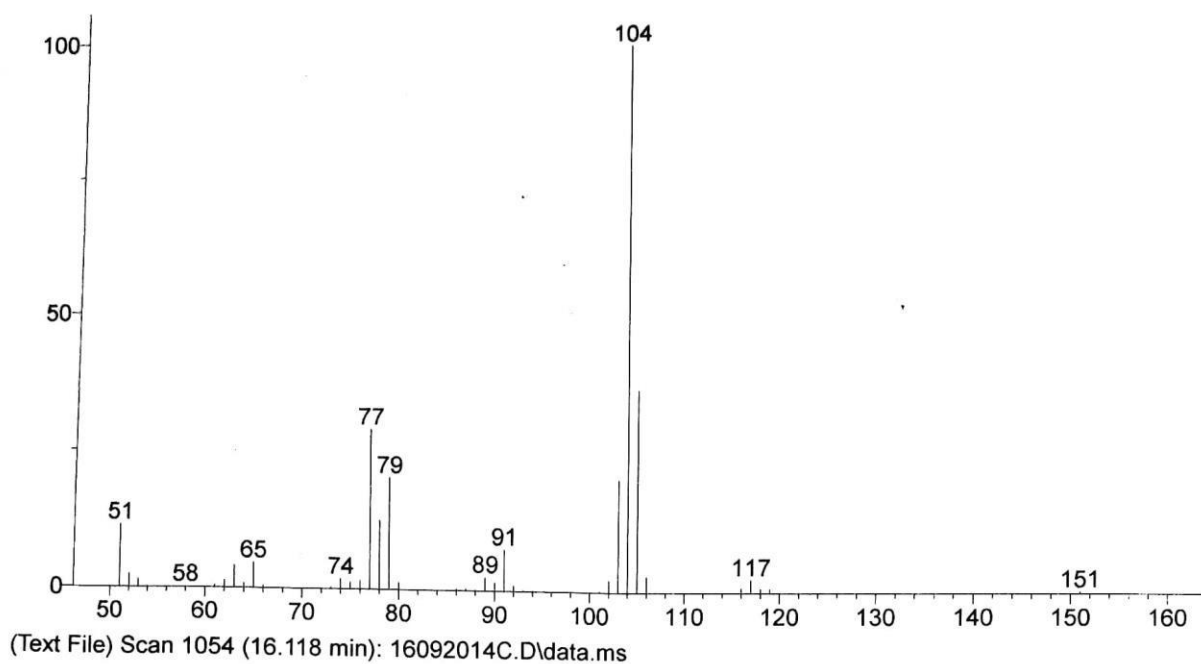
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Integrator: ChemStation

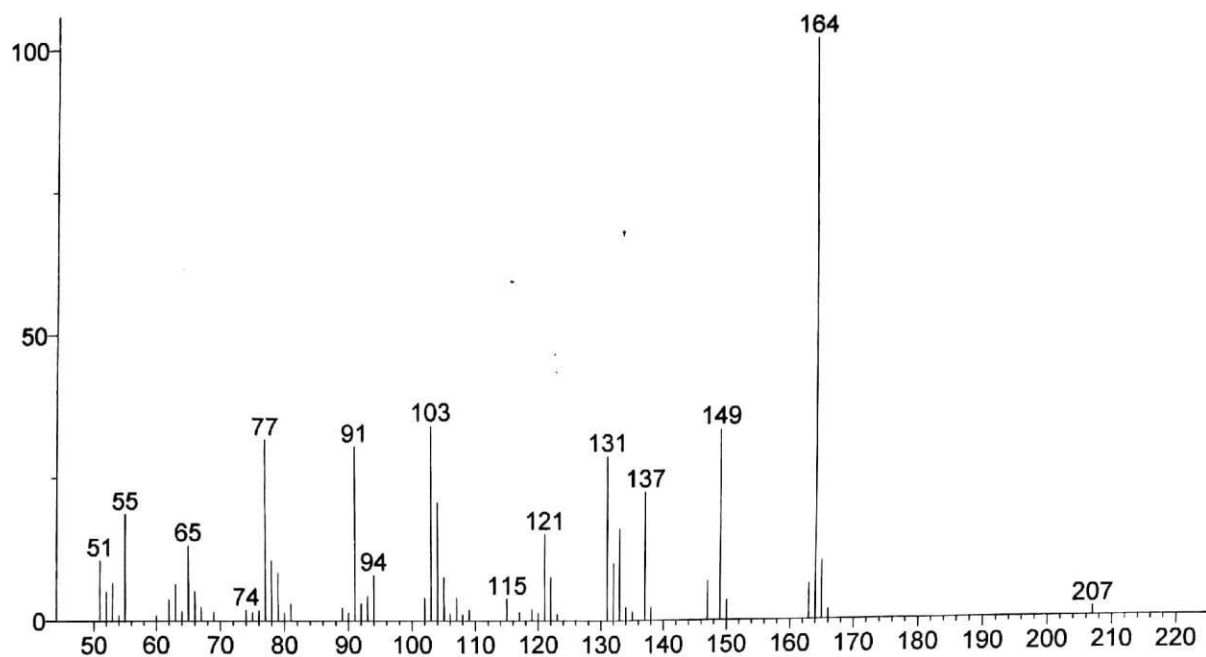
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Title :



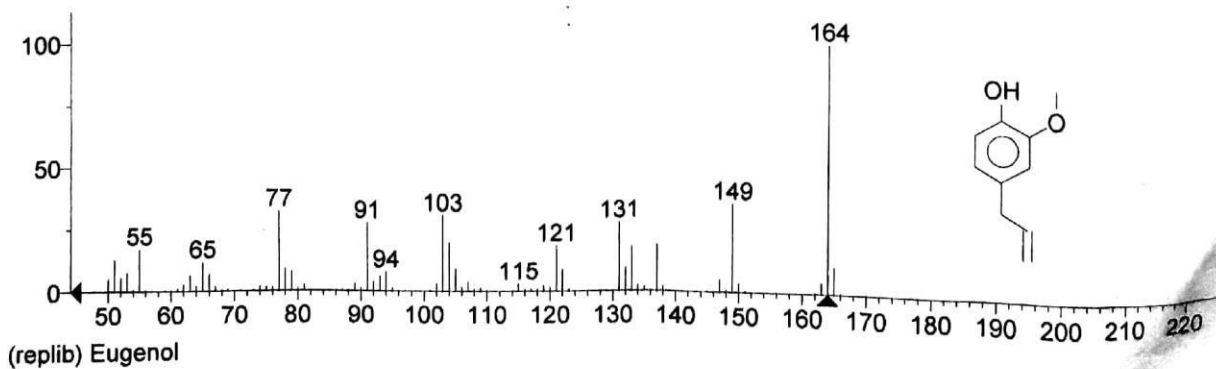
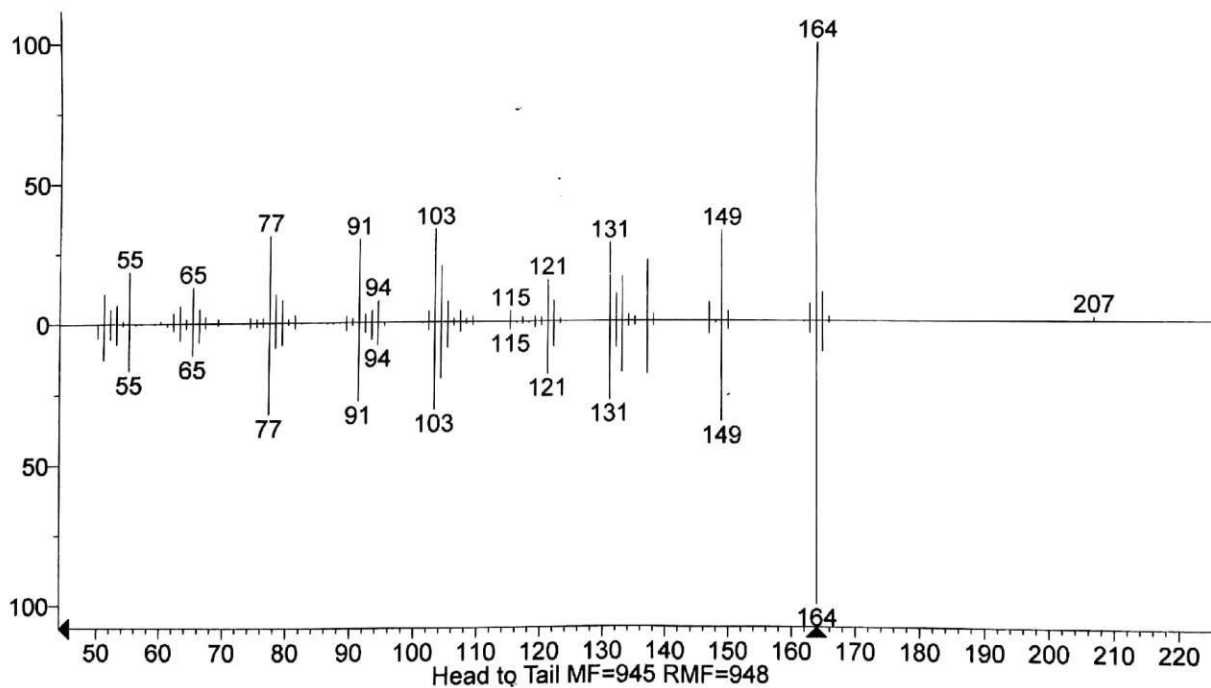
IBITOYE METHOD.M Tue Sep 16 16:00:13 2014

Page: 2





(Text File) Scan 1800 (20.386 min): 16092014C.D\data.ms



Name: Eugenol

Formula: C₁₀H₁₂O₂

MW: 164 Exact Mass: 164.08373 CAS#: 97-53-0 NIST#: 378793 ID#: 23453 DB: replib

Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB

Contributor: United States Army Criminal Investigation Laboratory (USACIL)

10 largest peaks:

164 999 | 149 358 | 77 325 | 103 312 | 131 281 |
91 279 | 104 201 | 137 189 | 121 188 | 133 183 |

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. Eugenenic 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. Allylguaiacol
26. 4-(2-Propenyl)-2-methoxyphenol
27. NSC 209525
28. Phenol, 2-methoxy-4-(2-propen-1-yl)-

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 µm

Data Type: Linear

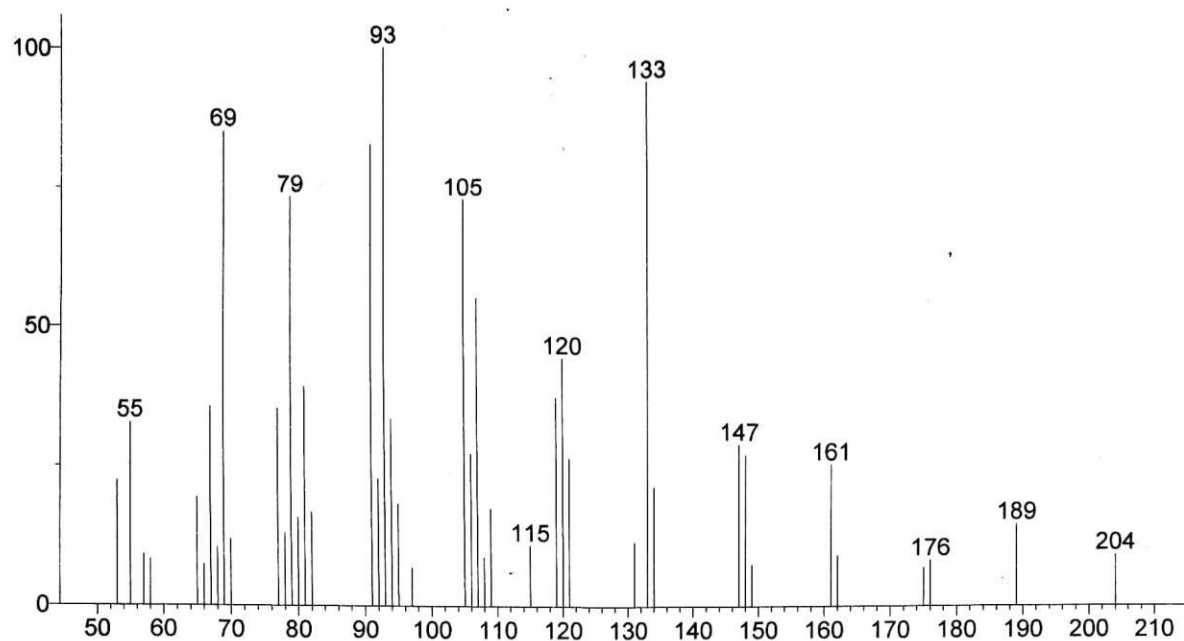
RI

Program Type: Ramp

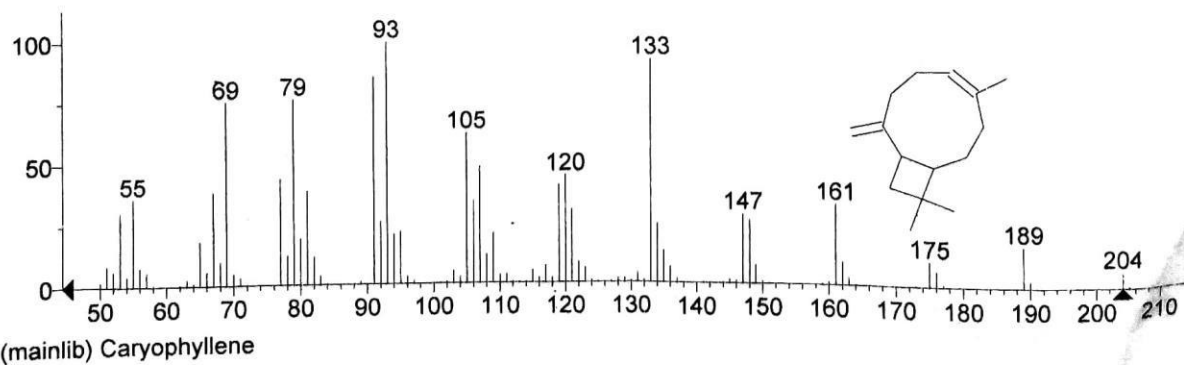
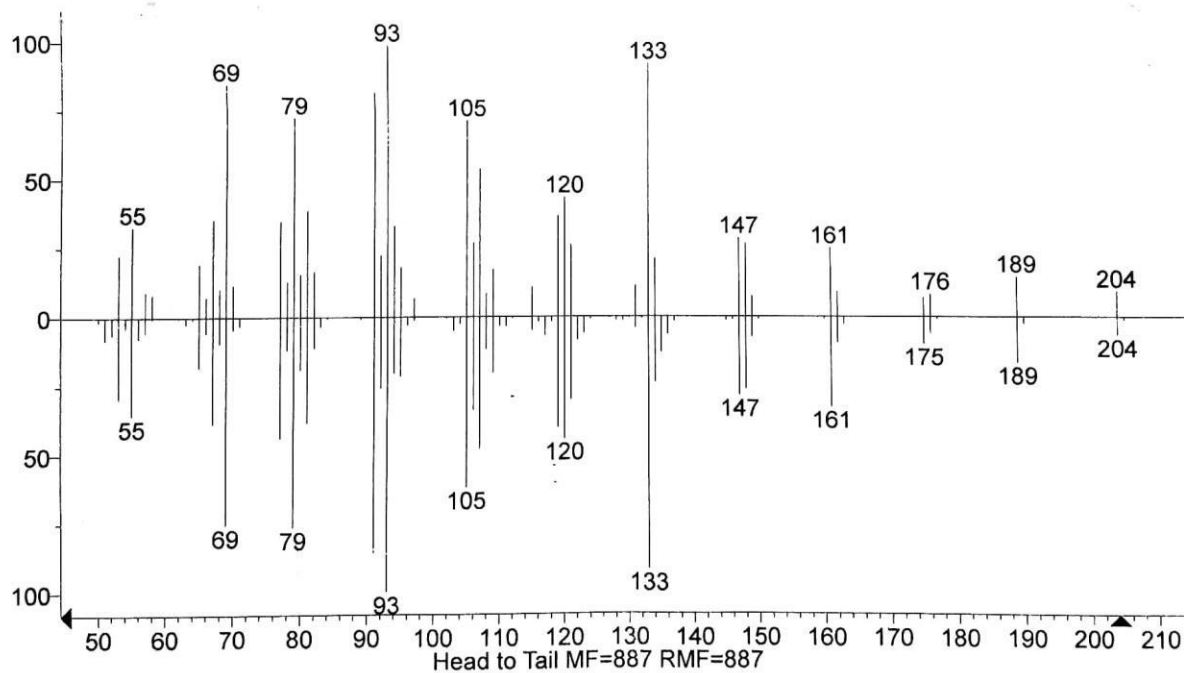
Start T: 60 C

End T: 220 C

Heat Rate: 2 K/min



(Text File) Scan 2590 (24.907 min): 16092014C.D\data.ms



(mainlib) Caryophyllene

Name: Caryophyllene

Formula: C₁₅H₂₄

MW: 204 Exact Mass: 204.1878 CAS#: 87-44-5 NIST#: 291486 ID#: 60555 DB: mainlib

Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS

Contributor: NIST Mass Spectrometry Data Center, 1998.

Related CAS#: 8007-38-3; 1407-53-0

10 largest peaks:

93 999 | 133 921 | 91 858 | 41 769 | 79 763 |
69 754 | 105 623 | 107 483 | 120 447 | 77 439 |

Synonyms:

1. Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]-
2. Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (E)-(1R,9S)-(-)-
3. β -Caryophyllen
4. β -Caryophyllene
5. trans-Caryophyllene
6. L-Caryophyllene
7. Bicyclo(7.2.0)undec-4-ene, 8-methylene-4,11,11-trimethyl-, (E)-(1R,9S)-(-)-
8. 8-Methylene-4,11,11-(trimethyl)bicyclo(7.2.0)undec-4-ene, (1R,4E,9S)-
9. beta-Caryophyllene
10. β -(E)-Caryophyllene
11. β -trans-Caryophyllene
12. Caryophyllene, (E)
13. E- β -Caryophyllene
14. (E)-Caryophyllene
15. trans- β -Caryophyllene
16. (-)-(E)-Caryophyllene
17. Caryophyllene B
18. NSC 11906

Estimated non-polar retention index (n-alkane scale):

Value: 1494 iu

Confidence interval (Hydrocarbons): 39(50%) 167(95%) iu

Retention index.

1. Value: 1424 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 μ m

Data Type: Linear

RI

Program Type: Ramp

Start T: 60 C

End T: 230 C

Heat Rate: 2 K/min

End Time: 30 min

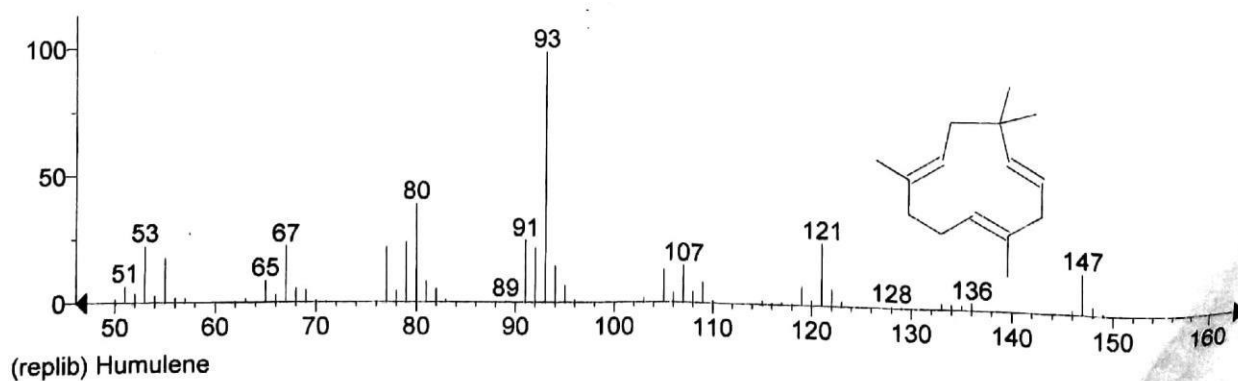
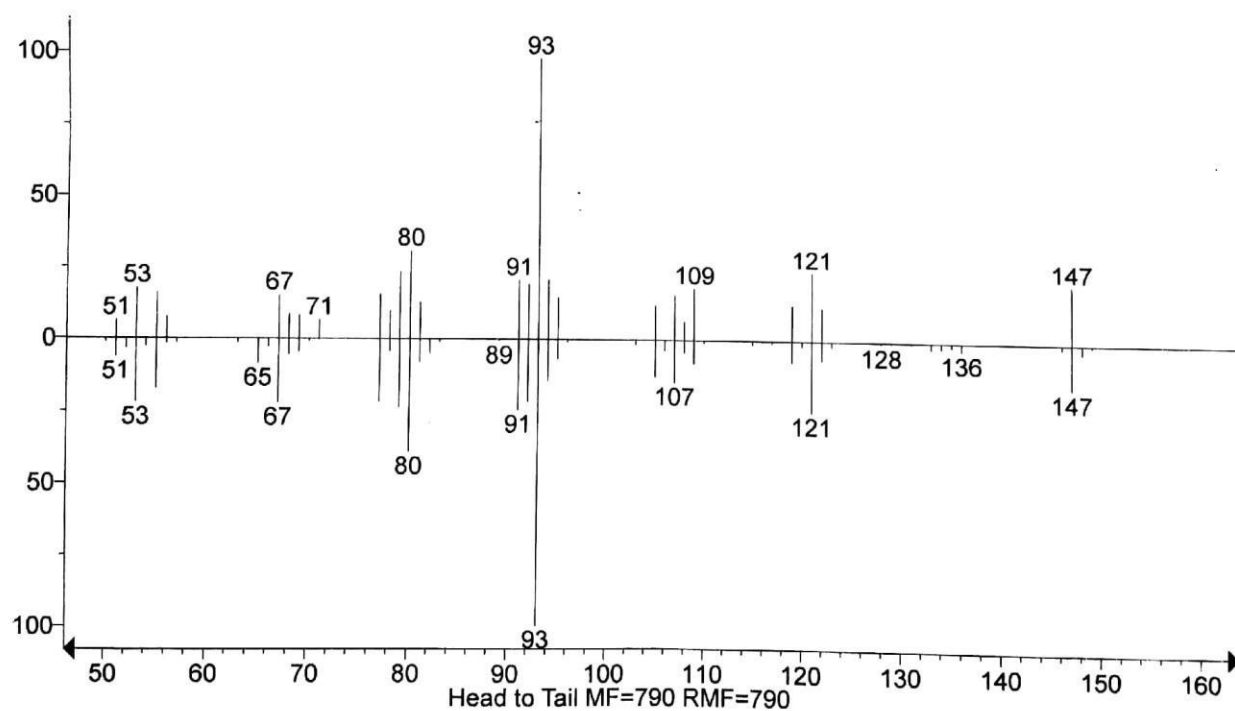
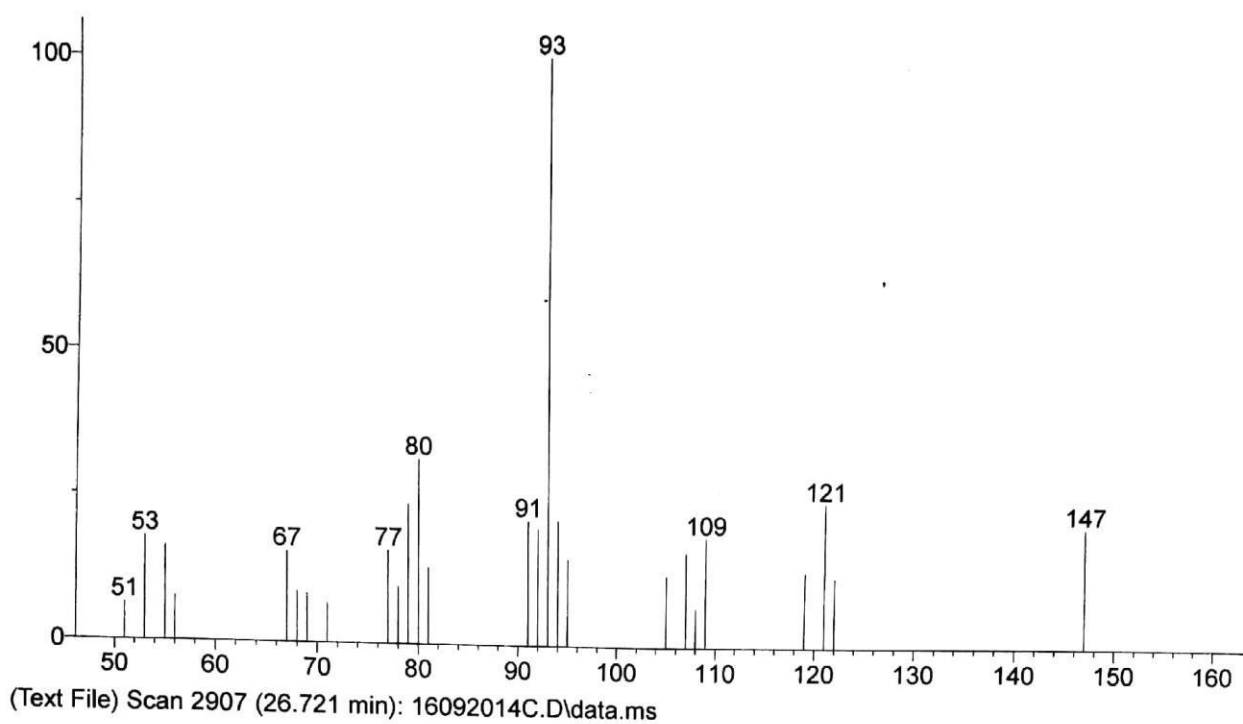
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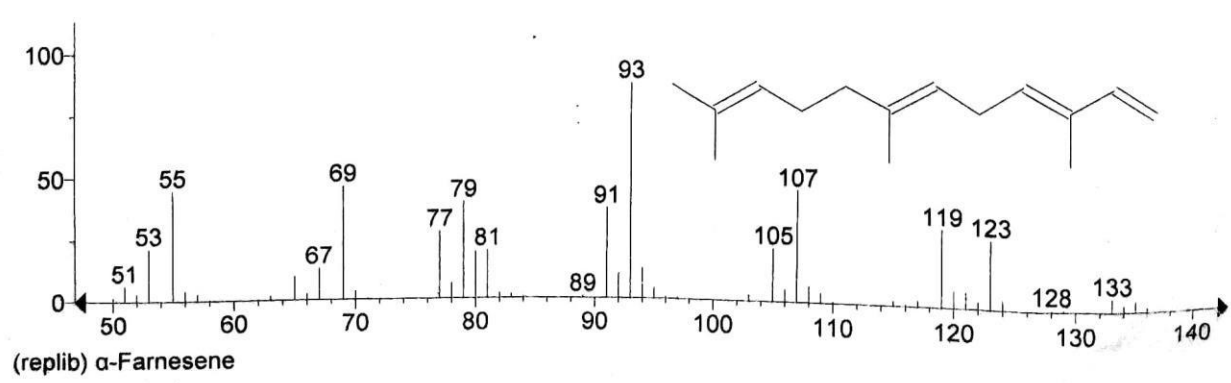
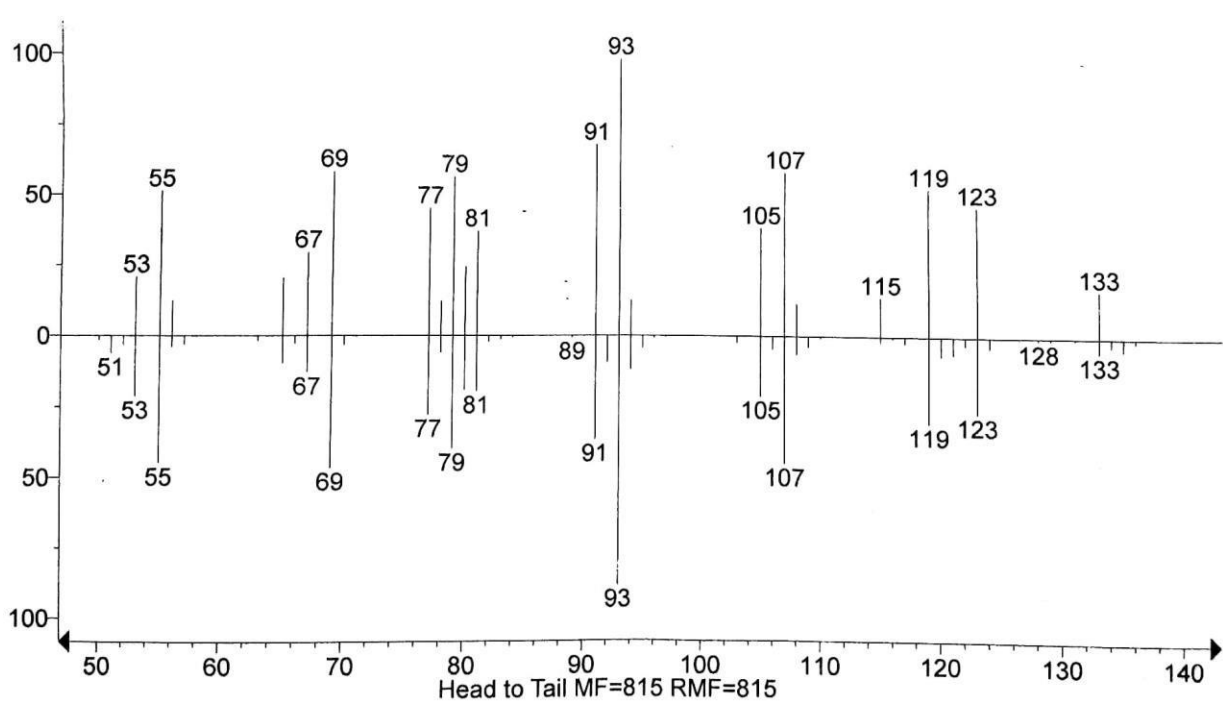
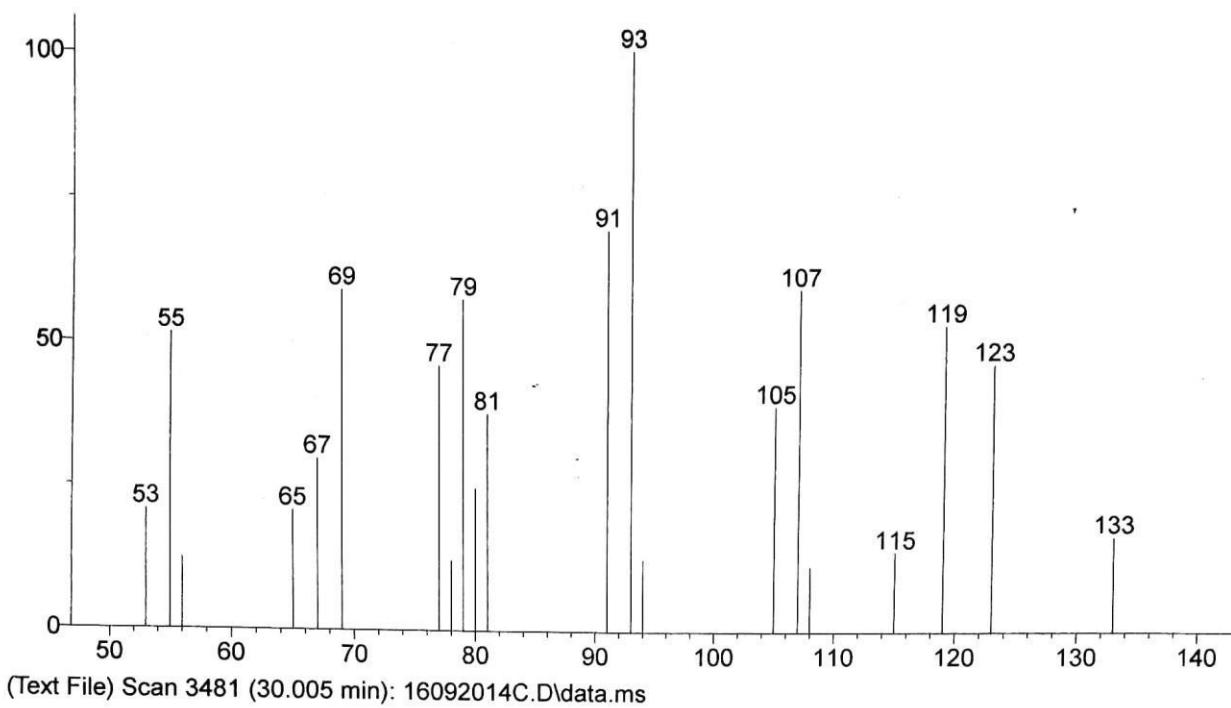
Bendahou, M.; Muselli, A.; Grignon-Dubois, M.; Benyoucef, M.; Desjobert, J.-M.; Bernardini, A.-F.; Costa, J.,
Antimicrobial activity and chemical composition of *Origanum glandulosum* Desf. essential oil and extract
obtained by microwave extraction: Comparison with hydrodistillation, Food Chem., 106, 2008, 132-139.

2.

Value: 1421 iu

Column Type: Capillary





Name: α -Farnesene

Formula: C₁₅H₂₄

MW: 204 Exact Mass: 204.1878 CAS#: 502-61-4 NIST#: 141113 ID#: 1267 DB: replib

Other DBs: Fine, TSCA, HODOC, EINECS

Contributor: Mark Whitten, Florida Museum of Natural History, U. of Florida

Related CAS#: 18452-58-9; 21499-64-9

10 largest peaks:

41 999	93 885	69 467	107 452	55 449
79 401	91 371	119 308	77 280	123 271

Synonyms:

1.1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (E,E)-

2.Farnesene

3.2,6,10-Trimethyl-2,6,9,11-dodecatetraene, trans-

4.3,7,11-Trimethyl-1,3,6,10-dodecatetraene, (trans,trans)-

5.(3E,6E)-3,7,11-Trimethyl-1,3,6,10-dodecatetraene #

6. α -E,E-Farnesene

7. α -Farnesene, (E,E)-

8. α -trans-Farnesene

9. α -trans,trans-Farnesene

10.(3E,6E)- α -Farnesene

11.(E,E)- α -Farnesene

12.alpha-Farnesene

13.trans- α -Farnesene

14.trans,trans- α -Farnesene

15.1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (3E,6E)-

16.trans-2,6,10-Trimethyl-2,6,9,11-dodecatetraene

17.trans-3,7,11-Trimethyl-1,3,6,10-dodecatetraene

Estimated non-polar retention index (n-alkane scale):

Value: 1458 iu

Confidence interval (Hydrocarbons): 39(50%) 167(95%) iu

Retention index.

1. Value: 1499 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 μ m

Data Type: Linear

RI

Program Type: Ramp

Start T: 60 C

End T: 220 C

Heat Rate: 2 K/min

End Time: 20 min

Source: Boti, J.

B.; Koukoua, G.; N'Guessan, T.Y.; Casanova, J., Chemical variability of *Conyza sumatrensis* and *Microglossa pyrifolia* from Cote d'Ivoire, *Flavour Fragr. J.*, 22, 2007, 27-31.

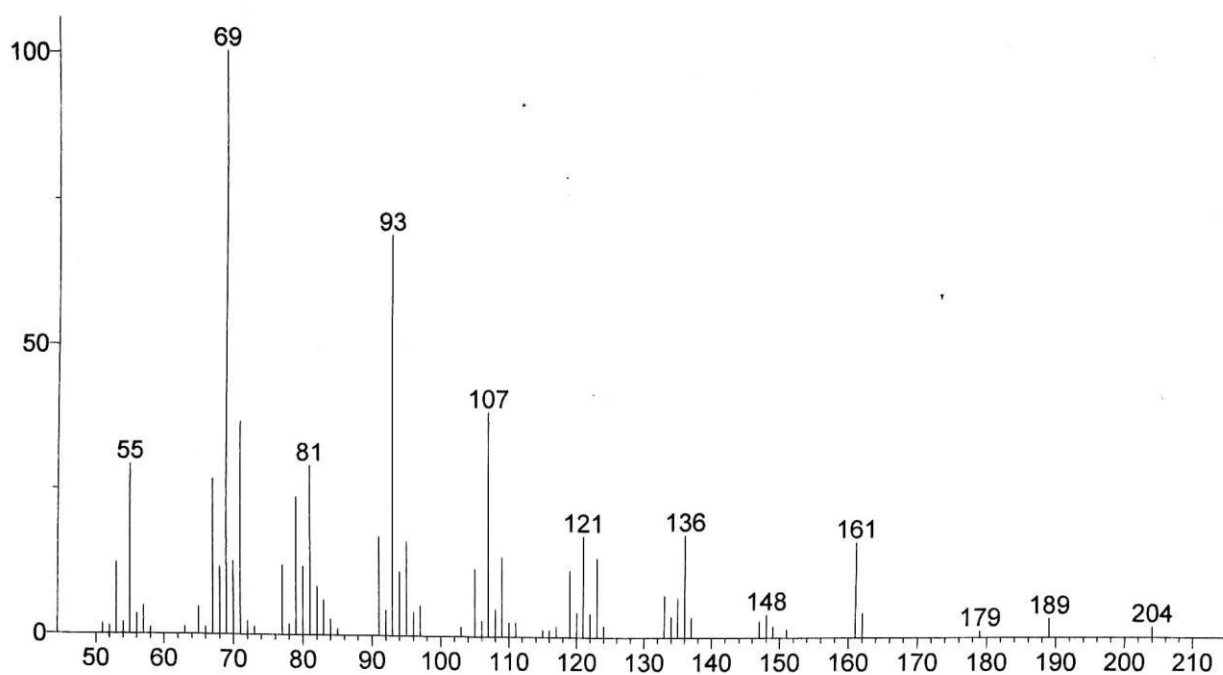
2. Value: 1496 iu

Column Type:

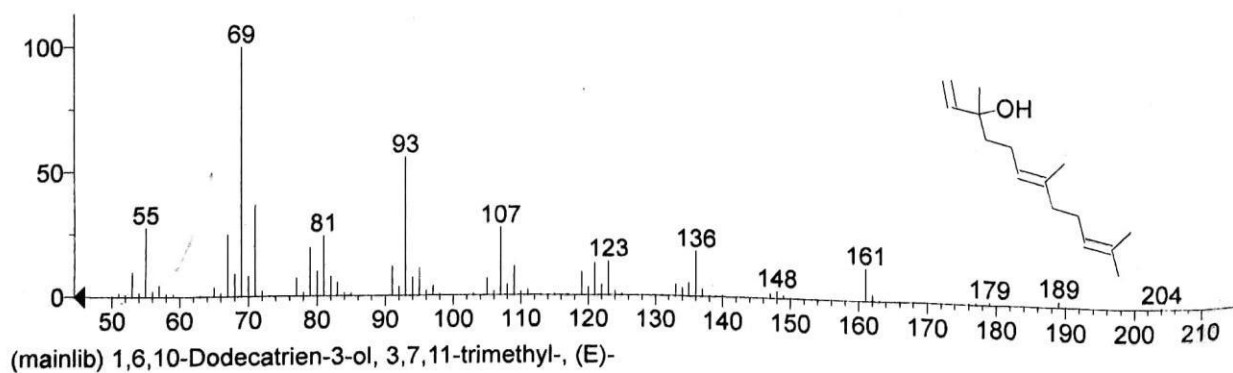
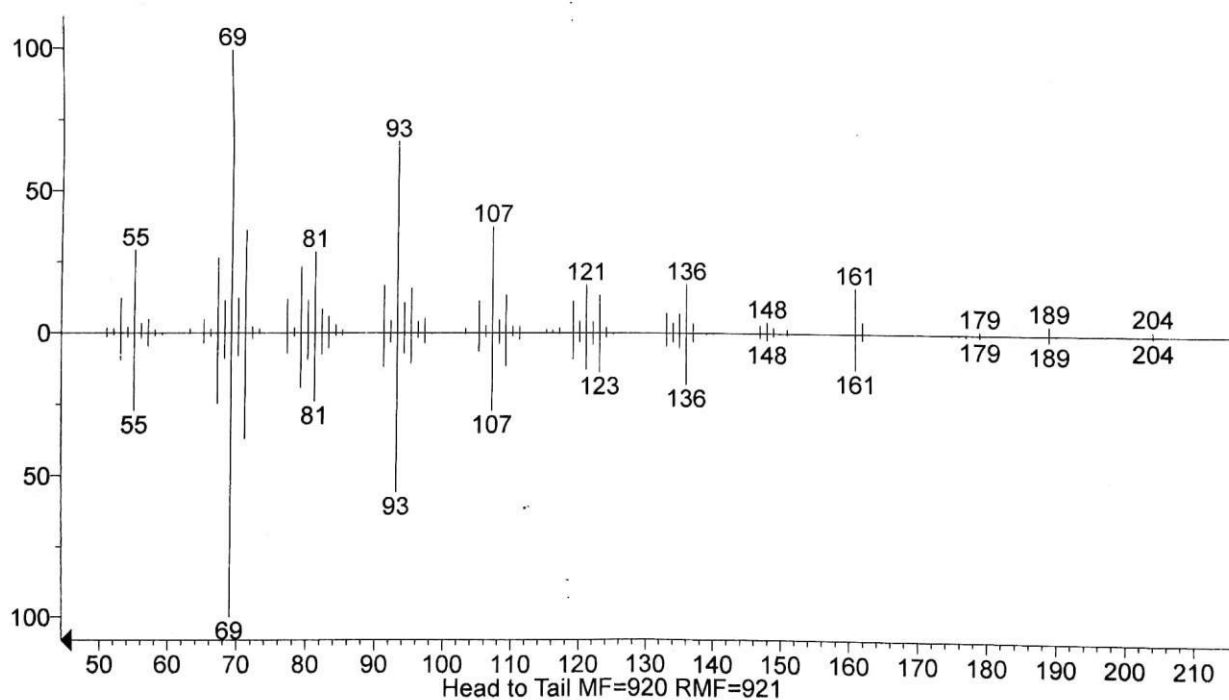
Capillary

Column Class: Standard non-polar

Active Phase: RTX-1



(Text File) Scan 3968 (32.792 min): 16092014C:D\data.ms



Name: 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-

Formula: C₁₅H₂₆O

MW: 222 Exact Mass: 222.198365 CAS#: 40716-66-3 NIST#: 108468 ID#: 31602 DB: mainlib

Other DBs: EINECS

Contributor: Chuck Anderson, Aldrich Chemical Co.

Related CAS#: 2211-29-2

10 largest peaks:

69 999	41 586	93 560	43 410	71 370
107 275	55 272	67 249	81 241	79 192

Synonyms:

1.(±)-trans-Nerolidol

2.(6E)-3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol #

3.(6E)-Nerolidol

4.E-Nerolidol

5.Nerolidol, E-

6.Nerolidol, trans

7.trans-Nerolidol

8.trans-3,7,11-Trimethyl-dodeca-1,6,10-trien-3-ol

9.3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol, (E)-

Estimated non-polar retention index (n-alkane scale):

Value: 1564 iu

Confidence interval (Alcohols): 41(50%) 176(95%) iu

Retention index.

1. Value: 1548 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 µm

Data Type: Linear

RI

Program Type: Ramp

Start T: 60 C

End T: 220 C

Heat Rate: 2 K/min

End Time: 20 min

Source: Boti, J.

B.; Koukoua, G.; N'Guessan, T.Y.; Casanova, J., Chemical variability of *Conyza sumatrensis* and *Microglossa pyrifolia* from Cote d'Ivoire, *Flavour Fragr. J.*, 22, 2007, 27-31.

2. Value: 1555 iu

Column Type:

Capillary

Column Class: Standard non-polar

Active Phase: CP-Sil PONA GB

Column Length: 100 m

Carrier

Gas: He

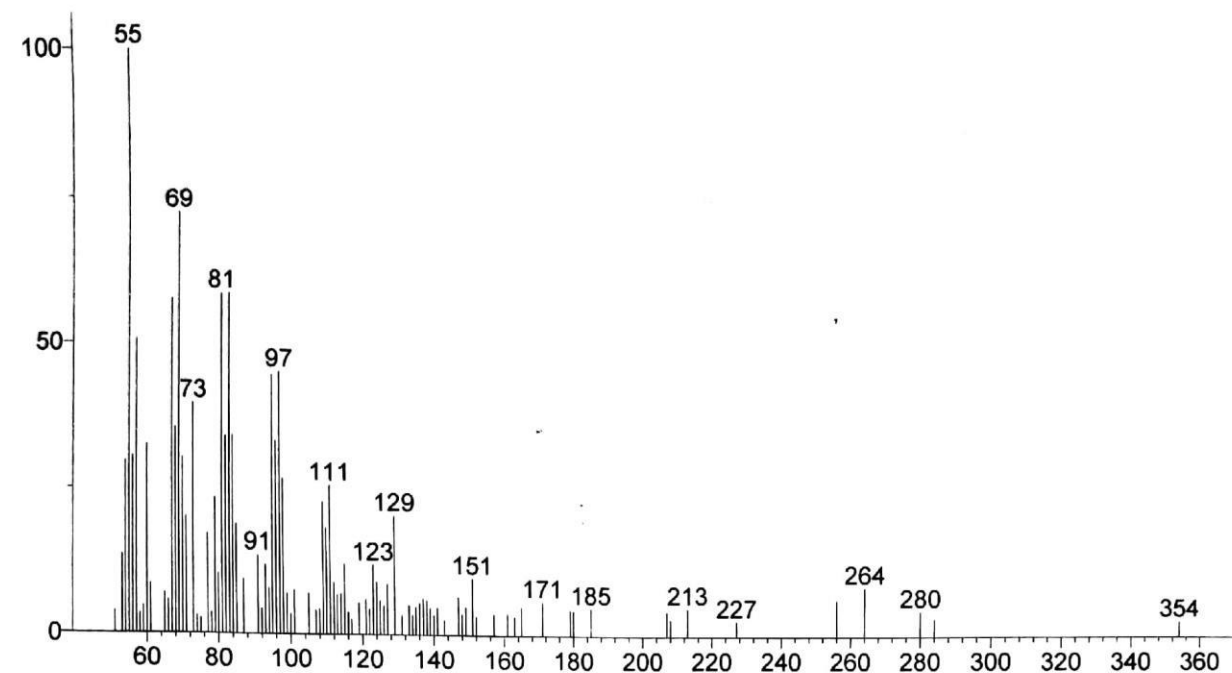
Column Diameter: 0.25 mm

Phase Thickness: 0.25 µm

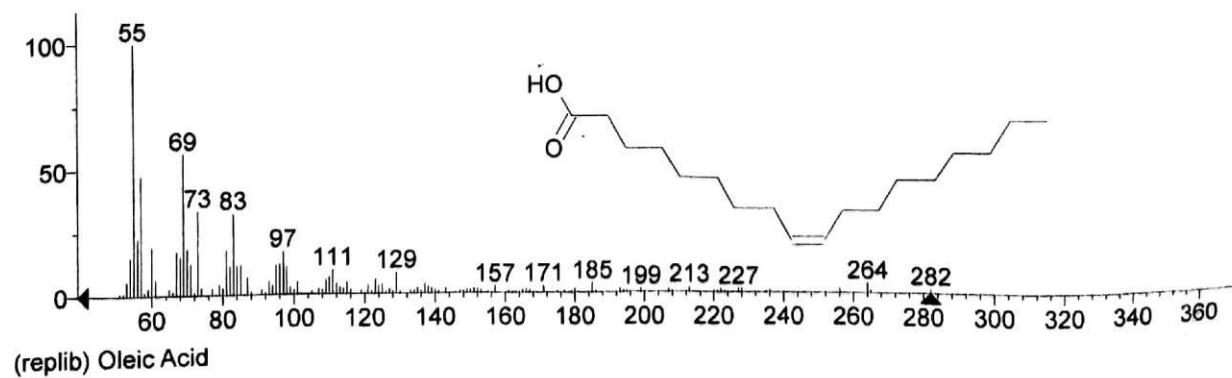
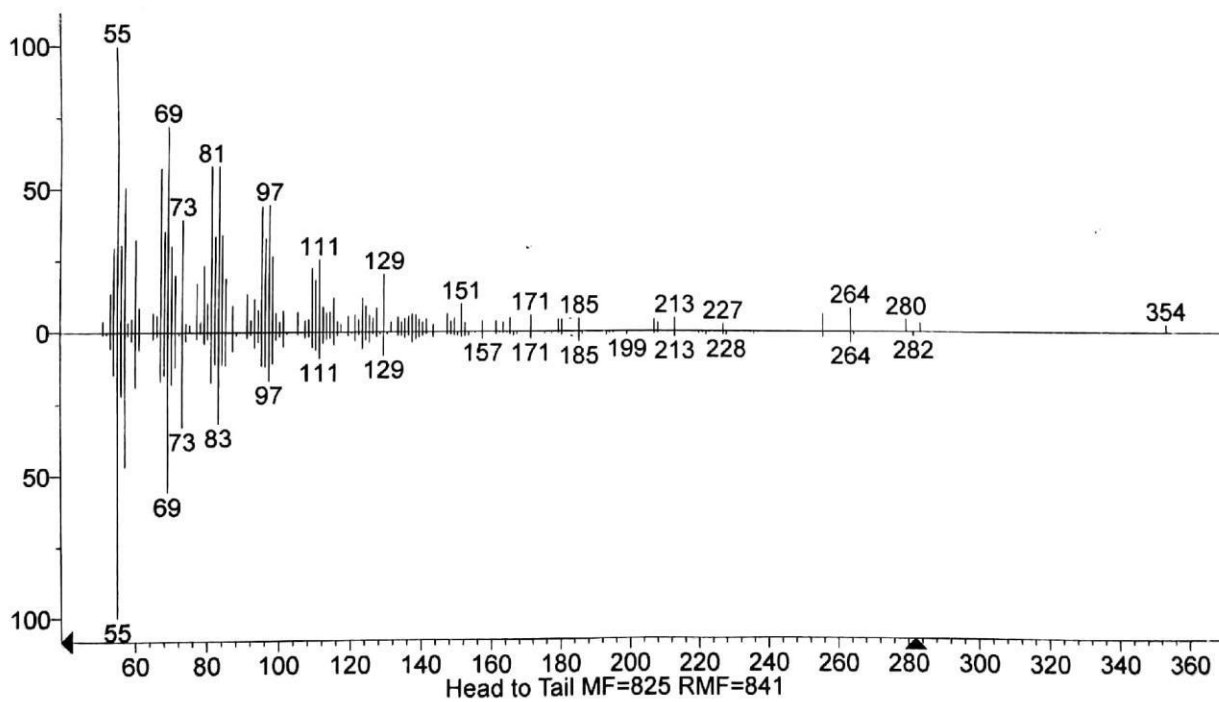
Data Type: Linear RI

Program Type:

Ramp



(Text File) Scan 8948 (61.287 min): 16092014C.D\data.ms



Name: Oleic Acid

Formula: C₁₈H₃₄O₂

MW: 282 Exact Mass: 282.25588 CAS#: 112-80-1 NIST#: 154664 ID#: 4486 DB: replib

Other DBs: TSCA, RTECS, USP, HODOC, NIH, EINECS, IRDB

Contributor: Chemical Concepts

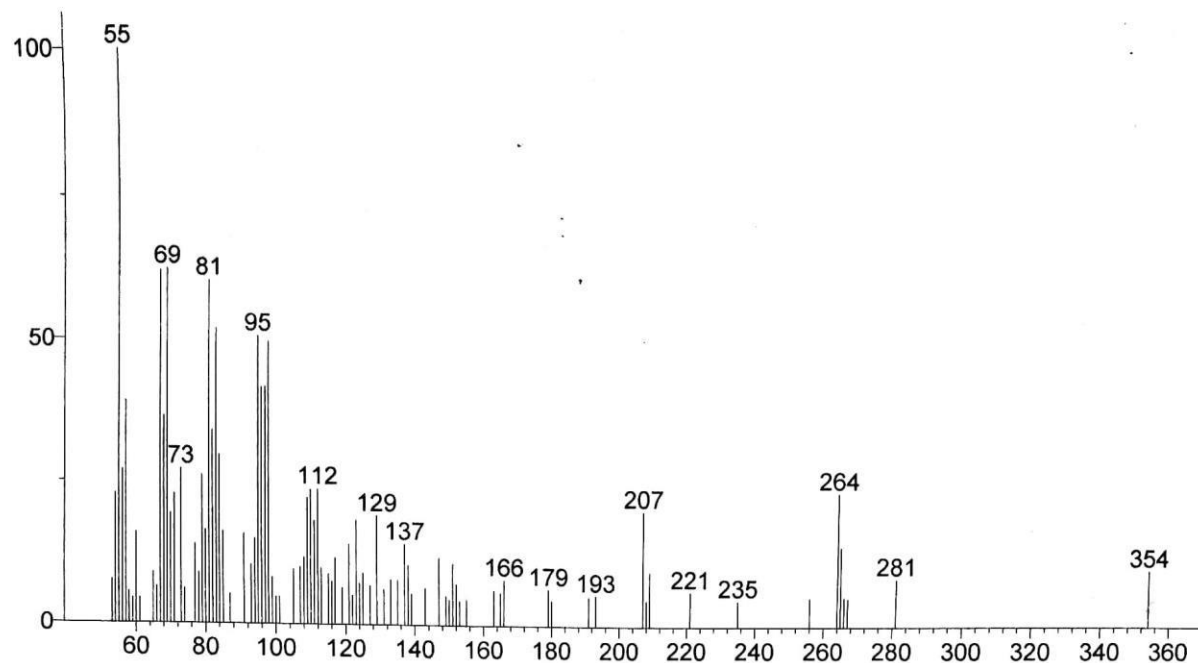
Related CAS#: 56833-51-3; 8046-01-3; 949900-16-7

10 largest peaks:

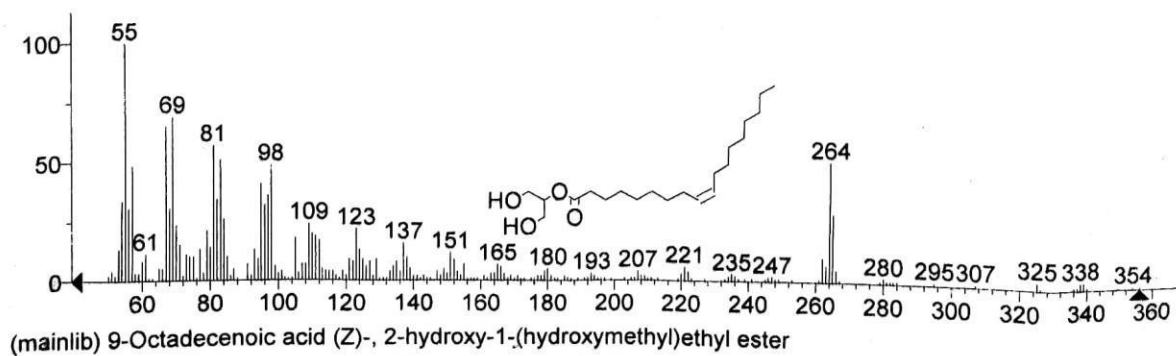
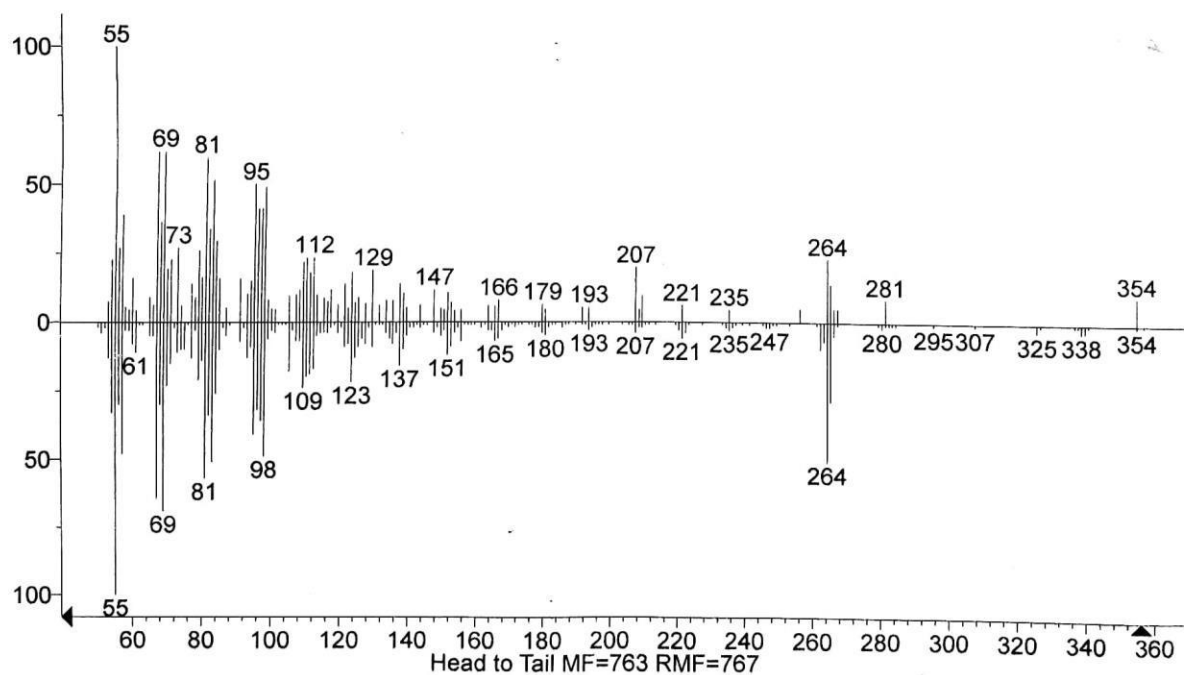
55 999	41 607	69 560	57 471	43 356
73 332	83 321	29 259	56 224	60 192

Synonyms:

1. 9-Octadecenoic acid (Z)-
2. DELTA.9-cis-Oleic acid
3. cis-Oleic Acid
4. cis-9-Octadecenoic Acid
5. Emersol 211
6. Emersol 220 White Oleic Acid
7. Emersol 221 Low Titer White Oleic Acid
8. Oelsauere
9. Oleine 7503
10. Pamolyn 100
11. Vopcolene 27
12. Wecoline OO
13. Z-9-Octadecenoic acid
14. cis-Octadec-9-enoic acid
15. cis-DELTA.9-octadecenoic acid
16. cis-DELTA.9-Octadecenoate
17. neo-Fat 90-04
18. neo-Fat 92-04
19. Century cd fatty acid
20. Elaidoic acid
21. Emersol 210
22. Emersol 213
23. Emersol 6321
24. Glycon RO
25. Glycon WO
26. Groco 2
27. Groco 4
28. Groco 5I
29. Groco 6
30. Hy-phi 1055
31. Hy-phi 1088
32. Hy-phi 2066
33. Hy-phi 2088
34. Hy-phi 2102
35. K 52
36. L'Acide oleique
37. Metaupon
38. Tego-oleic 130
39. 9-Octadecenoic acid, cis-
40. Elaic acid
41. Industrene 105
42. Industrene 205
43. Industrene 206
44. Oleinic acid
45. Pamolyn
46. Wochem no. 320
47. (Z)-9-Octadecanoic acid
48. Emersol 6313 NF



(Text File) Scan 11080 (73.486 min): 16092014C.D\data.ms



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

Formula: $C_{21}H_{40}O_4$

MW: 356 Exact Mass: 356.29266 CAS#: 3443-84-3 NIST#: 16061 ID#: 18035 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

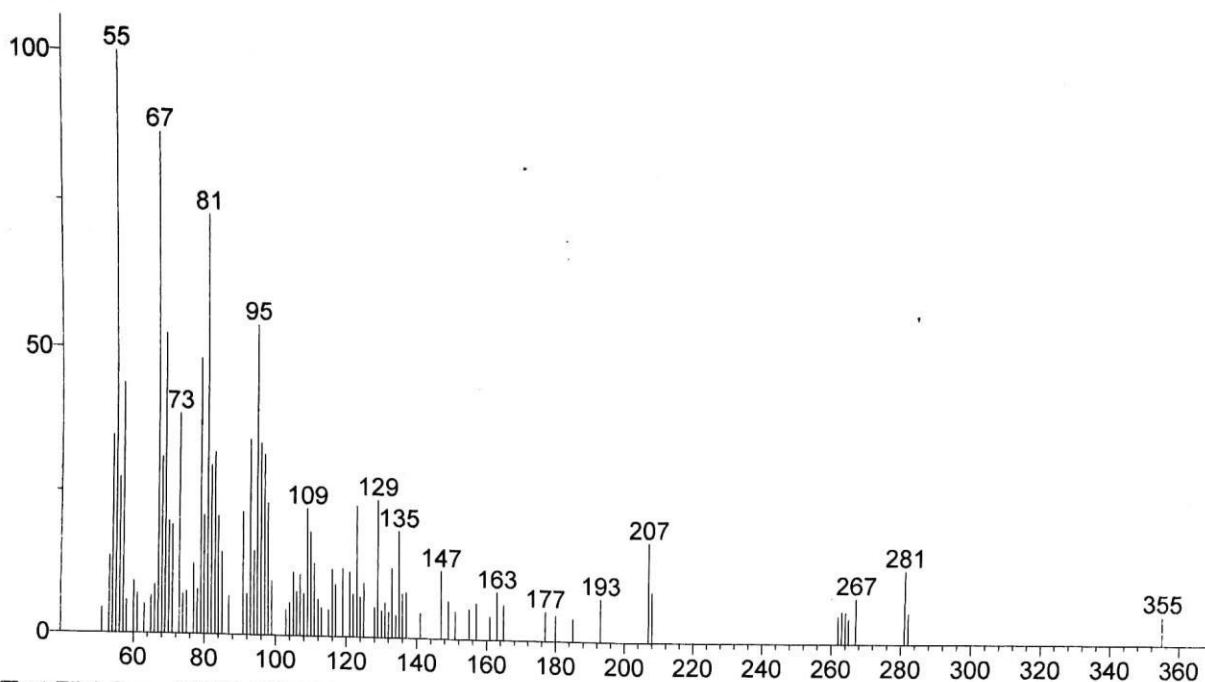
8. 2-Hydroxy-1-(hydroxymethyl)ethyl (9Z)-9-octadecenoate

9. β -Glyceryl monooleate

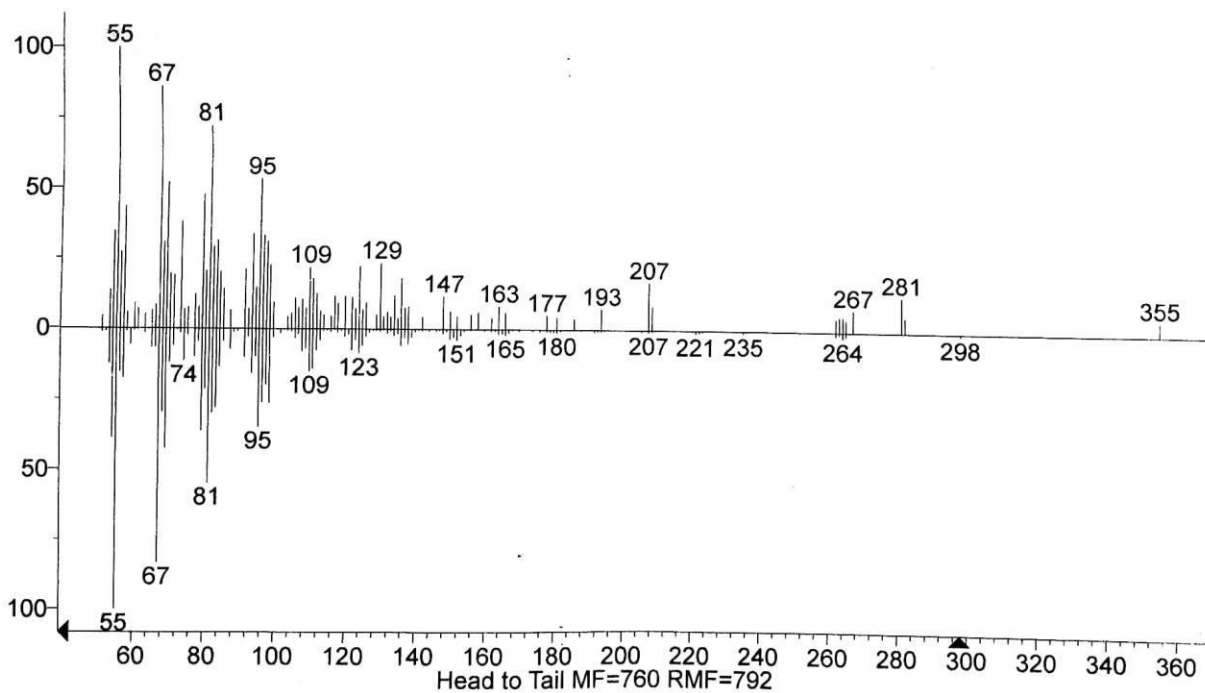
Estimated non-polar retention index (n-alkane scale):

Value: 2705 iu

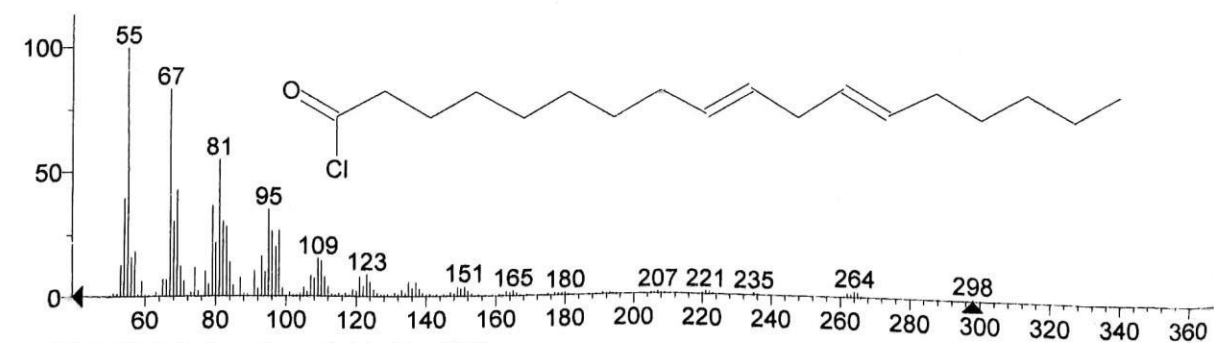
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) Scan 11356 (75.066 min): 16092014C.D\data.ms



Head to Tail MF=760 RMF=792



(replib) 9,12-Octadecadienoyl chloride, (Z,Z)-

Name: 9,12-Octadecadienoyl chloride, (Z,Z)-

Formula: $C_{18}H_{31}ClO$

MW: 298 Exact Mass: 298.206343 CAS#: 7459-33-8 NIST#: 76312 ID#: 4686 DB: replib

Other DBs: Fine, TSCA, NIH, EINECS

Contributor: RADIAN CORP

10 largest peaks:

55 999	67 832	41 754	81 549	69 426
54 389	79 362	43 355	95 350	82 299

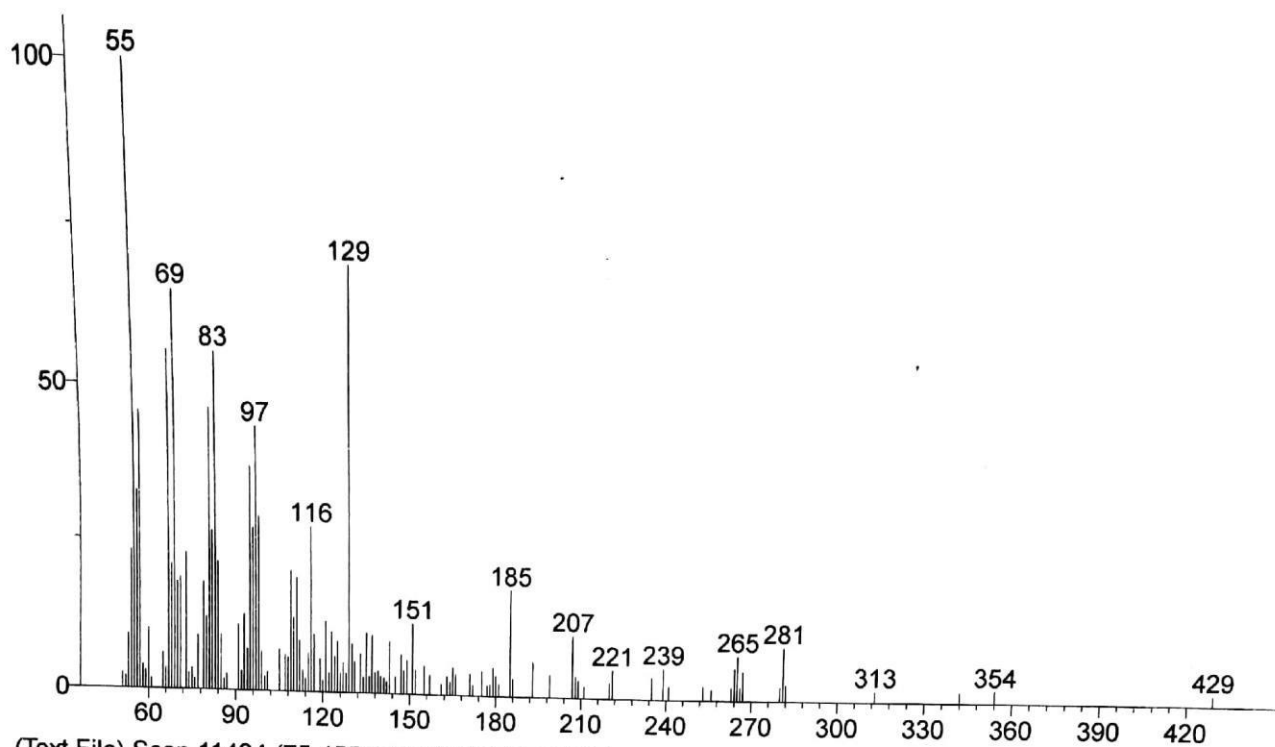
Synonyms:

1. Linoleoyl chloride
2. Lineoleoyl chloride
3. Linoleic acid chloride
4. (9E,12E)-9,12-Octadecadienoyl chloride #

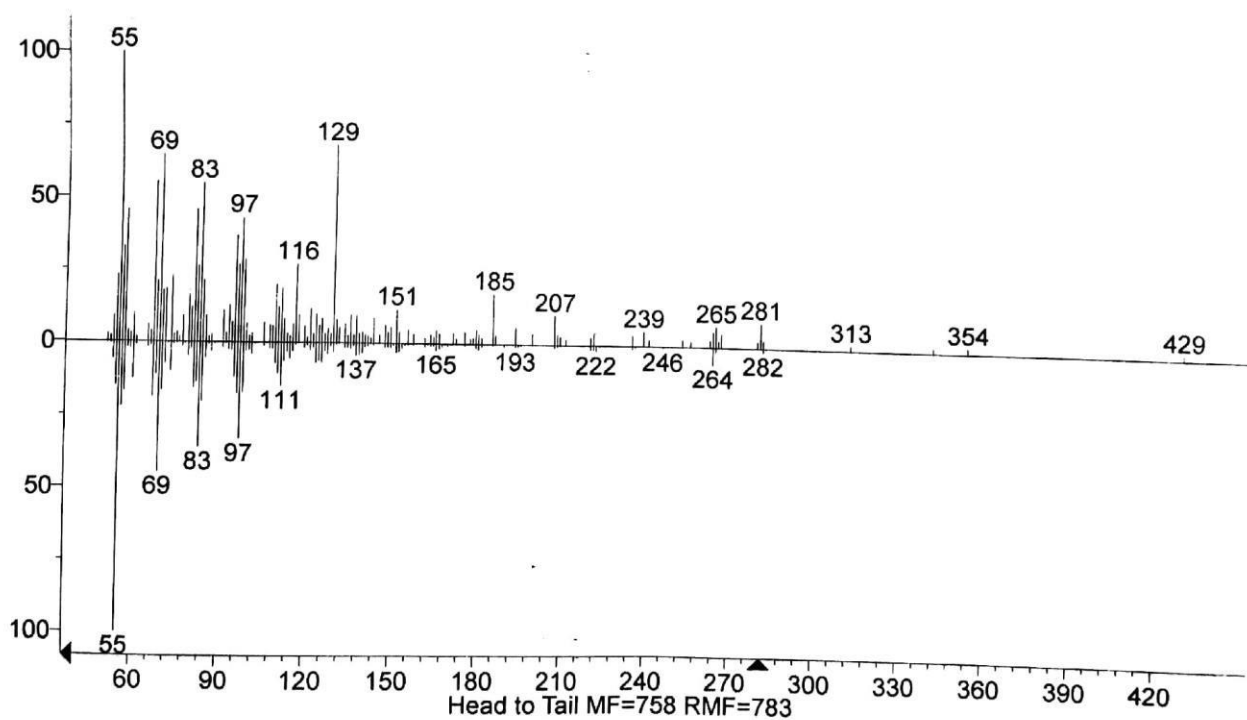
Estimated non-polar retention index (n-alkane scale):

Value: 2139 iu

Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu



(Text File) Scan 11424 (75.455 min): 16092014C.D\data.ms



Head to Tail MF=758 RMF=783



(mainlib) trans-13-Octadecenoic acid

Name: trans-13-Octadecenoic acid

Formula: C₁₈H₃₄O₂

MW: 282 Exact Mass: 282.25588 CAS#: 693-71-0 NIST#: 333615 ID#: 18062 DB: mainlib

Other DBs: None

Contributor: NIST Mass Spectrometry Data Center

10 largest peaks:

55 999	41 463	69 448	83 362	97 333
43 248	56 222	84 206	67 188	96 177

Synonyms:

no synonyms.

Estimated non-polar retention index (n-alkane scale):

Value: 2175 iu

Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

Retention index.

1. Value: 2163.6 iu

Column Type: Capillary

Column Class: Semi-standard non-polar

Active Phase: VF

-5MS

Column Length: 30 m

Carrier Gas: He

Column Diameter: 0.25 mm

Phase Thickness: 0.25 µm

Data

Type: Linear RI

Program Type: Complex

Description: Multi-step temperature program; T(initial)=60C; T(final)
=270C

Source: Tret'yakov, K.V., Retention Data. NIST Mass Spectrometry Data Center., 2007.

