Interpretation of GC MS Results

Dr. Dhia Falih Al-Fekaiki

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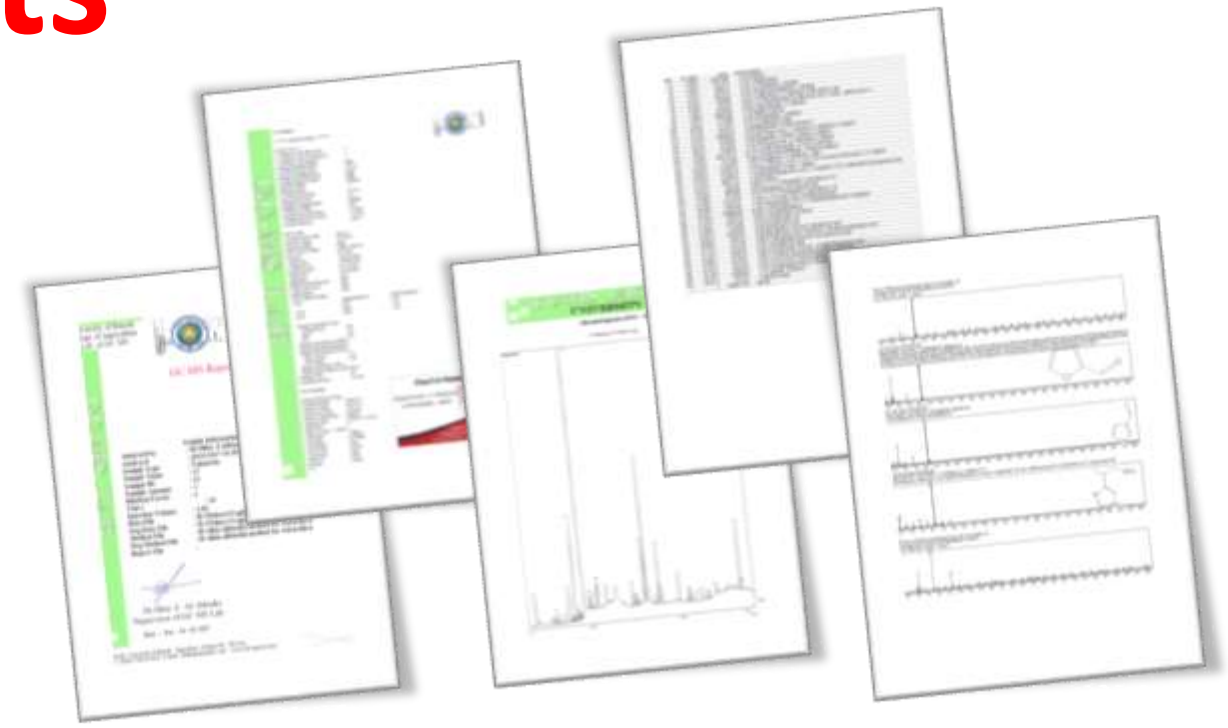
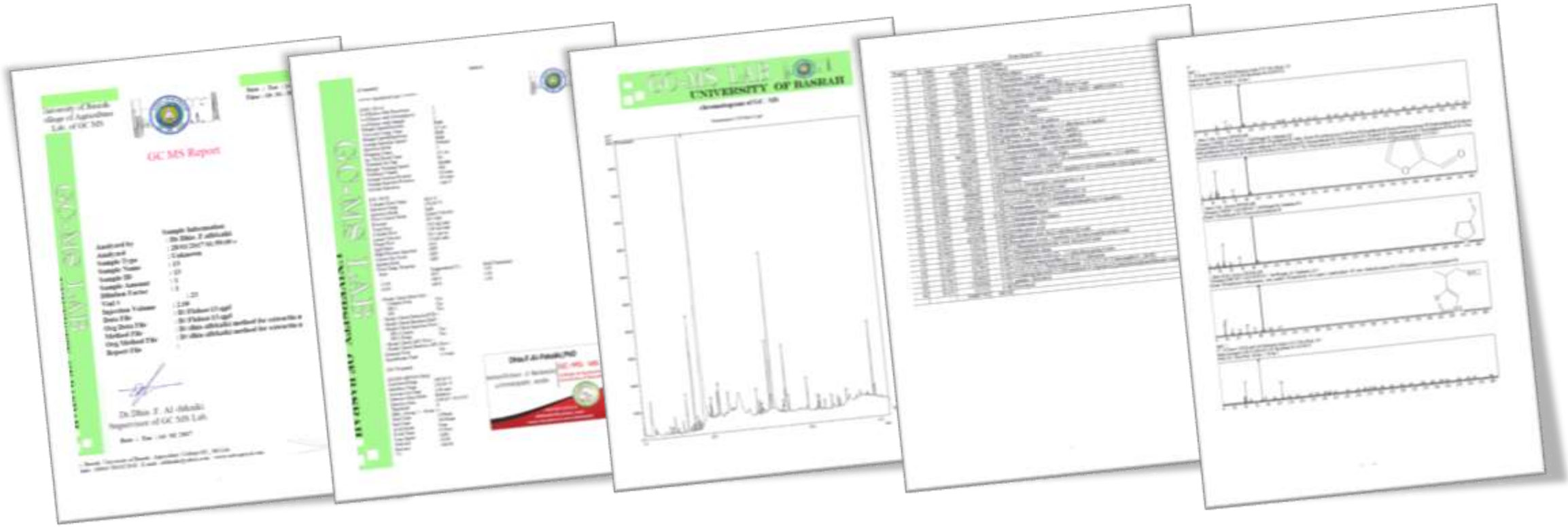
Iraq- Basrah

2017



GC MS Report



University of Basrah
College of Agriculture
Lab. of GC MS

Date : Tue : 14 / 02 /2017
Time : 10: 36 : 38

GC MS Report

GC-MS LAB
UNIVERSITY OF BASRAH

Sample Information

Analyzed by	**: Dr.Dhia .F.alfekaiki**
Analyzed	**: 28/01/2017 01:59:09 م**
Sample Type	**: Unknown**
Sample Name	**: 13**
Sample ID	**: 13**
Sample Amount	**: 1**
Dilution Factor	**: 1**
Vial #	**: 23**
Injection Volume	**: 2.00**
Data File	**: D:\Flahaa\13.qgd**
Org Data File	**: D:\Flahaa\13.qgd**
Method File	**: D:\dhia alfekaiki method for exteactin n**
Org Method File	**: D:\dhia alfekaiki method for exteactin n**
Report File	**:**

Dr.Dhia .F. Al -fekaiki
Supervisor of GC MS Lab.

Date : Tue : 14 / 02 /2017

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1

2

3

4

GC-MS LAB

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Method

[Comment]

——— Analytical Line 1 ———

[AOC-20i+s]

# of Rinses with Presolvent	:1
# of Rinses with Solvent(post)	:2
# of Rinses with Sample	:1
Plunger Speed(Suction)	:High
Viscosity Comp. Time	:0.2 sec
Plunger Speed(Injection)	:High
Syringe Insertion Speed	:High
Injection Mode	:Normal
Pumping Times	:5
Inj. Port Dwell Time	:0.3 sec
Terminal Air Gap	:No
Plunger Washing Speed	:High
Washing Volume	:8uL
Syringe Suction Position	:0.0 mm
Syringe Injection Position	:0.0 mm
Solvent Selection	:only C

[AOC-20i+s]

[GC-2010]

Column Oven Temp.	:40.0 °C
Injection Temp.	:250.00 °C
Injection Mode	:Split
Flow Control Mode	:Pressure
Pressure	:57.4 kPa
Total Flow	:37.3 mL/min
Column Flow	:1.11 mL/min
Linear Velocity	:38.0 cm/sec
Purge Flow	:3.0 mL/min
Split Ratio	:30.0
High Pressure Injection	:OFF
Carrier Gas Saver	:OFF
Splitter Hold	:OFF

[GC-2010]

Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	40.0	4.00
7.00	120.0	1.00
100.00	250.0	1.00

[GC Program]

< Ready Check Heat Unit >	
Column Oven	: Yes
SPL1	: Yes
MS	: Yes
< Ready Check Detector(FTD) >	
< Ready Check Baseline Drift >	
< Ready Check Injection Flow >	
SPL1 Carrier	: Yes
SPL1 Purge	: Yes
< Ready Check APC Flow >	
< Ready Check Detector APC Flow >	
External Wait	:No
Equilibrium Time	:1.0 min

[GC Program]

[GCMS-QP2010 Ultra]

IonSourceTemp	:200.00 °C
Interface Temp.	:250.00 °C
Solvent Cut Time	:3.00 min
Detector Gain Mode	:Relative
Detector Gain	:0.70 kV +0.10 kV
Threshold	:0
If(--Group 1 - Event 1--	
Start Time	:3.00min
End Time	:18.73min
ACQ Mode	:Scan
Event Time	:0.50sec
Scan Speed	:294
Start m/z	:30.00
End m/z	:170.00
!=)	

[MS-2010]

AOC-20i+s

1

GC and GCMS Autosampler System

[Comment]

====== Analytical Line 1 ======

[AOC-20i+s]

# of Rinses with Presolvent	:1
# of Rinses with Solvent(post)	:2
# of Rinses with Sample	:1
Plunger Speed(Suction)	:High
Viscosity Comp. Time	:0.2 sec
Plunger Speed(Injection)	:High
Syringe Insertion Speed	:High
Injection Mode	:Normal
Pumping Times	:5
Inj. Port Dwell Time	:0.3 sec
Terminal Air Gap	:No
Plunger Washing Speed	:Middle
Washing Volume	:8uL
Syringe Suction Position	:0.0 mm
Syringe Injection Position	:0.0 mm
Solvent Selection	:only C

GC -2010

2

[GC-2010]

Column Oven Temp.	:40.0 °C
Injection Temp.	:250.00 °C
Injection Mode	:Split
Flow Control Mode	:Linear Velocity
Pressure	:49.5 kPa
Total Flow	:34.0 mL/min
Column Flow	:1.00 mL/min
Linear Velocity	:36.1 cm/sec
Purge Flow	:3.0 mL/min
Split Ratio	:30.0
High Pressure Injection	:OFF
Carrier Gas Saver	:OFF
Splitter Hold	:OFF

Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
-	40.0	3.00
15.00	180.0	1.00
10.00	300.0	3.00

MS-2010

3

[GCMS-QP2010 Ultra]

IonSourceTemp	:200.00 °C
Interface Temp.	:250.00 °C
Solvent Cut Time	:3.00 min
Detector Gain Mode	:Relative
Detector Gain	:0.69 kV +0.10 kV
Threshold	:0
If(--Group 1 - Event 1--	
Start Time	:3.00min
End Time	:28.00min
ACQ Mode	:Scan
Event Time	:0.50sec
Scan Speed	:1000
Start m/z	:50.00
End m/z	:500.00

!=)

GC Program

Oven Temp. Program

Rate	Temperature(°C)	Hold Time(min)
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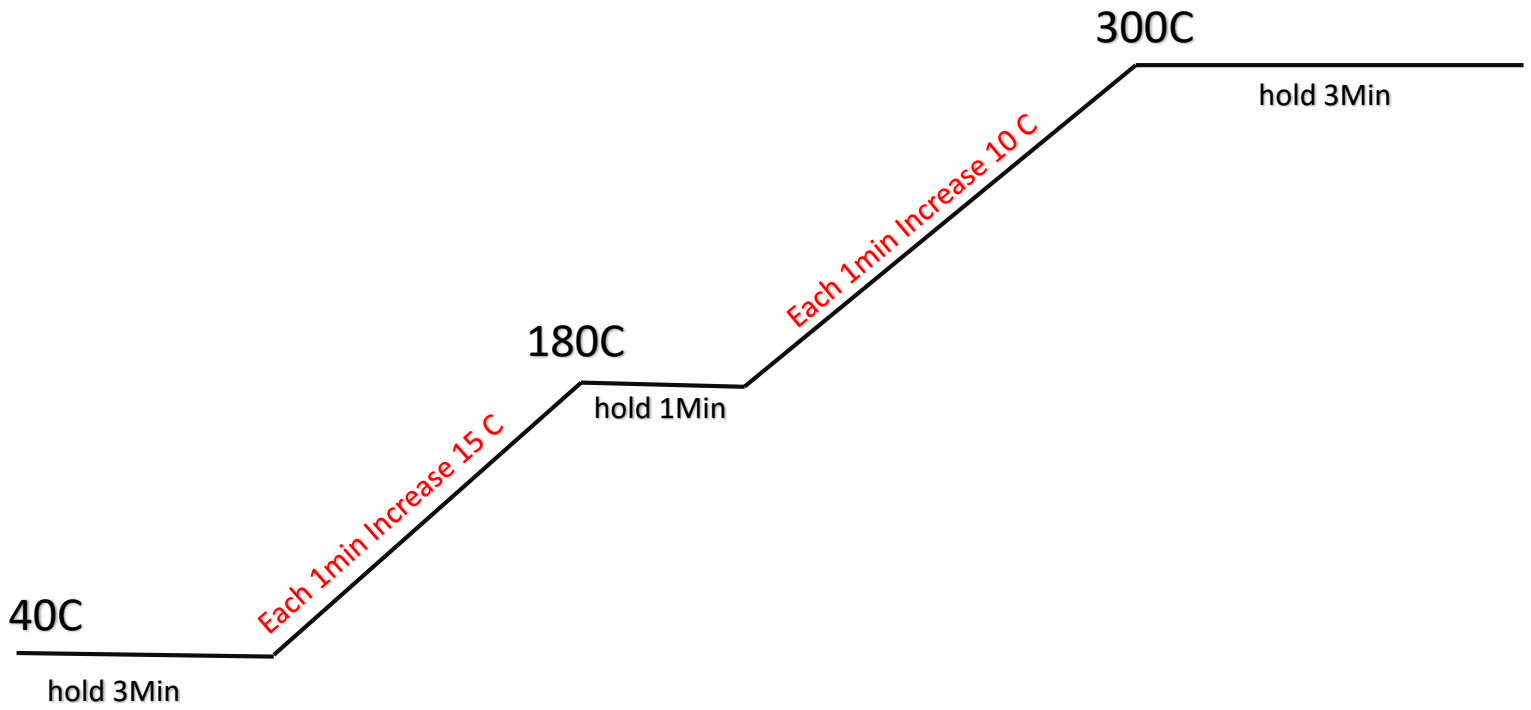
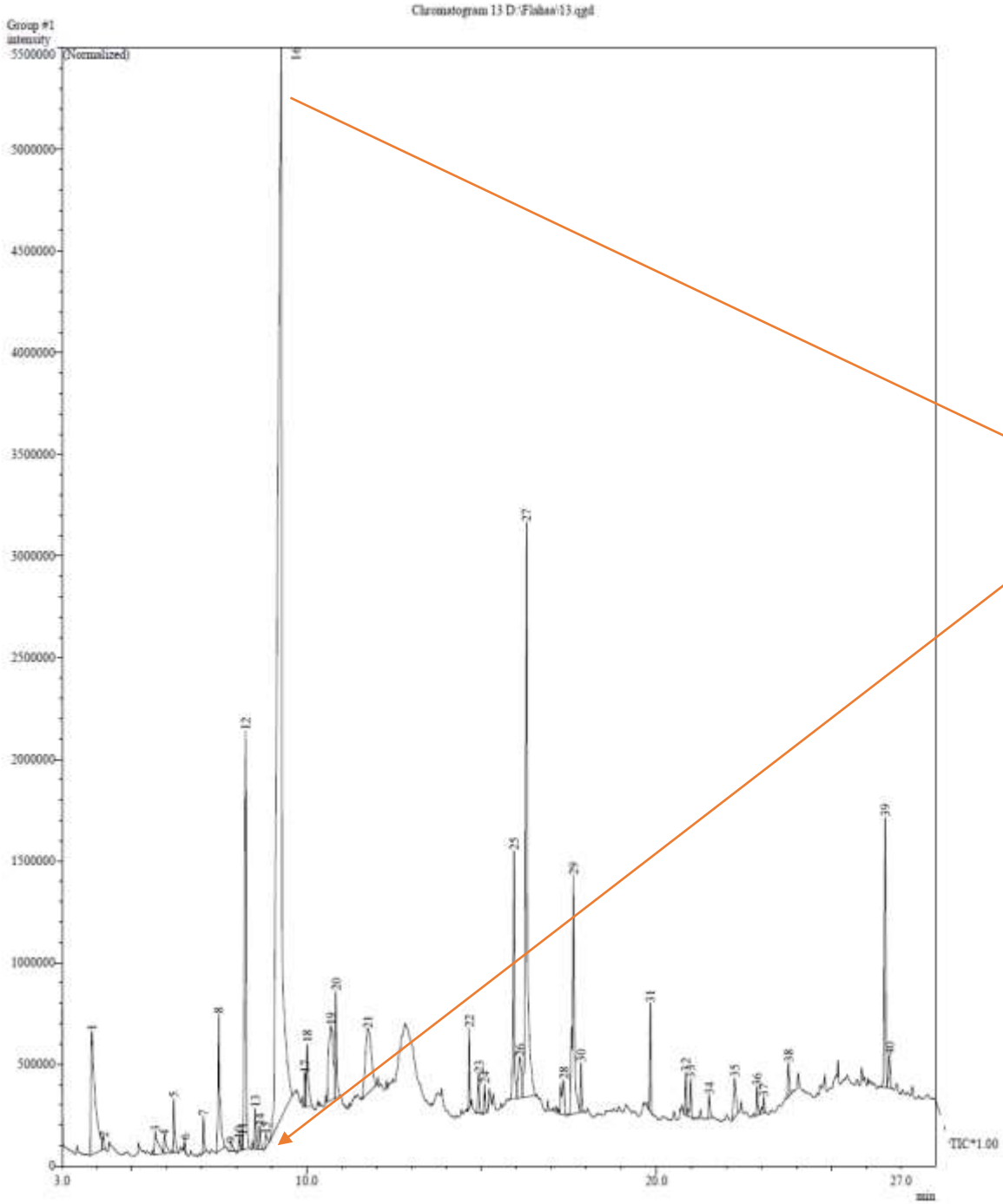
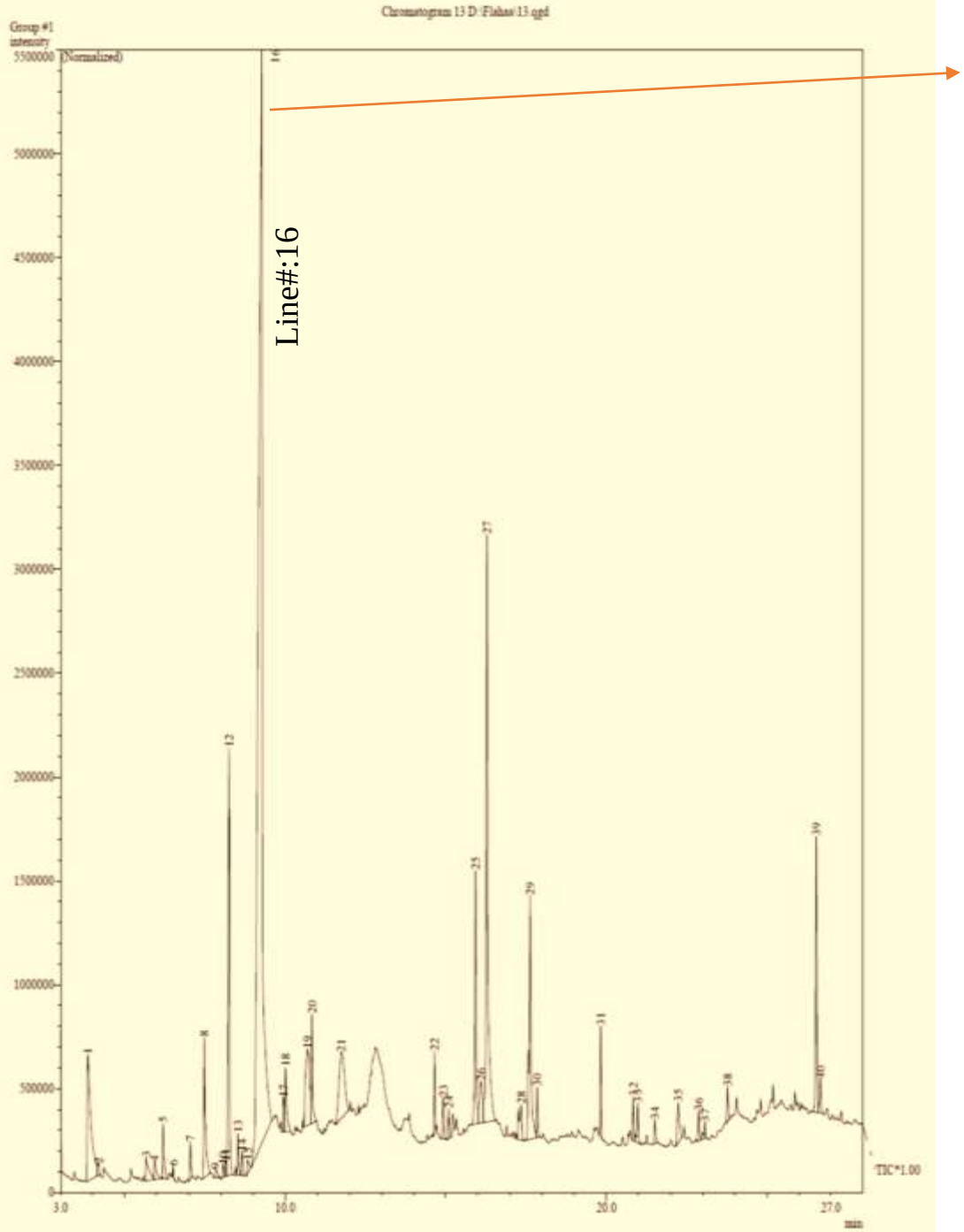
15.00	180.0	1.00
10.00	300.0	3.00





Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	3.849	4966708	4.65	Furfural
2	4.192	232117	0.22	2-Furfurylthiol
3	5.667	746855	0.70	2,5-Furandione, 3-methyl-
4	5.925	442595	0.41	2-Furancarboxaldehyde, 5-methyl-
5	6.193	783808	0.73	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one
6	6.508	94120	0.09	1,3,2-Oxazaborolane-4-carboxylic acid, 2-butyl-, methyl ester, L-
7	7.043	475609	0.44	2-Thiazolamine, 4,5-dihydro-
8	7.480	2408439	2.25	Methyl 2-furoate
9	7.817	175188	0.16	4-Pyrimidinol, 5-methoxy-
10	8.058	177121	0.17	4,4-Dimethyl octane
11	8.150	194331	0.18	Ethanamine, N-ethyl-N-nitroso-
12	8.249	6484893	6.07	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
13	8.525	475661	0.44	Pyrimidine, 4-chloro-5-ethoxy-2-methyl-
14	8.653	337019	0.32	4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-
15	8.825	270807	0.25	2,3-Dihydrooxazole, 2-t-butyl-3-pivaloyl-
16	9.266	46235225	43.25	2-Furancarboxaldehyde, 5-(hydroxymethyl)-
17	9.942	521548	0.49	Cyclohexane, 1,4-diethoxy-, trans-
18	10.010	1124035	1.05	2,13-Dibora-1,3,6,9,12,14,17,20-octaoxacyclodocosane, 2,13-diethyl-
19	10.692	3393625	3.17	Pyrimidine-4,6-diol, 5-methyl-
20	10.833	1328651	1.24	Hexadecaneperoxoic acid, 1,1-dimethyl-3-[(1-oxohexadecyl)oxy]propyl ester
21	11.742	3803175	3.56	D-Allose
22	14.651	736326	0.69	3,7,11,15-Tetramethyl-2-hexadecen-1-ol
23	14.926	669840	0.63	Hexanedioic acid, dioctyl ester
24	15.090	327200	0.31	3,7,11,15-Tetramethyl-2-hexadecen-1-ol
25	15.928	3376315	3.16	l-(+)-Ascorbic acid 2,6-dihexadecanoate
26	16.098	1366506	1.28	3-Pentanamine, N,N'-1,2-ethanediylidenebis[2,4-dimethyl-
27	16.285	10688640	10.00	3,4-Furandimethanol
28	17.350	965675	0.90	1-Tetradecanol, 14-chloro-
29	17.632	4759238	4.45	9-Octadecenal, (Z)-
30	17.849	531403	0.50	Octadecanoic acid
31	19.827	1050076	0.98	Hexanedioic acid, bis(2-ethylhexyl) ester
32	20.842	518217	0.48	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester
33	20.983	522759	0.49	1,2-Benzenedicarboxylic acid, diisooctyl ester
34	21.512	332474	0.31	2-Furaldehyde azine
35	22.242	956037	0.89	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester
36	22.881	427493	0.40	3-(2-Fluoro-benzylsulfanyl)-1H-[1,2,4]triazole
37	23.075	267113	0.25	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-
38	23.781	458433	0.43	Cyclopropylpyrrol4-[3-(1H-imidazol-4-yl)propoxy] phenylmorphomethanone oxime
39	26.545	3760966	3.52	.gamma.-Sitosterol
40	26.671	511551	0.48	Fucosterol
		106897792	100.00	



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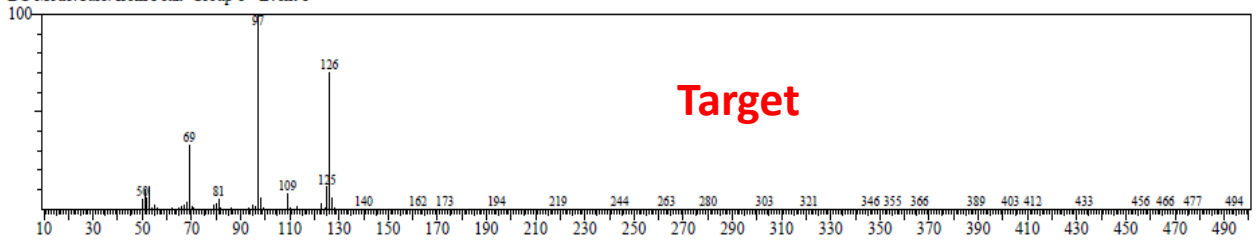
BG Mode:Calc. from Peak Group 1 - Event 1



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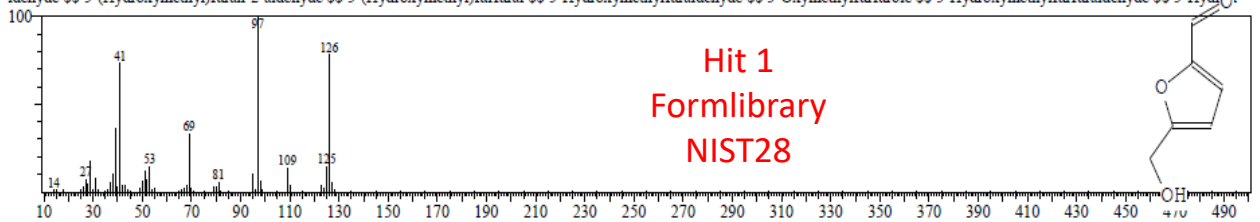
SI:96 Formula:C6H6O3 CAS:67-47-0 MolWeight:126 RetIndex:1163
CompName:2-Furancarboxaldehyde, 5-(hydroxymethyl)- $$ 2-Furaldehyde, 5-(hydroxymethyl)- $$ 5-Hydrxoymethylfurfural $$ Hydroxymethylfurfurole $$ HMF $$ 5-(Hyddroxymethyl)Furfurole $$ 5-(Hydroxymethyl)-2-formylfuran $$ 5-(Hydroxymethyl)-2-furaldehyde $$ 5-(Hydroxymethyl)-2-furancarbonal $$ 5-(Hydroxymethyl)-2-furfural $$ 5-(Hydroxymethyl)-2-furfuraldehyde $$ 5-(Hydroxymethyl)furan-2-aldehyde $$ 5-(Hydroxymethyl)furfural $$ 5-Hydroxymethylfuraldehyde $$ 5-Oxymethylfurfurole $$ 5-Hydroxymethylfurfuraldehyde $$ 5-Hydr:



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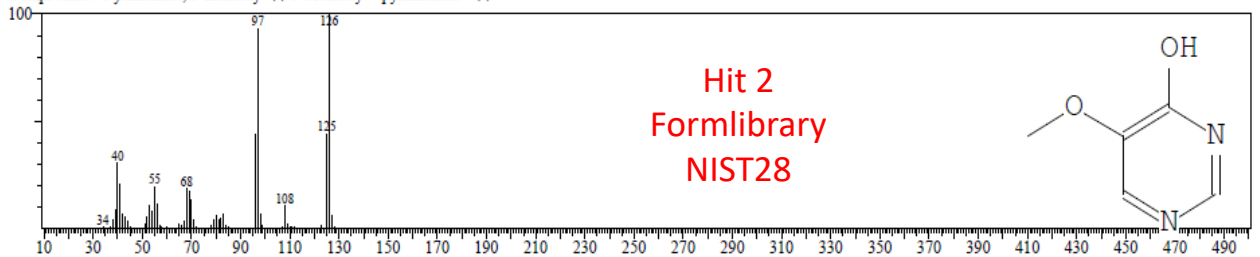
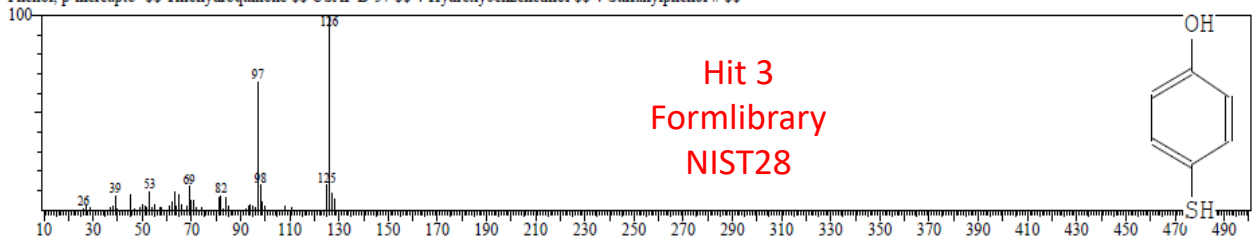
CompName:4-Pyrimidinol, 5-methoxy- $$ 5-Methoxy-4-pyrimidinol # $$



Hit#:3 Entry:6337 Library:NIST08.LIB
SI:81 Formula:C6H6OS CAS:637-89-8 MolWeight:126 RetIndex:1220
CompName:4-Mercaptophenol $$ p-Hydroxythiophenol $$ 4-Hydroxythiophenol $$ Phenol, 4-mercapto- $$ p-Mercaptophenol $$ Hydroquinone, monothio- $$ Monothiohydroquinone $$ Phenol, p-mercapto- $$ Thiohydroquinone $$ USAF B-57 $$ 4-Hydroxybenzenethiol $$ 4-Sulfanylphenol # $$

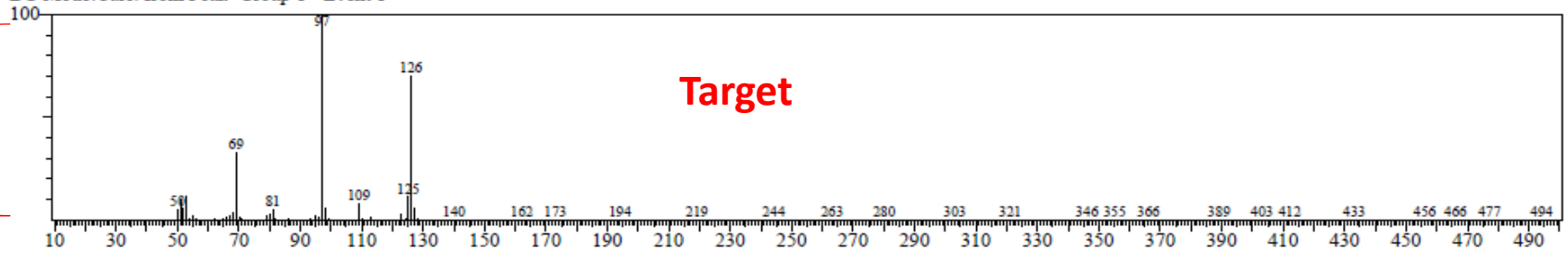


Mean of peak number

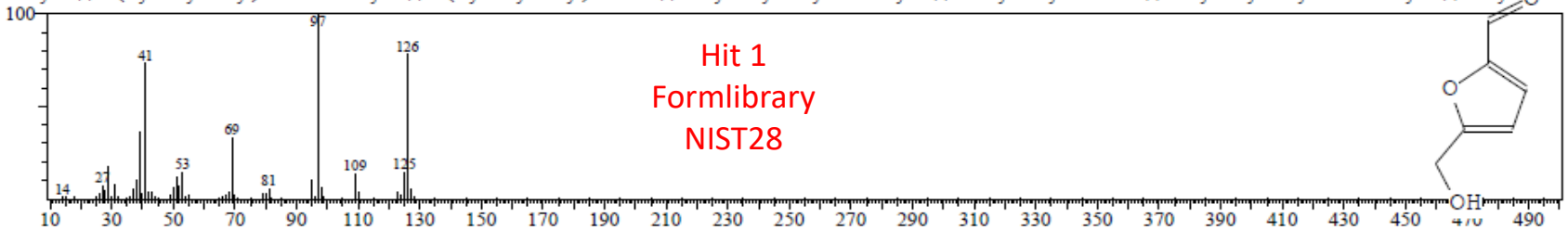
The compute 0f our samples

The computes which suggest from NIST Library

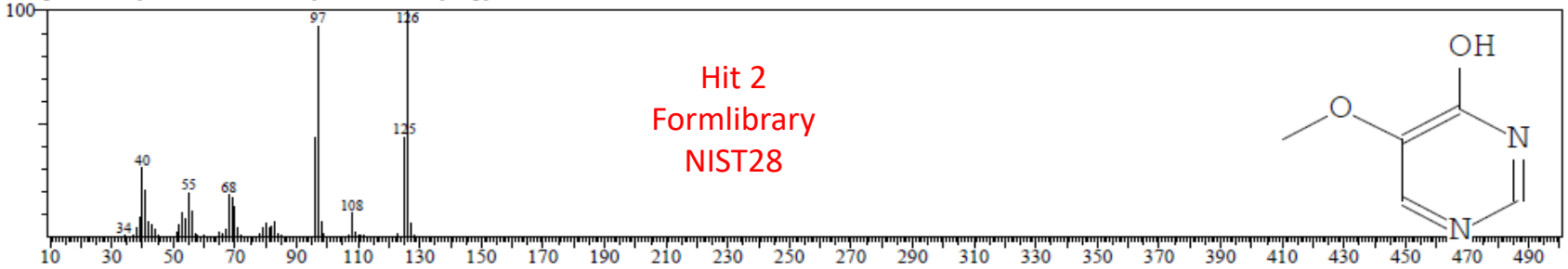
<< Target >>
Line#:16 R.Time:9.267(Scan#:753) Retention Index:1562 MassPeaks:220
RawMode:Averaged 9.258-9.275(752-754) BasePeak:97.05(1676012)
BG Mode:Calc. from Peak Group 1 - Event 1



Hit#:1 Entry:6349 Library:NIST08.LIB
SI:96 Formula:C6H6O3 CAS:67-47-0 MolWeight:126 RetIndex:1163
CompName:2-Furancarboxaldehyde, 5-(hydroxymethyl)- $$ 2-Furaldehyde, 5-(hydroxymethyl)- $$ 5-Hydrxoymethylfurfural $$ Hydroxymethylfurfurole $$ HMF $$ 5-(Hyddroxymethyl)Furfurole $$ 5-(Hydroxymethyl)-2-formylfuran $$ 5-(Hydroxymethyl)-2-furaldehyde $$ 5-(Hydroxymethyl)-2-furancarbonal $$ 5-(Hydroxymethyl)-2-furfural $$ 5-(Hydroxymethyl)-2-furfuraldehyde $$ 5-(Hydroxymethyl)furan-2-aldehyde $$ 5-(Hydroxymethyl)furfural $$ 5-Hydroxymethylfuraldehyde $$ 5-Oxymethylfurfurole $$ 5-Hydroxymethylfurfuraldehyde $$ 5-Hydr



Hit#:2 Entry:6323 Library:NIST08.LIB
SI:82 Formula:C5H6N2O2 CAS:695-87-4 MolWeight:126 RetIndex:1078
CompName:4-Pyrimidinol, 5-methoxy- $$ 5-Methoxy-4-pyrimidinol # $$



Hit#:3 Entry:6337 Library:NIST08.LIB
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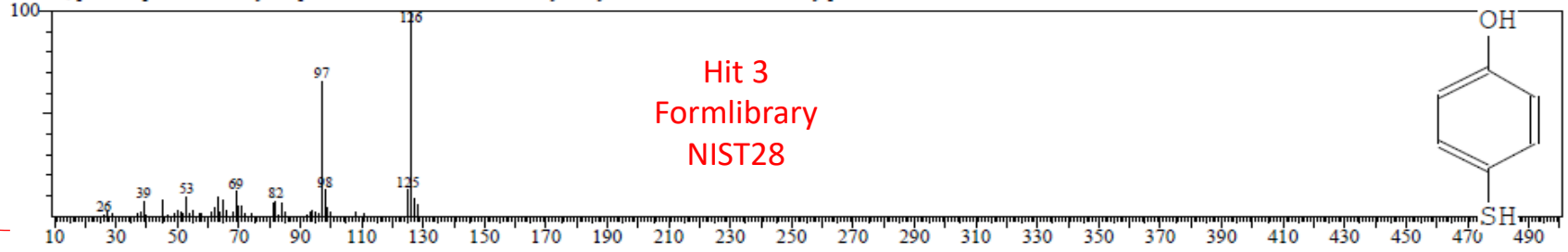

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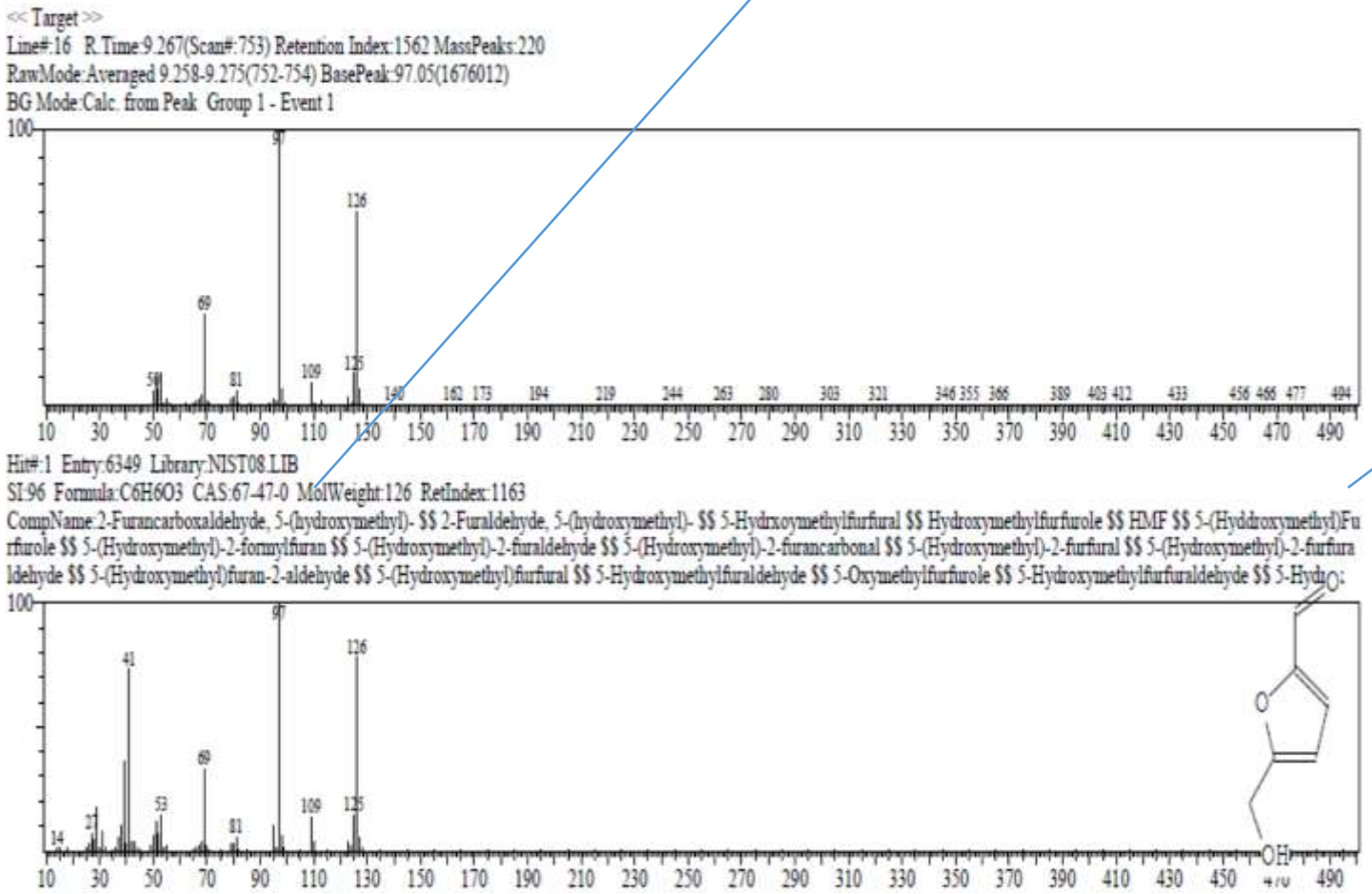
SI:96 Formula:C6H6O3 CAS:67-47-0 MolWeight:126 RetIndex:1163

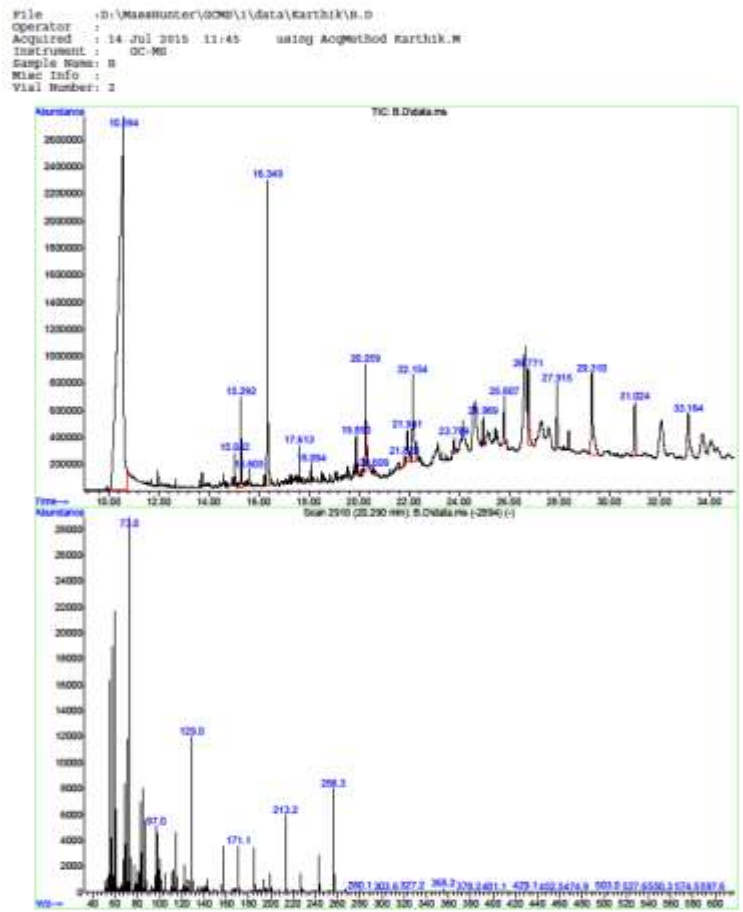


Synonyms:

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.Rcra waste number U125
29.2-Furylcarboxaldehyde
30.Qo furfural
31.Furan-2-aldehyde
32.Furan-2-carbaldehyde
33.NSC 8841

RESULTS AND DISCUSSION

Figure 1. The GC MS Graph of Kulathadi Kashayam



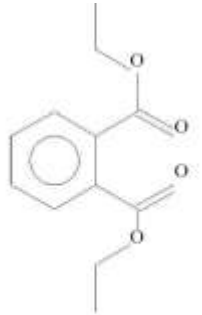
The GC MS data of Kulathadi Kashayam is shown in Table 1.

Table 1

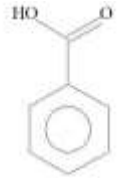
Sl No.	Retention Time (In Min)	Name of the Compound	Molecular formula	Molecular Weight	Peak (%)	(%) Probability
1	10.594	Benzoic acid	C7H6O2	122	62.236	46.1
2	15.042	Heptadecane, 2,6,10,15-tetramethyl-	C21H44	296	0.630	7.23
3	15.292	Phenol, 2,4-bis(1,1-dimethylethyl)-	C14H22O	206	1.967	60.5
4	15.605	Hexadecane	C16H34	226	0.394	7.97
5	16.349	Diethyl Phthalate	C12H14O4	222	7.362	68.6
6	17.613	Hexadecane, 2,6,11,15-tetramethyl-	C20H42	282	0.665	7.53
7	18.094	Heptadecane	C17H36	240	0.337	7.86
8	19.890	Nonadecane, 2-methyl-	C20H42	282	0.782	6.48
9	20.259	n-Hexadecanoic acid	C16H32O2	256	2.882	75.4
10	20.609	Heptadecane, 9-hexyl-	C23H48	324	0.314	15.7
11	21.823	Octadecane, 1,1'-[(1-methyl-1,2-ethanediyl)bis(oxy)]bis-	C39H80O2	496	0.401	7.79
12	21.941	Eicosane, 2-methyl-	C21H44	296	1.400	7.14
13	22.154	Octadecanoic acid	C18H36O2	284	3.519	73.3
14	23.799	Heptadecane, 9-hexyl-	C23H48	324	0.379	6.27
15	24.969	Eicosane, 10-methyl-	C21H44	296	0.564	10.5
16	25.807	Eicosane	C20H42	282	1.184	10.2
17	26.771	Heptacosane, 1-chloro-	C27H55Cl	414	2.801	16.5
18	27.915	Eicosane	C20H42	282	2.120	13.5
19	29.310	Tetratriacontane	C34H70	478	5.141	6.72
20	31.024	Eicosane	C20H42	242	2.529	7.65
21	33.164	Tetratriacontane	C34H70	478	1.822	9.52

The important biomolecules present in Kulathadi kashayam are represented by Figure no. 2 to 13.

Figure 2. Benzoic Acid



Name: Diethyl Phthalate
Formula: $C_{12}H_{14}O_4$
MW: 222



Name: Benzoic acid
Formula: $C_7H_6O_2$
MW: 122

Figure 3. Diethyl Phthalate

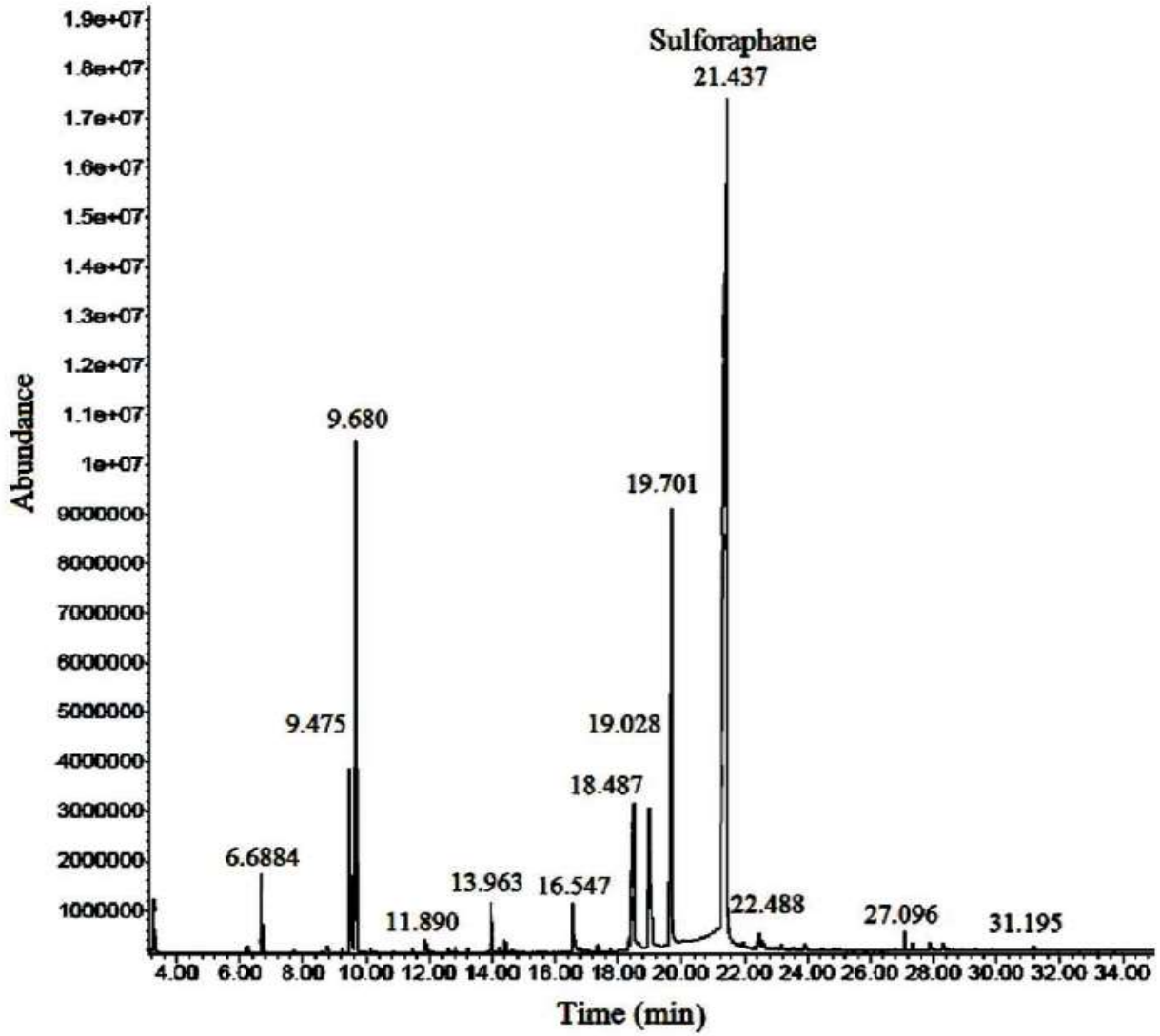


Fig. 3. Gas chromatogram of crude sulforaphane extracted from broccoli seed meal, conditions described in GC-MS section.

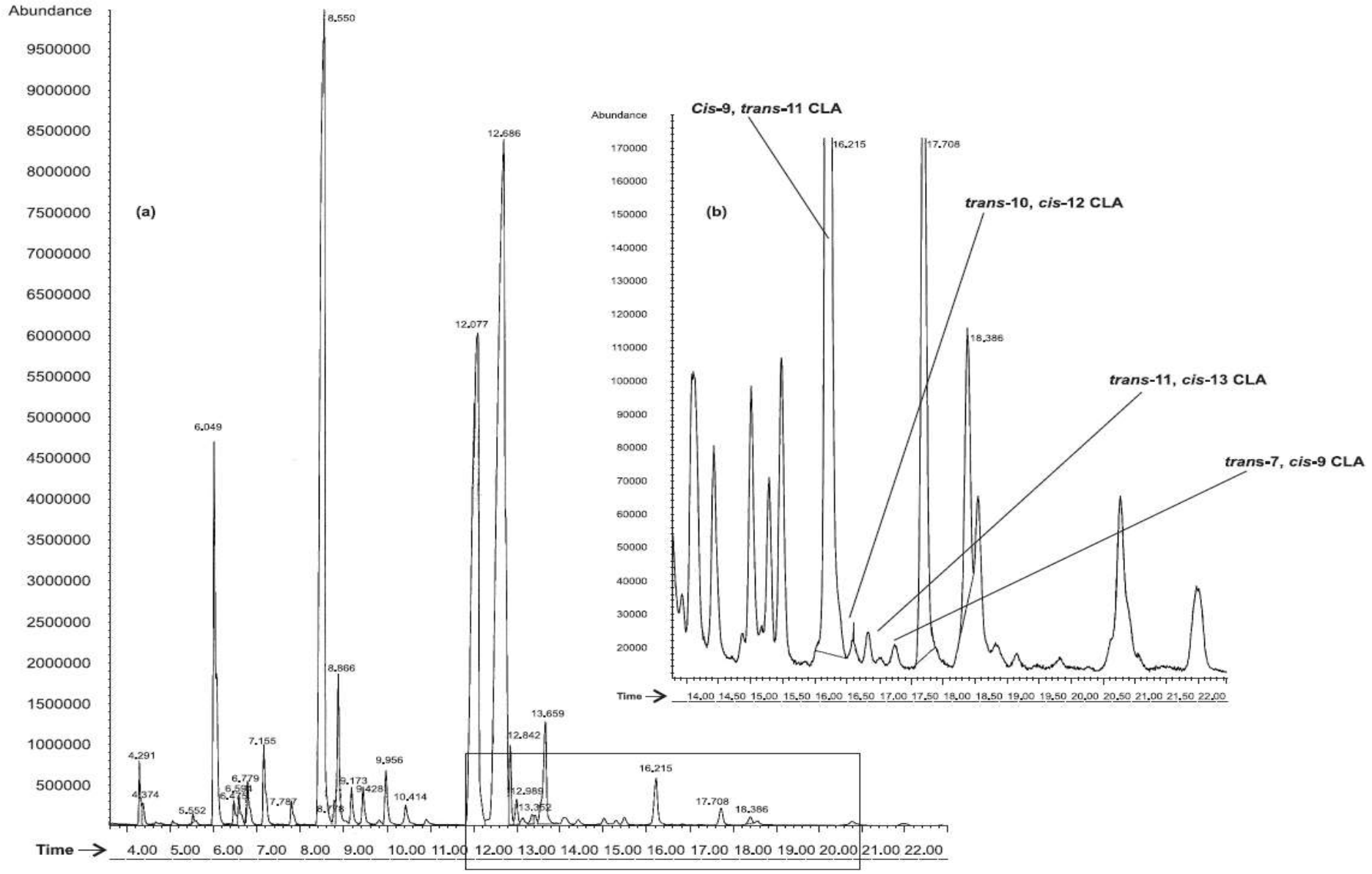


FIGURE 1. (a) Gas chromatogram of fatty acid methyl esters of a fresh butter fat sample separated on SP-2340 capillary column (60 m × 0.25 mm); see text for operating conditions. (b) Partially enlarged chromatogram showing the separation of *cis*- 9, *trans*-11; *trans*-10, *cis*-12; *trans*-11, *cis*-13; *trans*-7, *cis*-9 CLA isomers of the same fresh butter sample

5.3.2.1 Injection – Using the autosampler with a 10 µL syringe injection, perform three solvent washes from each wash bottle. Inject a 0.2 µL sample with a fast plunger speed, no sample washes, and 3 sample pumps.

5.3.2.2 Inlet – Run in split mode at 200 °C with a 100:1 split ratio.

5.3.2.3 Carrier gas – Helium.

5.3.2.4 Oven – Run a temperature program starting at 50.0 °C for 2.50 minutes. Then ramp at 10.0 °C per minute until 300 °C is obtained. Hold at 300 °C for 5.00 minutes.

5.3.2.5 Column – Use a (5 %-Phenyl)-methylpolysiloxane (such as a HP-5MS or DB-5MS) column which is 0.25 mm in diameter that is approximately 30 m long with a 0.25 µm film thickness. The column shall be kept at a constant flow of 0.6 mL/min.

5.3.2.6 Mass spectrometer – The transfer line temperature shall be set at 300 °C. The MS Quad temperature is set at 150 °C and the MS source is set at 230 °C. The MS shall be run in scan mode using the settings from the atune.u file with an electron multiplier offset of 200 eV. The mass scan range is 20.0 amu to 400.0 amu with a threshold abundance of 150. The mass spectrometer shall have a 2.50 minute solvent de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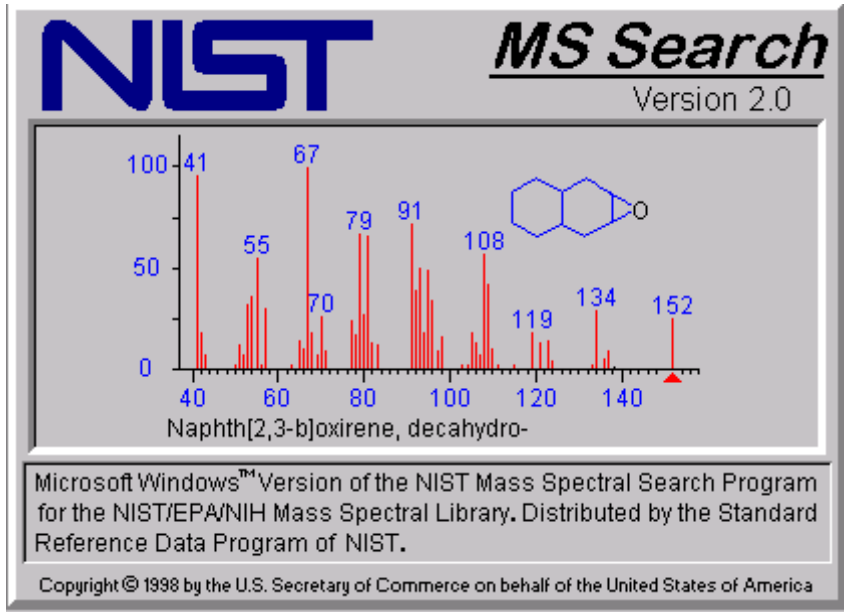
GC METHOD/RETENTION INDEX LIBRARY
Search Program and Data for Microsoft Windows XP (SP3), Vista, Windows 7, 8, 8.1, 10
NIST
• 404,045 Retention Indices of 99,400 Compounds on Polar and Non-polar Stationary Phase.
Contains All RI Data from the 2017 version of NIST/EPA/NIH MS Library
June 2017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Naphth[2,3-b]oxirene, decahydro-
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• Mass Spec Interpreter
• Amdis v.2.72
NIST
• 276,248 EI Mass Spectra of 242,466 Compounds with 242,463 Chemical Structures
• 387,463 Retention Indices of 82,868 Compounds
• 45,298 MS/MS Precursors
(NIST 2014)
June 2014


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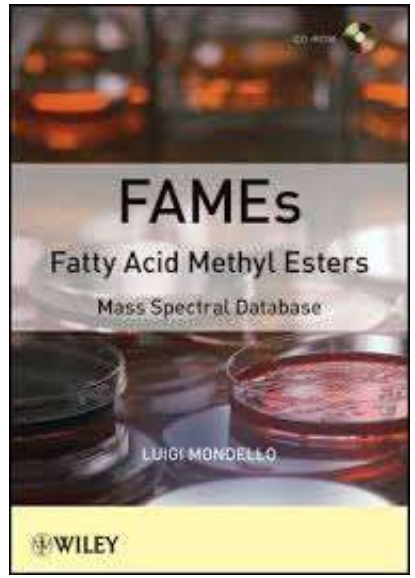
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Mass Spectral Database
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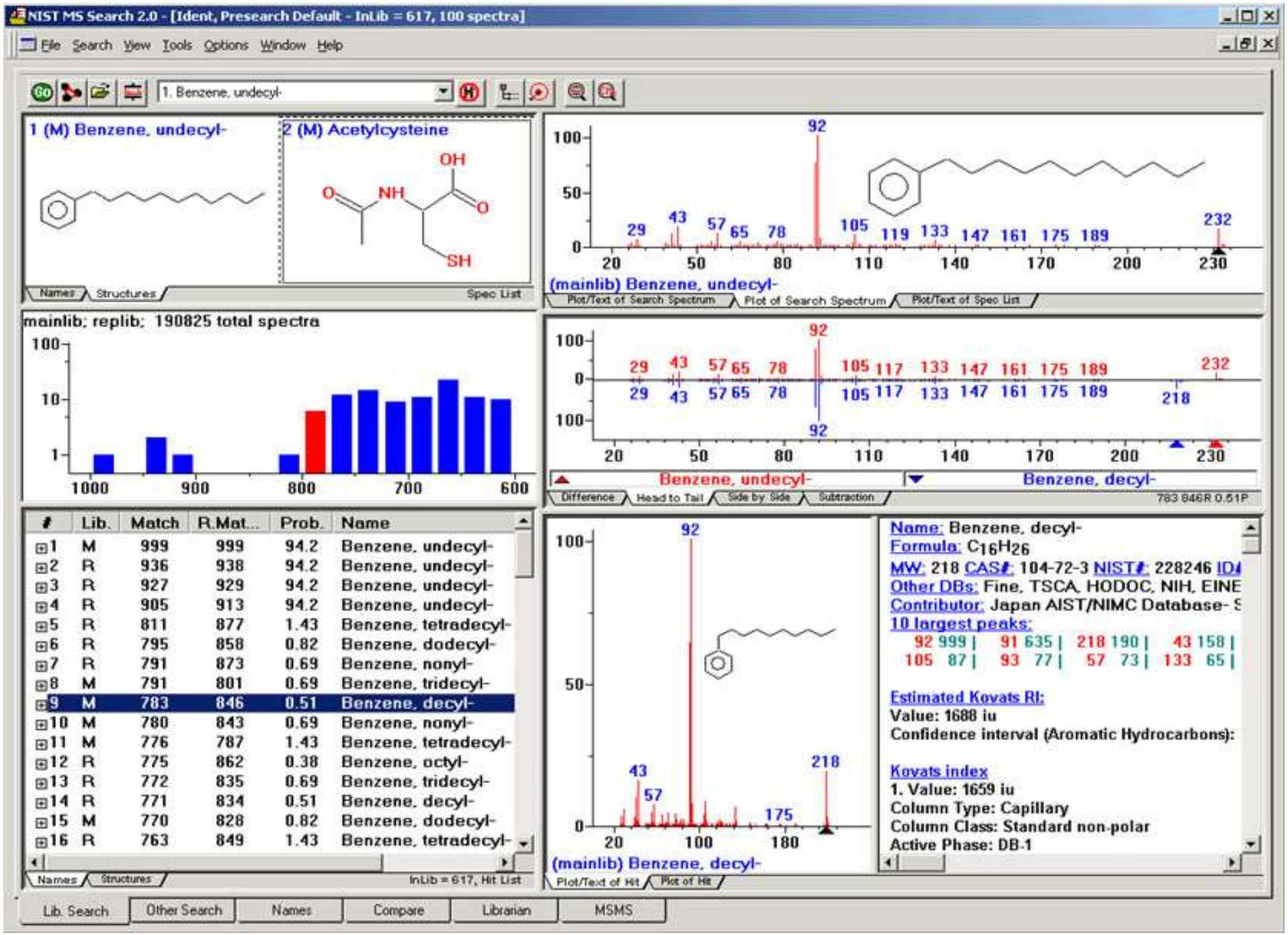
NIST MS Search 2.0 - [Ident, Presearch Default - InLib = 617, 100 spectra]
File Search View Tools Options Window Help
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1 (M) Benzene, undecyl-
2 (M) Acetylcysteine
OH
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Names Structures
Spec List
mainlib; replib; 190825 total spectra
100
10
1
1000 900 800 700 600
92
29 43 57 65 78 105 119 133 147 161 175 189 232
(mainlib) Benzene, undecyl-
Plot/Text of Search Spectrum
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Plot/Text of Spec List
92
29 43 57 65 78 105 117 133 147 161 175 189 232
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Benzene, undecyl-
Benzene, decyl-
Difference
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783 846R 0.51P
Lib. Match R.Mat... Prob. Name
1 M 999 999 94.2 Benzene, undecyl-
2 R 936 938 94.2 Benzene, undecyl-
3 R 927 929 94.2 Benzene, undecyl-
4 R 905 913 94.2 Benzene, undecyl-
5 R 811 877 1.43 Benzene, tetradecyl-
6 R 795 858 0.82 Benzene, dodecyl-
7 R 791 873 0.69 Benzene, nonyl-
8 M 791 801 0.69 Benzene, tridecyl-
9 M 783 846 0.51 Benzene, decyl-
10 M 780 843 0.69 Benzene, nonyl-
11 M 776 787 1.43 Benzene, tetradecyl-
12 R 775 862 0.38 Benzene, octyl-
13 R 772 835 0.69 Benzene, tridecyl-
14 R 771 834 0.51 Benzene, decyl-
15 M 770 828 0.82 Benzene, dodecyl-
16 R 763 849 1.43 Benzene, tetradecyl-
Names Structures
InLib = 617, Hit List
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Plot/Text of Hit
Plot of Hit
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MW: 218 CAS#: 104-72-3 NIST#: 228246 ID#
Other DBs: Fine, TSCA, HODOC, NIH, EINE
Contributor: Japan AIST/NIMC Database- S
10 largest peaks:
92 999 | 91 635 | 218 190 | 43 158 |
105 87 | 93 77 | 57 73 | 133 65 |
Estimated Kovats RI:
Value: 1688 iu
Confidence interval (Aromatic Hydrocarbons):
Kovats index
1. Value: 1659 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: DB-1
Lib. Search
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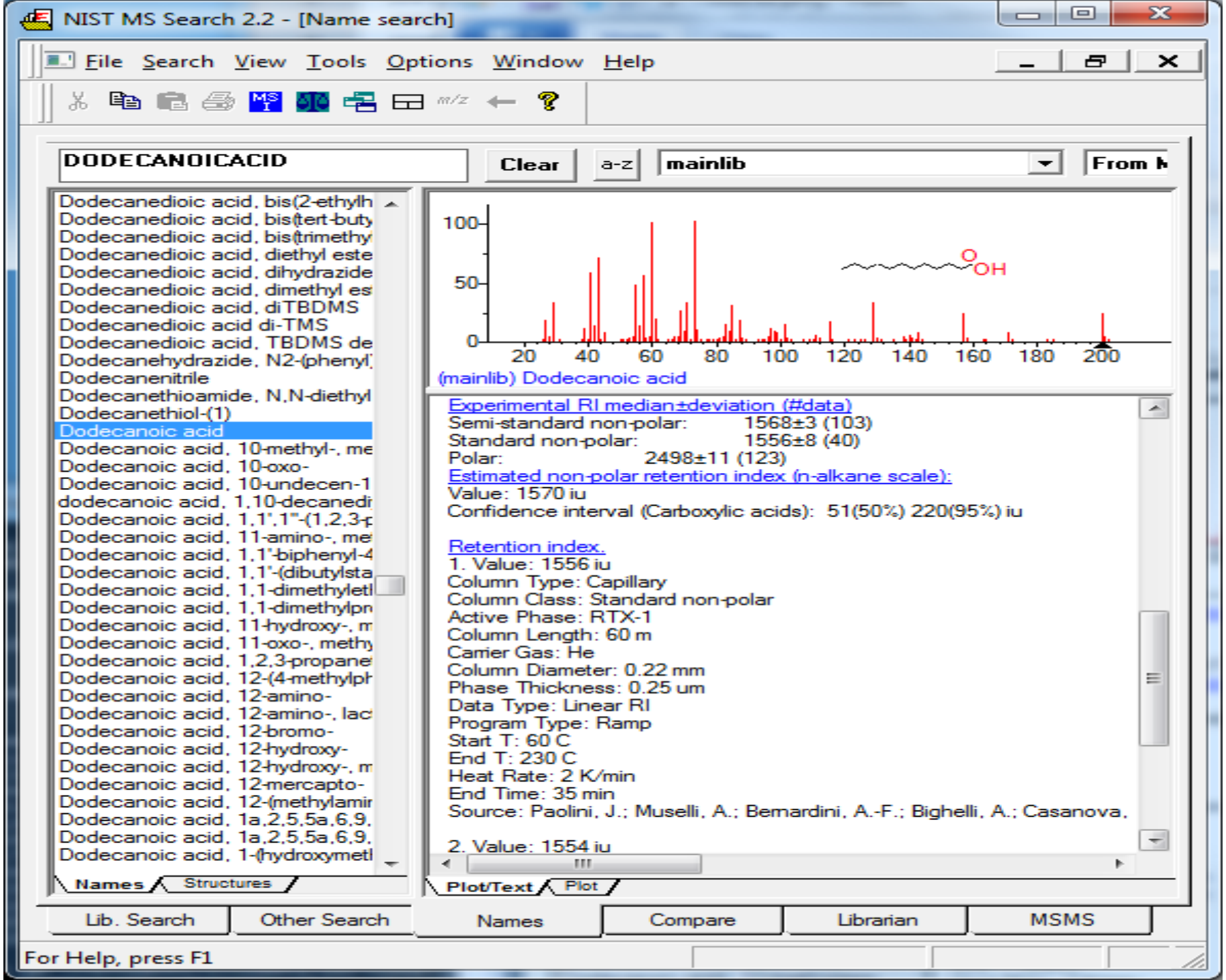
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File Search View Tools Options Window Help
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Dodecanedioic acid, bis(trimethy
Dodecanedioic acid, diethyl este
Dodecanedioic acid, dihydrazide
Dodecanedioic acid, dimethyl es
Dodecanedioic acid, diTBDMS
Dodecanedioic acid di-TMS
Dodecanedioic acid, TBDMS de
Dodecanehydrazide, N2-(phenyl
Dodecanenitrile
Dodecanethioamide, N,N-diethyl
Dodecanethiol-(1)
Dodecanoic acid
Dodecanoic acid, 10-methyl-, me
Dodecanoic acid, 10-oxo-
Dodecanoic acid, 10-undecen-1
dodecanoic acid, 1,10-decanedi
Dodecanoic acid, 1,1',1''-(1,2,3-p
Dodecanoic acid, 11-amino-, me
Dodecanoic acid, 1,1'-biphenyl-4
Dodecanoic acid, 1,1'-(dibutylsta
Dodecanoic acid, 1,1-dimethyletl
Dodecanoic acid, 1,1-dimethylpr
Dodecanoic acid, 11-hydroxy-, m
Dodecanoic acid, 11-oxo-, methy
Dodecanoic acid, 1,2,3-propane
Dodecanoic acid, 12-(4-methylph
Dodecanoic acid, 12-amino-
Dodecanoic acid, 12-amino-, lac
Dodecanoic acid, 12-bromo-
Dodecanoic acid, 12-hydroxy-
Dodecanoic acid, 12-hydroxy-, m
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Dodecanoic acid, 12-(methylamir
Dodecanoic acid, 1a,2,5,5a,6,9,
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Dodecanoic acid, 1-(hydroxymetl
Names
Structures
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20 40 60 80 100 120 140 160 180 200
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OH
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Standard non-polar: 1556±8 (40)
Polar: 2498±11 (123)
Estimated non-polar retention index (n-alkane scale):
Value: 1570 iu
Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu
Retention index.
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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,
2. Value: 1554 iu
Plot/Text
Plot
Lib. Search
Other Search
Names
Compare
Librarian
MSMS
For Help, press F1

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Food sciences- Biochemistry /enzymes

Thank you
Dr . Dhia alfekaiki