



CASE STUDY

Deformulate a Multilayer Film

PROBLEM

The goal of this analysis was to deformulate a multilayer film sample.

ANALYTICAL STRATEGY

A variety of techniques were used including, Optical Microscopy, Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), Pyrolysis Gas Chromatography Mass Spectrometry (PYMS) and Liquid Chromatography Mass Spectrometry (LCMS). The microscopy techniques were used to examine the separate layers and measure the thickness of the layers. The remaining techniques were used to identify the polymer types and additives found in the sample.

CONCLUSIONS

Three layers were observed in which the major components observed were consistent with polyethylene and Nylon 6. A series of antioxidants and slip agents were also identified.

Read the following report to see the full analysis.

Material Solutions. Uncompromising Integrity.



Final Report

Company Name
Client Name

Date:

Released by:
Dr. Mark Jordi
President
Jordi Labs LLC

Report Number: J6604

Company Name Confidential



WEB: www.jordilabs.com

EMAIL: info@jordilabs.com



Date

Client Name
Company Name

P: xxx-xxx-xxx
E: xxxxx@xxxx.com

Dear Client,

Please find enclosed the test results for your sample described as:

1. Multilayer Film

The following tests were performed:

1. Optical Microscopy (OM)
2. Scanning Electron Microscopy (SEM)
3. Fourier Transform Infrared Spectroscopy (FTIR)
4. Pyrolysis Gas Chromatography Mass Spectrometry (PYMS)
5. Liquid Chromatography Mass Spectrometry (LCMS)

Objective

The goal of this analysis was to deformulate a multilayer film sample.

Summary of Results

Scanning Electron Microscopy (SEM) reveals that the film is formed from three layers. The first layer is a $\sim 40\mu\text{m}$ perforated layer. A backing layer is attached to this which is also $\sim 40\mu\text{m}$ thick. A final smooth layer is attached which is $\sim 20\mu\text{m}$.

Optical microscopy images can distinguish only two layers: one perforated layer and one smooth layer (**Figure 1**). The perforated layer can be easily separated from the smooth layer, which suggests the two layers were thermally welded together without an adhesive.

The test results by Fourier Transform Infrared Spectroscopy (FTIR) and Pyrolysis Gas Chromatography Mass Spectrometry (PYMS) show two polymer types. The perforated and middle layers of the film are most consistent with polyethylene and the smooth backing layer

of the film is most consistent with Nylon 6. A UV absorber, Tinuvin 328, is also detected by PYMS.

LCMS analysis confirmed the identification of the smooth layer as nylon 6 and identified a series of additives including antioxidants and slip agents. The slip agents Ethylene bis(stearamide) and erucylamide were observed. The heat stabilized Irgafos 168 was also detected.

Individual Test Results

A summary of the individual test results is provided below. All accompanying data, including spectra, has been included in the data section of this report.

Optical Microscopy

The sample was analyzed using optical microscopy in order to gain a general overview of the physical characteristics of the material. The film shows an array of elliptical features. These features appear to be holes through the top polymeric layer. The polymer extends outward from the edges of each ellipse. The holes do not extend through the sample. The opposite side is a smooth polymeric material. The perforations were approximately .725 mm in length.

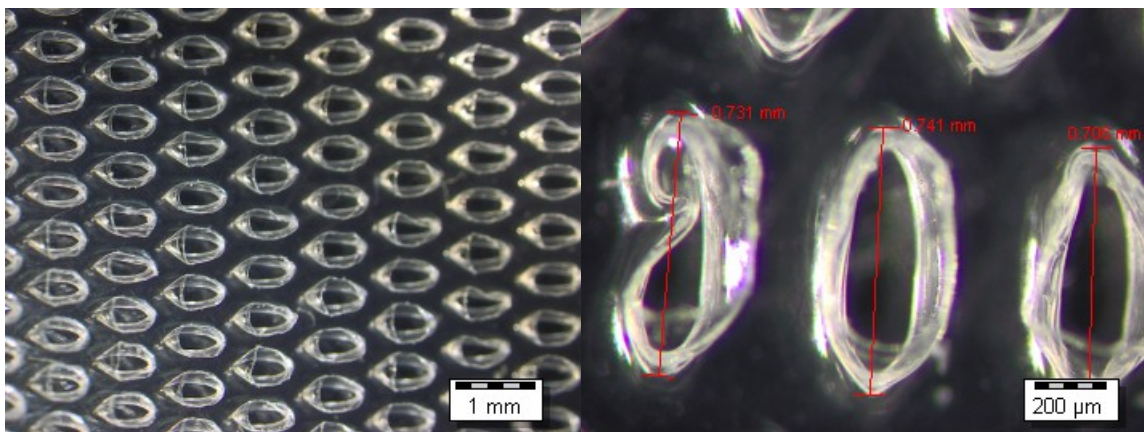


Figure 1: Images of the ‘perforated’ side of the film.

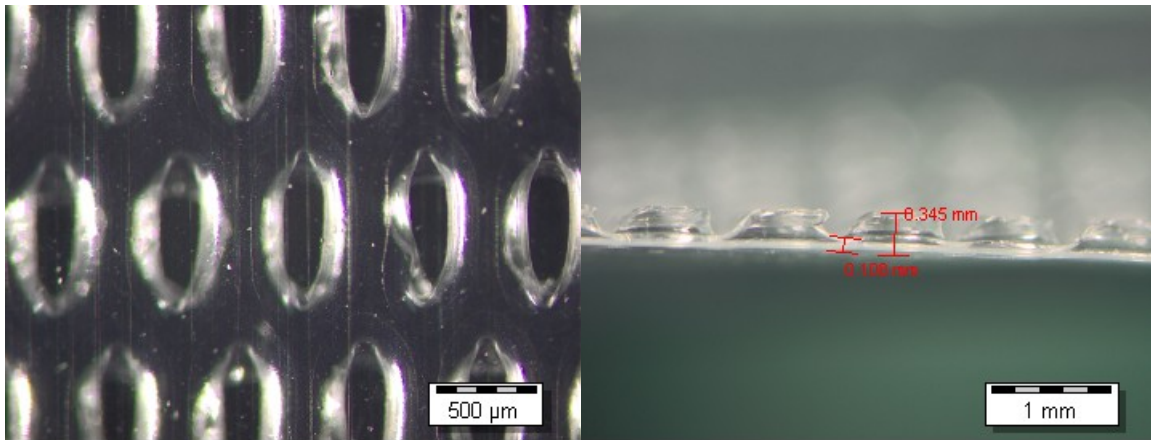


Figure 2: Image of the 'smooth' side (left) and a cross-sectional view (right) of the multilayer film.

When manipulated, the sample layers are found to require little force to separate the perforated layer from the smooth layer. Visual inspection showed no evidence of an adhesive between the layers. The perforated layer can be easily removed. The perforations were observed to extend completely through the top layer.

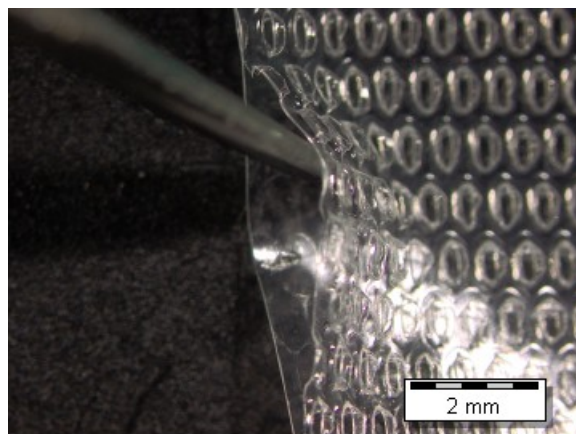


Figure 3: Image of separated layers.

SEM

The sample was also analyzed by scanning electron microscopy. The sample was prepared by imbedding the film in an epoxy and then cross sectioning the material. The electron microscope allows for a large increase in resolution as compared to the optical microscope and also allows for identification of the elemental composition using x-ray spectroscopy.

The collected micrographs show similar dimensions as compared to measurements made by optical microscopy. The sample shows a total of 3 layers, a 'perforated' layer, another similar solid layer, and a third thinner layer on the opposite surface.

Figure 4 includes backscattered electron micrographs of the sample cross-section. In backscattered mode, the brightness of a particular spot on the sample is related to the average atomic number of the elements present in that region. Heavier elements create more backscattered electrons and therefore are brighter regions in the backscattered electron image.

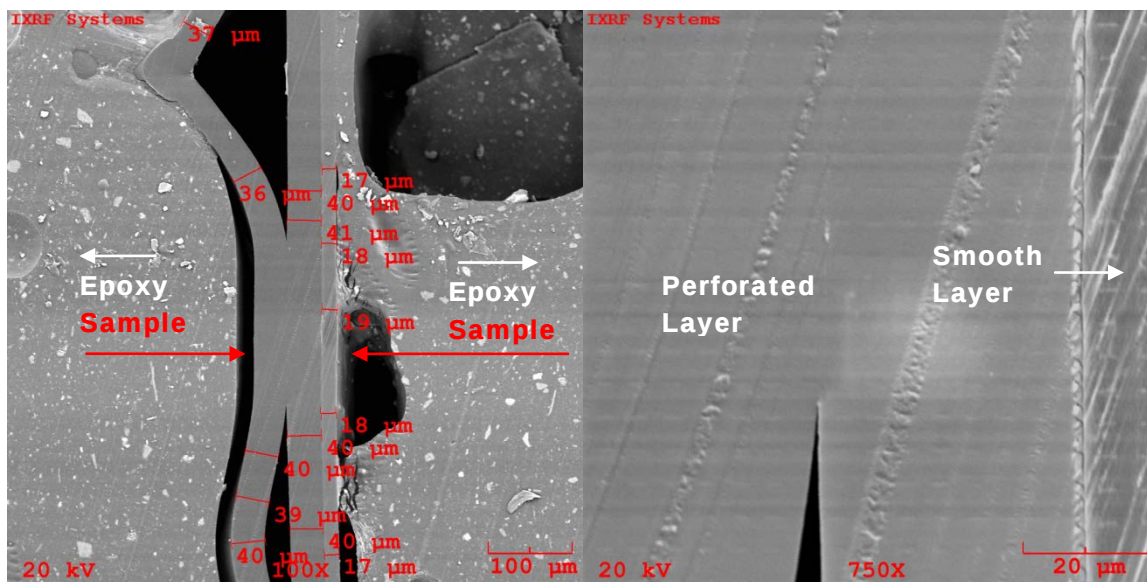


Figure 4: Backscattered electron micrographs of the cross-section of the sample.

Energy dispersive x-ray spectroscopy was used in order to investigate the samples for any inorganics (fillers, pigments, etc.). The spectra collected show only carbon and oxygen in the sample. Additional metals are detected; however the x-ray dot maps constructed indicate that they are impurities in the epoxy used to mount the sample.

25082

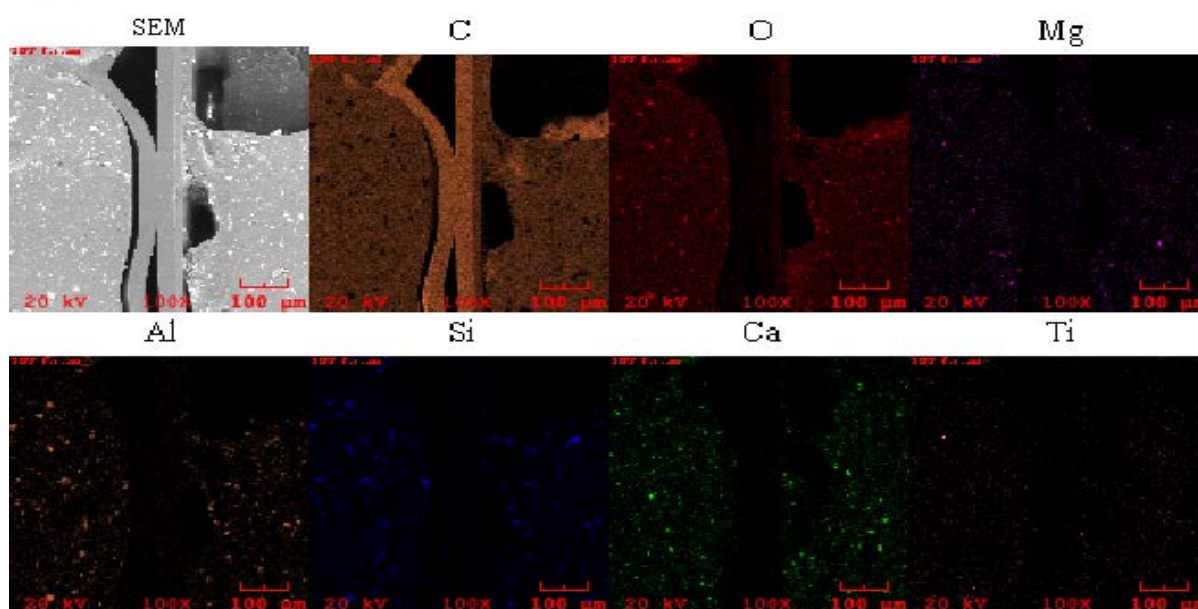


Figure 5: Elemental dot maps for the low magnification image (left image in **Figure 4**).

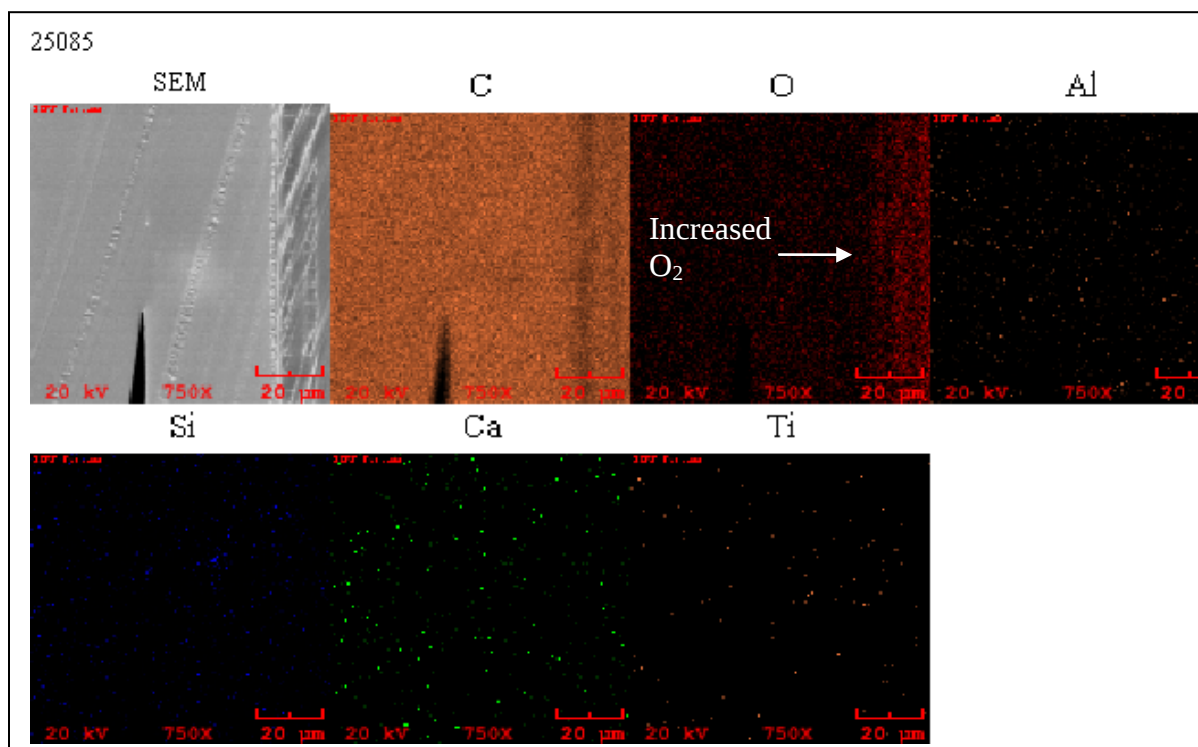


Figure 6: Elemental dot maps for the high-magnification image (right image in **Figure 4**).

If the elemental dot map for the high magnification image is closely examined, a slightly increased concentration of oxygen is observed in layer 3. This suggests that layer 3 is composed of a polymer containing oxygen.

FTIR

FTIR is a valuable polymer characterization tool which utilizes characteristic bond vibrations to probe the functional groups present in a sample. Collection of an FTIR spectrum can be used for identification of the bulk sample component. FTIR is generally limited to sample components which are present at approximately 5% or higher. It is generally not preferred for complex mixture.

The FTIR spectra collected from each of the sample layers was compared with a database of approximately 20,000 spectra of polymers and additives. This methodology treats the FTIR spectra collected as a fingerprint for a particular polymer or additive. Two compounds having the same FTIR spectra are in most cases comprised of the same bulk material. In the case that a suitable match cannot be found, the chemical data (functional groups) can be used in conjunction with other methods (such as PYMS) to reach confident identification.

The perforated layer and the front side of the smooth layer show FTIR spectra most consistent with polyethylene. The spectrum of polyethylene is relatively simple, containing only a few peaks. The peaks observed are tabulated in **Table 1** and represent the -CH stretching, -CH₂ bending, and -CH₂ rocking vibration modes. A comparison of the spectrum with our reference database of over 23,000 compounds produced a best match of ROCK F T WAX which has the same repeat unit as polyethylene.

Table 1	
FTIR identification of the 'perforated' layer of the sample	
IR Frequency (cm⁻¹)	Functional Group
2918	CH ₂ asymmetrical stretching
2850	CH ₂ symmetrical stretching
1466	CH ₂ scissoring
720	CH ₂ rocking

The backside of the smooth layer shows an FTIR spectrum most consistent with Nylon 6 (polycaprolactam). Polyamides show characteristic bands near 3200 cm⁻¹ (NH stretch), 1540 and 1635 cm⁻¹ (Amide I & II bands). A comparison of the spectrum with our reference database of over 23,000 compounds produced a best match of BLUE C NYLON 10V*UNMODIFIED NYLON 6/6. Nylon 6,6 and Nylon 6 have very similar spectra. PYMS was used to make a more definitive identification.

Table 2 FTIR identification of the 'smooth' layer of the sample	
IR Frequency (cm ⁻¹)	Functional Group
3300	NH stretching
2918	CH ₂ asymmetrical stretching
2850	CH ₂ symmetrical stretching
1635	C=O stretching Amide I
1541	NH bending Amide II
1466	CH ₂ scissoring
1412	CN stretching
720	CH ₂ rocking

PYMS

Analysis by PY-GCMS was conducted using a double shot technique. The double shot experiment consists of heating the sample to release volatiles which were then cryogenically trapped and then analyzed by GCMS. Following completion of the 1st pass analysis, the remaining portion of the sample was then heated above the decomposition temperature rapidly and pyrolyzed components were passed into a gas chromatography column and analyzed by mass spectroscopy.

Prominent peaks found in PY-GCMS typically include fragments of the polymer as well as monomer, antioxidants and other additives. Sample peaks were compared with over 796,613 reference compounds using the NIST/EPA/NIH mass spectral search program.

Results

The PYMS data collected is well correlated with the FTIR data. The PYMS 1st pass chromatogram is characterized by a relatively intense peak identified as caprolactam (Nylon 6 monomer). The caprolactam dimer is also observed. In addition, the common polymer additive, Tinuvin 328, is detected. TINUVIN 328 is a UV absorber of the hydroxyphenylbenzotriazole class designed for coatings. Because of its extended UV absorption, TINUVIN 328 provides efficient protection to coatings and light sensitive substrates.

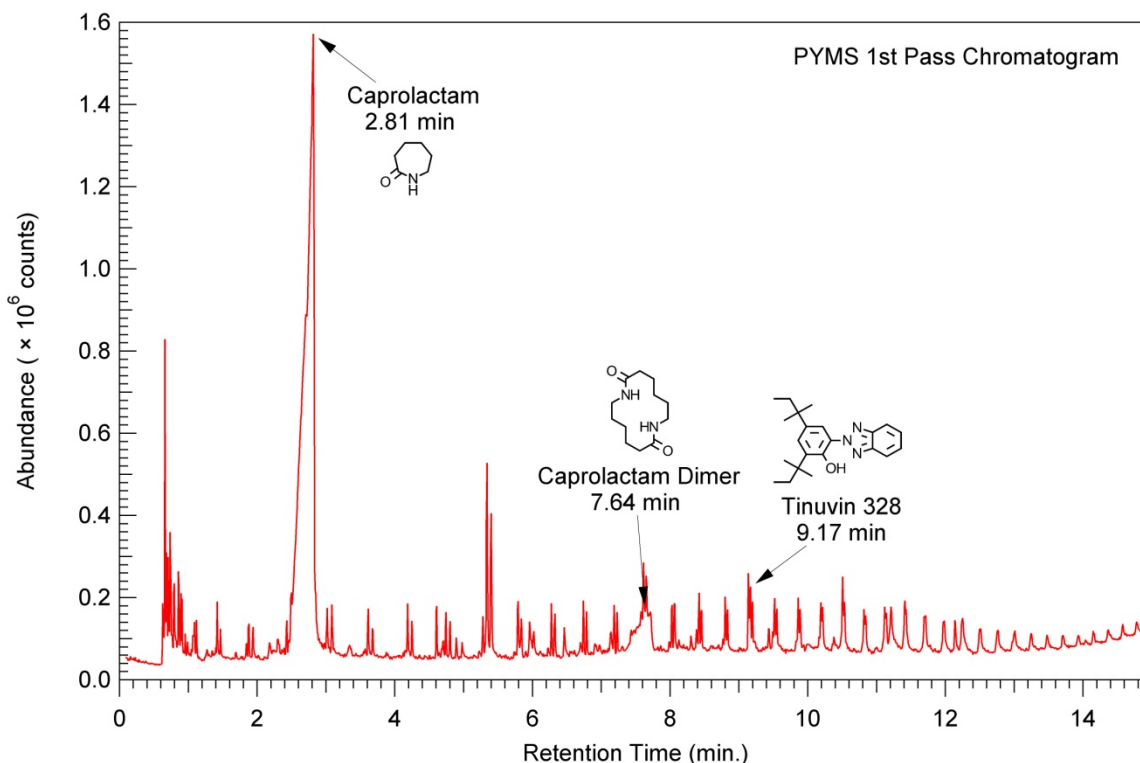


Figure 7: PYMS 1st pass chromatogram collected from the sample.

The PYMS second pass chromatogram shows a large number of peaks with the pattern characteristic of a series of linear alkanes. The mass spectra observed are all consistent with various, mostly linear, alkane fragments. This is the typical behavior of polyethylene. The polyethylene fragments dominated the chromatogram of the both the 1st and 2nd heating passes. This suggests that polyethylene is the majority of the material.

No evidence of an adhesive was observed in the data collected.

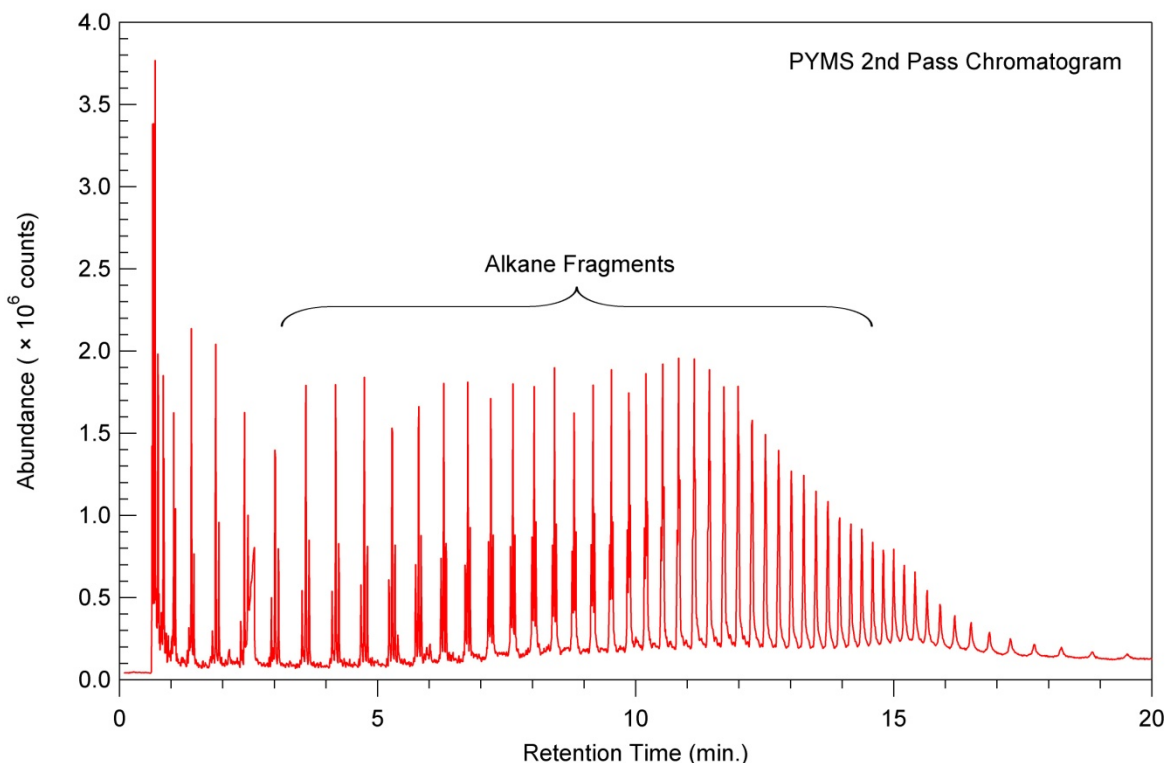


Figure 8: PYMS 2nd pass chromatogram collected from the sample.

LCMS

Background: QTOF-LCMS combines high mass accuracy time of flight mass spectroscopy with the power of a liquid chromatography separation to provide detailed information about the elemental composition of unknowns.

The presence of an additional quadrupole mass spectrometer (Q) provides the added capability to perform fragmentation experiments. This increases the confidence of unknown identification. It is preferable that a standard of the suspected unknown be analyzed under identical conditions as the sample. If the fragmentation patterns, high accuracy mass data, isotope patterns and LC retention times match for the unknown and standard then there is a very high probability that the identification is correct. It is possible to gain significant information about the structure of an unknown, even in cases in which standards are not available by using the molecular formula generation (MFG) algorithms contained in the Mass Hunter qualitative software.

LCMS requires that the molecule of interest be ionized. Thus, data is typically plotted in positive and negative modes indicating the charge on the ions. Ion formation is accomplished through the formation of a molecular adduct using a charge carrying species. Typical charge carriers in positive ion mode include H^+ , Na^+ , K^+ , NH_4^+ etc. Thus the observed mass is typically the mass of the compound plus the mass of the charge carrier.

The nature of the mobile phase and the ionization conditions determine the ions formed. In negative ion, the loss of hydrogen is generally observed which results in the loss of one mass unit (1.0078 amu). Other transformations are also possible including dehydration, dimer formation, etc.

A number of plots are used to aid in interpreting QTOF-LCMS data. This includes Base Peak Chromatograms (BPC), Extracted Ion Chromatograms (EIC), Extracted Compound Chromatograms (ECC), Mass spectra (MS) and Product Ion Spectra (MSMS). A BPC is formed by plotting the most intense ion at a given retention time. This spectrum is particularly useful for identifying the retention time of unknowns. EICs are formed by plotting a single mass at all retention times. This could be considered a plot of peak intensity (~compound concentration) for a single compound (and its isomers) versus retention time. ECC's are the sum of all the ions determined to be related to a single compound.

MS spectra plot the observed masses and their intensities at a single retention time. MS/MS spectra show the fragmentation pattern for a single compound. Mass Spectra plot the mass to charge ratio (m/z) and not the mass of the compound.

Molecular Formula Generation (MFG) was used to identify the best matching elemental composition for the unknown unique components. It is generally observed that, as the mass increases, the number of potential elemental formulas of matching mass increases exponentially.

Molecular Formula Generation (MFG) was used to identify the best matching elemental composition for the unknown unique components. It is generally observed that, as the mass increases, the number of potential elemental formulas of matching mass increases exponentially.

Sample preparation: A 200 mg portion of the sample (all three layers included) was extracted for LCMS analysis. The extract was filtered prior to injection. This extraction procedure is generally able to extract most small molecule polymer additives and contaminants.

Results: The sample was analyzed in positive mode. Positive mode will show compounds which are able to form adducts that can carry a positive charge. Common adducts observed in positive mode include $[M+H]^+$, $[M+NH_4]^+$, and $[M+Na]^+$. The positive mode chromatogram collected is shown in **Figure 9**.

Various nylon 6 oligomers and additives including antioxidants and slip agents were found in the sample. The summary of LCMS identification results in positive mode is listed in **Table 3**.

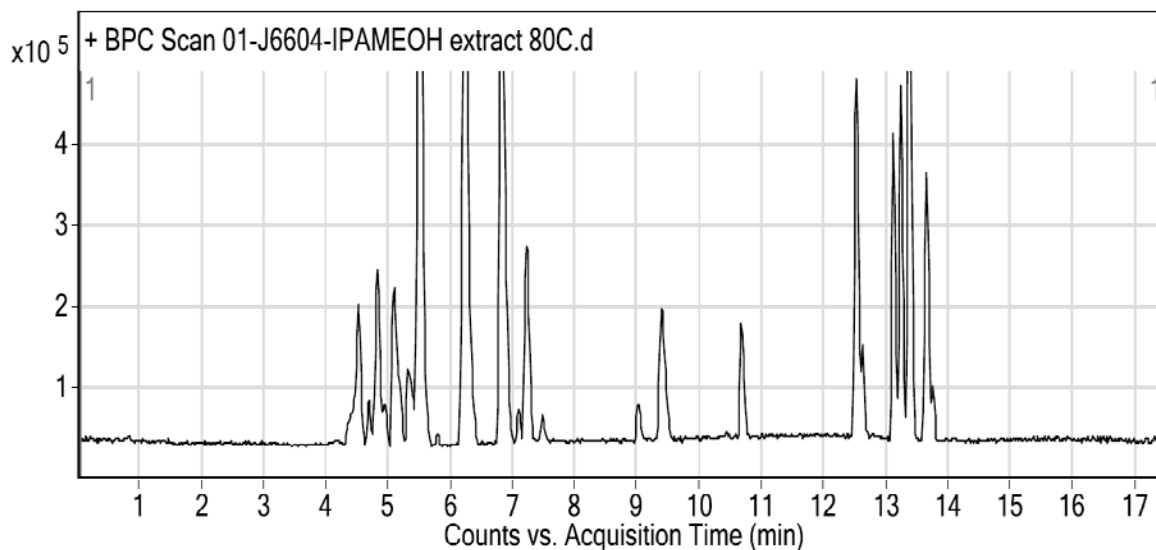


Figure 9: The LCMS base peak chromatogram (BPC) of the sample *Multilayer Film* in positive mode.

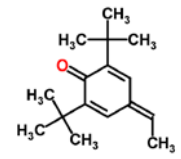
Table 3 Summary of LCMS Identification Results In Positive Mode				
Best Match	RT (min)	m/z	Species	Calculated m/z
Tricaprolactam $C_{18}H_{33}N_3O_3$	5.545	340.2602	$[M+H]^+$	240.2595
Dow Ecosurf 2A1 Component C4-PPG5-PEG2-OH $C_{23}H_{48}O_8$	6.274	453.3441	$[M+H]^+$	453.3422
Pentacaprolactam $C_{30}H_{55}N_5O_5$	6.832	566.4285	$[M+H]^+$	566.4276
Dioctylamine $C_{16}H_{35}N$	7.067	242.2842	$[M+H]^+$	242.2842
Hexacaprolactam $C_{36}H_{66}N_6O_6$	7.221	679.5120	$[M+H]^+$	679.5117
Heptacaprolactam $C_{42}H_{77}N_7O_7$	7.472	396.8024	$[M+2H]^{2+}$	396.8018
		792.5950	$[M+H]^+$	792.5957
 (Oxidized BHEB) $C_{16}H_{24}O$	10.654	233.1900	$[M+H]^+$	233.1900
Erucylamide	12.638	338.3416	$[M+H]^+$	338.3417

Table 3 Summary of LCMS Identification Results In Positive Mode				
Best Match	RT (min)	m/z	Species	Calculated m/z
C ₂₂ H ₄₃ NO				
Ethylene bis(stearamide) C ₃₈ H ₇₆ N ₂ O ₂	13.092	593.5983	[M+H] ⁺	593.5980
Ethylene bis (nonadecylamide) C ₄₀ H ₈₀ N ₂ O ₂	13.222	621.6297	[M+H] ⁺	621.6293
Oxidized Irgafos 168 C ₄₂ H ₆₃ O ₄ P	13.383	663.4545	[M+H] ⁺	663.4537
C ₃₆ H ₆₄ N ₈ O ₆	13.618	705.5011	[M+H] ⁺	705.5022
Irgafos 168 C ₄₂ H ₆₃ O ₃ P	13.383	647.4583	[M+H] ⁺	647.4588

Analysis Conditions

Experimental conditions are provided here.

Closing Comments

Deformulation of an unknown material is intended to provide a best estimate of the chemical nature of the sample. All chemical structures are supported by the evidence presented but are subject to revision upon receipt of additional evidence. Additional factors such as material processing conditions may also affect final material properties.

Jordi Labs' reports are issued solely for the use of the clients to whom they are addressed. No quotations from reports or use of the Jordi name is permitted except as authorized in writing. The liability of Jordi Labs with respect to the services rendered shall be limited to the amount of consideration paid for such services and do not include any consequential damages. Jordi Labs specializes in polymer testing and has 30 years experience doing complete polymer reformulations. We are one of the few labs in the country specialized in this type of testing. We will work closely with you to help explain your test results and solve your problem. We appreciate your business and are looking forward to speaking with you concerning these results.

Sincerely,

Kevin Rowland

Kevin Rowland, M.S.
Senior Chemist
Jordi Labs LLC

Mark Jordi

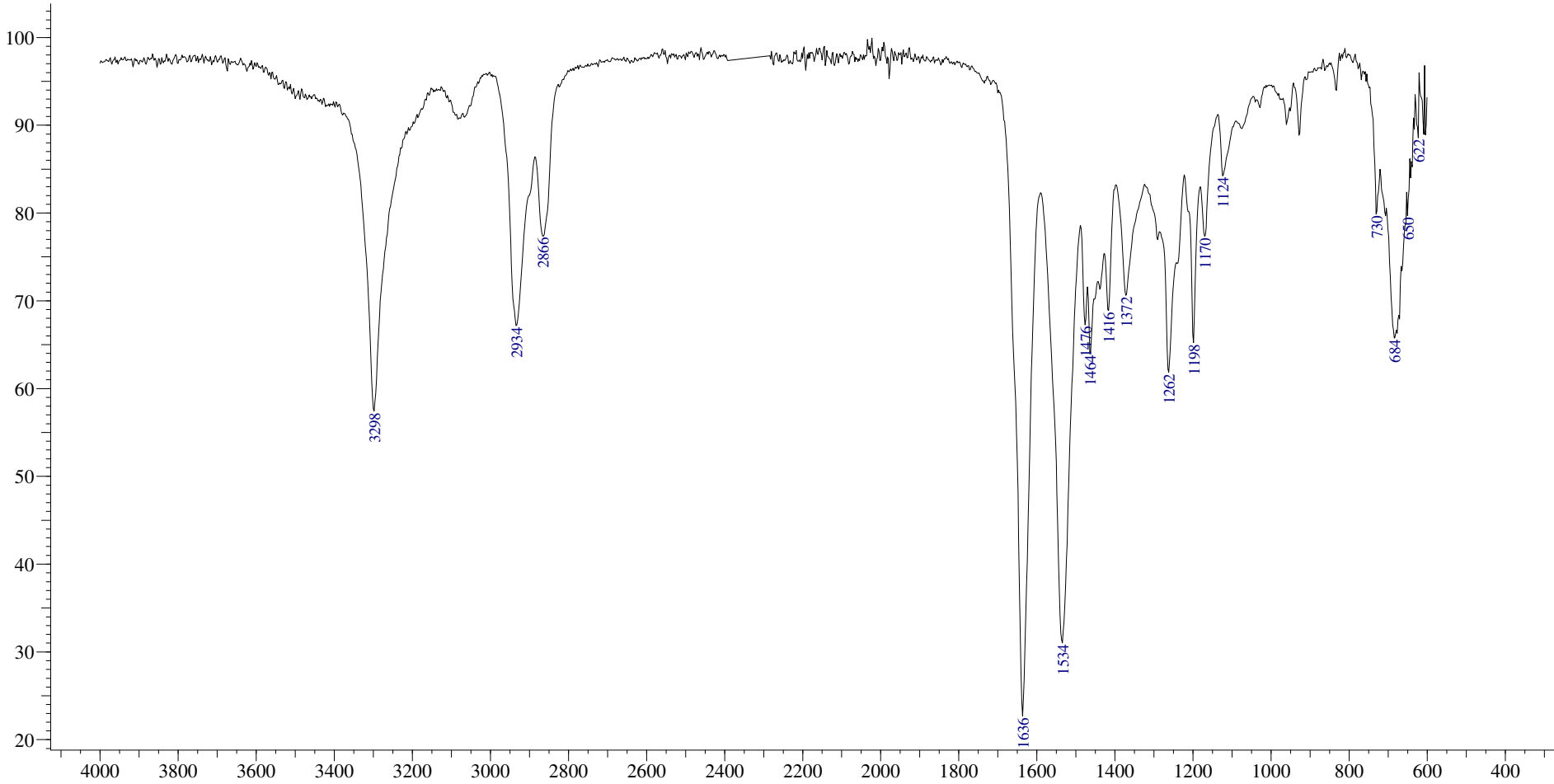
Mark Jordi, Ph. D.
President
Jordi Labs LLC

Appendix

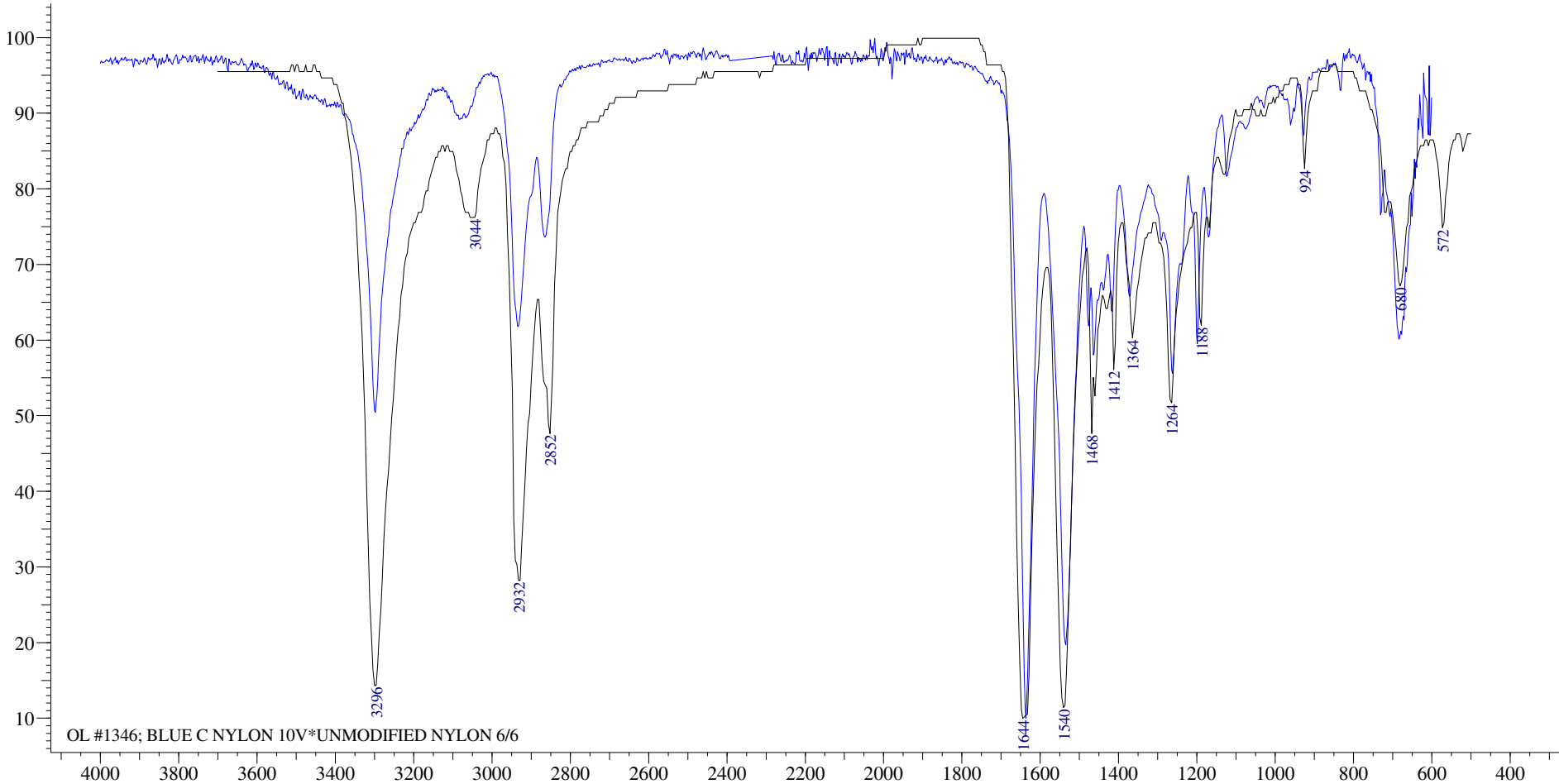
- Pages 16 - 36 FTIR Data
- Pages 37 - 132 PYMS Data
- Pages 133 - 147 LCMS Data

FTIR Data

Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.

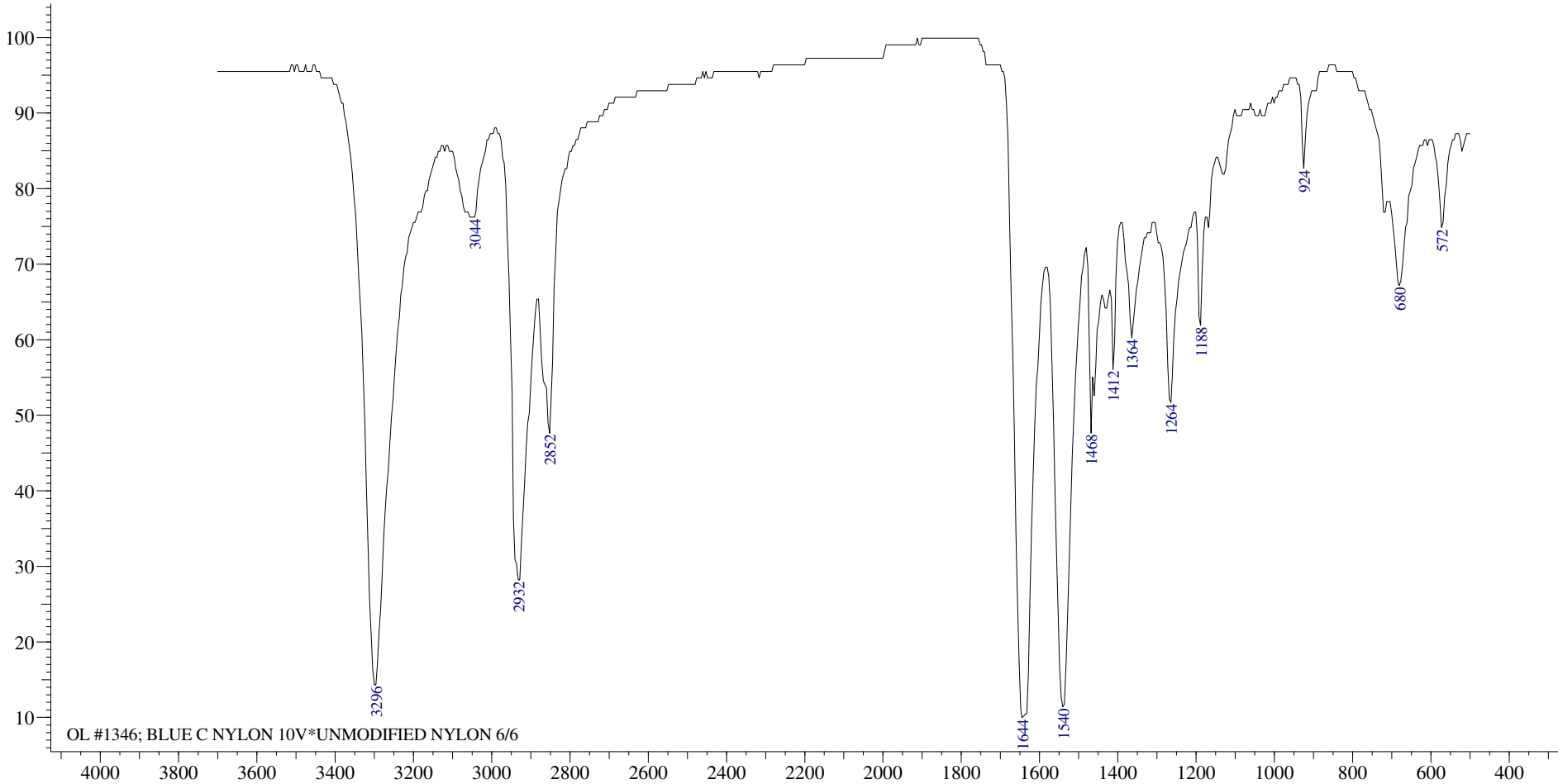


Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.



Name(s): BLUE C NYLON 10V*UNMODIFIED NYLON 6/6
Source Of Sample: MONSANTO POLYMER PRODUCTS COMPANY
Technique: FILM (CAST FROM FORMIC ACID)
Classification: Polymers: POLYAMIDES

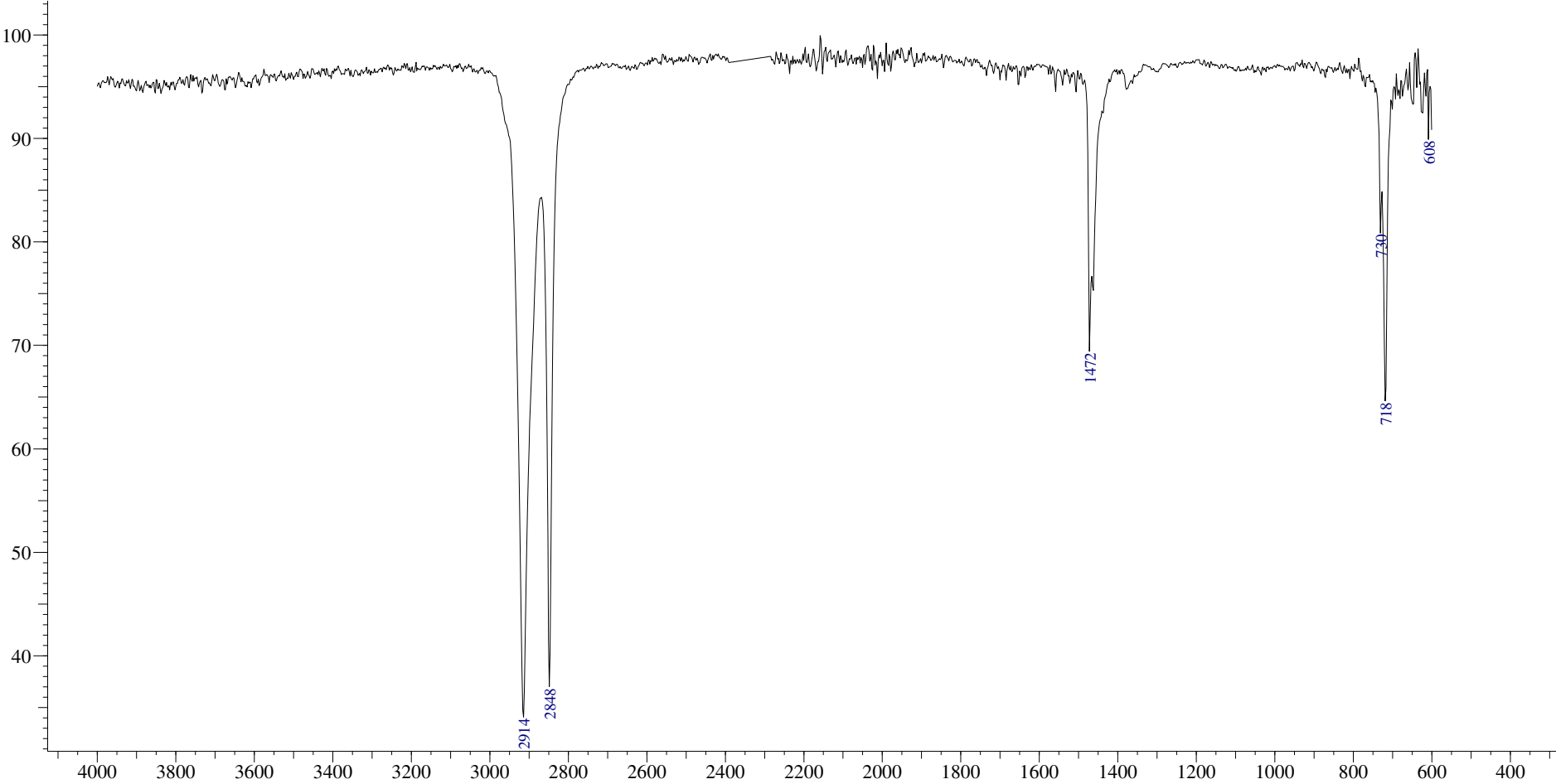
Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.



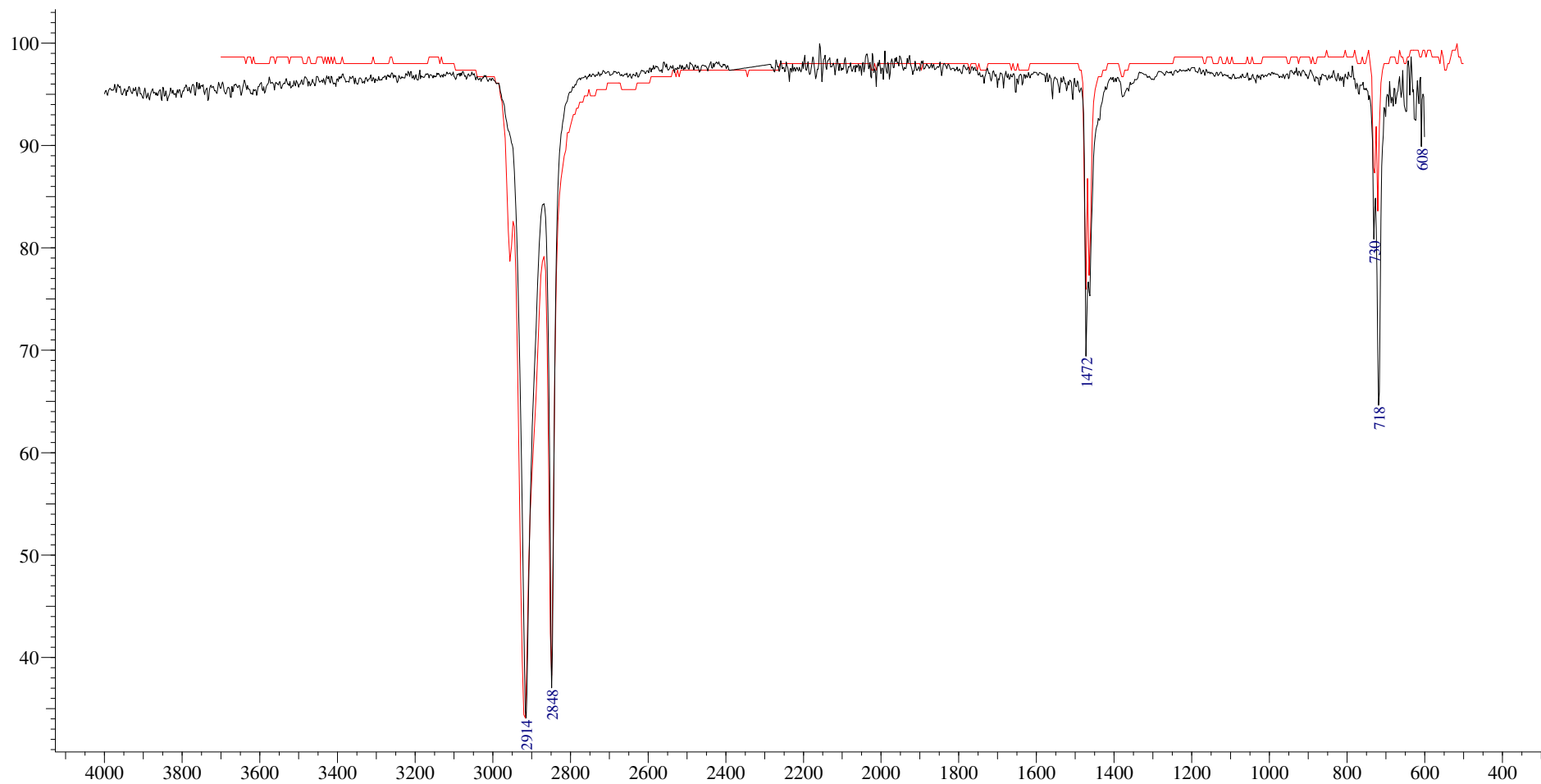
Name(s): BLUE C NYLON 10V*UNMODIFIED NYLON 6/6
Source Of Sample: MONSANTO POLYMER PRODUCTS COMPANY
Technique: FILM (CAST FROM FORMIC ACID)
Classification: Polymers: POLYAMIDES

Index	HQI	Chemical Name	Spectrum
OL #1375	681.78	BCI NYLON 1107-P40*NYLON 11, PLASTICIZED	
QF #424	668.76	N ² ,N ⁶ -DIBENZOYL-DL-LYSINE	
OL #1370	666.69	ULTRAMID S3 NYLON 6/10*POLYMERIC HEXAM...	
OL #1368	661.21	BCI NYLON LX-3250*POLYHEXAMETHYLENE AD...	
CL #1975	659.76	CARTARETIN F-8 CATIONIC	
Z777 #202	659.29	PT24.7501 NYLON 6,12 GRILON CR9	
CL #1974	658.48	CARTARETIN F-4 CATIONIC	
Z777 #191	654.61	PT20.4102 POLYAMIDE 6 BEETLE	
Z777 #199	654.61	PT22.5601 POLYAMIDE 6,6 BEETLE	
OL #1395	653.95	COMER-7*POLYAMIDE/ESTER RESIN	
Z777 #148	652.01	PP82.26801.NYLON 4/6 STANYL	
CL #289	648.66	CASCOLOID ST-56 NONIONIC*CASEIN DERIVE...	
OL #1354	647.38	NYLON 4*A POLYMER OF 2-PYRROLIDONE	
AS #104	647.30	ZETOL	
OL #1355	646.81	DURETHAN BK 31 F*NYLON 6(EPSILON-CAPRO...	
Z777 #43	645.98	PP22.5602 NYLON 6,6 MARANYL@ @	
OL #1358	643.95	NYPEL 2314*NYLON TYPE 6	
OL #1363	642.09	ULTRAMID A3HG5*NYLON TYPE 6/6	
Z777 #44	641.80	PP22.6701 NYLON 6,6 ZYTELLON P0%CCLTF=	
OL #1346	641.70	BLUE C NYLON 10V*UNMODIFIED NYLON 6/6	
Z777 #190	640.50	PT20.4101 NYLON 6 DURETHAN B	
Z777 #204	639.01	PT26.8101 POLYAMIDE 11 RILSAN	

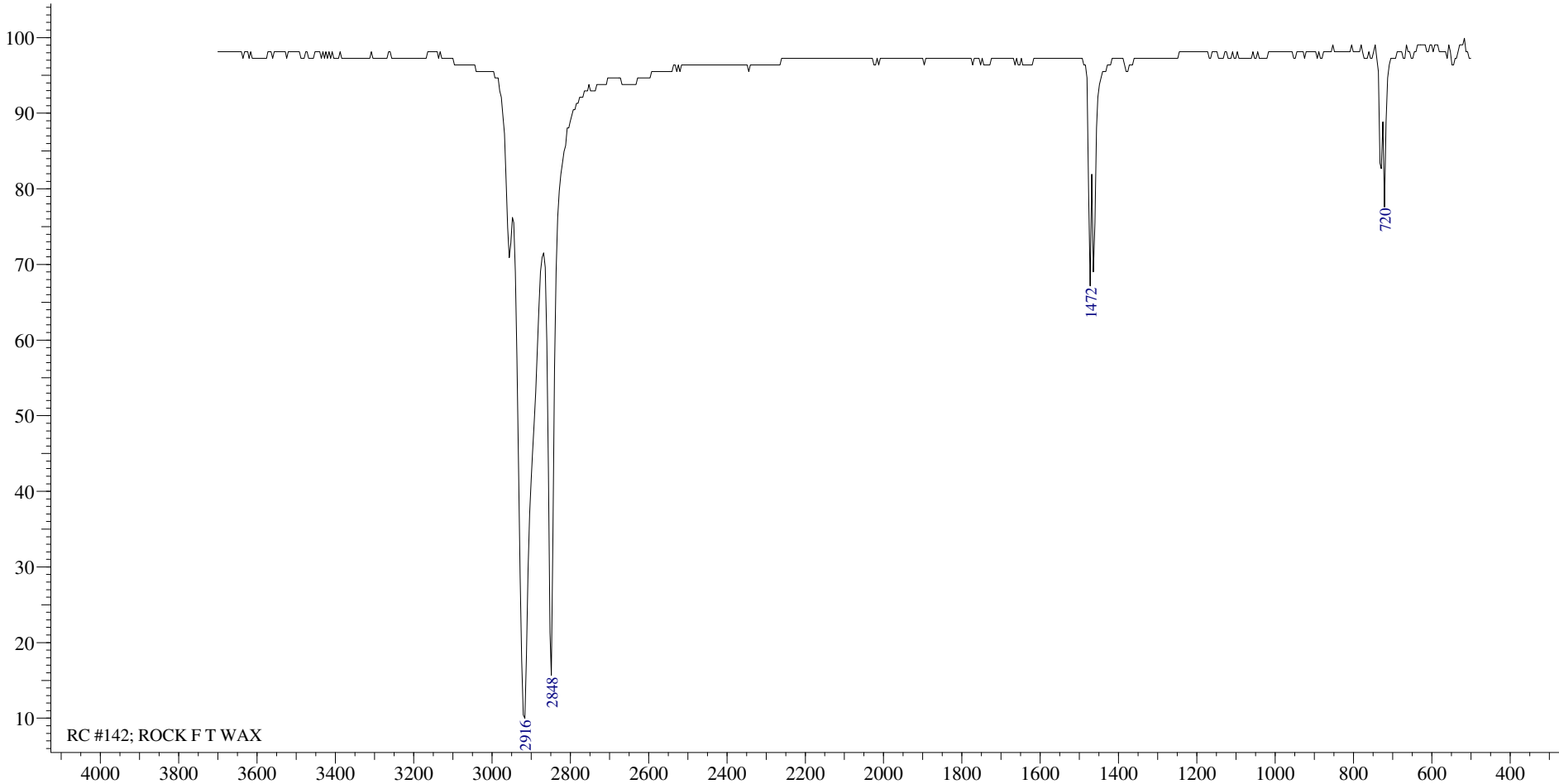
Index	HQI	Chemical Name	Spectrum
OM #1117	637.90	CARTARETIN F-23	
OM #1185	637.43	AMBERLITE IRA-60	
AS #103	636.72	ZETEN	



Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.



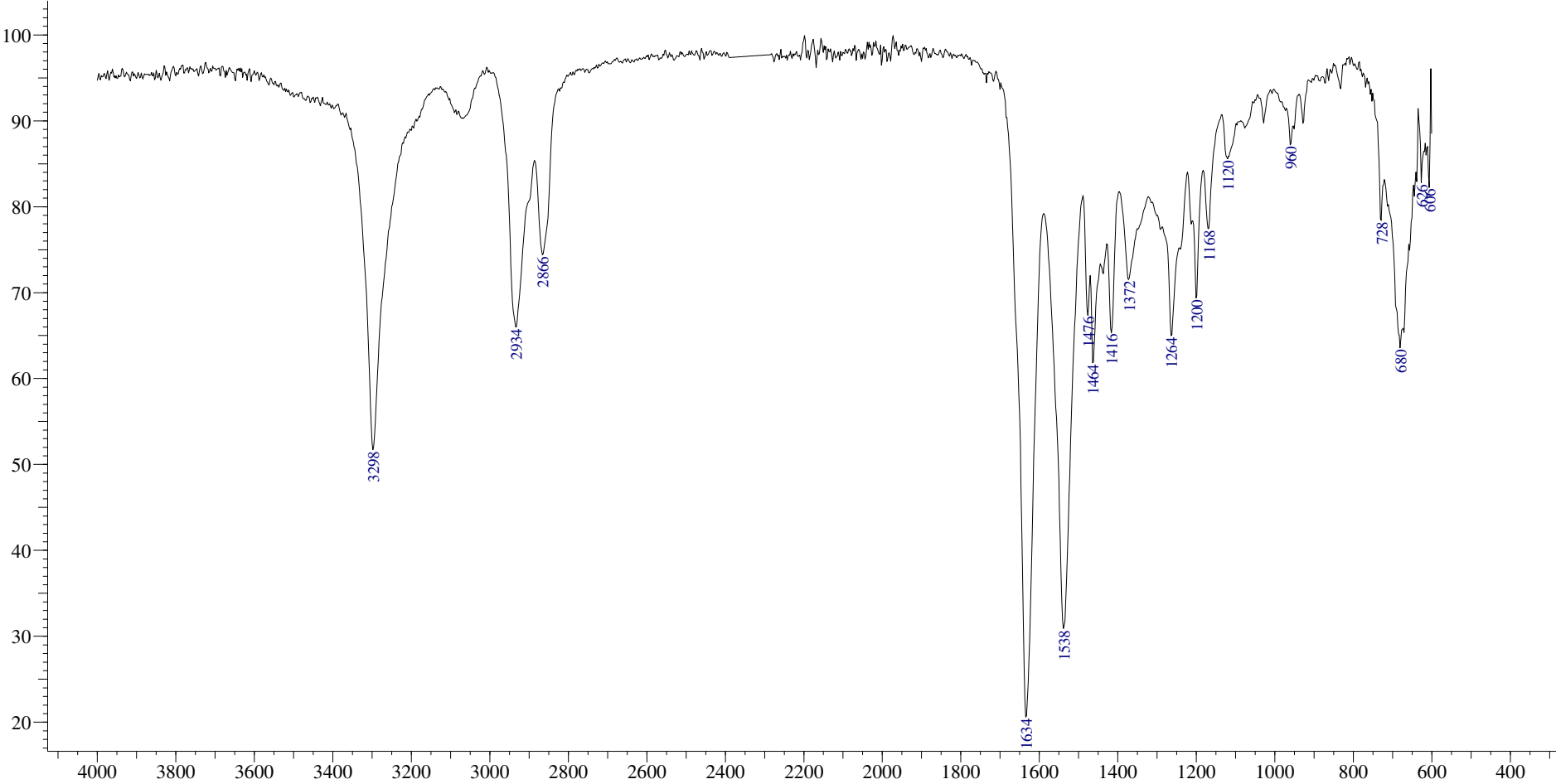
Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.



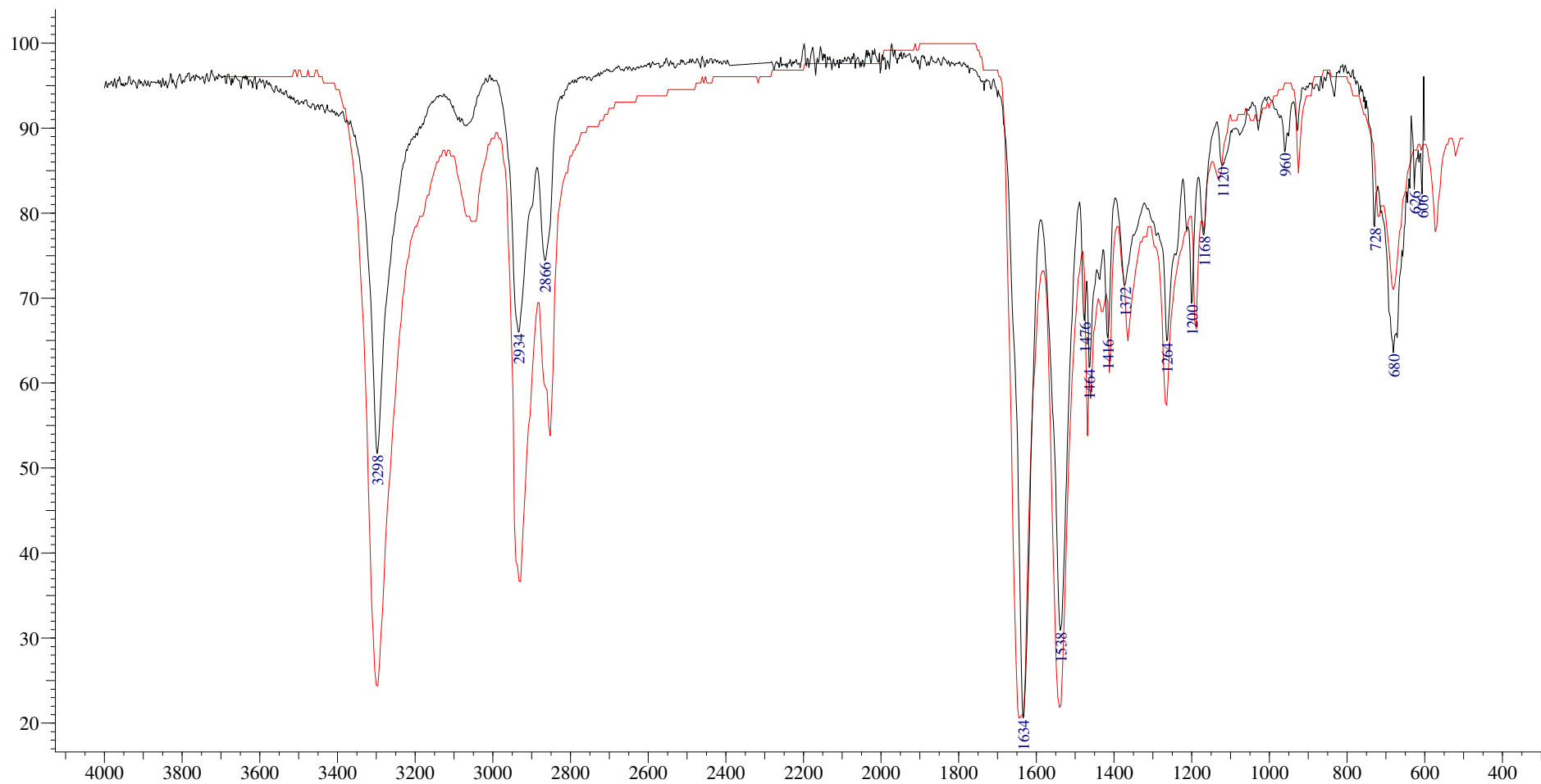
Name(s):	ROCK F T WAX
Melting Point:	98.8889
Comments:	Physical Description: WHITE WAX Chemical Description: ROCK F T WAX
Source Of Sample:	INTERNATIONAL WAX REFINING COMPANY, INC., VALLEY STREAM, NEW YORK
Technique:	MELT (CRYSTALLINE PHASE)
Use:	VERY HARD WITH PENETRATION VALUE CLOSE TO CARNAUBA WAX
Classification:	Rubber Chemicals: ANTIOXIDANT

Index	HQI	Chemical Name	Spectrum
AS #1858	753.83	DAF 618 FILM FORMULATED WITH AN ADHESI...	
AS #930	751.79	LIQUI WAX	
OL #63	747.49	BAYLON V22H764*LOW DENSITY POLYETHYLENE	
OL #4	747.39	PARVAN 4550, F.N. 3519*REFINED PARAFFI...	
OM #46	737.64	PETROLITE C-4040	
OL #33	730.88	POLY EM 12*ANIONIC POLYETHYLENE EMULSION	
RC #142	729.51	ROCK F T WAX	
CL #380	726.70	AMMONYX 2200 CATIONIC*DITALLOW DIMETHY...	
PL #1491	725.83	EPOLENE C-13 : HIGH MOLECULAR WEIGHT P...	
OL #47	724.91	POLY EM 40*PH STABLE ANIONIC POLYETHYL...	
OL #29	719.54	RIGIDEX TYPE 50*HIGH DENSITY POLYETHYL...	
RC #143	718.43	SUNOLITE 127	
CL #454	716.82	BARLOX 18S BIODEGRADABLE*STEARYL DIMET...	
AS #700	716.72	EASTOBOND A-39	
PL #669	714.66	STANDAMUL STC-25 : STEARALKONIUM CHLORIDE	
OM #13	710.08	HOSTALEN GK9050 HO	
CL #356	709.69	LISSOLAMINE A CATIONIC*CETYL TRIMETHYL...	
QF #97	709.55	HEPTACOSANE	
OL #2	707.95	PARVAN 3150, F.N. 3502*REFINED PARAFFI...	
SR #167	707.95	PARVAN 3150, F.N. 3502*REFINED PARAFFI...	
SR #167	707.95	PARVAN 3150, F.N. 3502*REFINED PARAFFI...	
SR #167	707.95	PARVAN 3150, F.N. 3502*REFINED PARAFFI...	

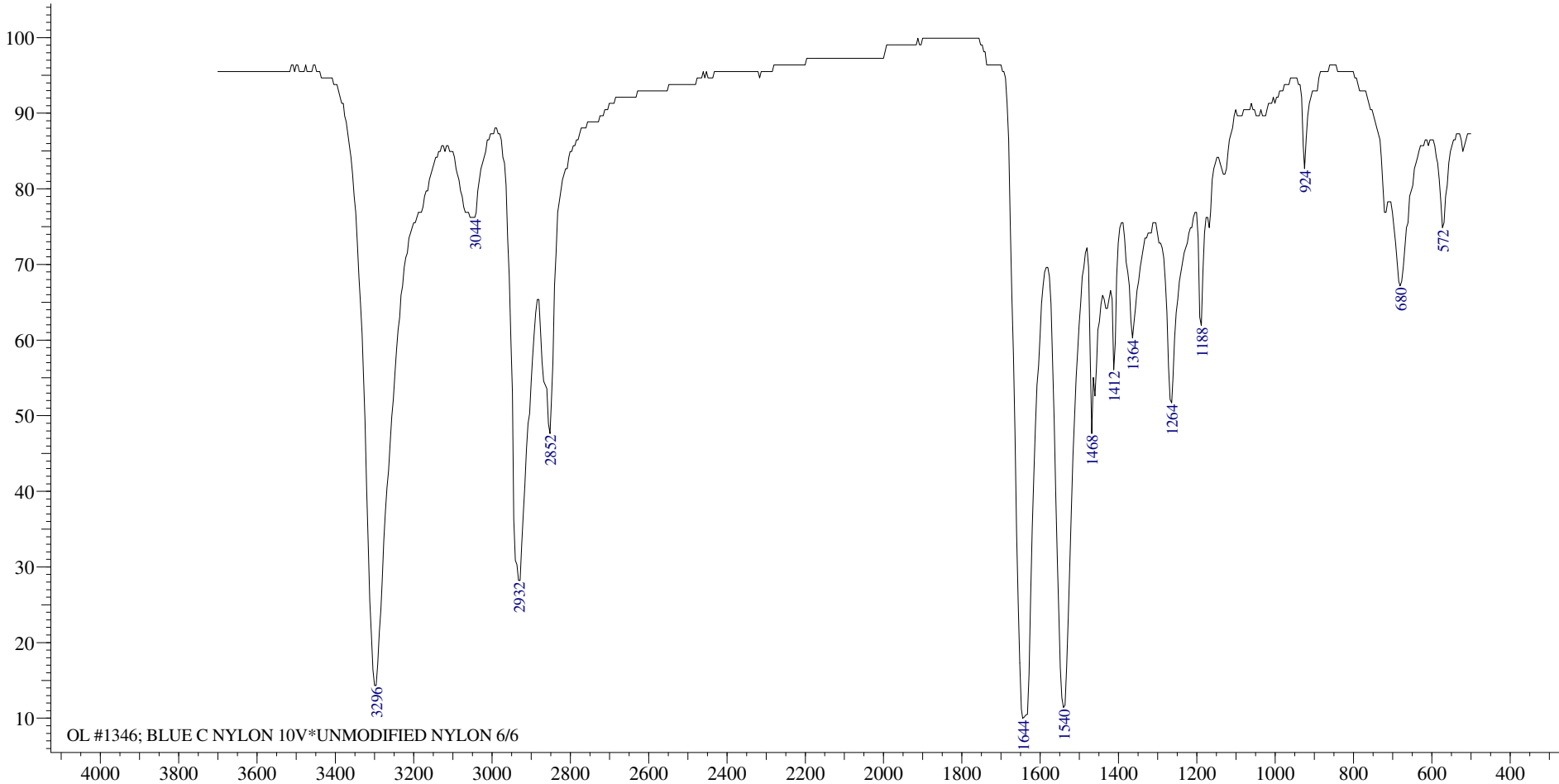
Index	HQI	Chemical Name	Spectrum
OM #19	707.49	PETROTHENE NL 409-00	
AS #1860	705.24	DAF 709 LOW MELT TEMPERATURE, LOW VISC...	
PL #832	702.82	KEMAMINE Q-1902-C : DIMETHYL DIARACHID...	



Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.

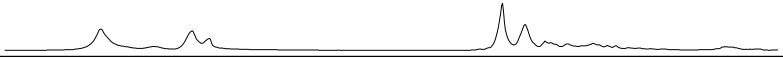
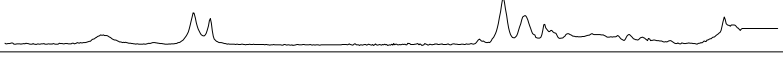


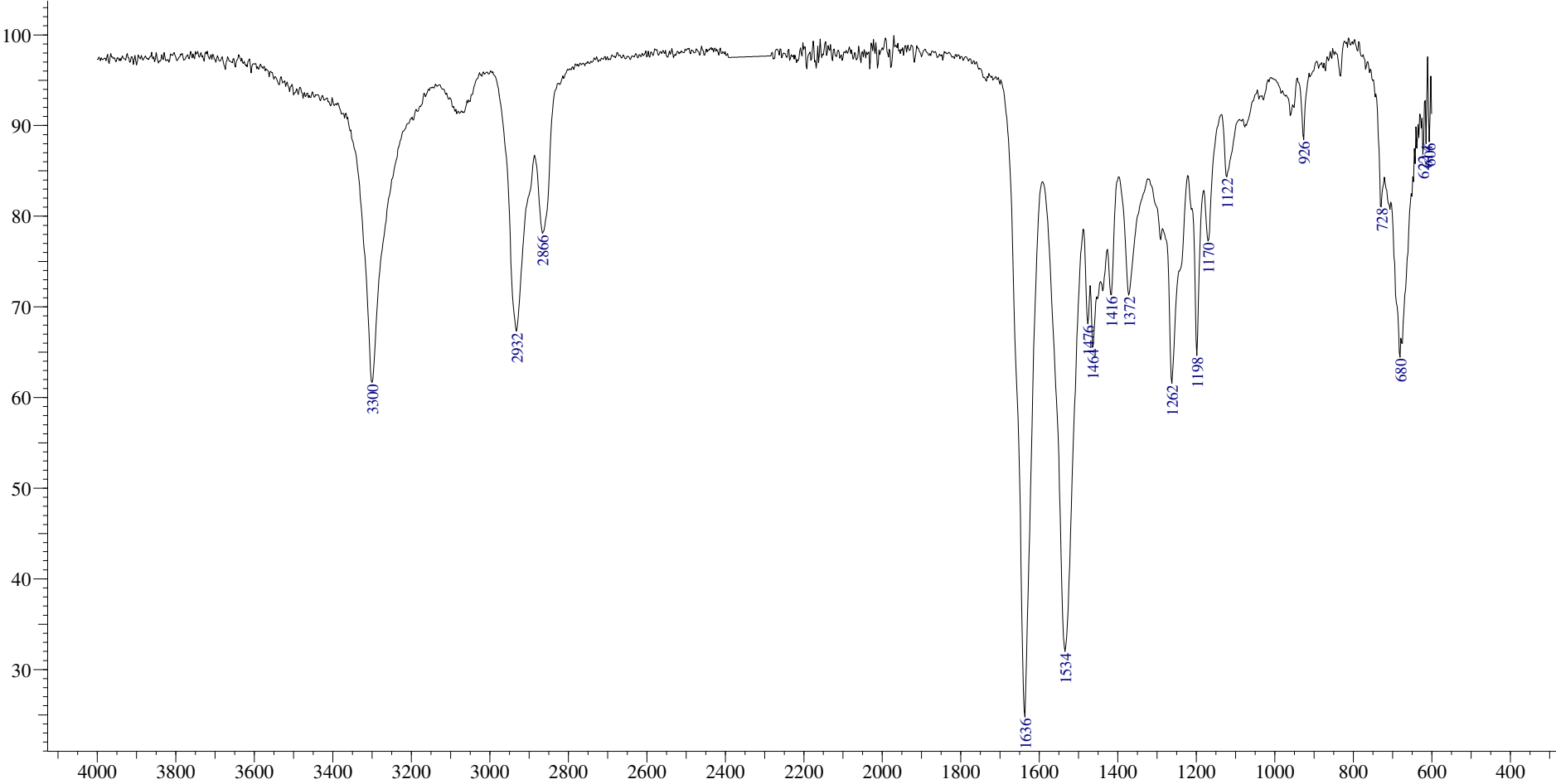
Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.



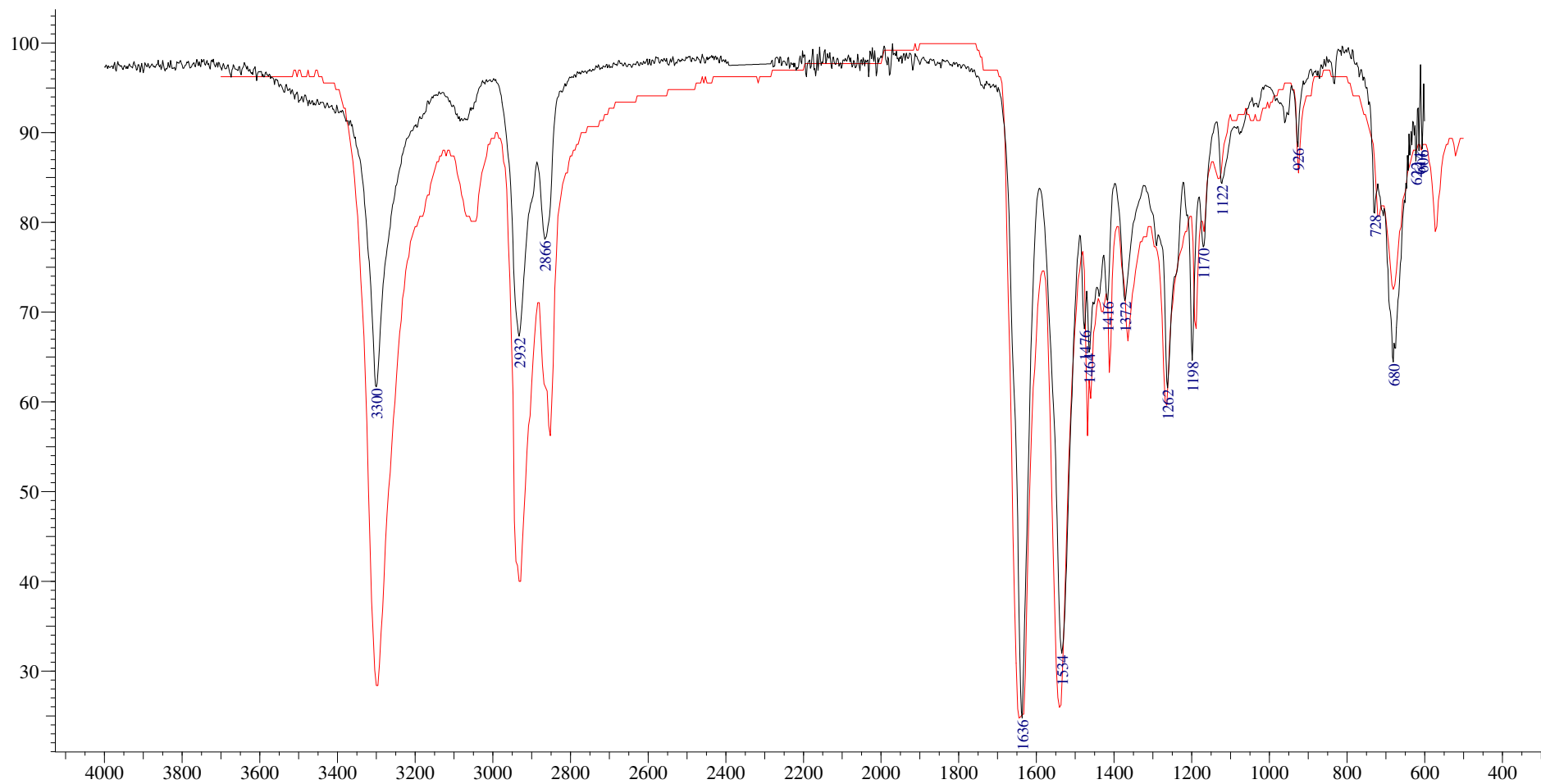
Name(s): BLUE C NYLON 10V*UNMODIFIED NYLON 6/6
Source Of Sample: MONSANTO POLYMER PRODUCTS COMPANY
Technique: FILM (CAST FROM FORMIC ACID)
Classification: Polymers: POLYAMIDES

Index	HQI	Chemical Name	Spectrum
OL #1368	765.42	BCI NYLON LX-3250*POLYHEXAMETHYLENE AD...	
OL #1362	751.60	BCI NYLON LX-3314*POLYHEXAMETHYLENE AD...	
OM #1099	730.11	CELANESE N-186	
OL #1346	728.52	BLUE C NYLON 10V*UNMODIFIED NYLON 6/6	
OL #1363	728.00	ULTRAMID A3HG5*NYLON TYPE 6/6	
OL #1367	722.46	NYPEL 1714*NYLON 6, 6/6 ALLOY	
OL #1358	718.73	NYPEL 2314*NYLON TYPE 6	
OL #1366	705.04	MONOCAST NYLON 901 TYPE 6/6	
OM #1059	699.86	ASHLENE 520	
OL #1370	697.99	ULTRAMID S3 NYLON 6/10*POLYMERIC HEXAM...	
OM #693	696.78	GILLINER 1109	
OM #1078	695.44	ANTRON 24 (TYPE 815) (VERY BRIGHT LUSTER)	
OM #1140	695.14	NY-80	
OM #1042	693.09	AKULON S223-G7	
OM #1137	692.25	RTP 283 TFE 13	
Z777 #201	692.23	PT22.6702 NYLON 6,6 RESIN ZYTEL	
OM #1058	686.80	ASHLENE 60M	
Z777 #599	683.11	J6292 Arekema PEBAX 7233 Natural Lot# ...	
Z777 #601	681.63	J6292 PEBAX 7233 Pantone 295C Lot# T10...	
AS #1928	679.95	FUS-O-BOND N-00 POLYAMIDE HOT- MELT AD...	
OL #1356	678.32	NYPEL 2315*NYLON TYPE 6	
OM #1113	678.10	NYLATRON 1018	

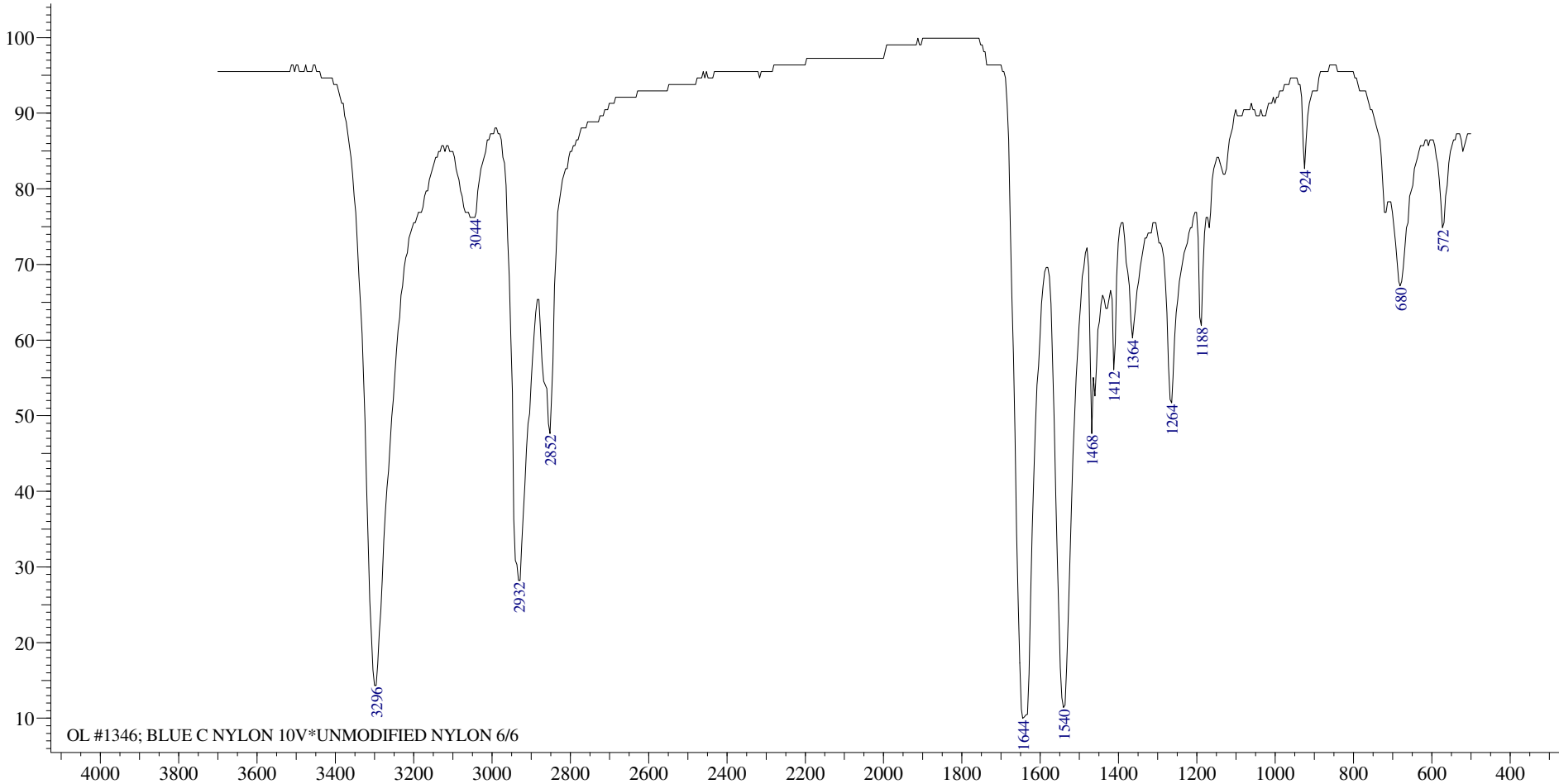
Index	HQI	Chemical Name	Spectrum
OM #1089	675.52	GRILAMID W7615	
OM #1139	675.34	THERMOFIL N11-25NG-0945	
Z777 #600	675.12	J6292 PEBAX 72D (7233) Lot# T106173	



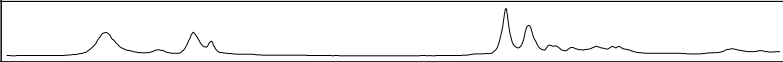
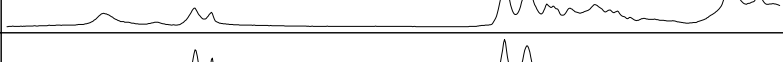
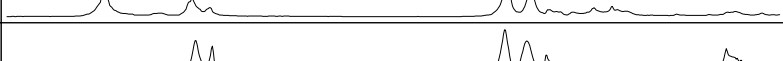
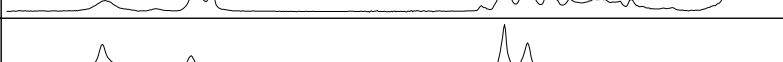
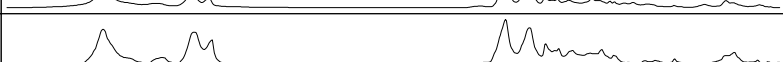
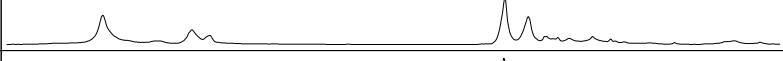
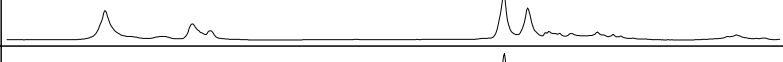
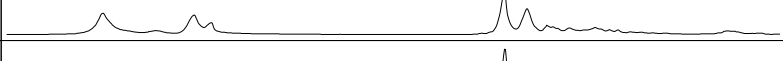
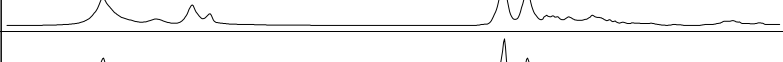
Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.

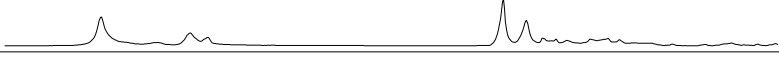


Copr. © 1980, 1981-1993 Sadtler. All Rights Reserved.

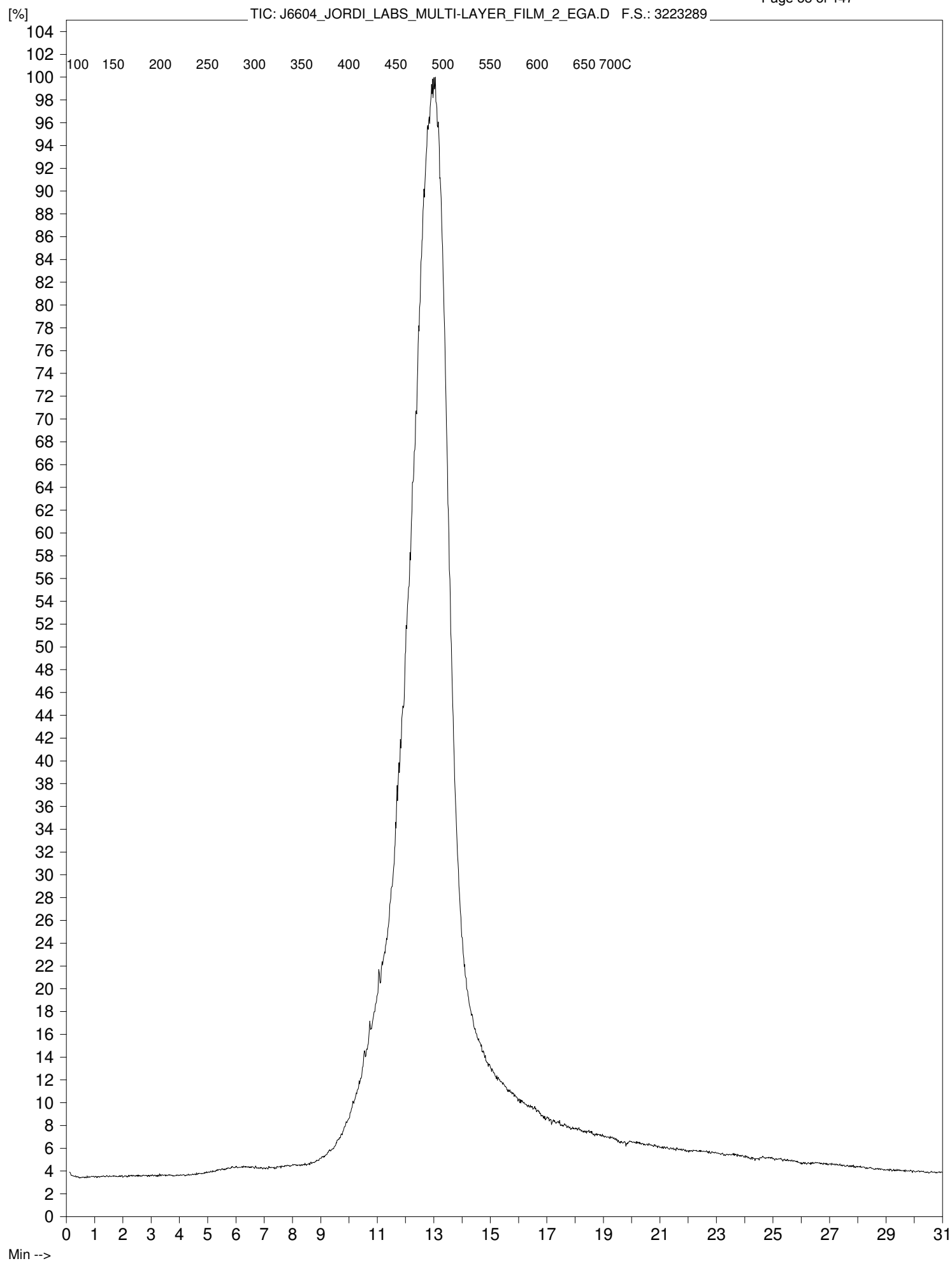


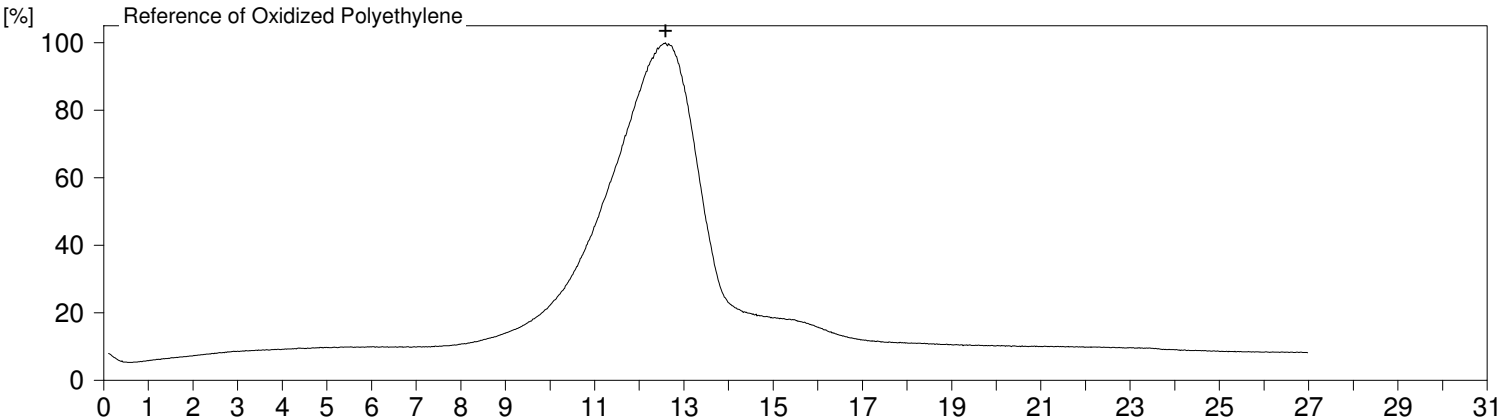
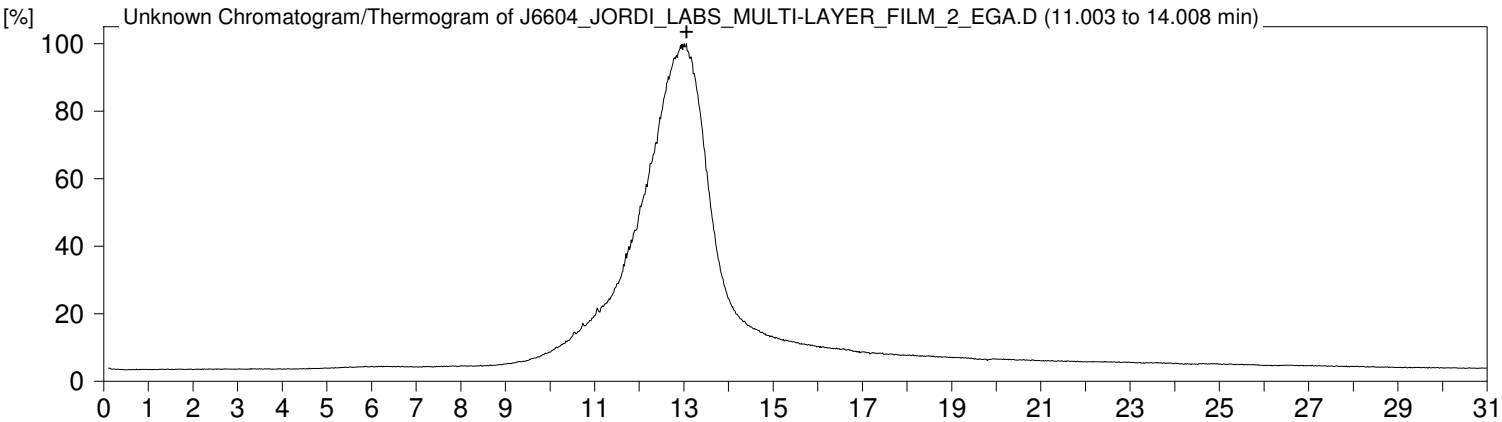
Name(s): BLUE C NYLON 10V*UNMODIFIED NYLON 6/6
Source Of Sample: MONSANTO POLYMER PRODUCTS COMPANY
Technique: FILM (CAST FROM FORMIC ACID)
Classification: Polymers: POLYAMIDES

Index	HQI	Chemical Name	Spectrum
OL #1368	729.89	BCI NYLON LX-3250*POLYHEXAMETHYLENE AD...	
OL #1367	719.50	NYPEL 1714*NYLON 6, 6/6 ALLOY	
OL #1358	714.03	NYPEL 2314*NYLON TYPE 6	
OL #1363	712.12	ULTRAMID A3HG5*NYLON TYPE 6/6	
OM #1099	708.35	CELANESE N-186	
OL #1346	706.70	BLUE C NYLON 10V*UNMODIFIED NYLON 6/6	
AS #1928	703.68	FUS-O-BOND N-00 POLYAMIDE HOT- MELT AD...	
Z777 #599	702.77	J6292 Arekema PEBAX 7233 Natural Lot# ...	
OL #1362	695.58	BCI NYLON LX-3314*POLYHEXAMETHYLENE AD...	
Z777 #601	692.90	J6292 PEBAX 7233 Pantone 295C Lot# T10...	
OM #693	691.33	GILLINER 1109	
OL #1370	688.99	ULTRAMID S3 NYLON 6/10*POLYMERIC HEXAM...	
OM #1140	680.17	NY-80	
Z777 #600	678.75	J6292 PEBAX 72D (7233) Lot# T106173	
OL #1366	675.74	MONOCAST NYLON 901 TYPE 6/6	
OM #521	675.49	PEBAX 6312 MN 00	
OM #1059	674.75	ASHLENE 520	
OL #1356	673.48	NYPEL 2315*NYLON TYPE 6	
OM #1139	671.93	THERMOFIL N11-25NG-0945	
OM #1078	671.37	ANTRON 24 (TYPE 815) (VERY BRIGHT LUSTER)	
OM #1153	671.04	NY-50	
OM #1104	669.89	THERMOCOMP PC-1006	

Index	HQI	Chemical Name	Spectrum
OM #1089	669.52	GRILAMID W7615	
OM #1037	668.93	AKULON M138-H	
OM #1137	664.42	RTP 283 TFE 13	

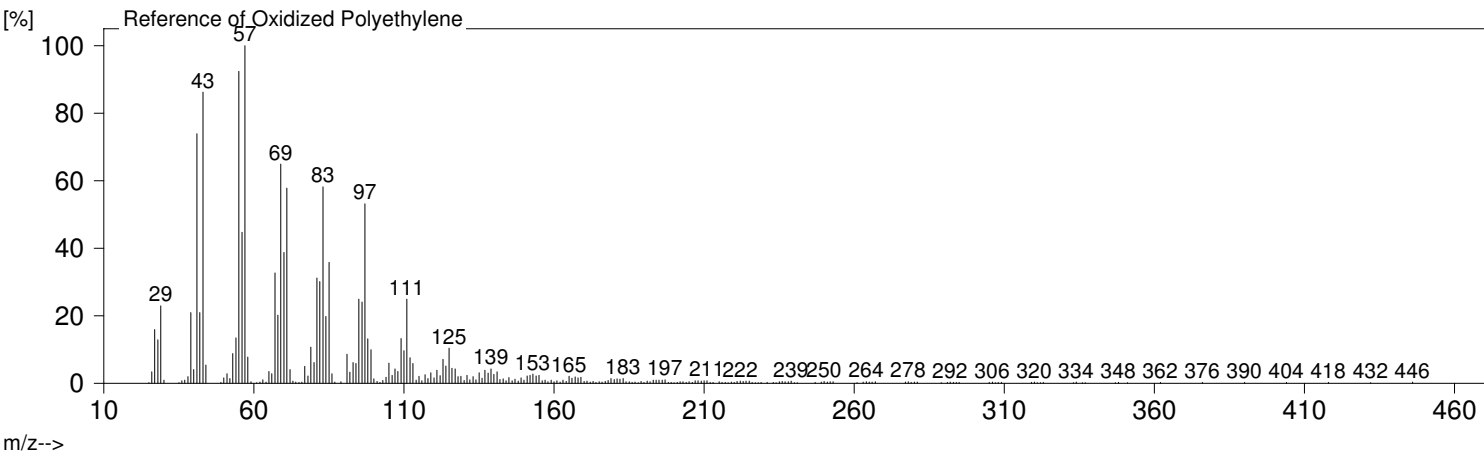
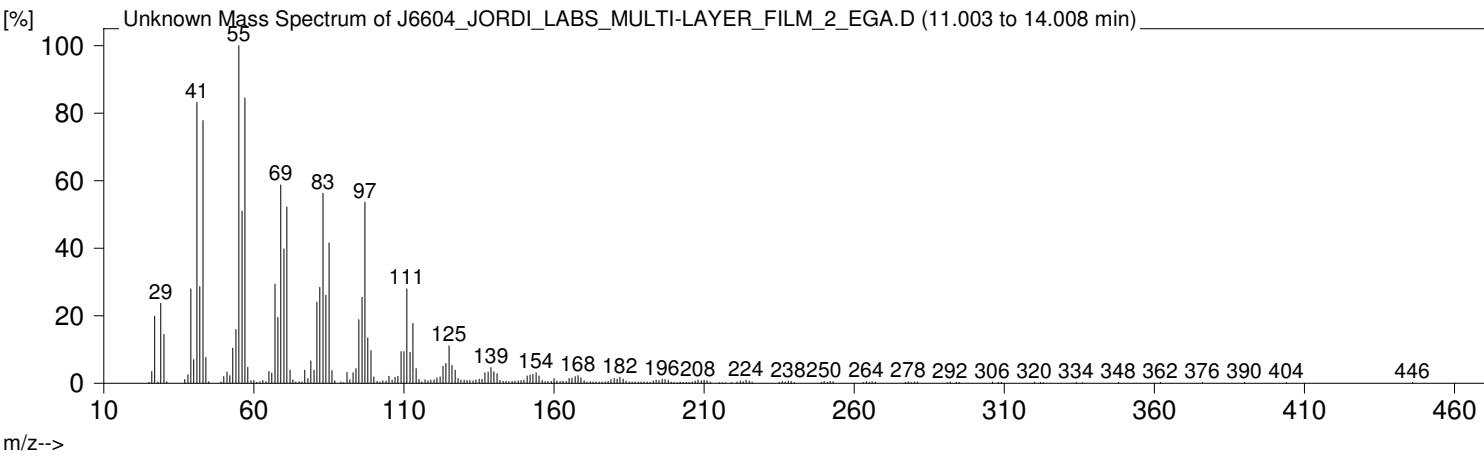
PYMS Data



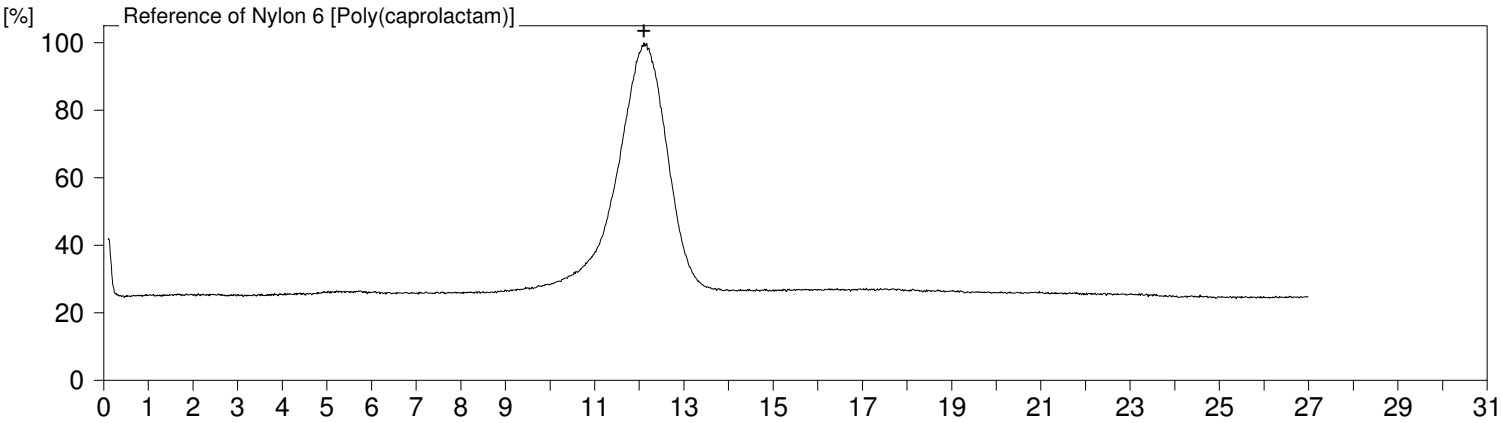
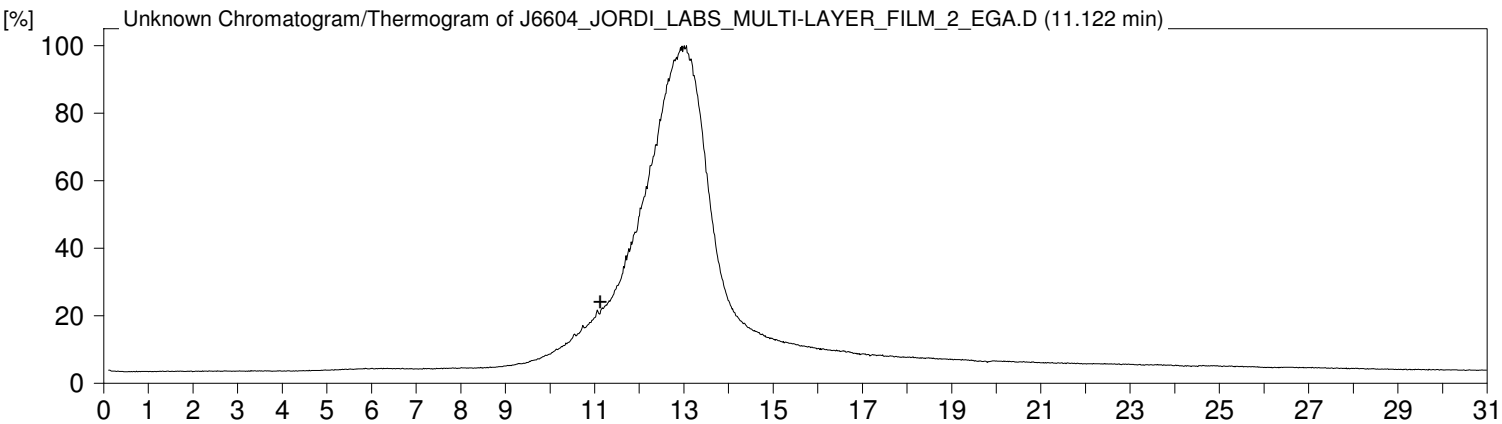


Min -->

Polymer / Additive		Entry ID	Start [C]	Top [C]	End [C]	Qual [%]
1	Oxidized Polyethylene		445	477	513	97
2	Polyethylene, low density		457	509	533	96
3	Polyethylene HD		467	499	527	96
4	Polyethylene LD		445	492	520	96
5	Ethylene / Propylene Copolymer; 60% Ethylene		460	505	535	95
6	Polyethylene, high density		474	512	535	95
7	Polyethylene, oxidized, Acid number 16mg KOH/g		446	498	525	95
8	Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (12.6-		478	491	520	94
9	Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (11.0-		430	466	520	94
10	Ethylene / Acrylic Acid Copolymer; Acrylic Acid Content 15% (9.5-14.0		385	490	520	94
11	Ethylene / Acrylic Acid Copolymer; Acrylic Acid Content 15% (13.0-14.		447	490	520	94
12	Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	459	94
13	Ethylene/Acrylic Acid		400	490	535	93
14	Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	512	92

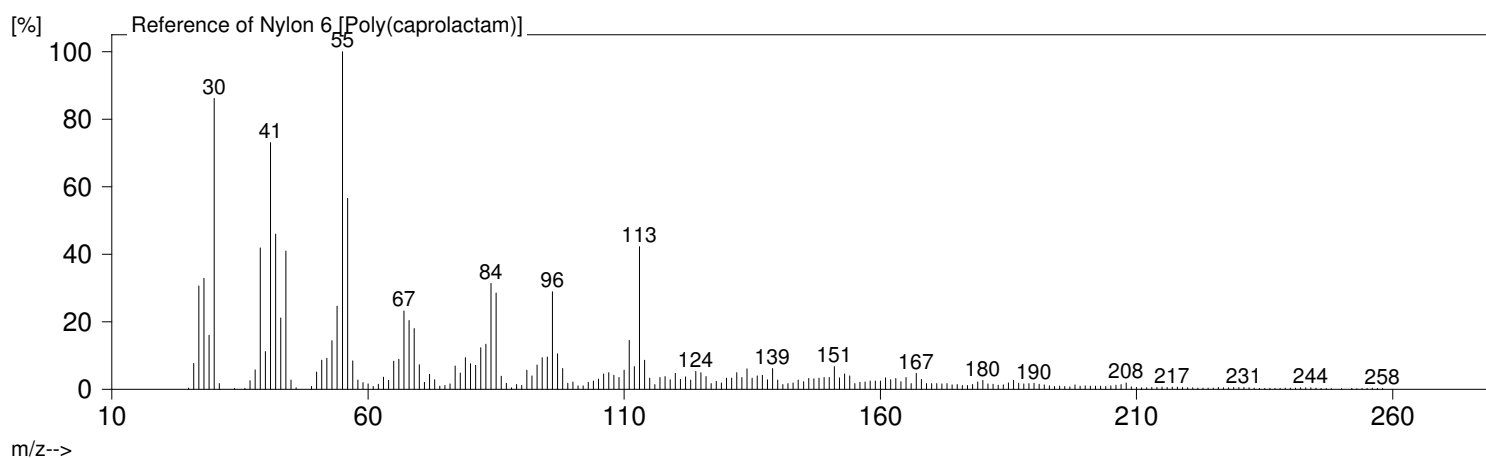
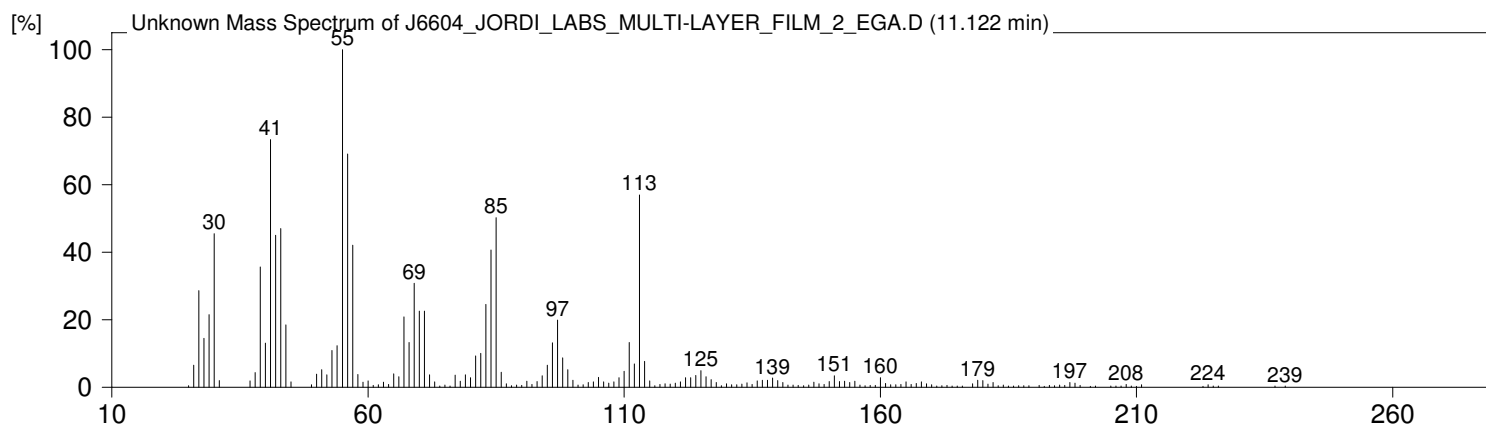


Polymer / Additive		Entry ID	Start [C]	Top [C]	End [C]	Qual [%]
1	Oxidized Polyethylene		445	477	513	97
2	Polyethylene, low density		457	509	533	96
3	Polyethylene HD		467	499	527	96
4	Polyethylene LD		445	492	520	96
5	Ethylene / Propylene Copolymer; 60% Ethylene		460	505	535	95
6	Polyethylene, high density		474	512	535	95
7	Polyethylene, oxidized, Acid number 16mg KOH/g		446	498	525	95
8	Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (12.6-		478	491	520	94
9	Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (11.0-		430	466	520	94
10	Ethylene / Acrylic Acid Copolymer; Acrylic Acid Content 15% (9.5-14.0		385	490	520	94
11	Ethylene / Acrylic Acid Copolymer; Acrylic Acid Content 15% (13.0-14.		447	490	520	94
12	Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	459	94
13	Ethylene/Acrylic Acid		400	490	535	93
14	Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	512	92



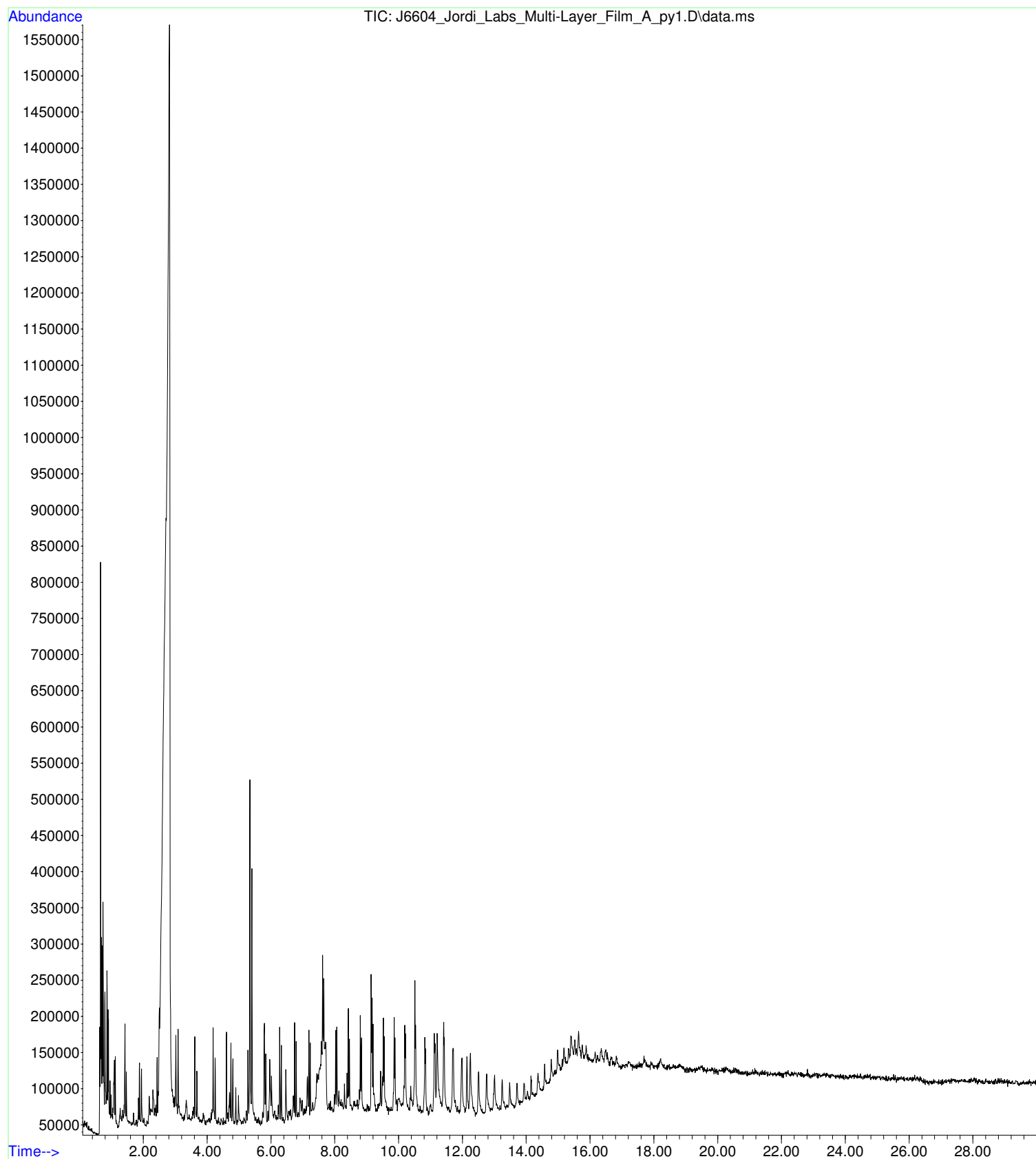
Min -->

Polymer / Additive		Entry ID	Start [C]	Top [C]	End [C]	Qual [%]
1	Nylon 6 [Poly(caprolactam)]		440	463	484	83
2	SP^2 #27 Cryoground Nylon 6 (Polycaprolactam)		430	466	490	80
3	SP^2 Nylon 6 [Poly(caprolactam)] Pellet		430	469	490	79
4	Brugglen C10 Cast Nylon catalyst 17-19% Sodiumcaprolactamate in cap		400	410	415	79
5	Broggolen C10 Cast Nylon catalyst 17-19% Sodiumcaprolactamate in ca		115	129	415	78
6	Bruggolen C10 Cast Nylon catalyst		115	129	166	77
7	Irganox 565		280	362	535	71
8	Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	459	71
9	Nylon 6/12 [Poly(hexamethylene dodecanediamide)]		451	481	507	71
10	Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (11.0-		430	466	473	70
11	Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (11.0-		430	466	520	69
12	Nylon 12 [Poly(lauryllactam)]		445	487	512	69
13	Oxidized Polyethylene		445	477	513	67
14	Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	512	67



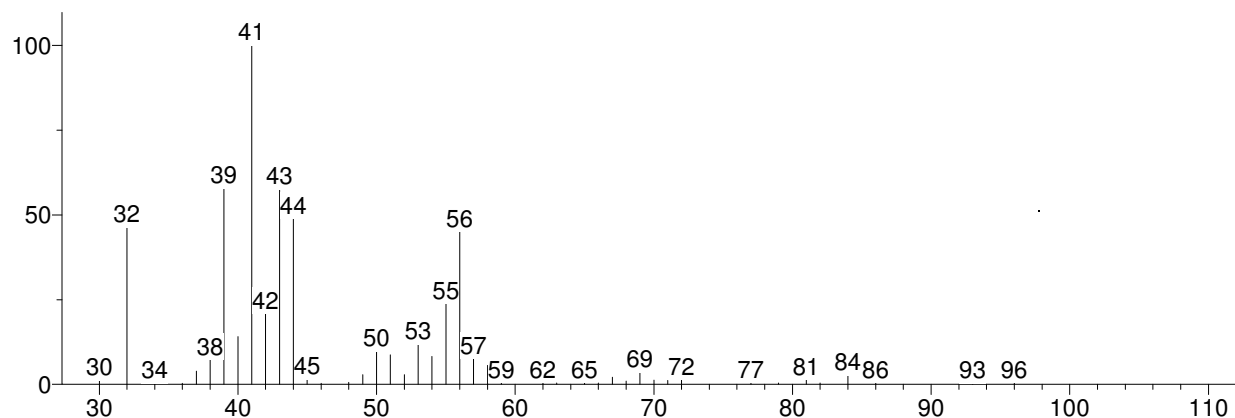
Polymer / Additive	Entry ID	Start [C]	Top [C]	End [C]	Qual [%]
1 Nylon 6 [Poly(caprolactam)]		440	463	484	83
2 SP^2 #27 Cryoground Nylon 6 (Polycaprolactam)		430	466	490	80
3 SP^2 Nylon 6 [Poly(caprolactam)] Pellet		430	469	490	79
4 Brugglen C10 Cast Nylon catalyst 17-19% Sodiumcaprolactamate in cap		400	410	415	79
5 Broggolen C10 Cast Nylon catalyst 17-19% Sodiumcaprolactamate in ca		115	129	415	78
6 Bruggolen C10 Cast Nylon catalyst		115	129	166	77
7 Irganox 565		280	362	535	71
8 Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	459	71
9 Nylon 6/12 [Poly(hexamethylene dodecanediamide)]		451	481	507	71
10 Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (11.0-		430	466	473	70
11 Ethylene / Ethyl Acrylate Copolymer; Ethyl Acrylate Content 18% (11.0-		430	466	520	69
12 Nylon 12 [Poly(lauryllactam)]		445	487	512	69
13 Oxidized Polyethylene		445	477	513	67
14 Ethylene / Methacrylic Acid Copolymer; Methacrylic Acid Content 12%		430	448	512	67

File :C:\msdchem\1\DATA\2012\Temp\040512\J6604_Jordi_Labs_Multi-La
... yer_Film_A_py1.D
Operator : Mark Jordi
Instrument : Instrument #1
Acquired : 9 Apr 2012 9:14 using AcqMethod PYMS.M
Sample Name: J6604 Jordi Labs Multi-Layer Film
Misc Info : J6604 Jordi Labs Multi-Layer Film

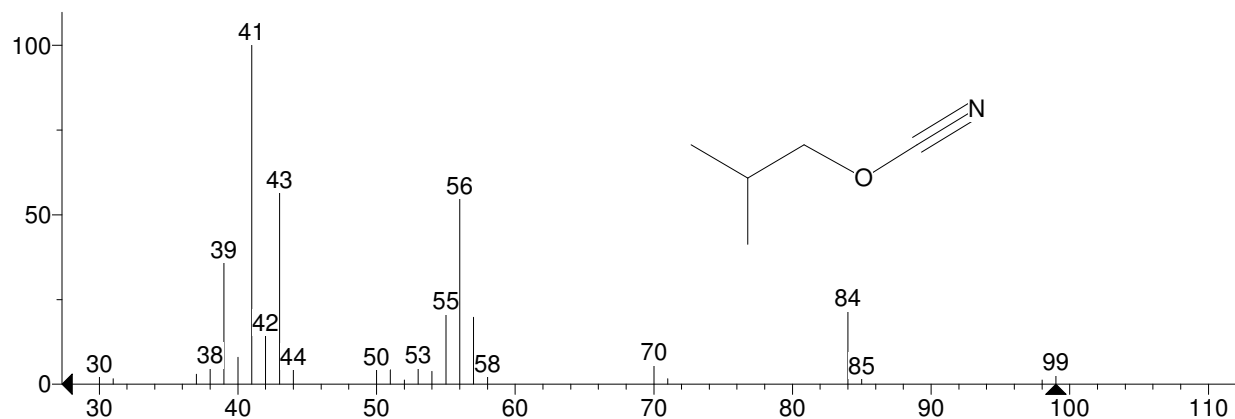


** Search Report Page 1 of 1 **

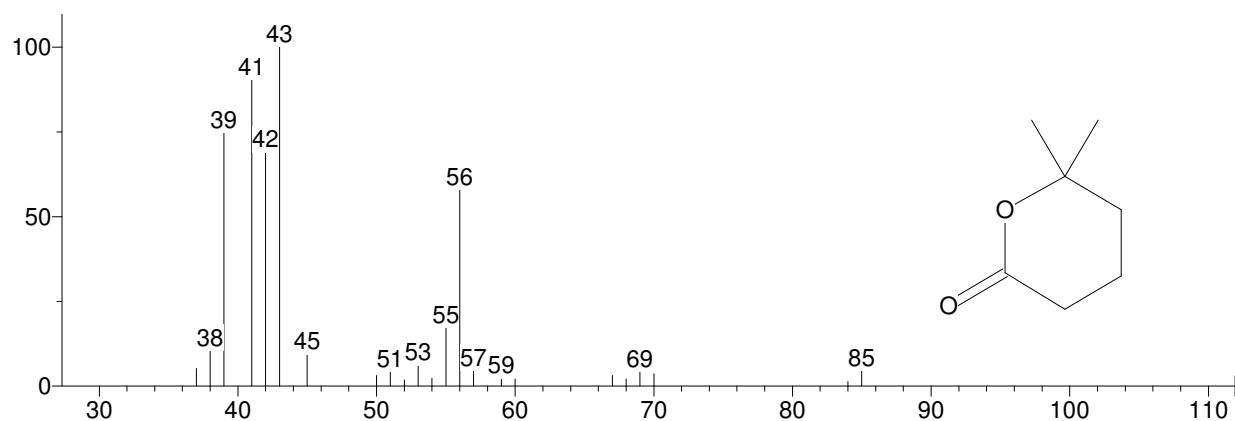
Unknown: Scan 79 (0.683 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms
Compound in Library Factor = -709



Hit 1 : Cyanic acid, 2-methylpropyl ester
C₅H₉NO; MF: 756; RMF: 811; Prob 18.0%; CAS: 1768-25-8; Lib: mainlib; ID: 2242.

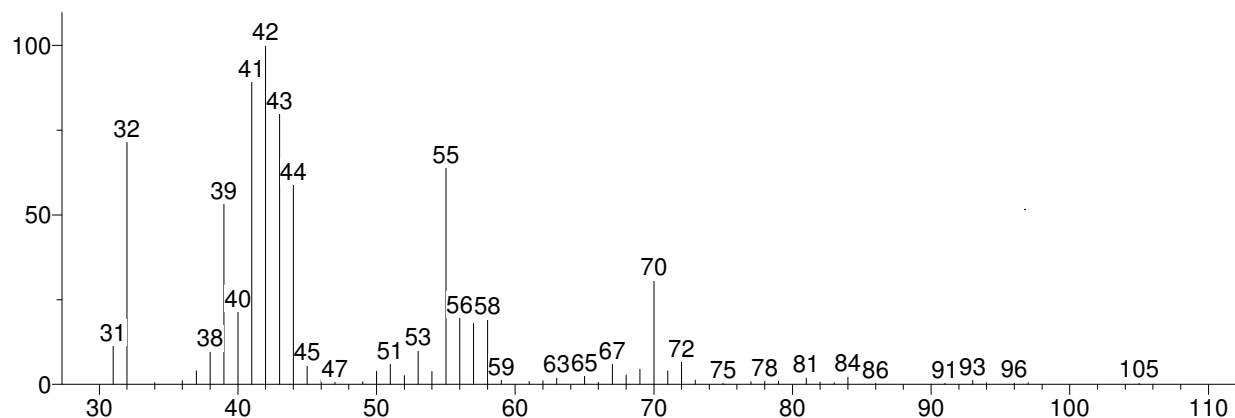


Hit 2 : 2H-Pyran-2-one, tetrahydro-6,6-dimethyl-
C₇H₁₂O₂; MF: 748; RMF: 843; Prob 13.5%; CAS: 2610-95-9; Lib: mainlib; ID: 5443.

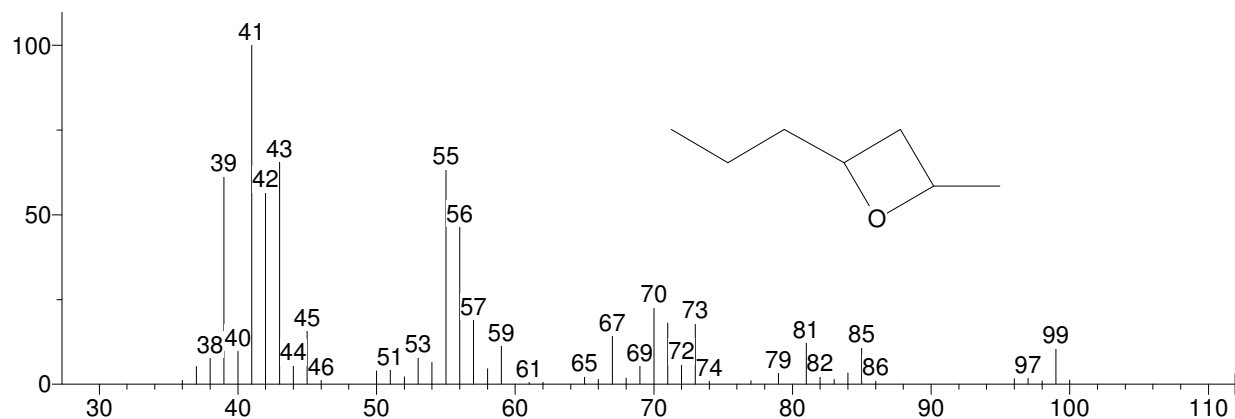


** Search Report Page 1 of 1 **

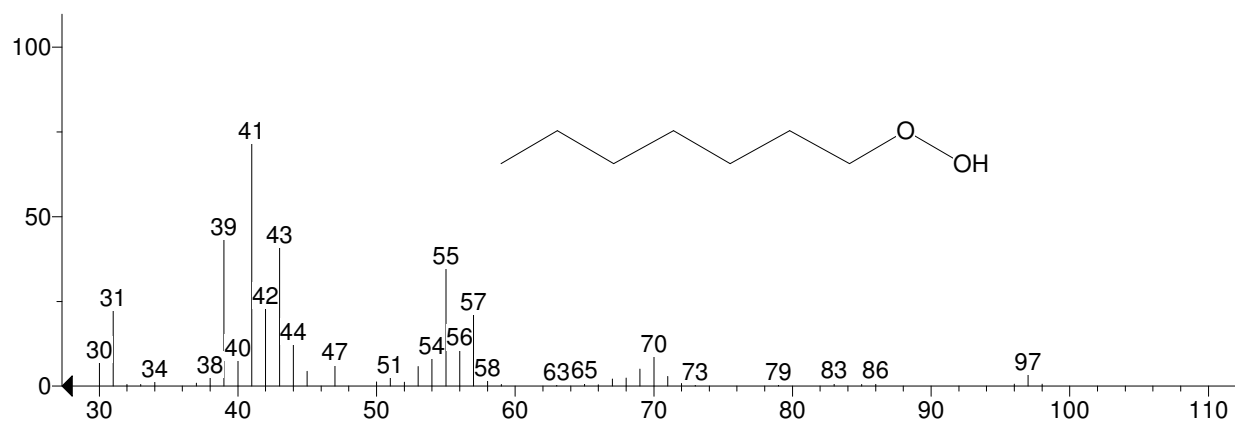
Unknown: Scan 82 (0.706 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms
Compound in Library Factor = -825



Hit 1 : Oxetane, 2-methyl-4-propyl-
C₇H₁₄O; MF: 729; RMF: 736; Prob 9.65%; CAS: 7045-79-6; Lib: mainlib; ID: 2216.

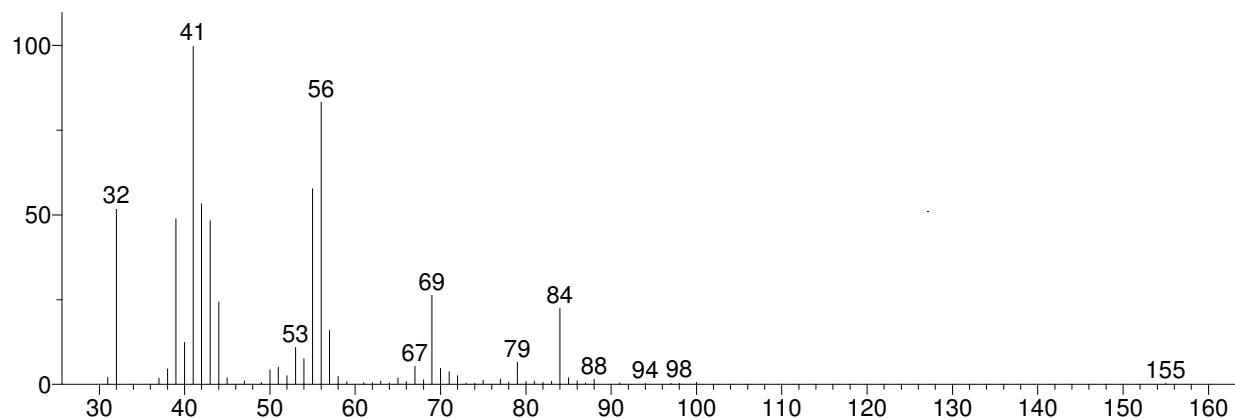


Hit 2 : Hydroperoxide, heptyl
C₇H₁₆O₂; MF: 728; RMF: 743; Prob 9.28%; CAS: 764-81-8; Lib: mainlib; ID: 357.

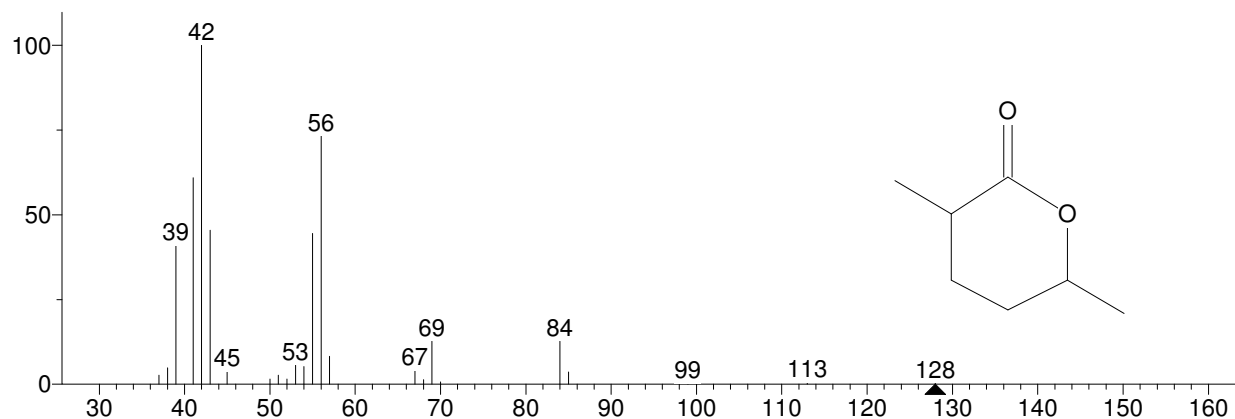


** Search Report Page 1 of 1 **

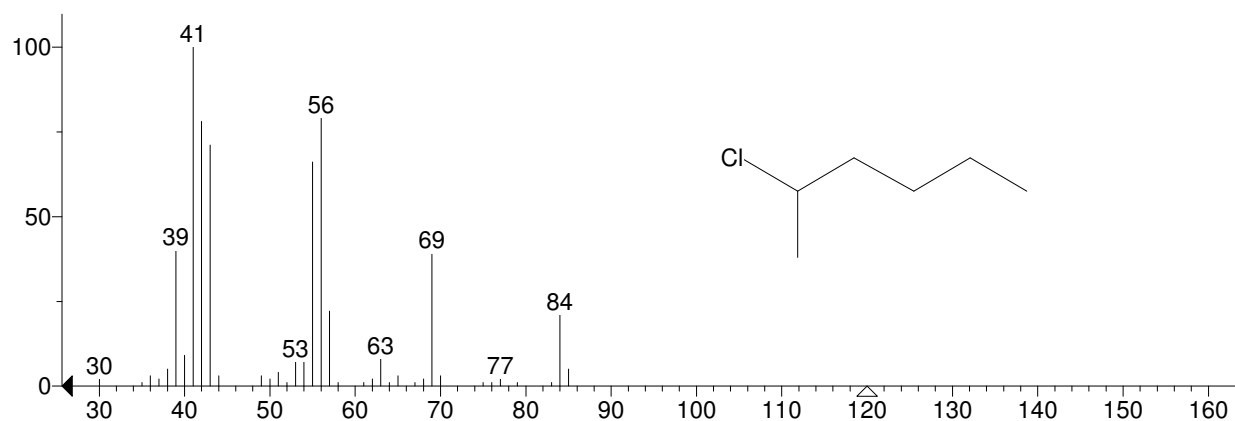
Unknown: Scan 86 (0.736 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms
Compound in Library Factor = -509



Hit 1 : 2H-Pyran-2-one, tetrahydro-3,6-dimethyl-
C₇H₁₂O₂; MF: 800; RMF: 877; Prob 9.05%; CAS: 3720-22-7; Lib: replib; ID: 1405.

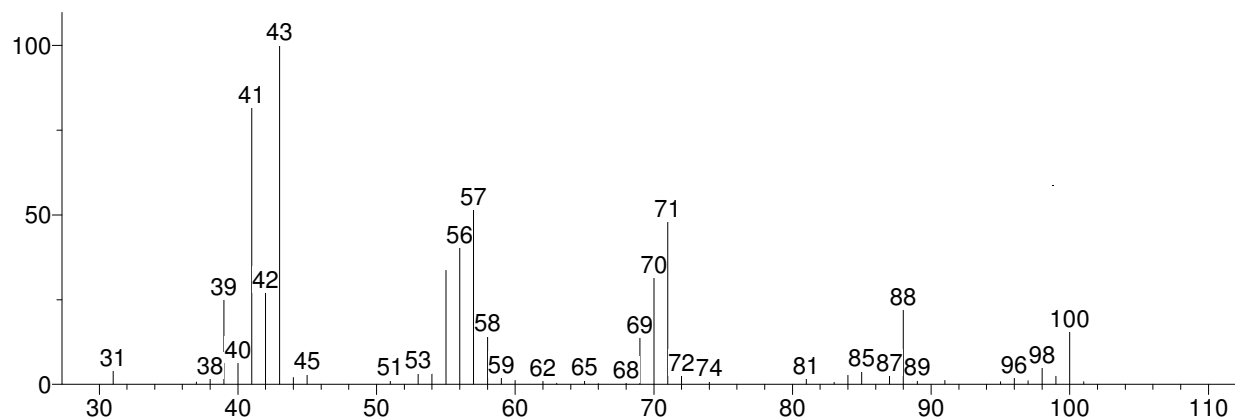


Hit 2 : Hexane, 2-chloro-
C₆H₁₃Cl; MF: 796; RMF: 849; Prob 7.65%; CAS: 638-28-8; Lib: replib; ID: 712.

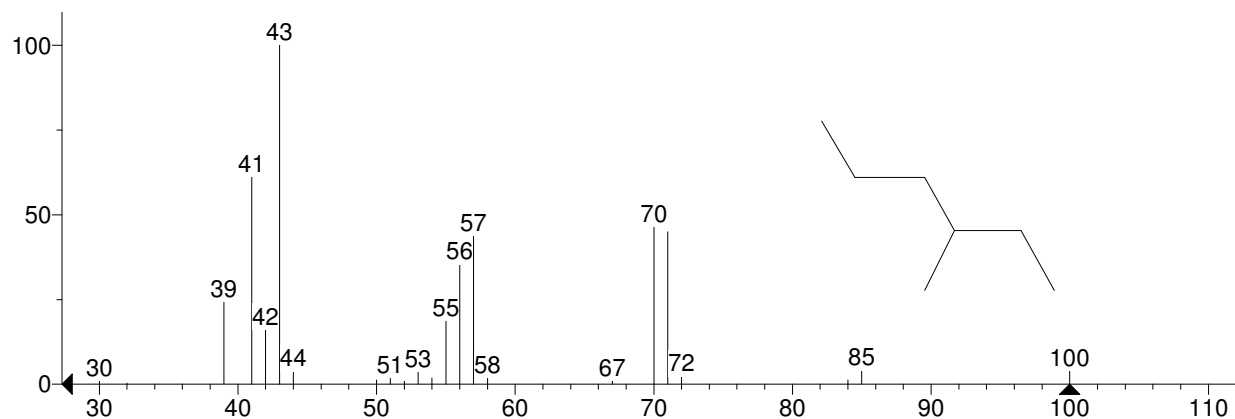


** Search Report Page 1 of 1 **

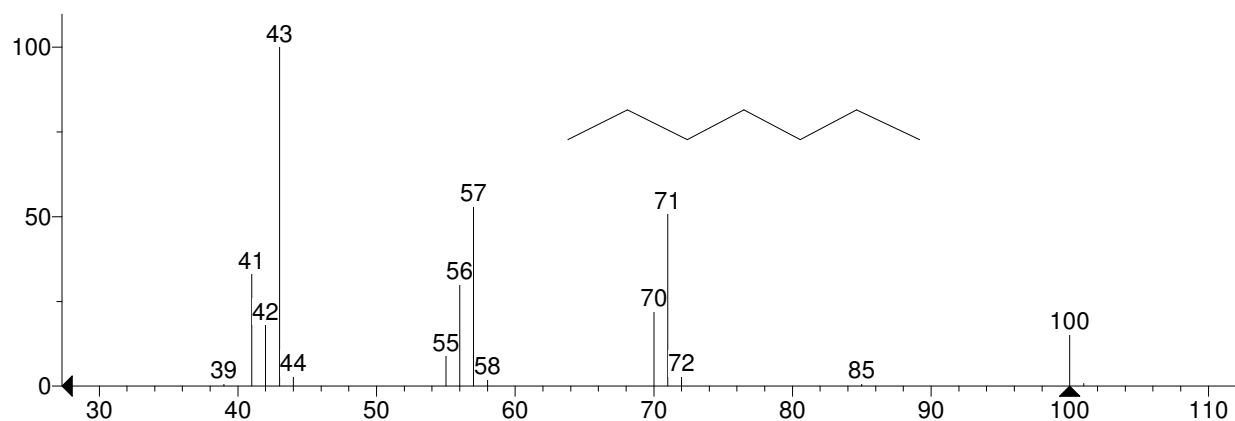
Unknown: Scan 94 (0.796 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-91)
Compound in Library Factor = -520



Hit 1 : Hexane, 3-methyl-
C₇H₁₆; MF: 785; RMF: 888; Prob 24.6%; CAS: 589-34-4; Lib: replib; ID: 1745.

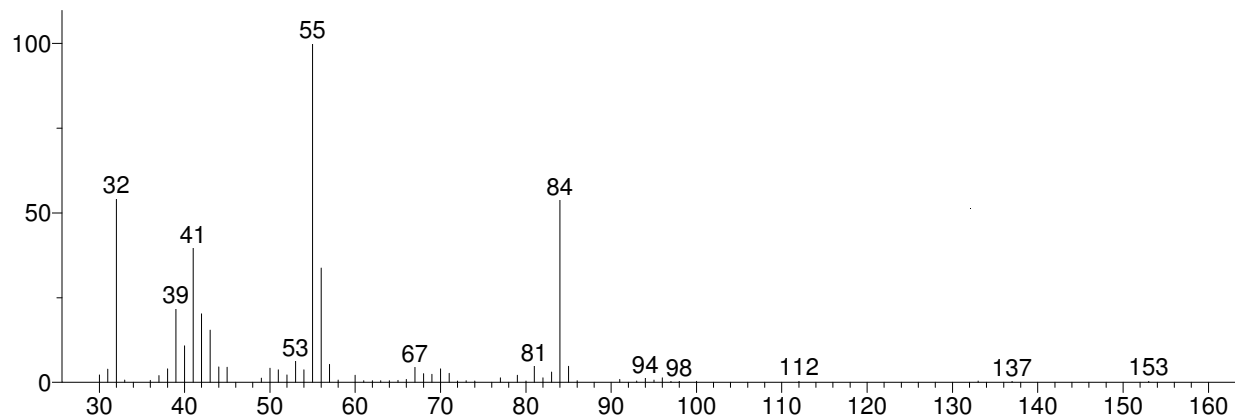


Hit 2 : Heptane
C₇H₁₆; MF: 766; RMF: 877; Prob 11.9%; CAS: 142-82-5; Lib: replib; ID: 2155.

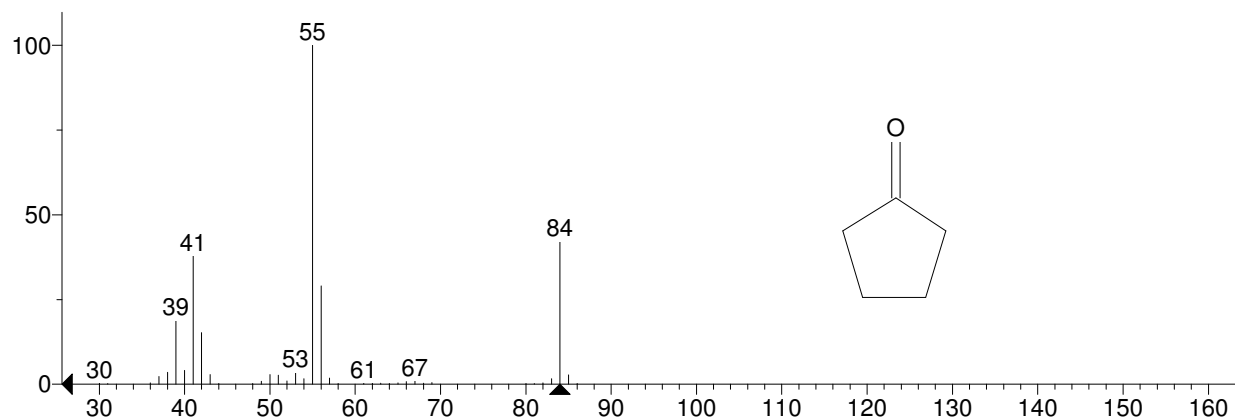


** Search Report Page 1 of 1 **

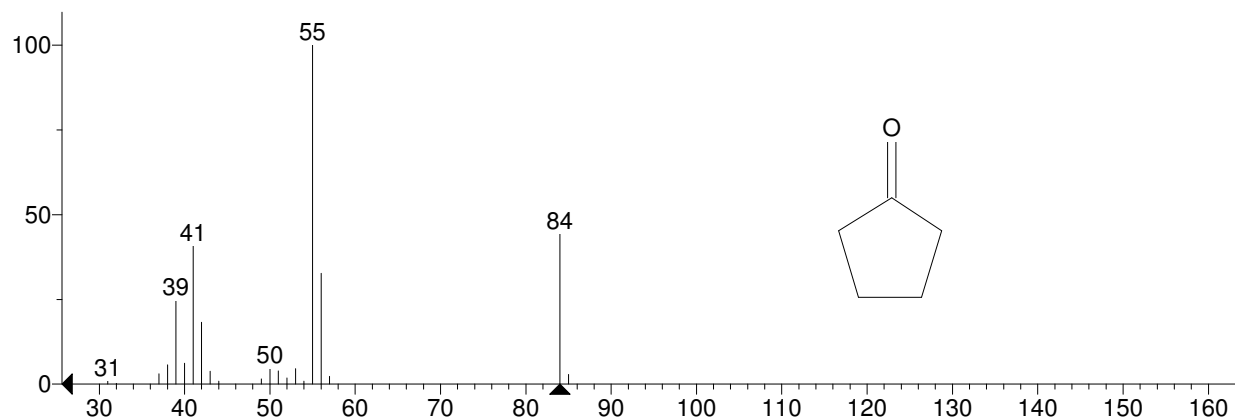
Unknown: Scan 103 (0.864 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms
Compound in Library Factor = -458



Hit 1 : Cyclopentanone
C5H8O; MF: 778; RMF: 866; Prob 28.8%; CAS: 120-92-3; Lib: mainlib; ID: 17101.

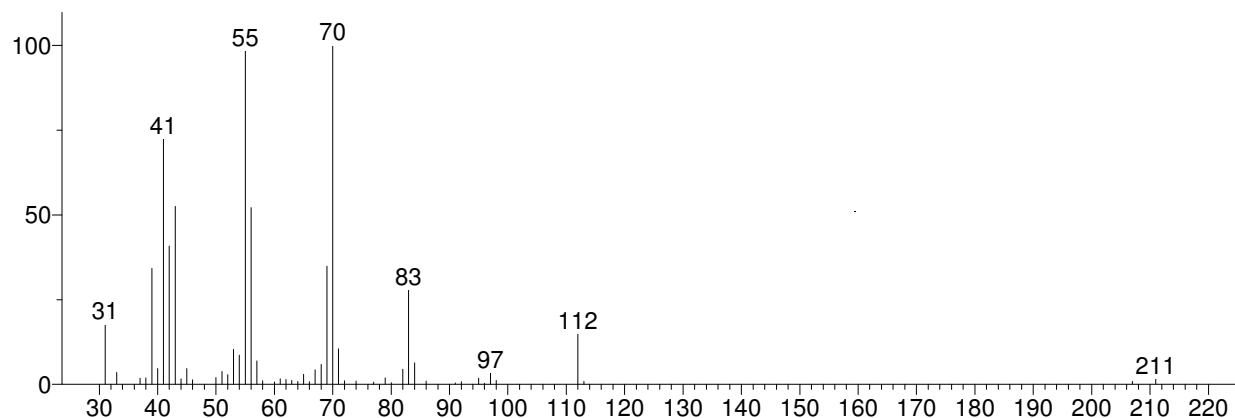


Hit 2 : Cyclopentanone
C5H8O; MF: 770; RMF: 845; Prob 28.8%; CAS: 120-92-3; Lib: replib; ID: 4118.



** Search Report Page 1 of 1 **

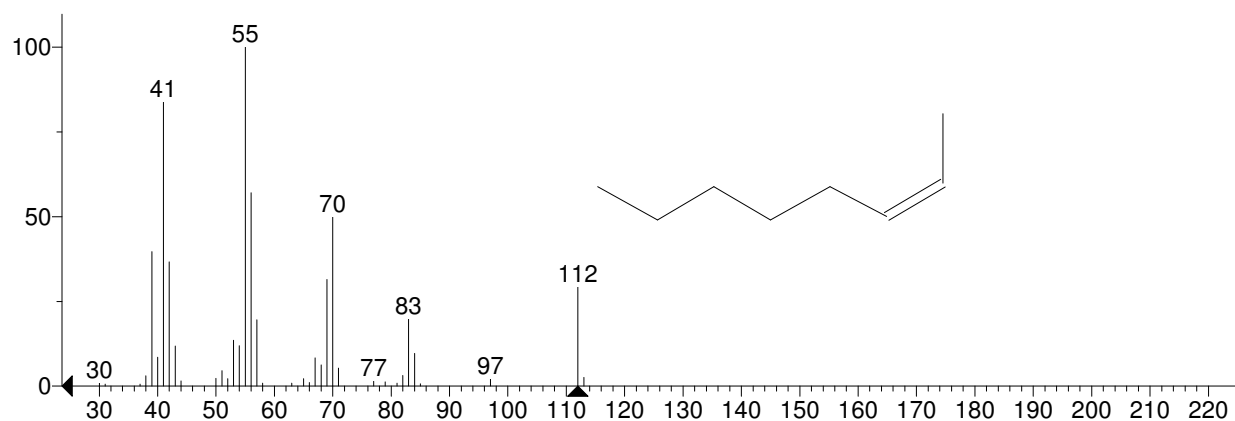
Unknown: Scan 107 (0.894 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-105)
Compound in Library Factor = -331



Hit 1 : 2-Octene
C₈H₁₆; MF: 849; RMF: 880; Prob 9.58%; CAS: 111-67-1; Lib: replib; ID: 4194.

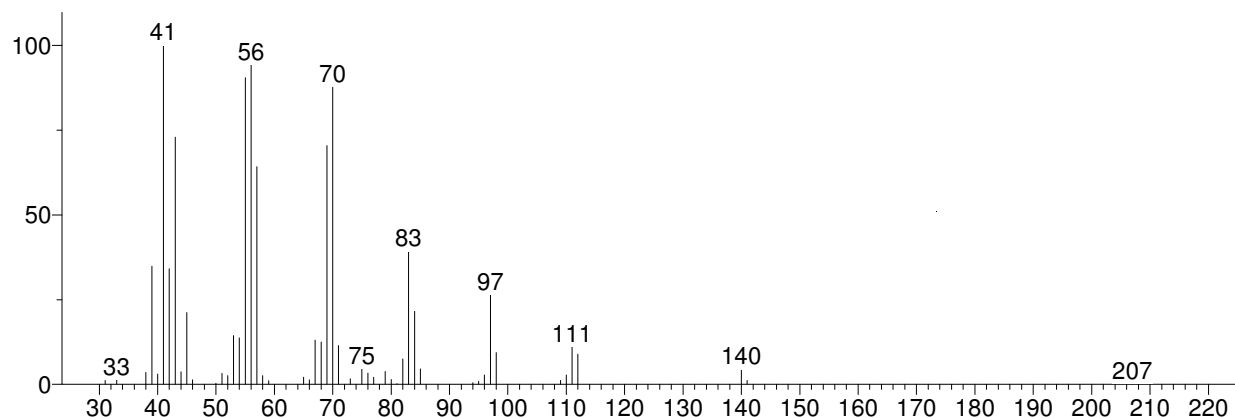


Hit 2 : 2-Octene, (Z)-
C₈H₁₆; MF: 837; RMF: 862; Prob 6.38%; CAS: 7642-04-8; Lib: replib; ID: 4208.

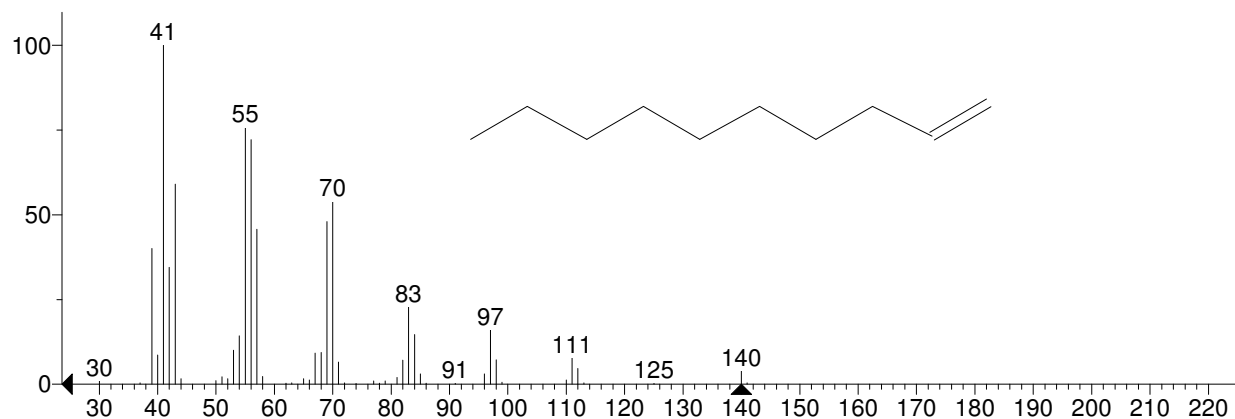


** Search Report Page 1 of 1 **

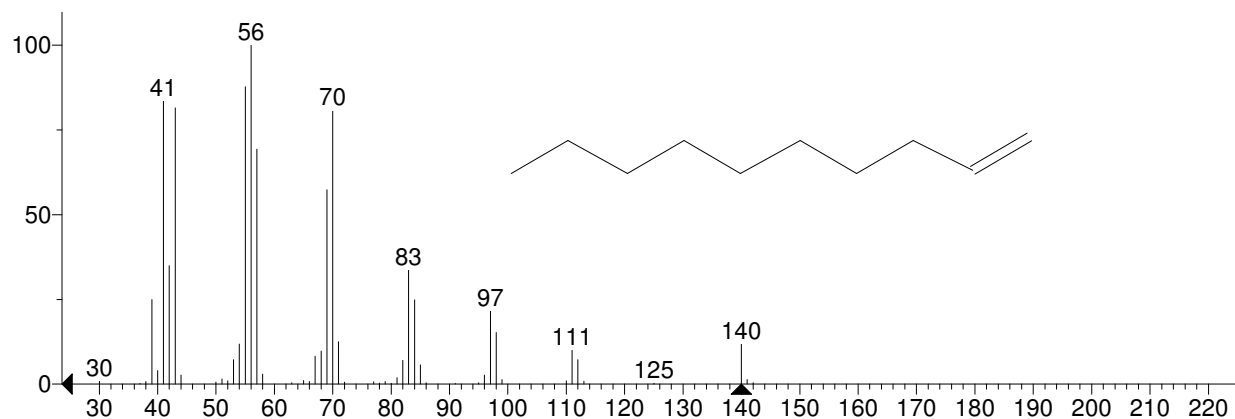
Unknown: Scan 177 (1.421 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-173)
Compound in Library Factor = -168



Hit 1 : 1-Decene
C₁₀H₂₀; MF: 885; RMF: 908; Prob 14.0%; CAS: 872-05-9; Lib: replib; ID: 896.

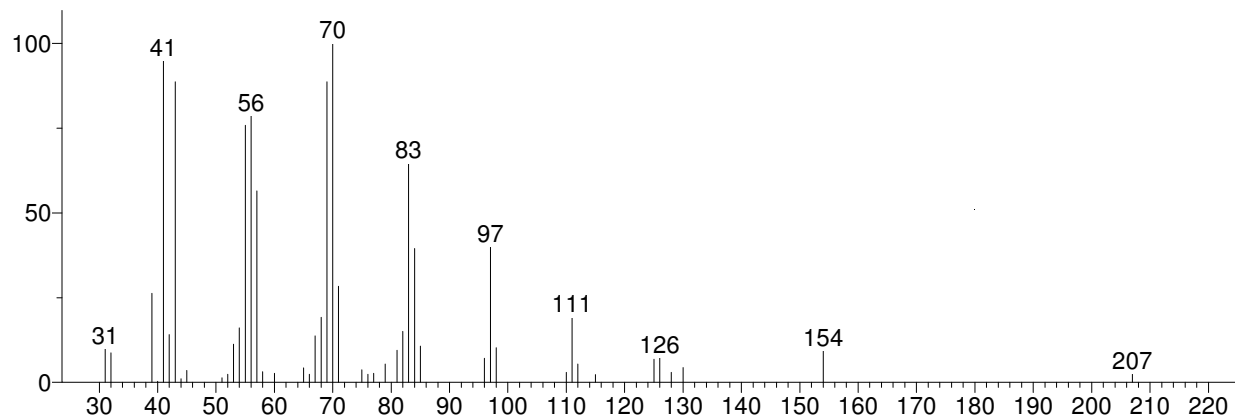


Hit 2 : 1-Decene
C₁₀H₂₀; MF: 866; RMF: 885; Prob 14.0%; CAS: 872-05-9; Lib: mainlib; ID: 20152.

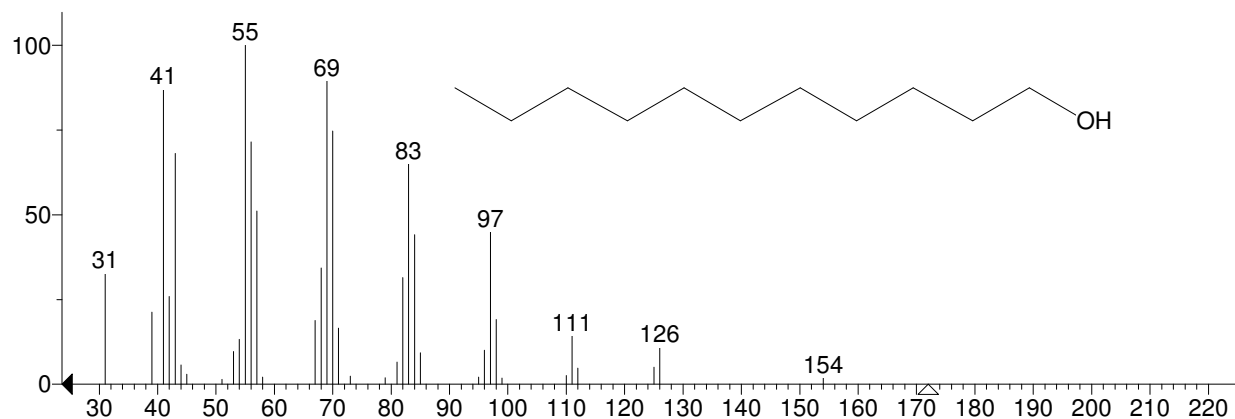


** Search Report Page 1 of 1 **

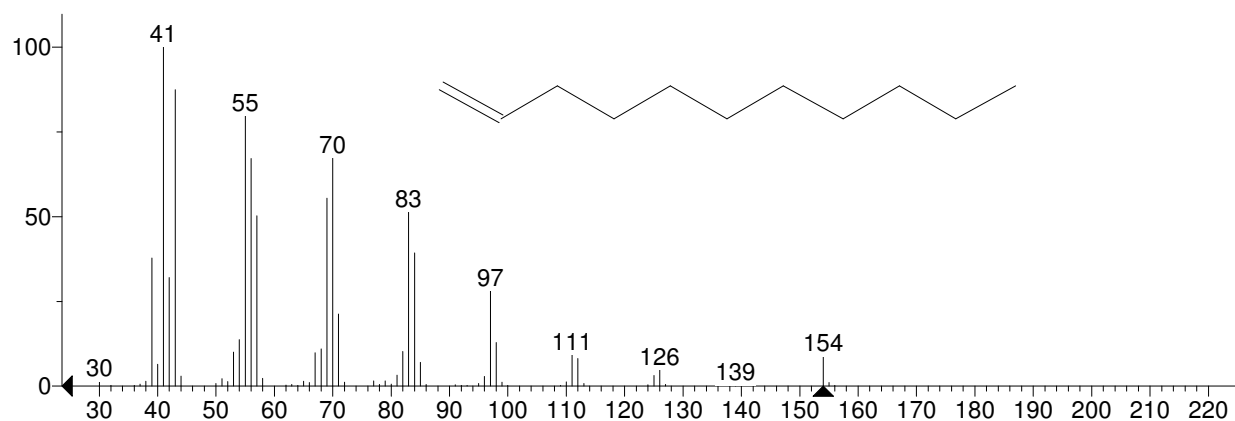
Unknown: Scan 238 (1.881 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-235)
Compound in Library Factor = -246



Hit 1 : 1-Undecanol
C₁₁H₂₄O; MF: 866; RMF: 893; Prob 4.71%; CAS: 112-42-5; Lib: mainlib; ID: 18199.

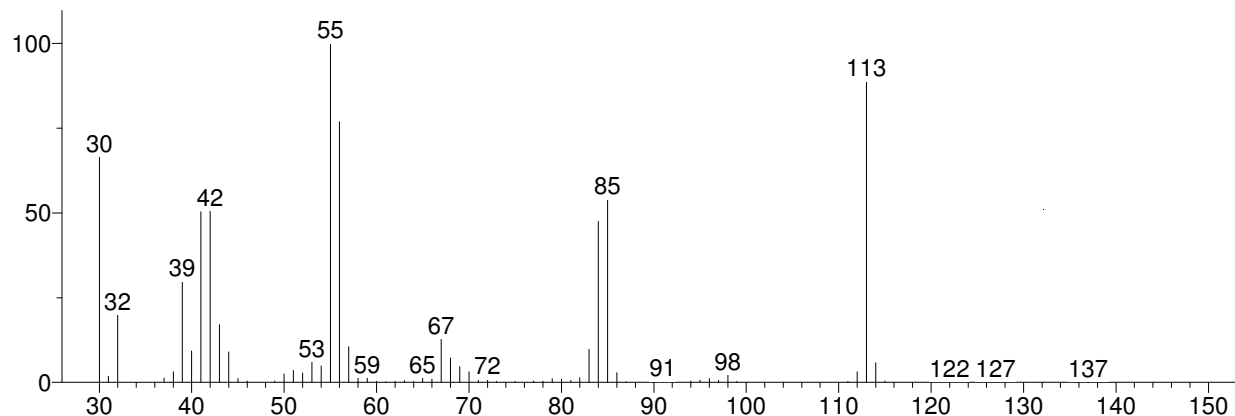


Hit 2 : 1-Undecene
C₁₁H₂₂; MF: 865; RMF: 888; Prob 4.52%; CAS: 821-95-4; Lib: replib; ID: 825.

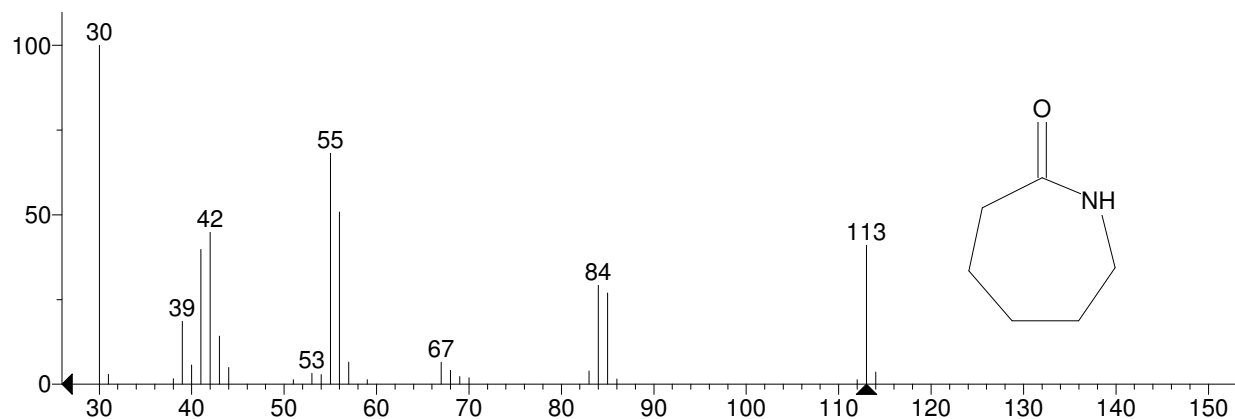


** Search Report Page 1 of 1 **

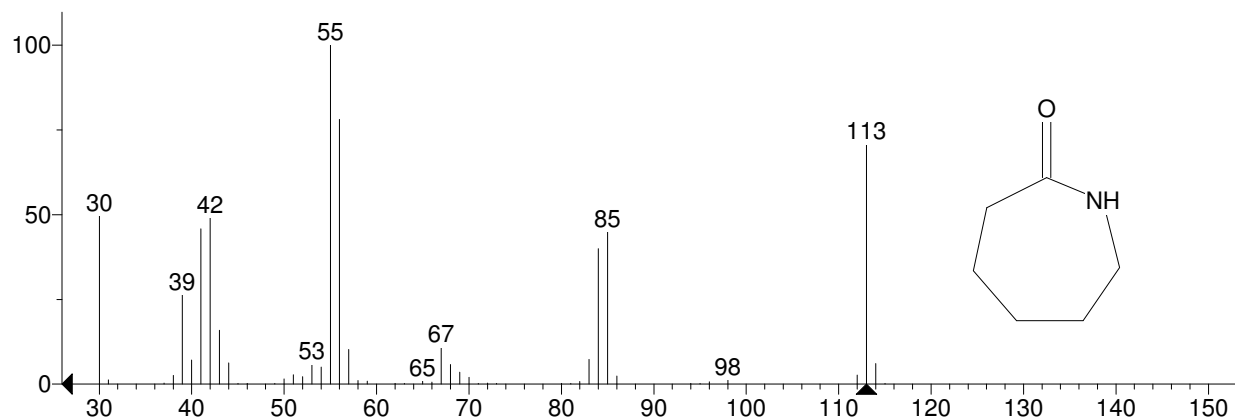
Unknown: Scan 349 (2.717 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms
Compound in Library Factor = 316



Hit 1 : Caprolactam
C₆H₁₁NO; MF: 922; RMF: 952; Prob 86.4%; CAS: 105-60-2; Lib: replib; ID: 413.

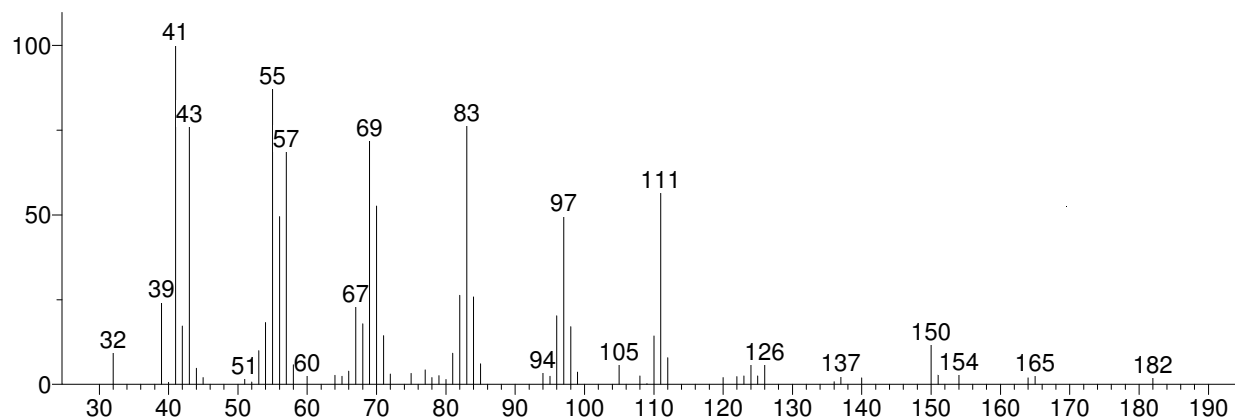


Hit 2 : Caprolactam
C₆H₁₁NO; MF: 904; RMF: 915; Prob 86.4%; CAS: 105-60-2; Lib: replib; ID: 4436.

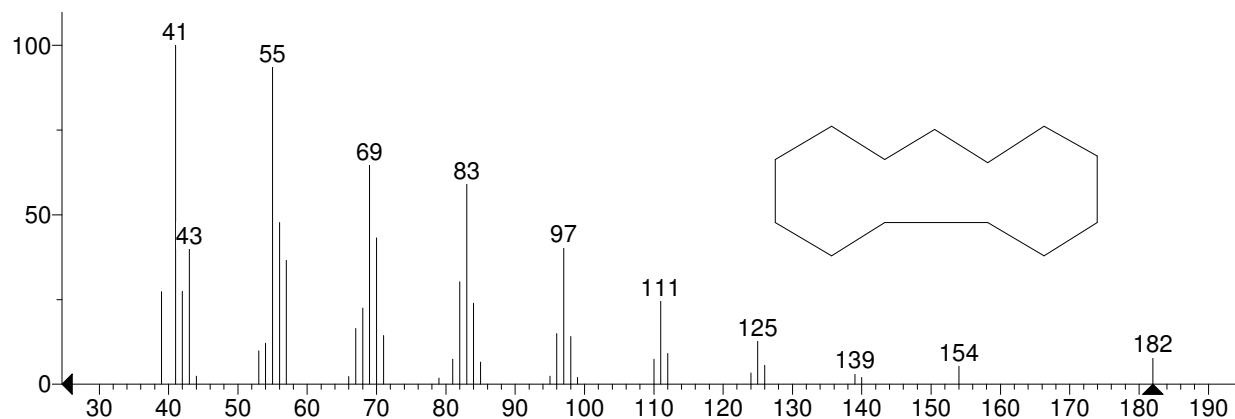


** Search Report Page 1 of 1 **

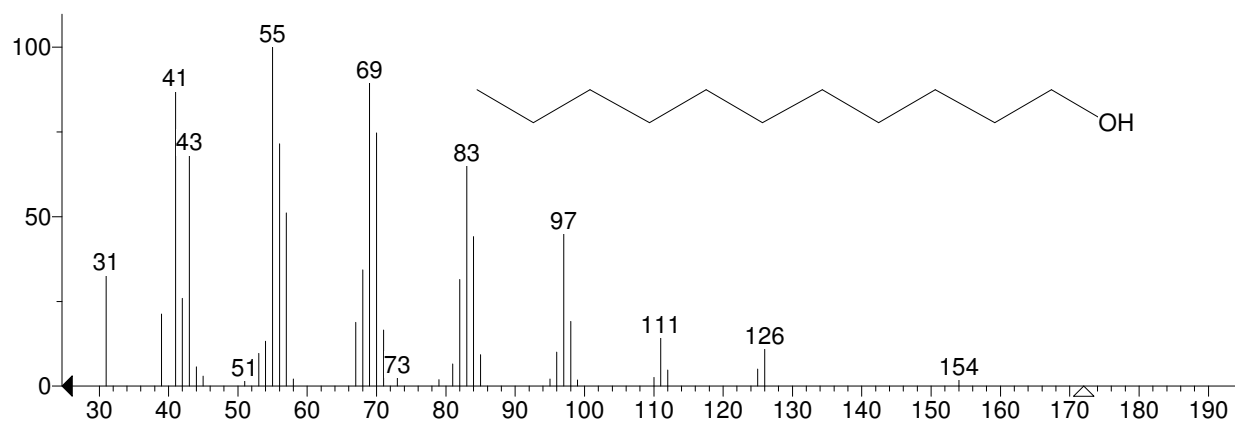
Unknown: Scan 389 (3.019 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-384)
Compound in Library Factor = -367



Hit 1 : Cyclotridecane
C₁₃H₂₆; MF: 829; RMF: 887; Prob 9.61%; CAS: 295-02-3; Lib: mainlib; ID: 2603.

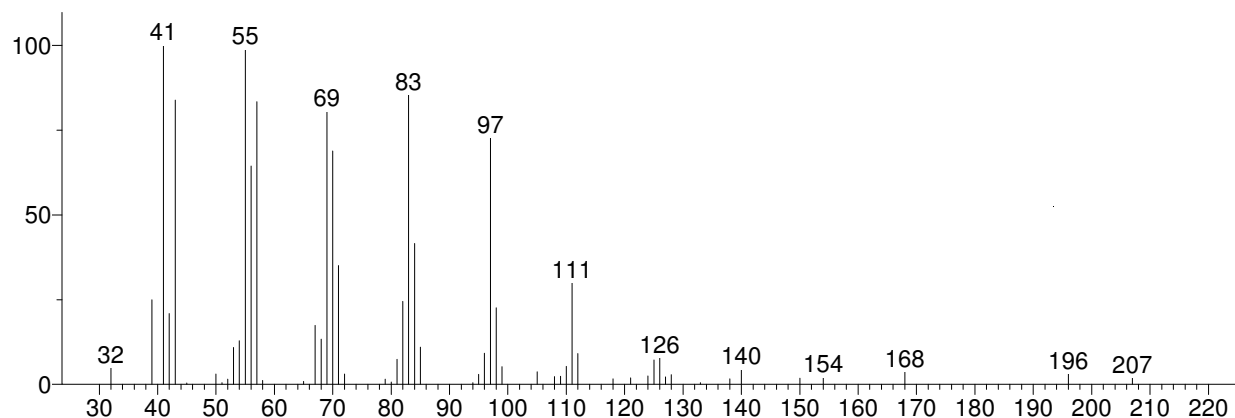


Hit 2 : 1-Undecanol
C₁₁H₂₄O; MF: 821; RMF: 884; Prob 7.17%; CAS: 112-42-5; Lib: mainlib; ID: 18199.

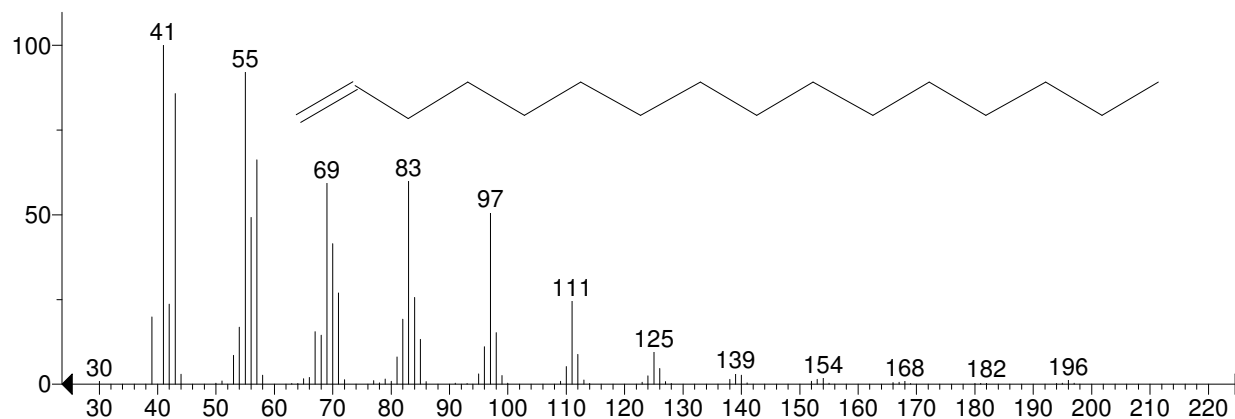


** Search Report Page 1 of 1 **

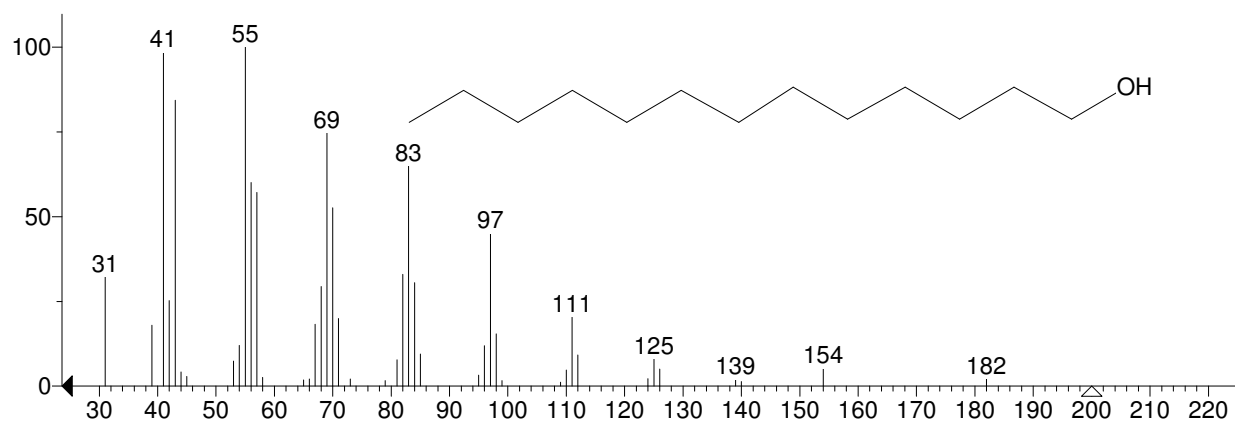
Unknown: Scan 468 (3.614 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-461)
Compound in Library Factor = -297



Hit 1 : 1-Hexadecene
C₁₆H₃₂; MF: 879; RMF: 896; Prob 4.02%; CAS: 629-73-2; Lib: replib; ID: 885.

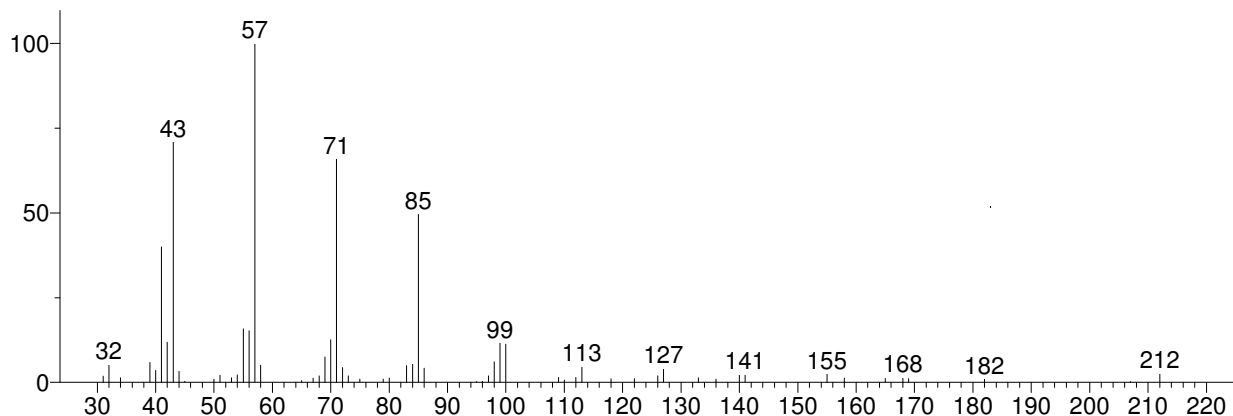


Hit 2 : n-Tridecan-1-ol
C₁₃H₂₈O; MF: 875; RMF: 907; Prob 3.40%; CAS: 112-70-9; Lib: mainlib; ID: 17267.

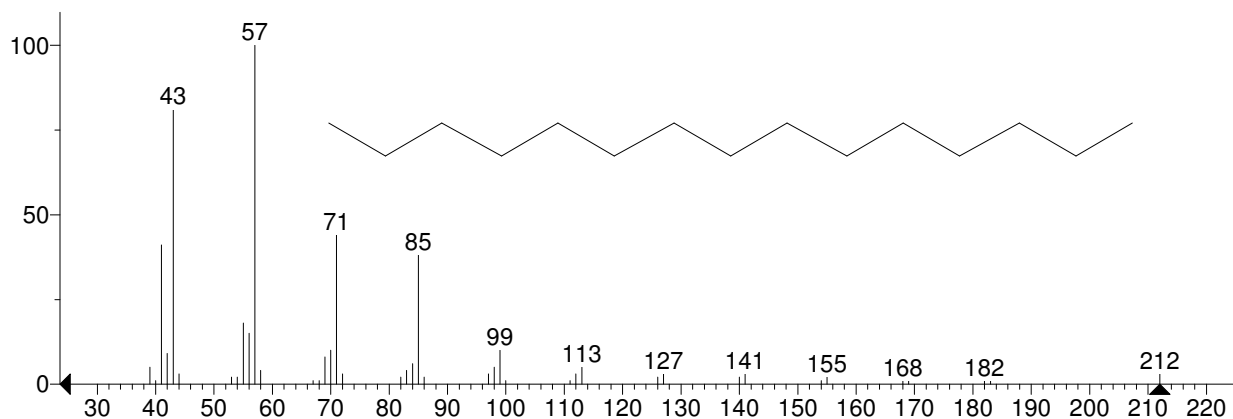


** Search Report Page 1 of 1 **

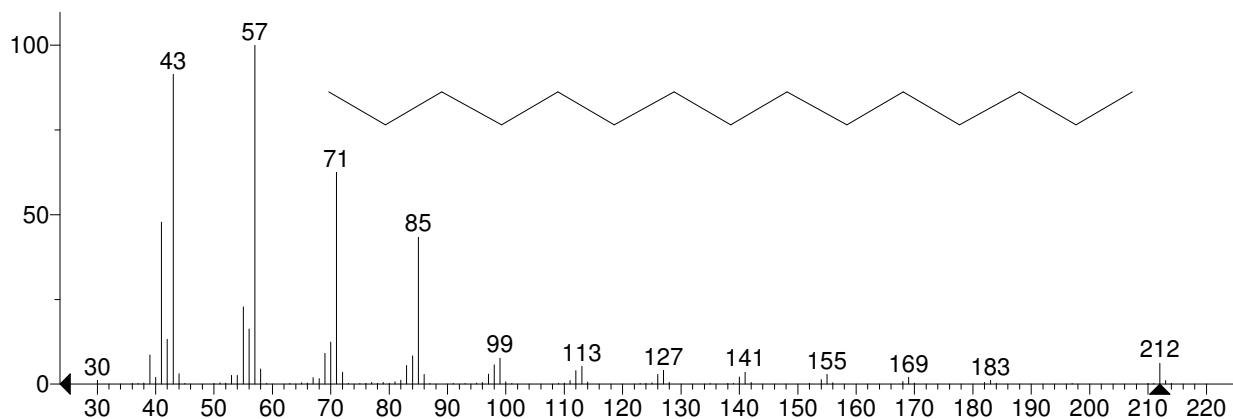
Unknown: Scan 552 (4.247 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-567)
Compound in Library Factor = -190



Hit 1 : Pentadecane
C₁₅H₃₂; MF: 865; RMF: 897; Prob 26.6%; CAS: 629-62-9; Lib: replib; ID: 5523.

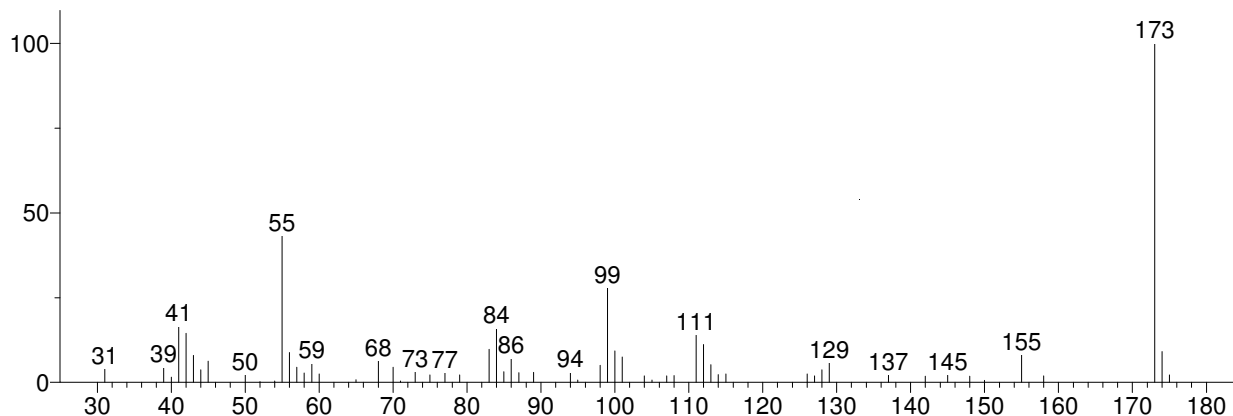


Hit 2 : Pentadecane
C₁₅H₃₂; MF: 832; RMF: 855; Prob 26.6%; CAS: 629-62-9; Lib: replib; ID: 5524.

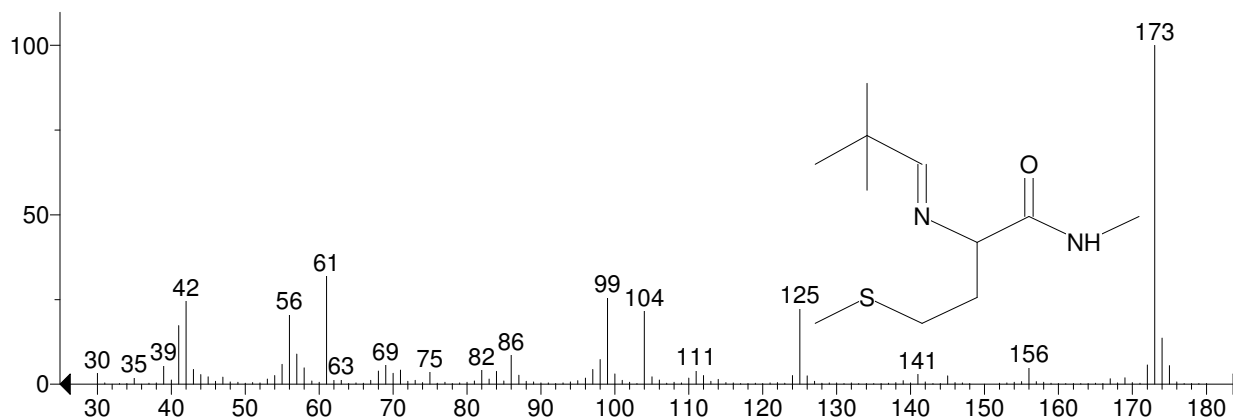


** Search Report Page 1 of 1 **

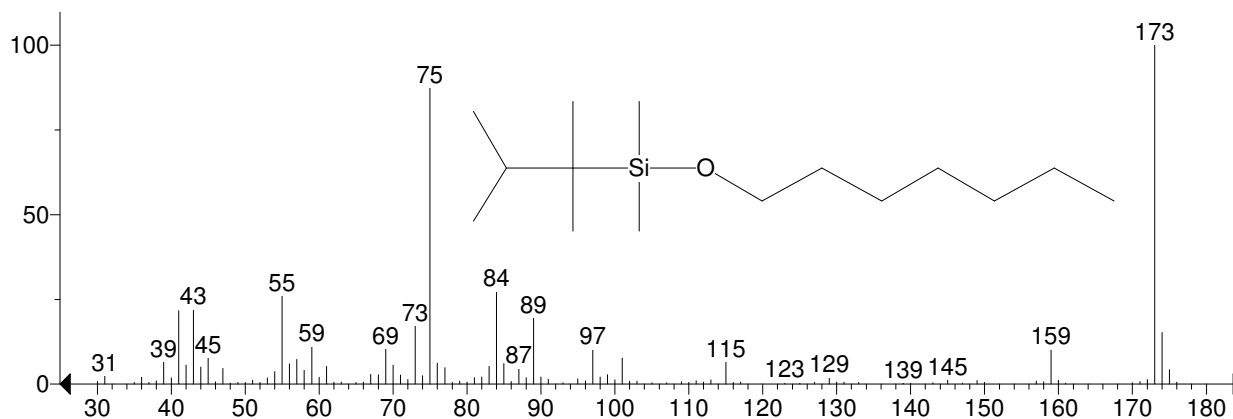
Unknown: Scan 601 (4.616 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-591)
Compound in Library Factor = -988



Hit 1 : Butanamide, N-methyl-4-(methylthio)-2-(2,2-dimethylpropylidene)amino-
C₁₁H₂₂N₂OS; MF: 637; RMF: 640; Prob 46.1%; CAS: 97443-86-2; Lib: mainlib; ID: 128211.

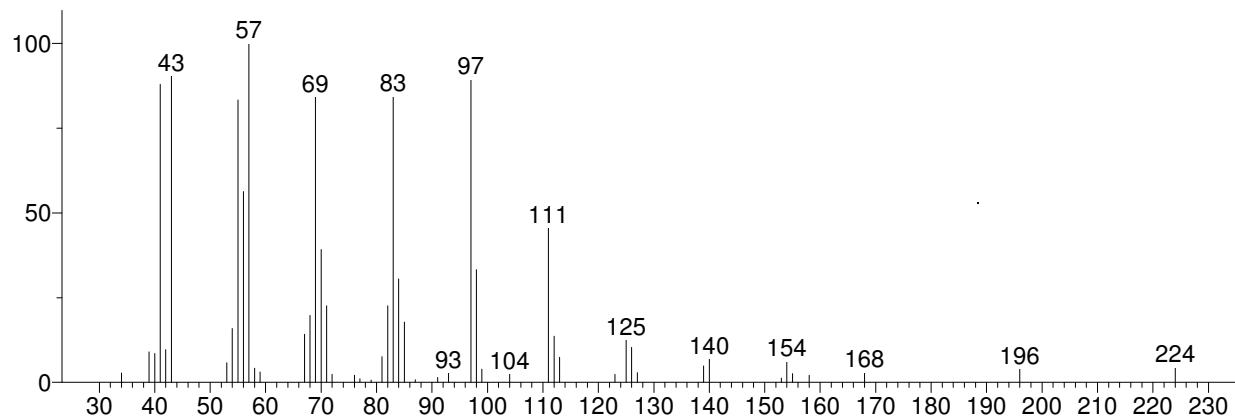


Hit 2 : 1-Dimethylhexylsilyloxyheptane
C₁₅H₃₄OSi; MF: 607; RMF: 643; Prob 12.8%; Lib: mainlib; ID: 128278.

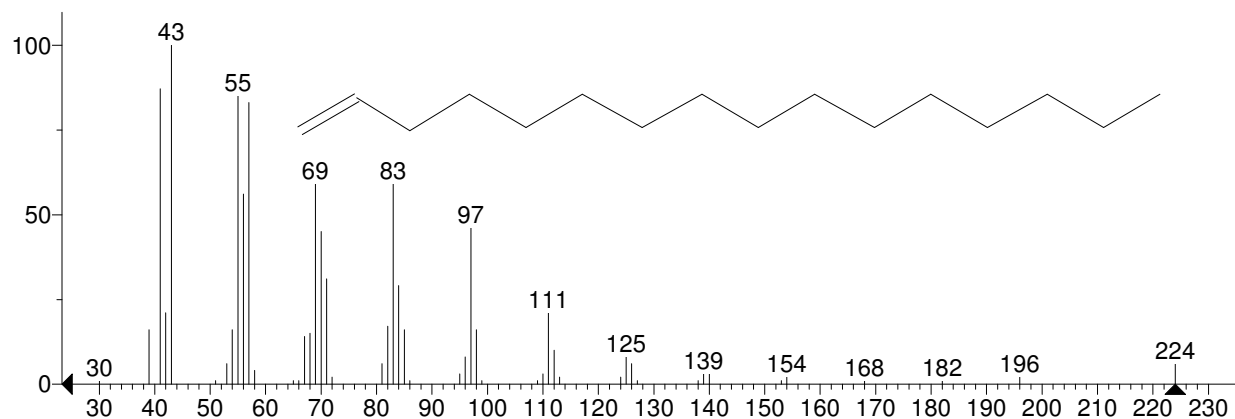


** Search Report Page 1 of 1 **

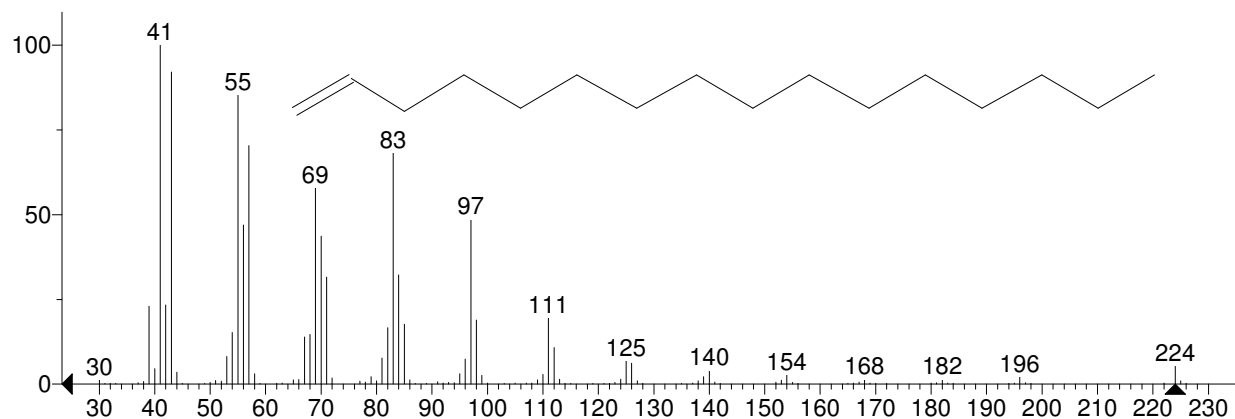
Unknown: Scan 618 (4.744 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-613)
Compound in Library Factor = -246



Hit 1 : 1-Hexadecene
C16H32; MF: 866; RMF: 884; Prob 6.50%; CAS: 629-73-2; Lib: mainlib; ID: 5641.

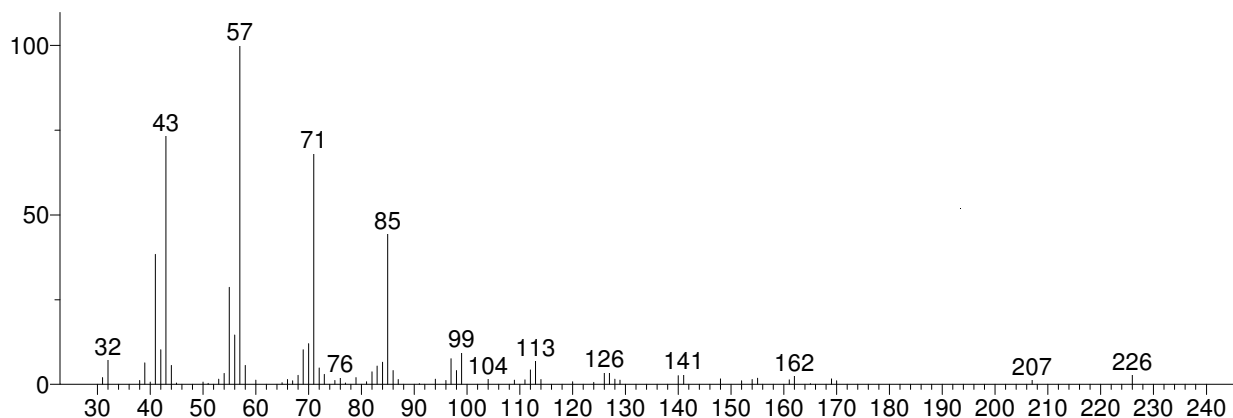


Hit 2 : 1-Hexadecene
C16H32; MF: 863; RMF: 870; Prob 6.50%; CAS: 629-73-2; Lib: replib; ID: 829.

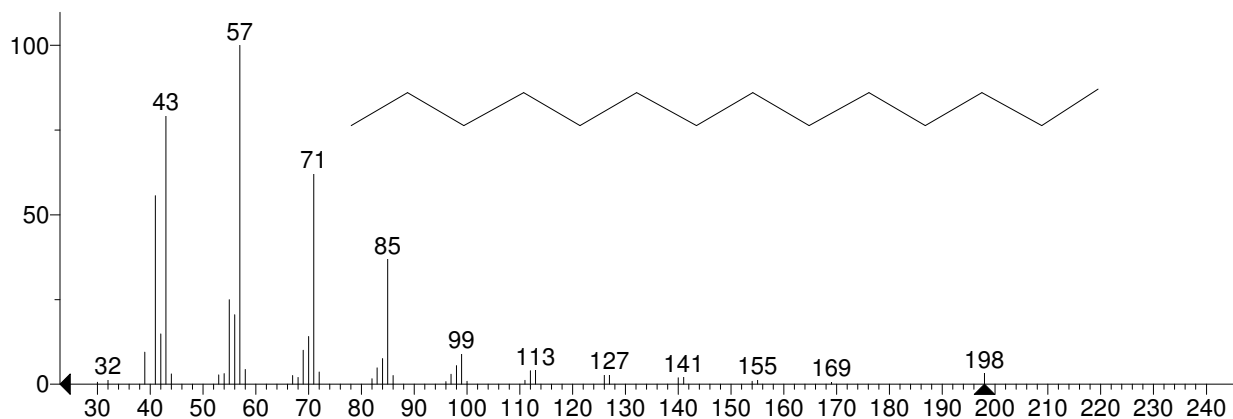


** Search Report Page 1 of 1 **

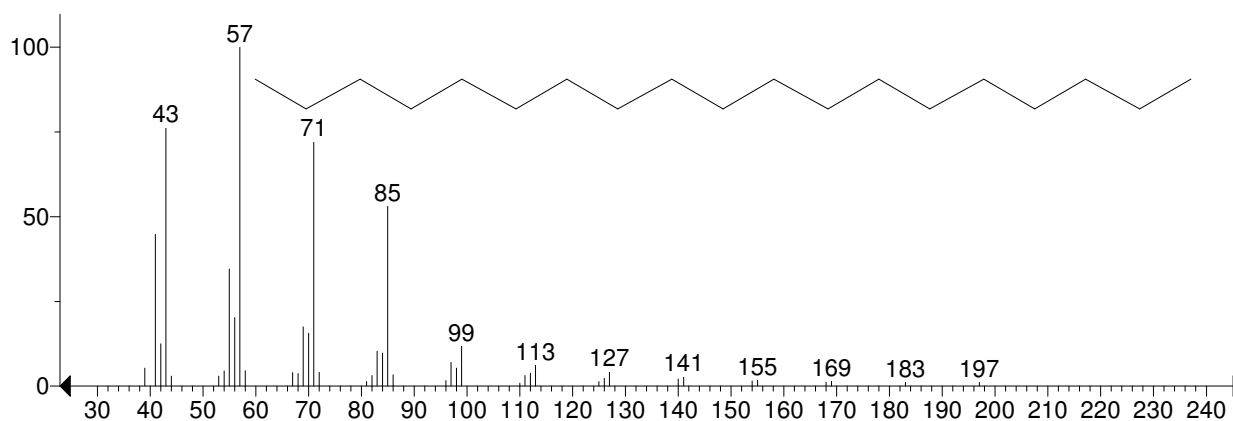
Unknown: Scan 625 (4.797 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-632)
Compound in Library Factor = -331



Hit 1 : Tetradecane
C₁₄H₃₀; MF: 844; RMF: 910; Prob 13.1%; CAS: 629-59-4; Lib: replib; ID: 5511.

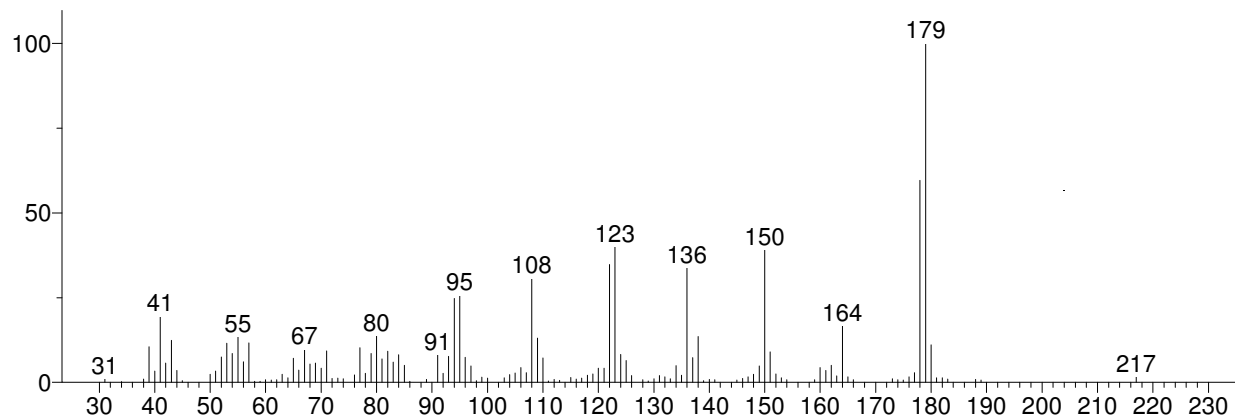


Hit 2 : Nonadecane
C₁₉H₄₀; MF: 840; RMF: 907; Prob 11.1%; CAS: 629-92-5; Lib: replib; ID: 5533.

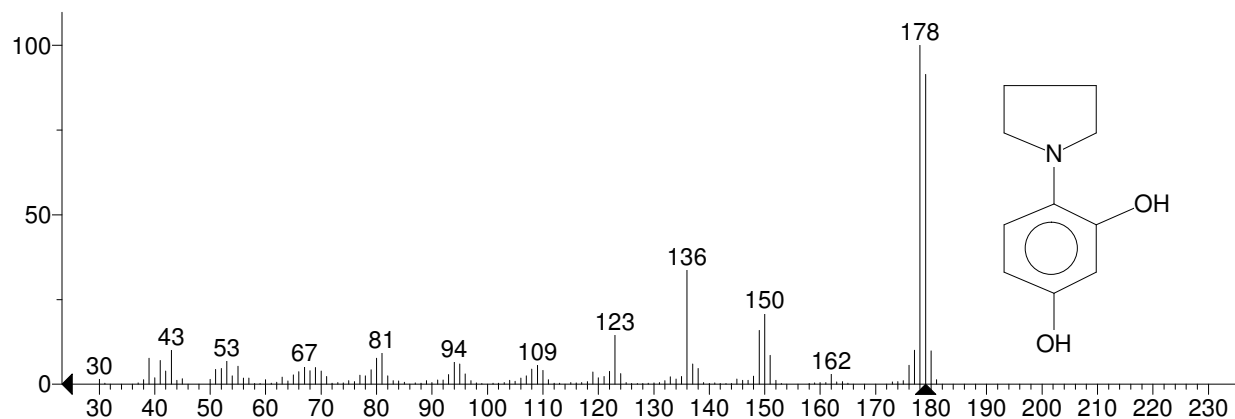


** Search Report Page 1 of 1 **

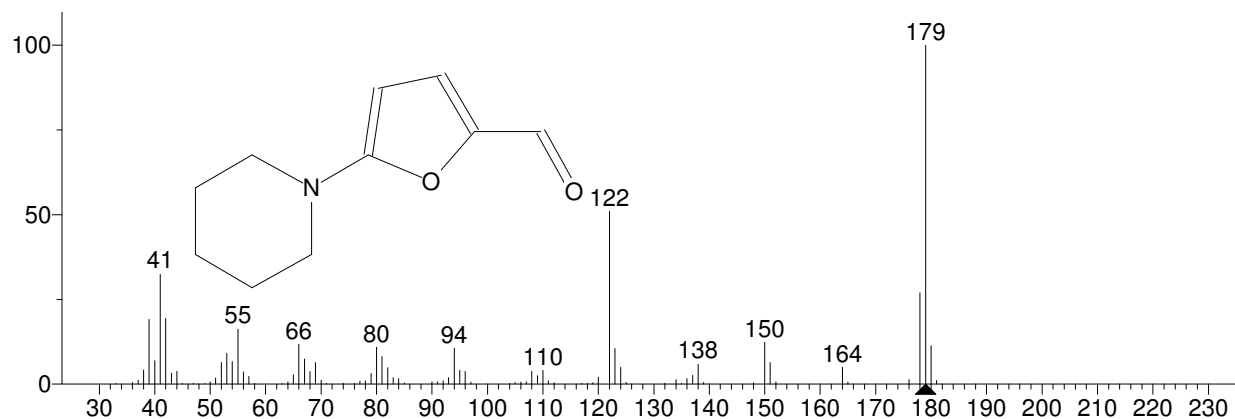
Unknown: Scan 698 (5.347 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-692)
Compound in Library Factor = -399



Hit 1 : 4-Pyrrolidin-1-yl-benzene-1,3-diol
C₁₀H₁₃NO₂; MF: 765; RMF: 771; Prob 52.5%; Lib: mainlib; ID: 132169.

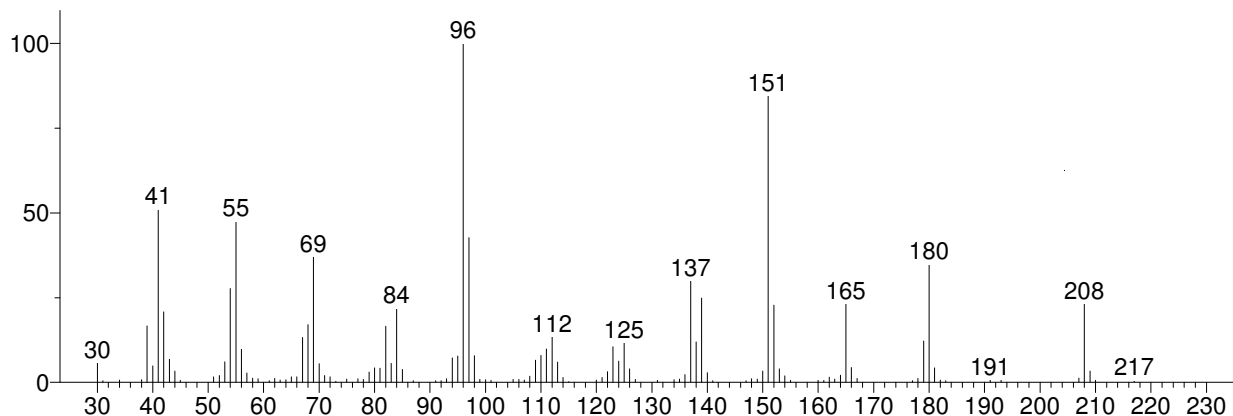


Hit 2 : Furan-2-carboxaldehyde, 5-(1-piperidyl)-
C₁₀H₁₃NO₂; MF: 722; RMF: 764; Prob 11.6%; CAS: 22868-60-6; Lib: mainlib; ID: 132584.

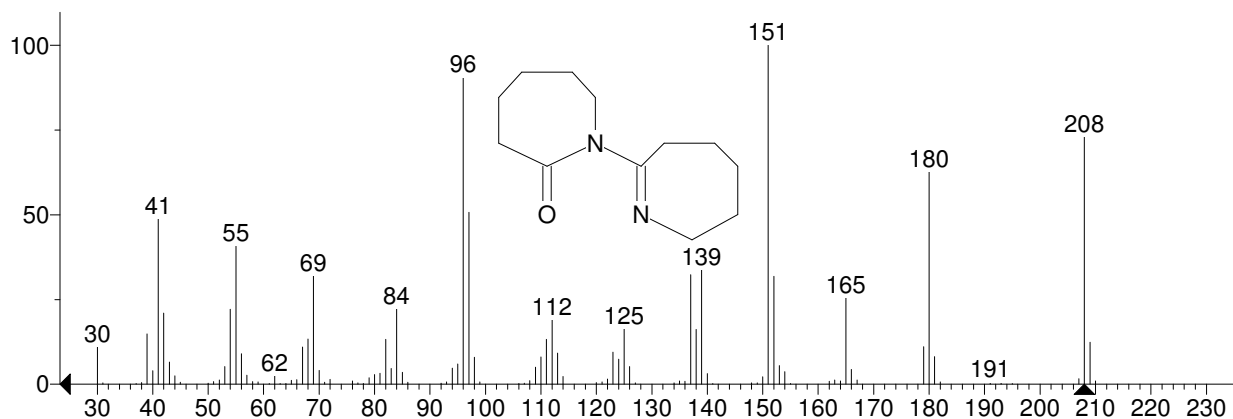


** Search Report Page 1 of 1 **

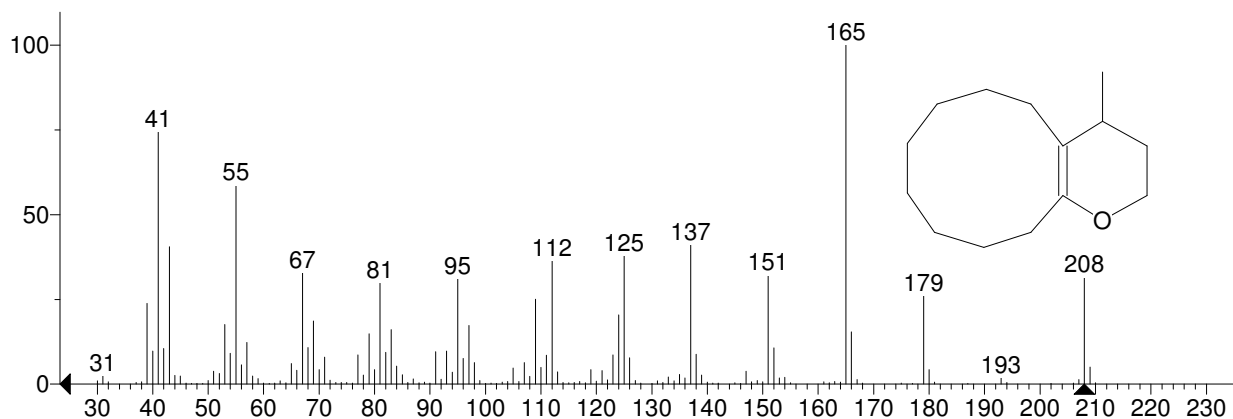
Unknown: Scan 705 (5.400 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-726)
Compound in Library Factor = 391



Hit 1 : 2H-Azepin-2-one, hexahydro-1-(3,4,5,6-tetrahydro-2H-azepin-7-yl)-
C₁₂H₂₀N₂O; MF: 881; RMF: 887; Prob 91.4%; CAS: 22993-71-1; Lib: mainlib; ID: 112495.

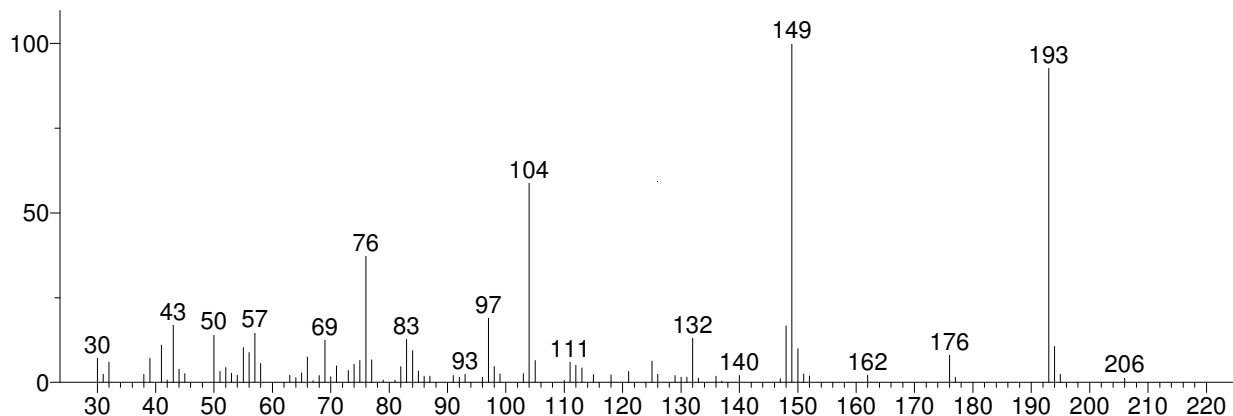


Hit 2 : 2H-Cyclodeca[b]pyran, 3,4,5,6,7,8,9,10,11,12-decahydro-4-methyl-
C₁₄H₂₄O; MF: 658; RMF: 661; Prob 0.91%; CAS: 74685-51-1; Lib: mainlib; ID: 122556.

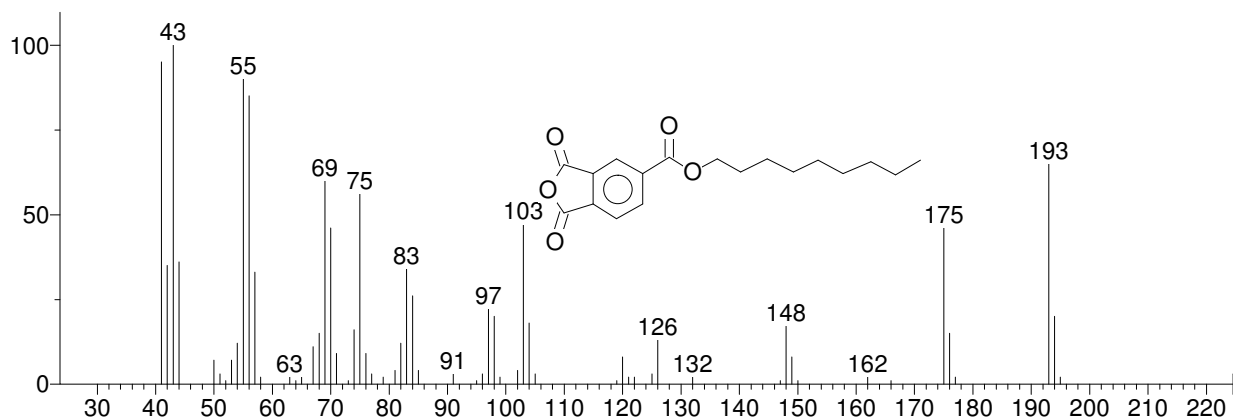


** Search Report Page 1 of 1 **

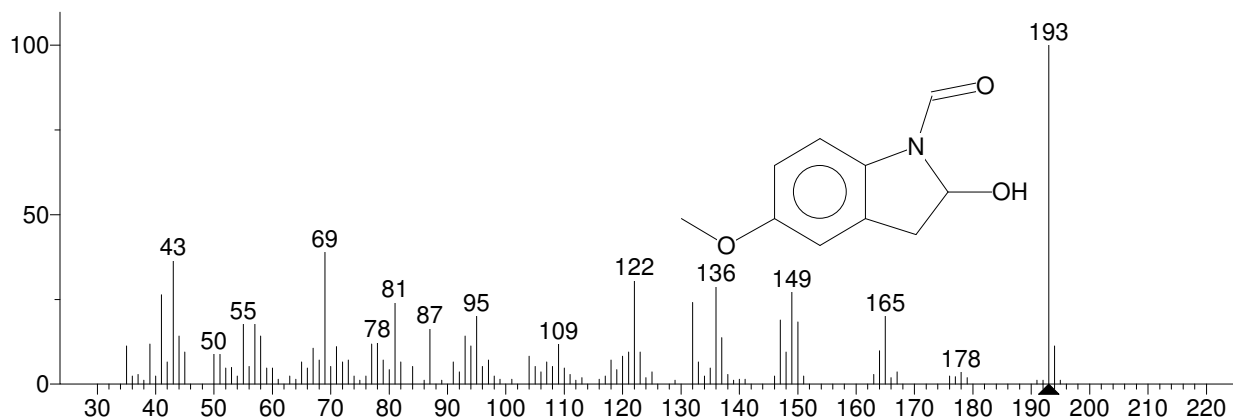
Unknown: Scan 758 (5.799 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-751)
Compound in Library Factor = -1589



Hit 1 : 1,2,4-Benzenetricarboxylic acid, cyclic 1,2-anhydride, nonyl ester
C₁₈H₂₂O₅; MF: 553; RMF: 577; Prob 8.43%; CAS: 33975-30-3; Lib: replib; ID: 1668.

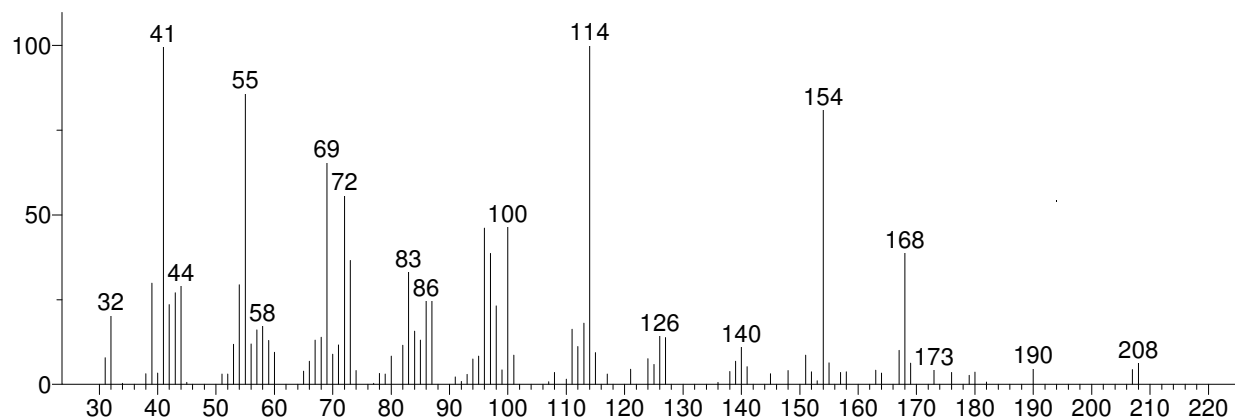


Hit 2 : 1-Indolinecarboxaldehyde, 2-hydroxy-5-methoxy-
C₁₀H₁₁NO₃; MF: 550; RMF: 565; Prob 7.45%; CAS: 13303-70-3; Lib: mainlib; ID: 141854.

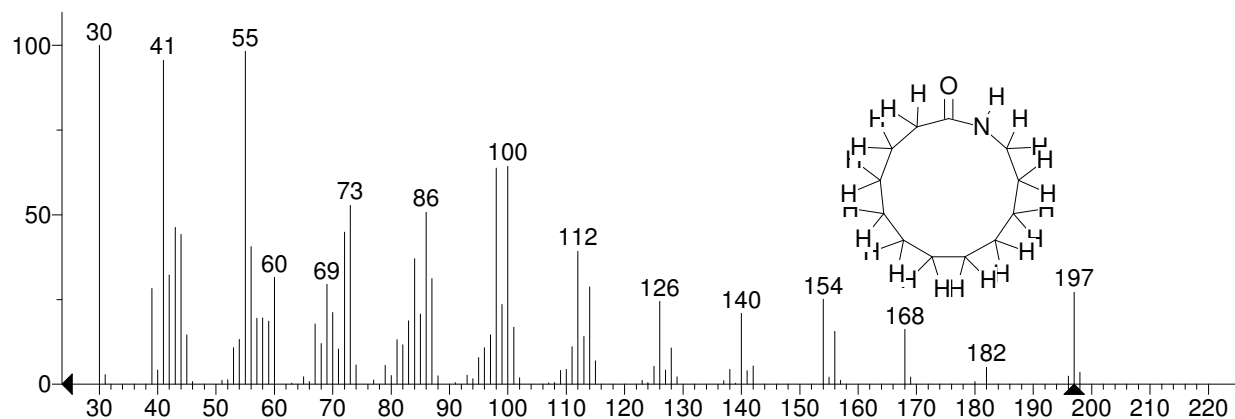


** Search Report Page 1 of 1 **

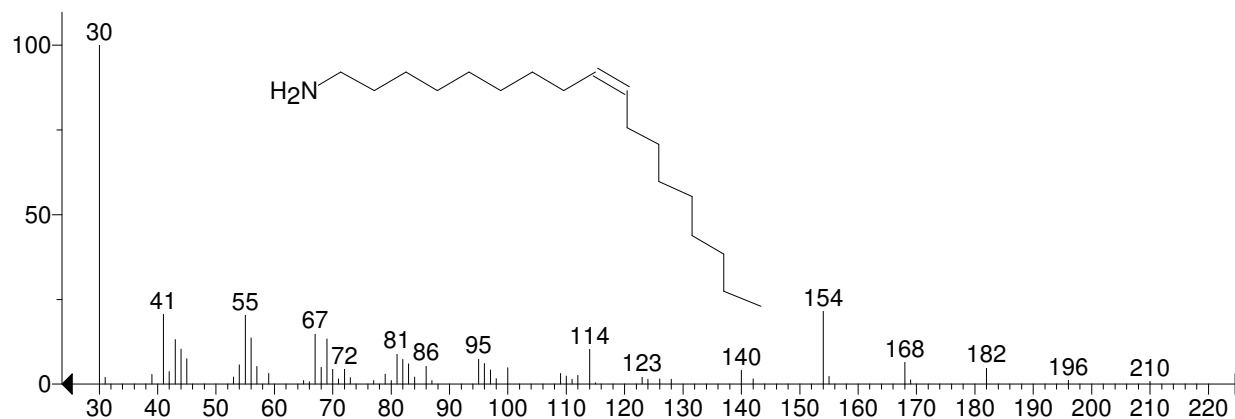
Unknown: Scan 780 (5.965 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-773)
Compound in Library Factor = -988



Hit 1 : Azacyclotridecan-2-one
C₁₂H₂₃NO; MF: 635; RMF: 679; Prob 30.7%; CAS: 947-04-6; Lib: replib; ID: 411.

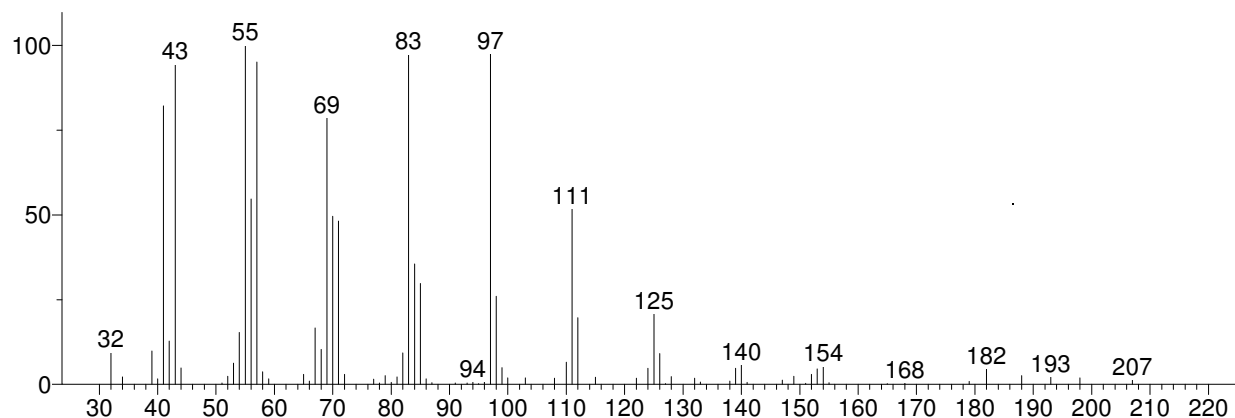


Hit 2 : Oleylamine
C₁₈H₃₇N; MF: 603; RMF: 704; Prob 8.19%; CAS: 112-90-3; Lib: mainlib; ID: 1259.

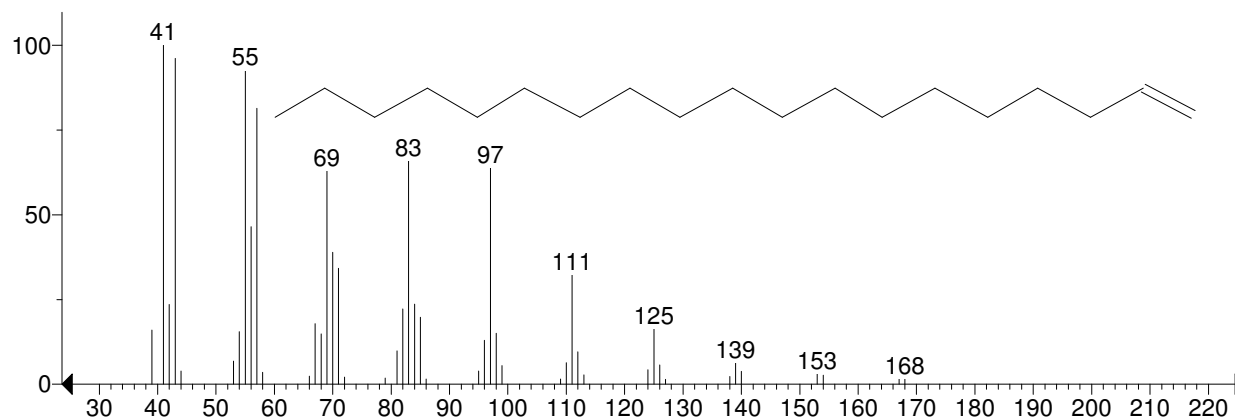


** Search Report Page 1 of 1 **

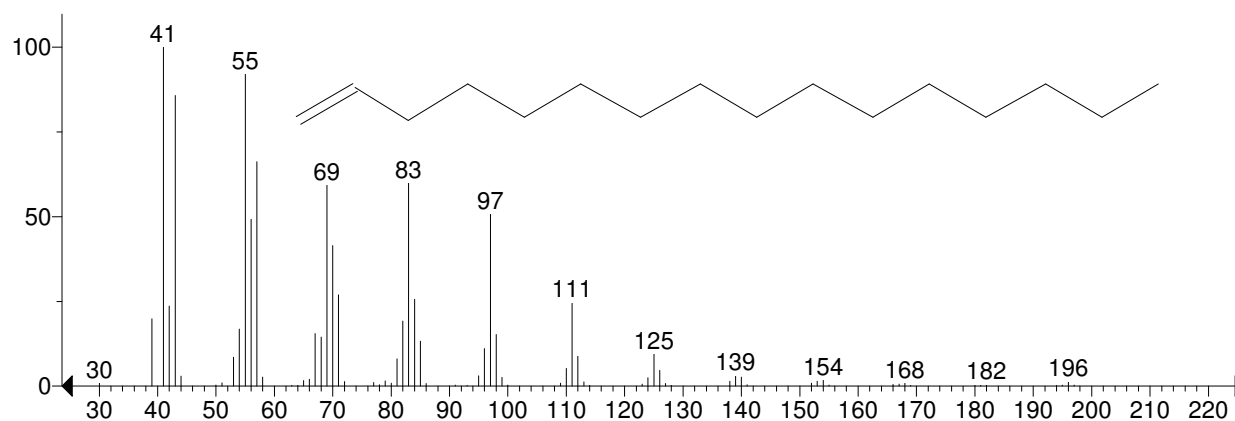
Unknown: Scan 821 (6.274 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-815)
Compound in Library Factor = -493



Hit 1 : 1-Nonadecene
C₁₉H₃₈; MF: 837; RMF: 876; Prob 4.54%; CAS: 18435-45-5; Lib: replib; ID: 818.

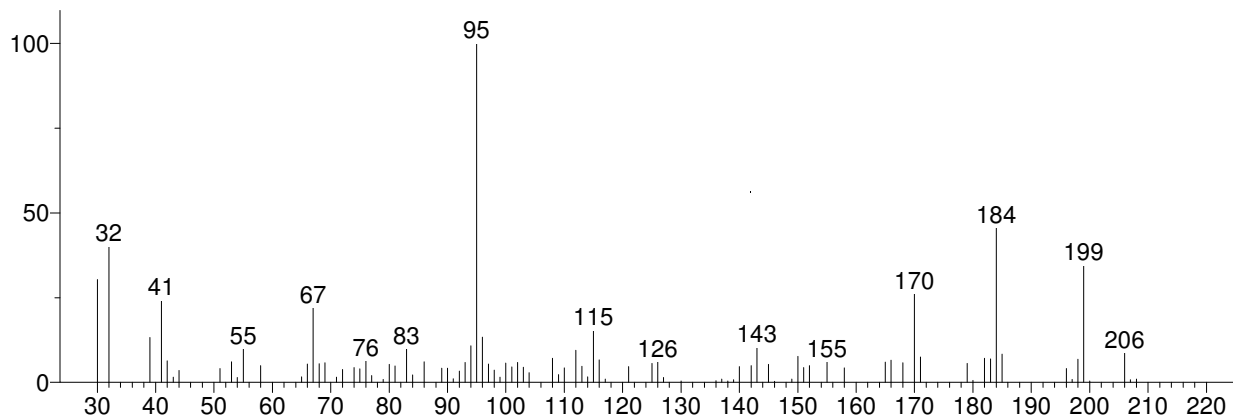


Hit 2 : 1-Hexadecene
C₁₆H₃₂; MF: 836; RMF: 862; Prob 4.36%; CAS: 629-73-2; Lib: replib; ID: 885.

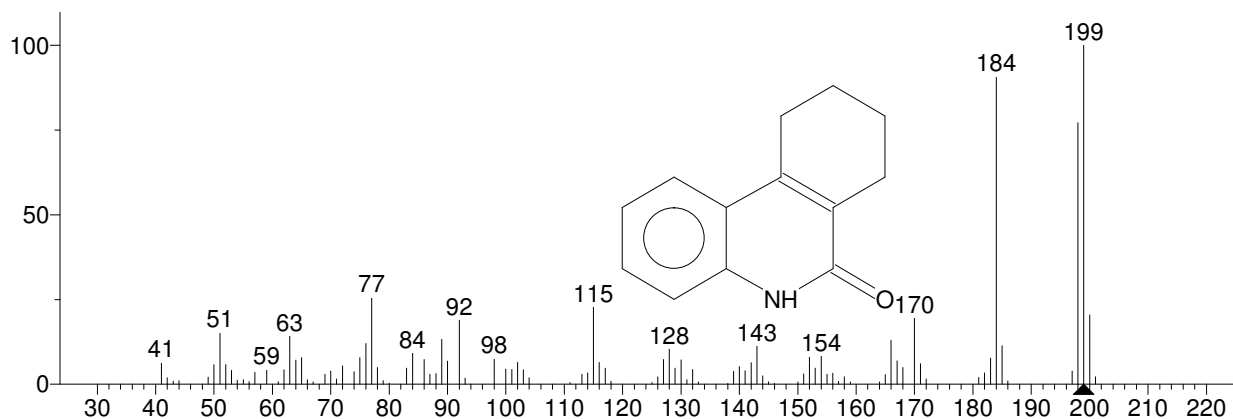


** Search Report Page 1 of 1 **

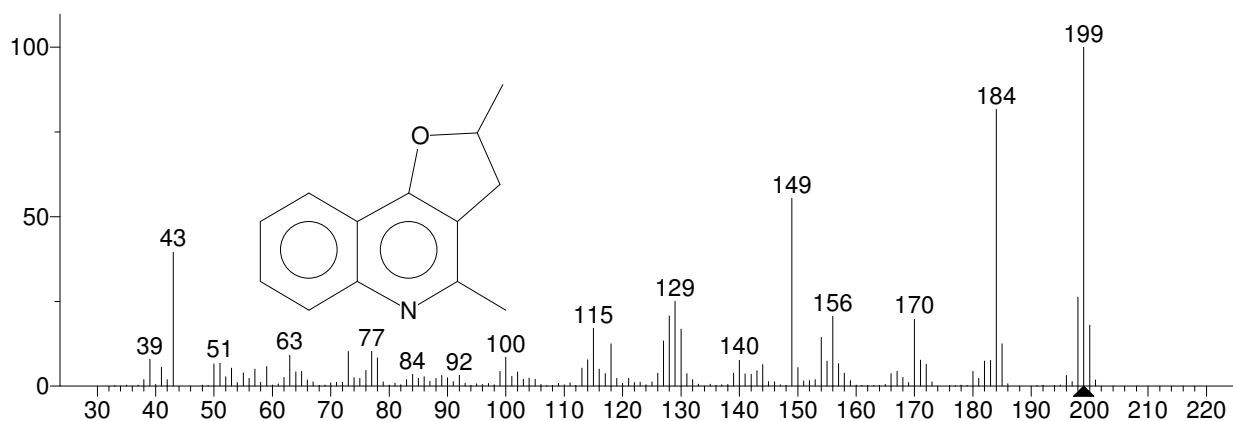
Unknown: Scan 848 (6.478 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-869)
Compound in Library Factor = -1275



Hit 1 : 7,8,9,10-Tetrahydro-6(5H)-phenanthridinone
C₁₃H₁₃NO; MF: 535; RMF: 649; Prob 35.6%; CAS: 4514-04-9; Lib: replib; ID: 24274.

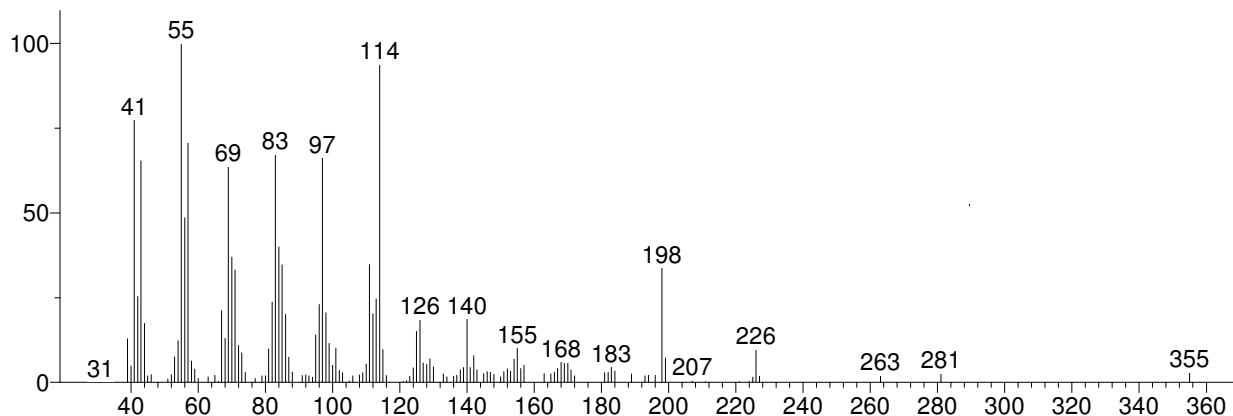


Hit 2 : Furo[3,2-c]quinoline, 2,3-dihydro-2,4-dimethyl-
C₁₃H₁₃NO; MF: 509; RMF: 529; Prob 10.7%; CAS: 1136-32-9; Lib: mainlib; ID: 145200.

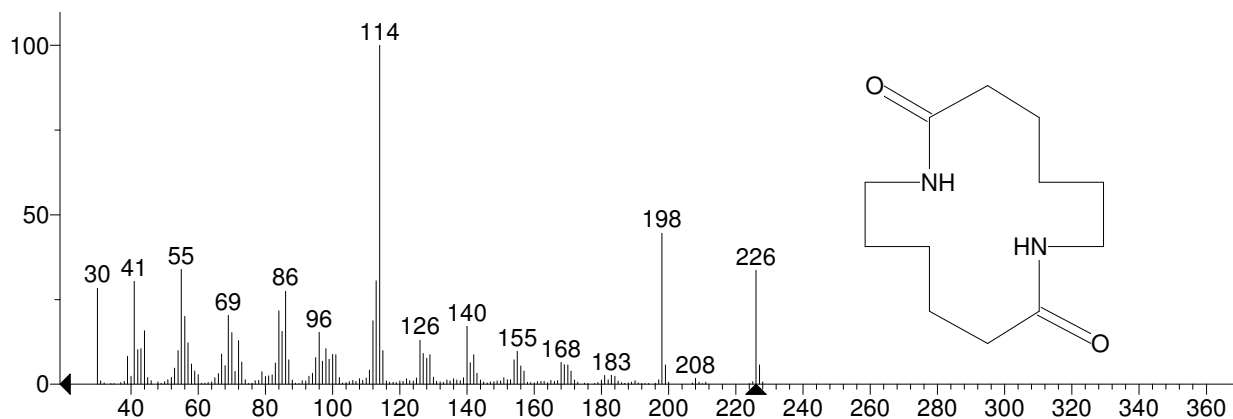


** Search Report Page 1 of 1 **

Unknown: Scan 1000 (7.623 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-967)
Compound in Library Factor = -399



Hit 1 : 1,8-Diazacyclotetradecane-2,9-dione
C₁₂H₂₂N₂O₂; MF: 769; RMF: 777; Prob 29.7%; CAS: 5776-79-4; Lib: mainlib; ID: 77439.

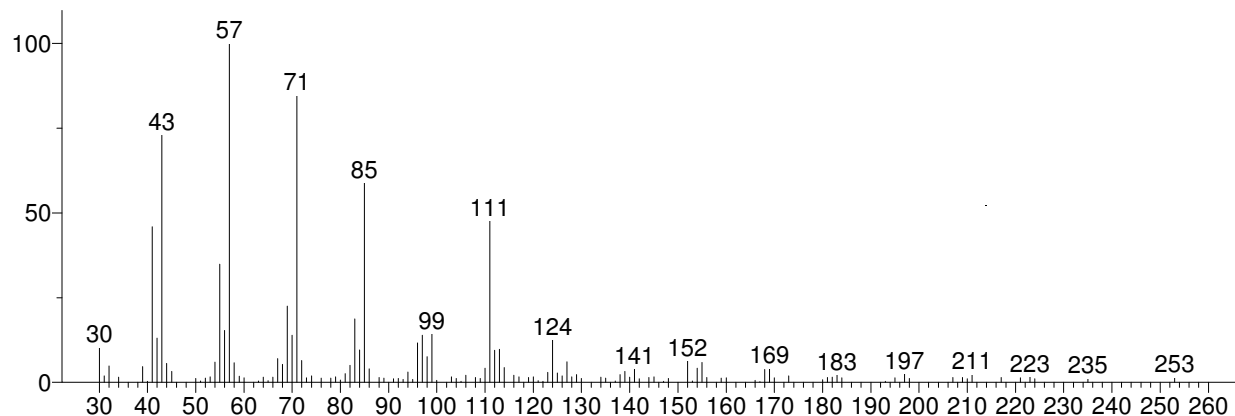


Hit 2 : 1-Dodecanol, 3,7,11-trimethyl-
C₁₅H₃₂O; MF: 721; RMF: 767; Prob 6.15%; CAS: 6750-34-1; Lib: replib; ID: 5710.

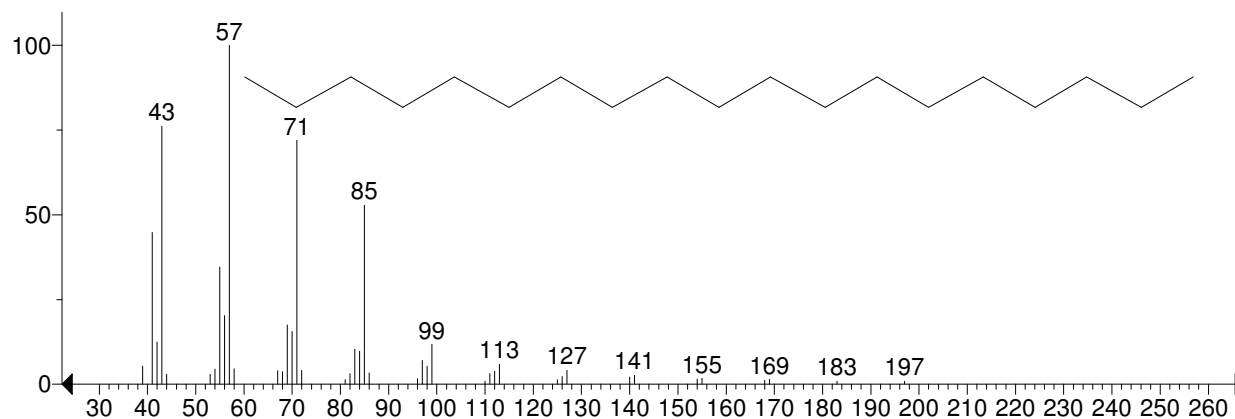


** Search Report Page 1 of 1 **

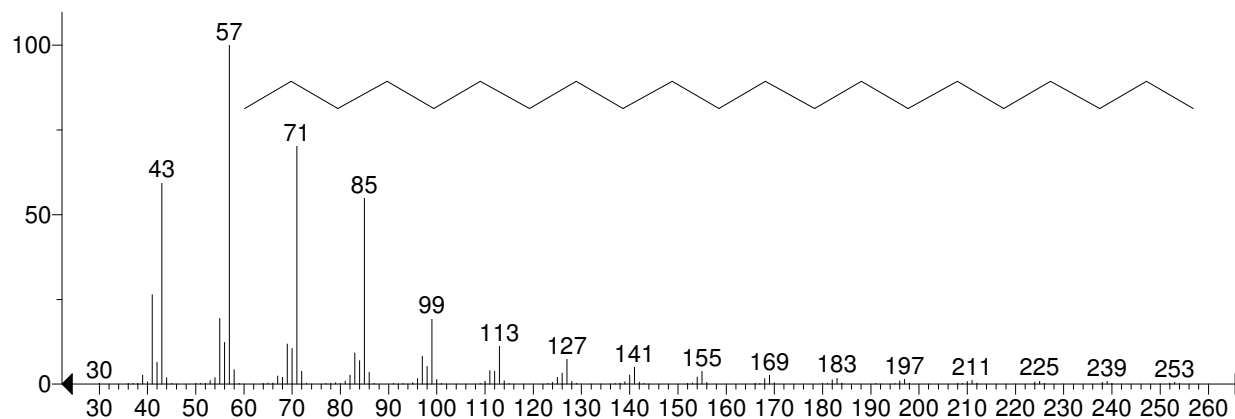
Unknown: Scan 1058 (8.060 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1045)
Compound in Library Factor = -816



Hit 1 : Nonadecane
C₁₉H₄₀; MF: 735; RMF: 862; Prob 5.61%; CAS: 629-92-5; Lib: replib; ID: 5533.

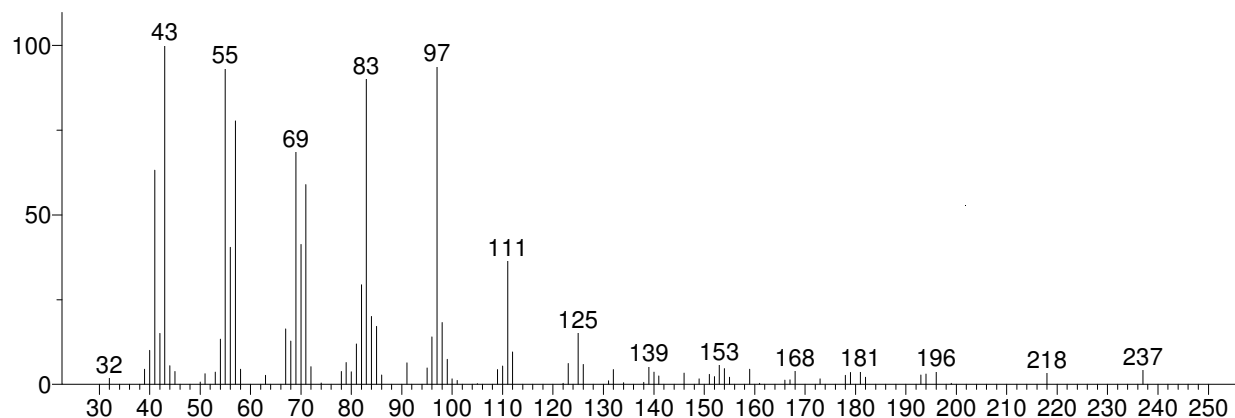


Hit 2 : Heneicosane
C₂₁H₄₄; MF: 720; RMF: 780; Prob 3.40%; CAS: 629-94-7; Lib: replib; ID: 5753.

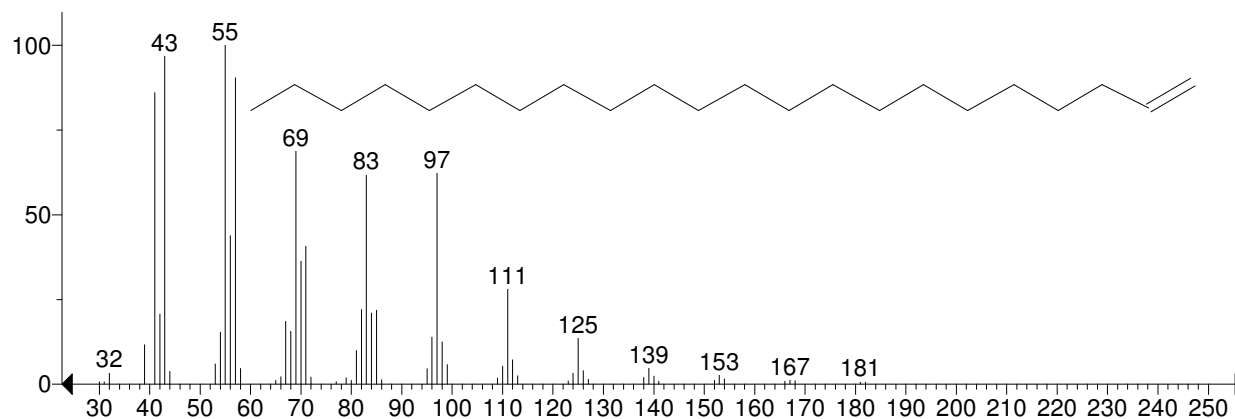


** Search Report Page 1 of 1 **

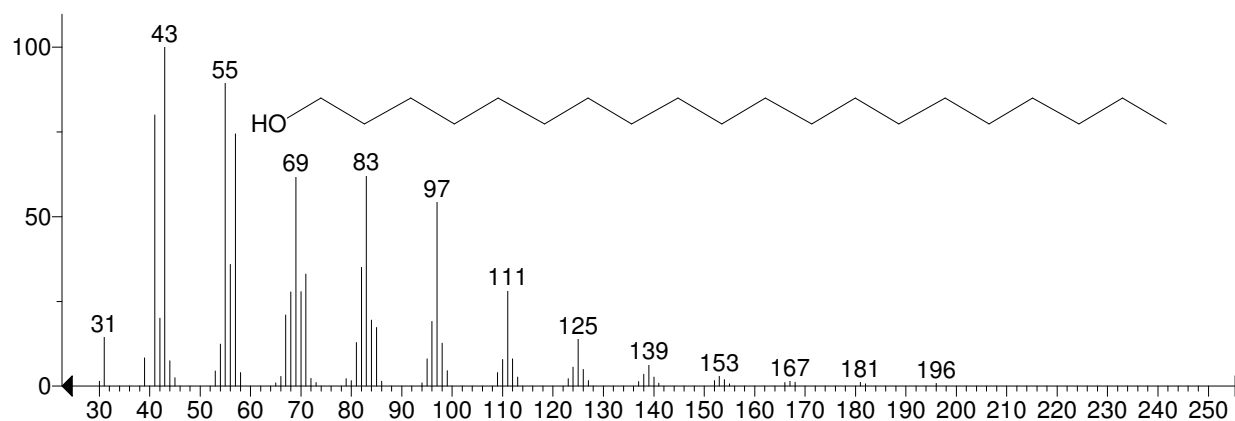
Unknown: Scan 1105 (8.414 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1129)
Compound in Library Factor = -493



Hit 1 : 1-Docosene
C₂₂H₄₄; MF: 836; RMF: 898; Prob 5.71%; CAS: 1599-67-3; Lib: replib; ID: 4382.

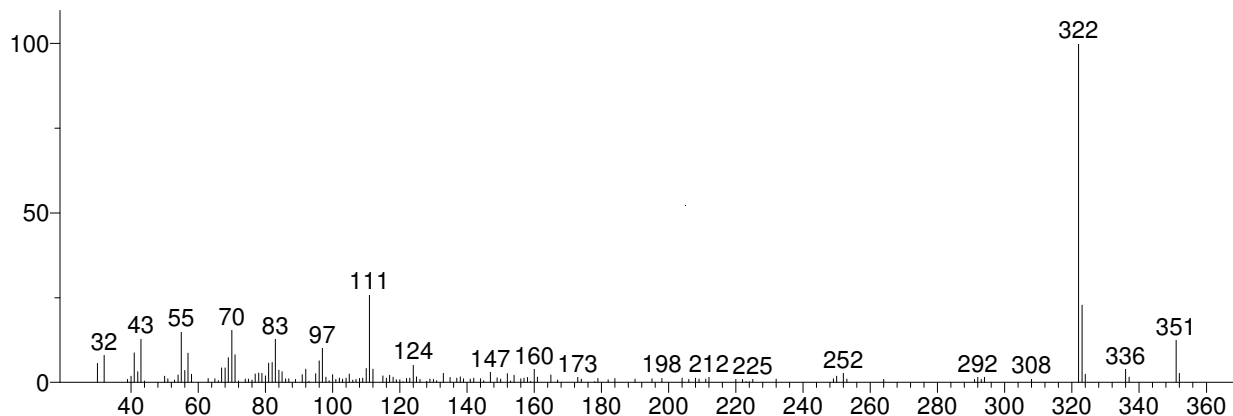


Hit 2 : 1-Eicosanol
C₂₀H₄₂O; MF: 833; RMF: 887; Prob 5.04%; CAS: 629-96-9; Lib: replib; ID: 1938.

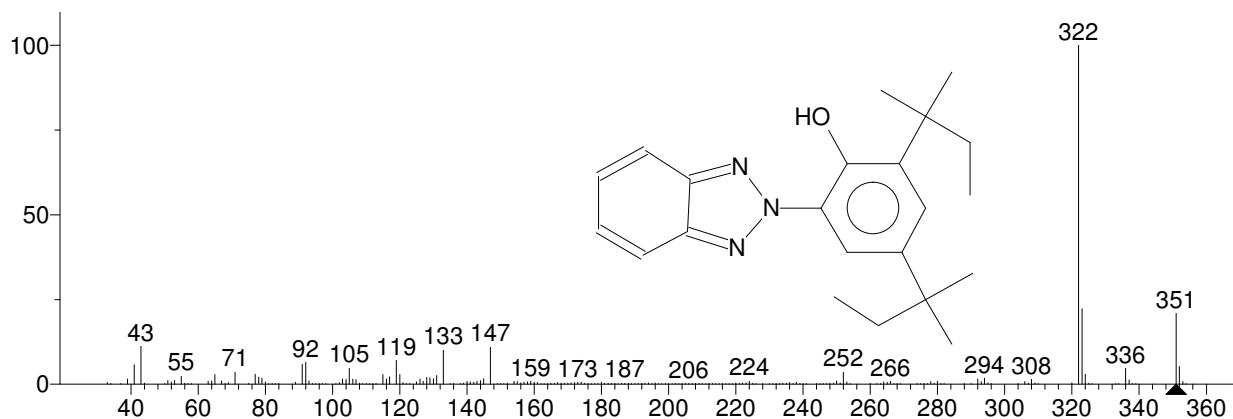


** Search Report Page 1 of 1 **

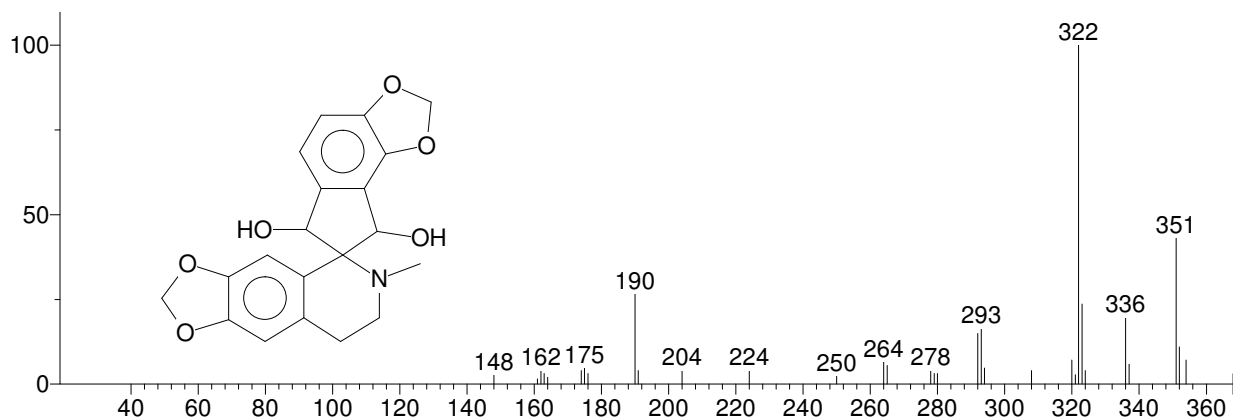
Unknown: Scan 1203 (9.153 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1194)
Compound in Library Factor = -333



Hit 1 : Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-
C₂₂H₂₉N₃O; MF: 717; RMF: 765; Prob 74.3%; CAS: 25973-55-1; Lib: mainlib; ID: 181524.

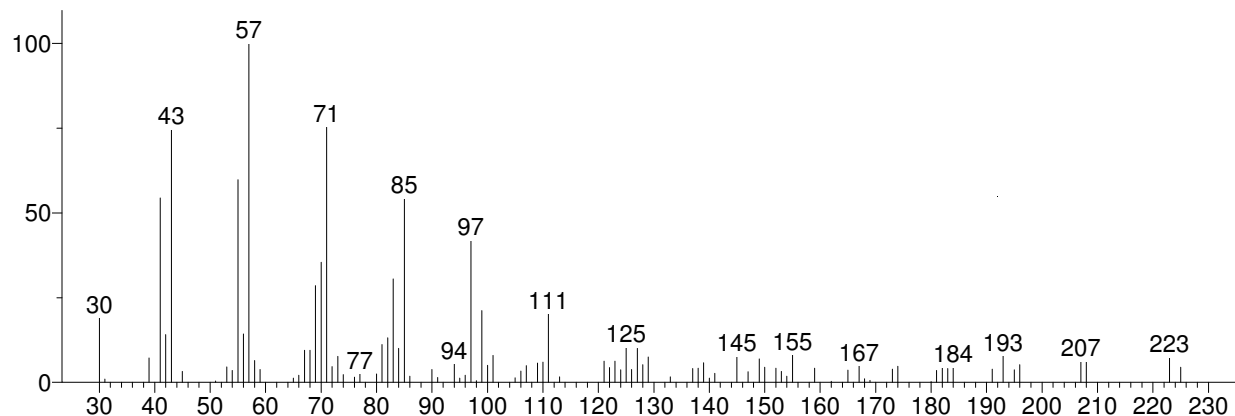


Hit 2 : Ochrobirine
C₂₀H₁₉NO₆; MF: 682; RMF: 743; Prob 18.7%; CAS: 24181-64-4; Lib: mainlib; ID: 181542.

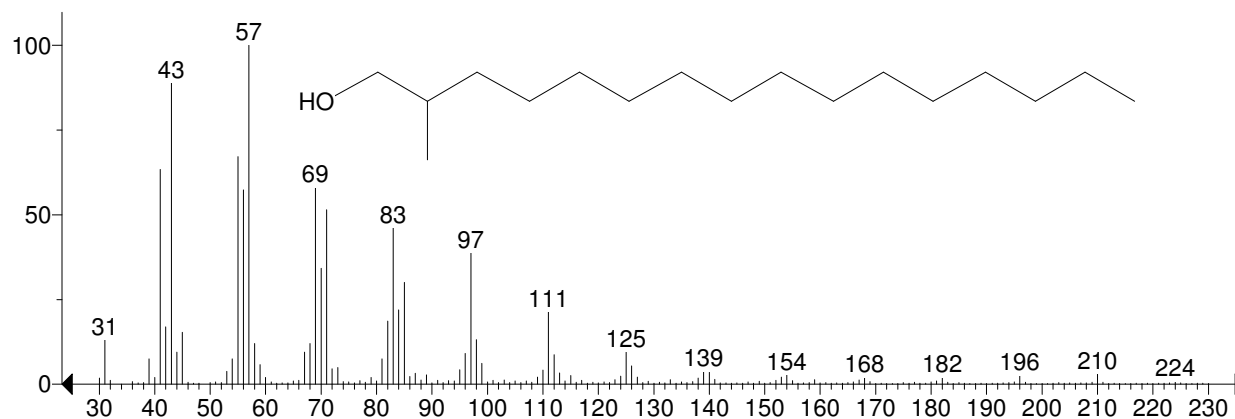


** Search Report Page 1 of 1 **

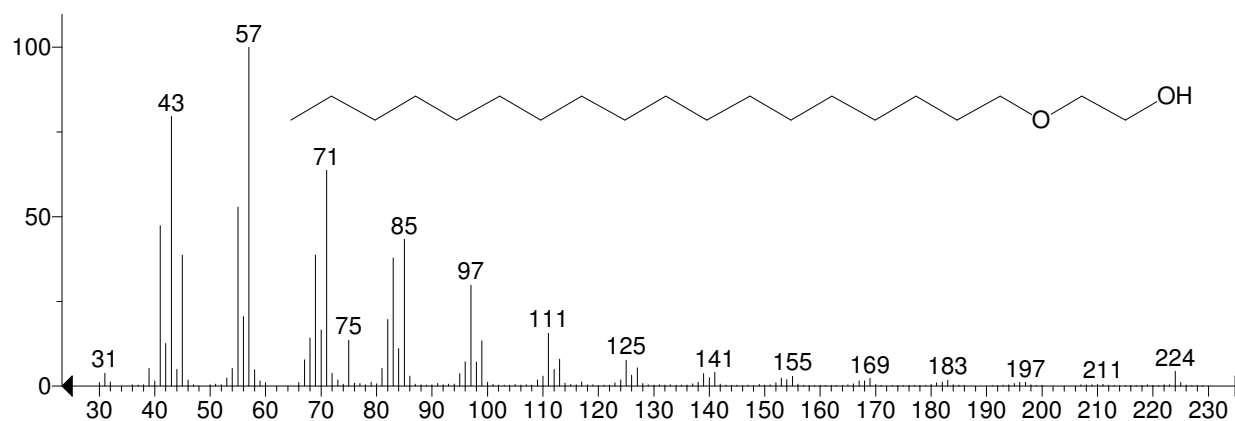
Unknown: Scan 1254 (9.537 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1232)
Compound in Library Factor = -1149



Hit 1 : 1-Hexadecanol, 2-methyl-
C₁₇H₃₆O; MF: 674; RMF: 674; Prob 5.09%; CAS: 2490-48-4; Lib: mainlib; ID: 21789.

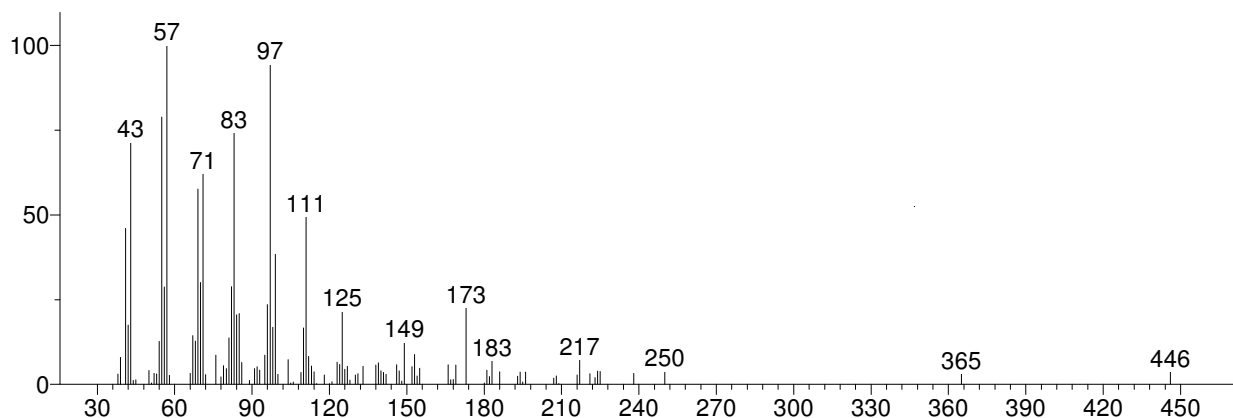


Hit 2 : Ethanol, 2-(octadecyloxy)-
C₂₀H₄₂O₂; MF: 673; RMF: 673; Prob 4.89%; CAS: 2136-72-3; Lib: mainlib; ID: 21971.

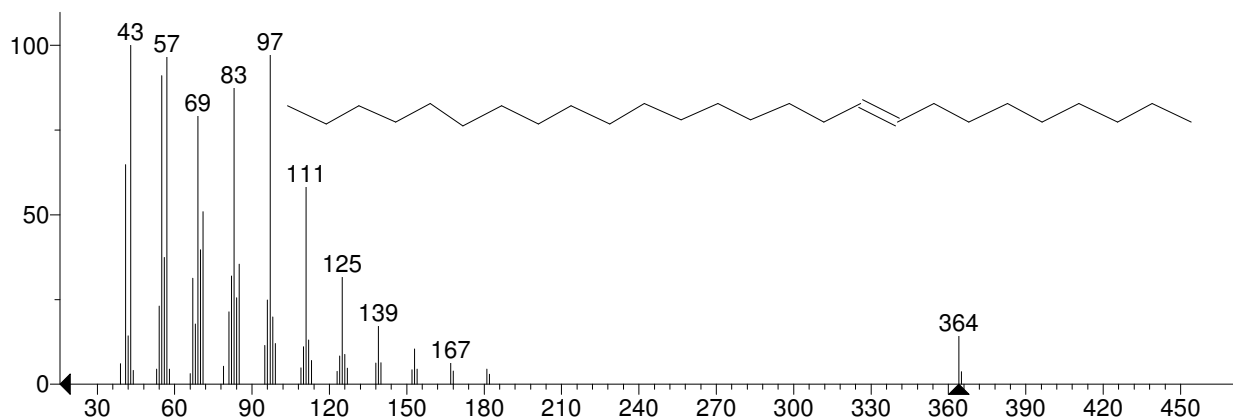


** Search Report Page 1 of 1 **

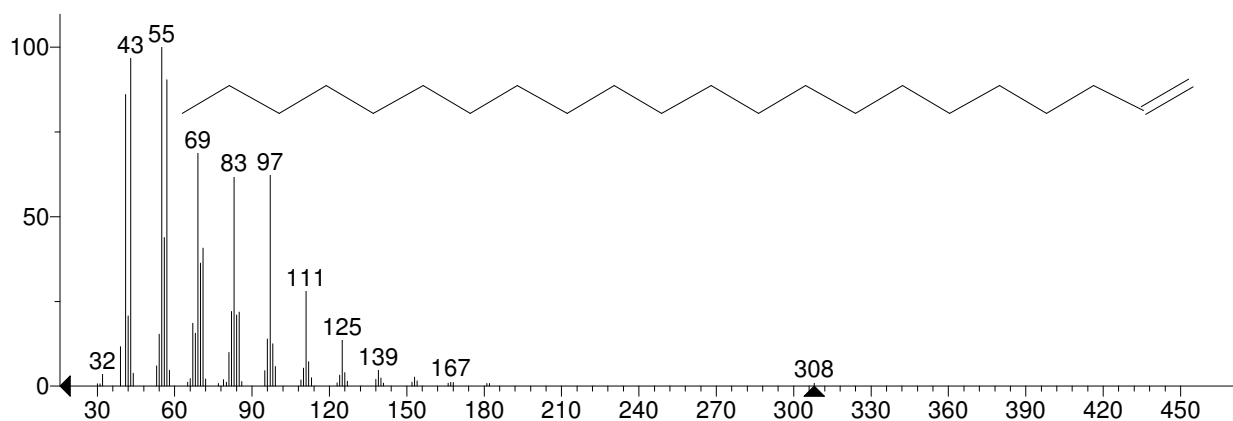
Unknown: Scan 1342 (10.200 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1331)
Compound in Library Factor = -1120



Hit 1 : 9-Hexacosene
C₂₆H₅₂; MF: 734; RMF: 876; Prob 4.78%; CAS: 71502-22-2; Lib: mainlib; ID: 9578.

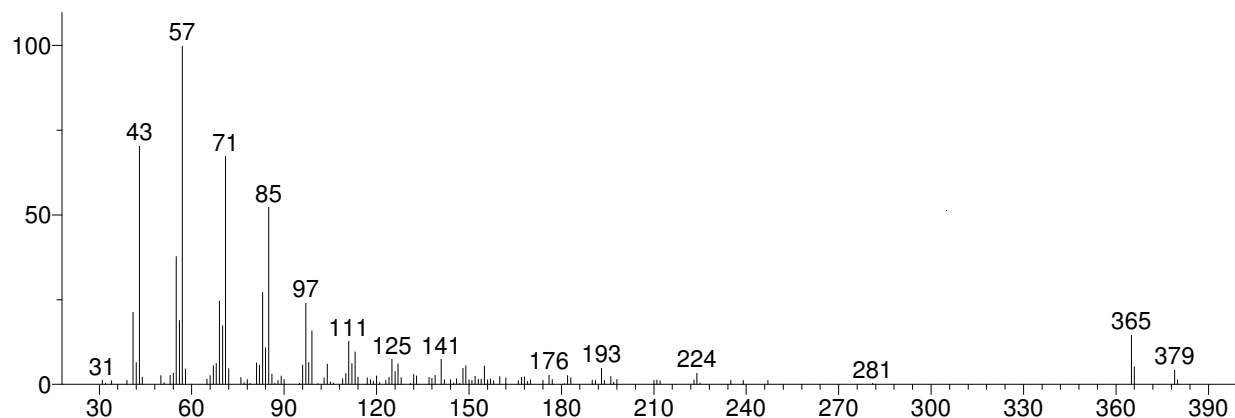


Hit 2 : 1-Docosene
C₂₂H₄₄; MF: 725; RMF: 858; Prob 3.47%; CAS: 1599-67-3; Lib: replib; ID: 4382.

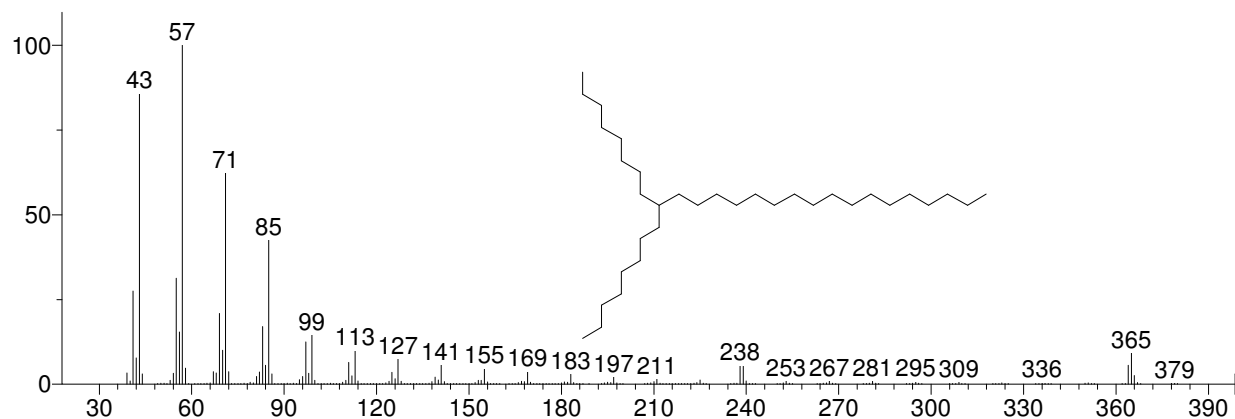


** Search Report Page 1 of 1 **

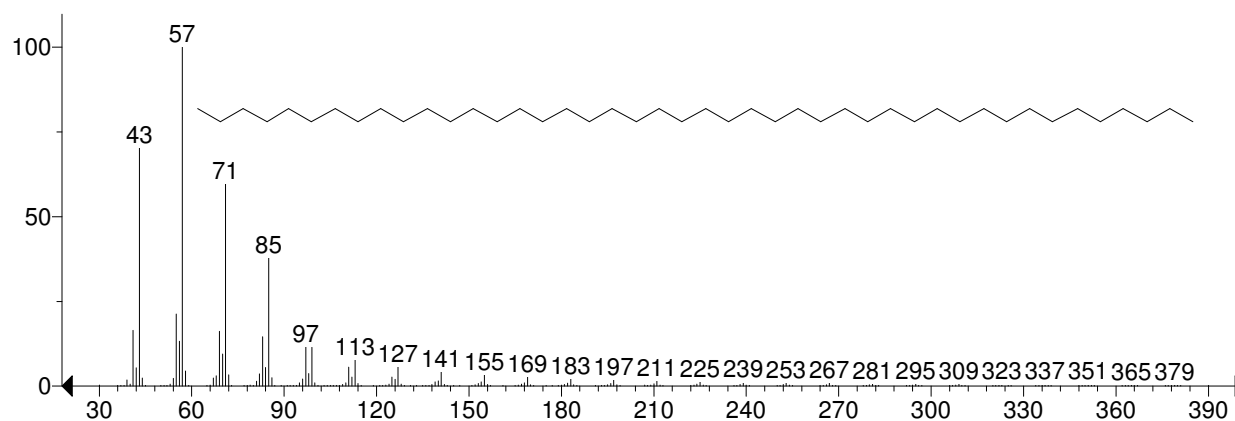
Unknown: Scan 1386 (10.532 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1374)
Compound in Library Factor = -1006



Hit 1 : Hexacosane, 9-octyl-
C₃₄H₇₀; MF: 700; RMF: 705; Prob 8.03%; CAS: 55429-83-9; Lib: mainlib; ID: 21998.

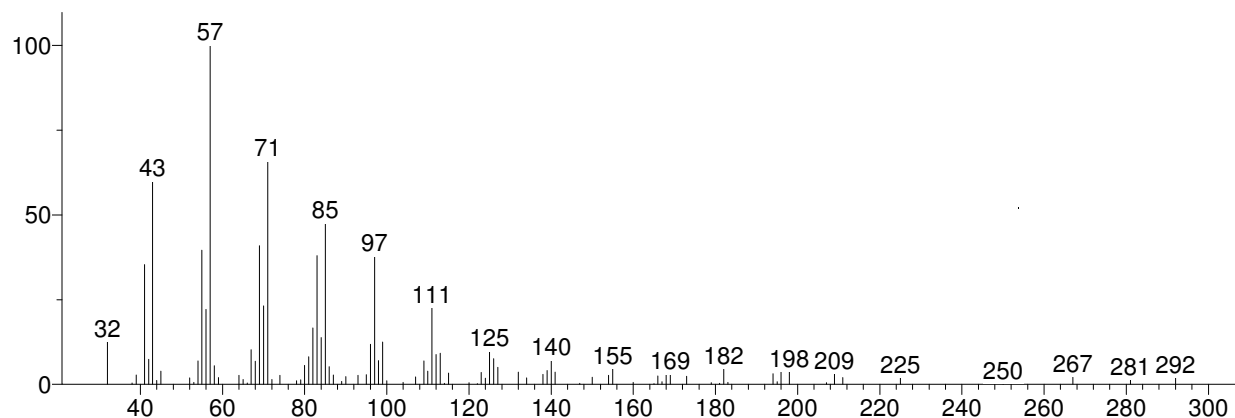


Hit 2 : Tetratetracontane
C₄₄H₉₀; MF: 689; RMF: 725; Prob 5.51%; CAS: 7098-22-8; Lib: replib; ID: 5520.

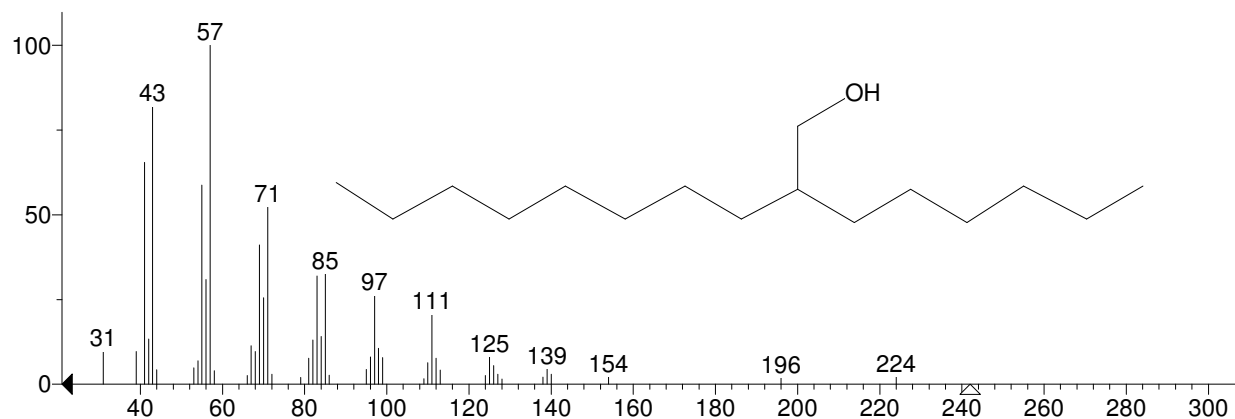


** Search Report Page 1 of 1 **

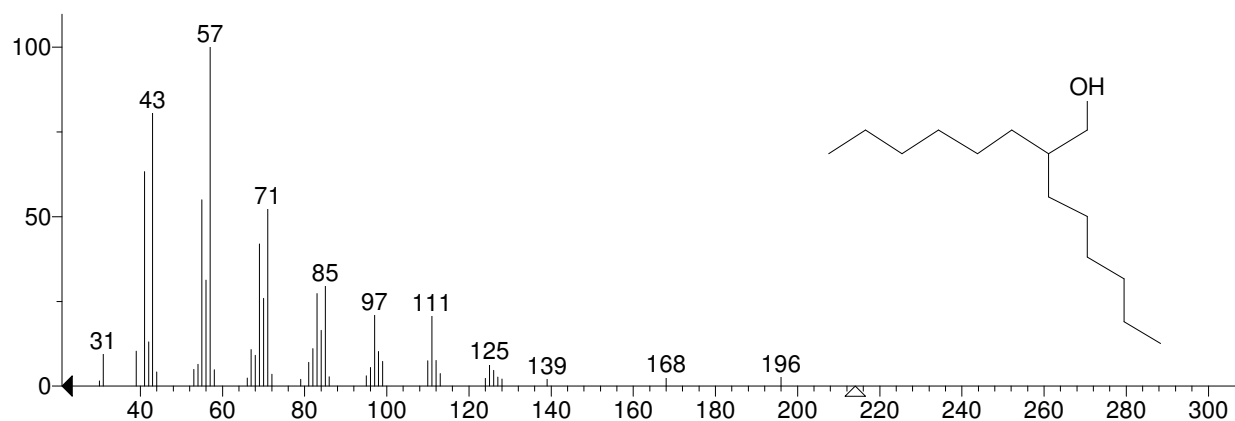
Unknown: Scan 1426 (10.833 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1414)
Compound in Library Factor = -625



Hit 1 : 1-Decanol, 2-hexyl-
C₁₆H₃₄O; MF: 770; RMF: 877; Prob 7.17%; CAS: 2425-77-6; Lib: replib; ID: 5417.

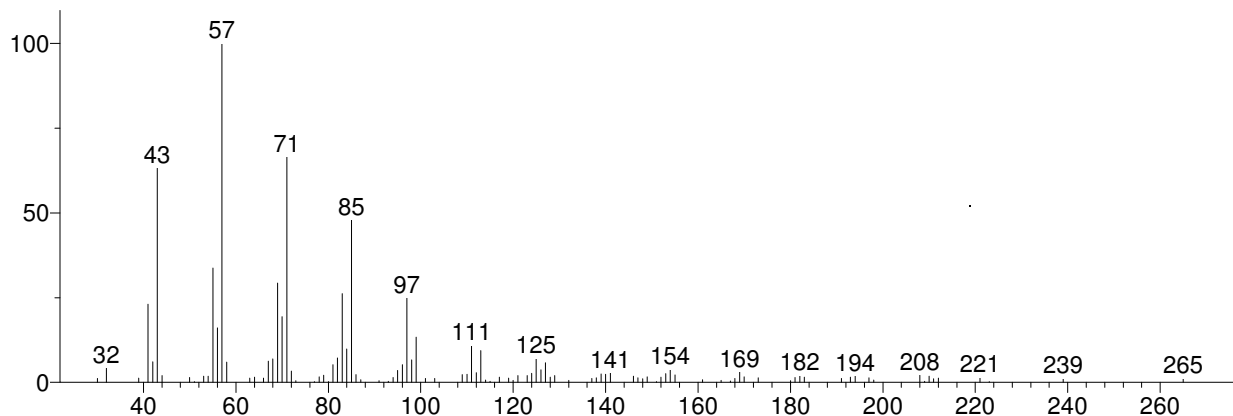


Hit 2 : 2-Hexyl-1-octanol
C₁₄H₃₀O; MF: 760; RMF: 885; Prob 5.06%; CAS: 19780-79-1; Lib: mainlib; ID: 21735.

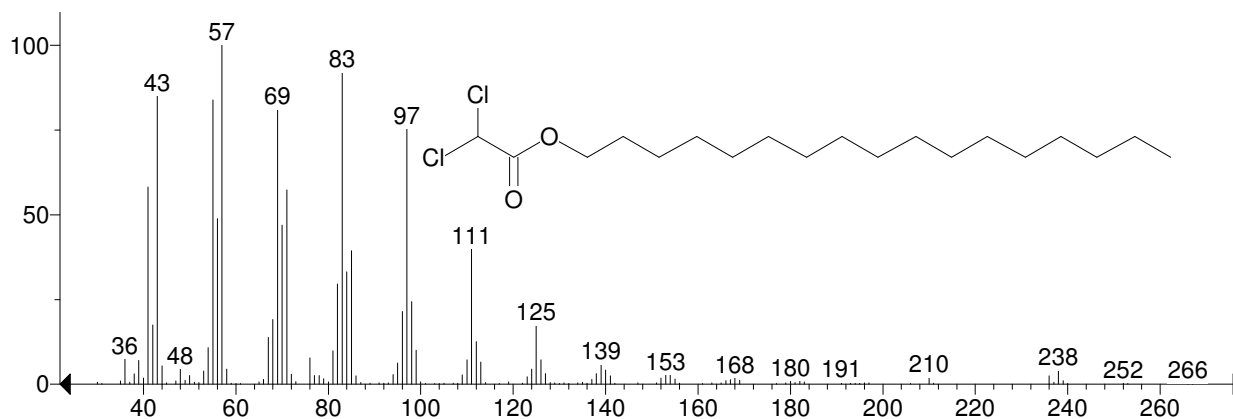


** Search Report Page 1 of 1 **

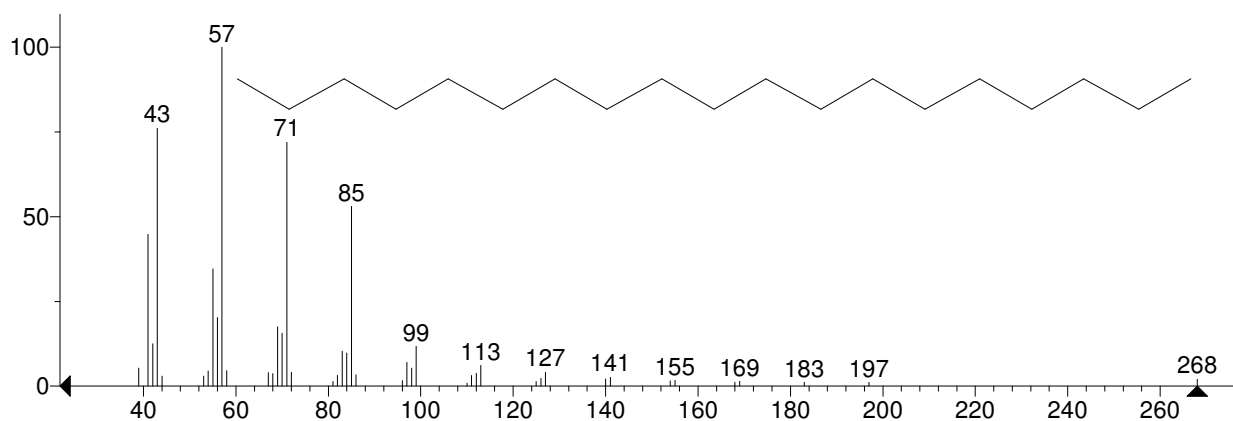
Unknown: Scan 1467 (11.142 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1456)
Compound in Library Factor = -811



Hit 1 : Dichloroacetic acid, heptadecyl ester
C₁₉H₃₆Cl₂O₂; MF: 772; RMF: 802; Prob 3.24%; Lib: mainlib; ID: 23051.

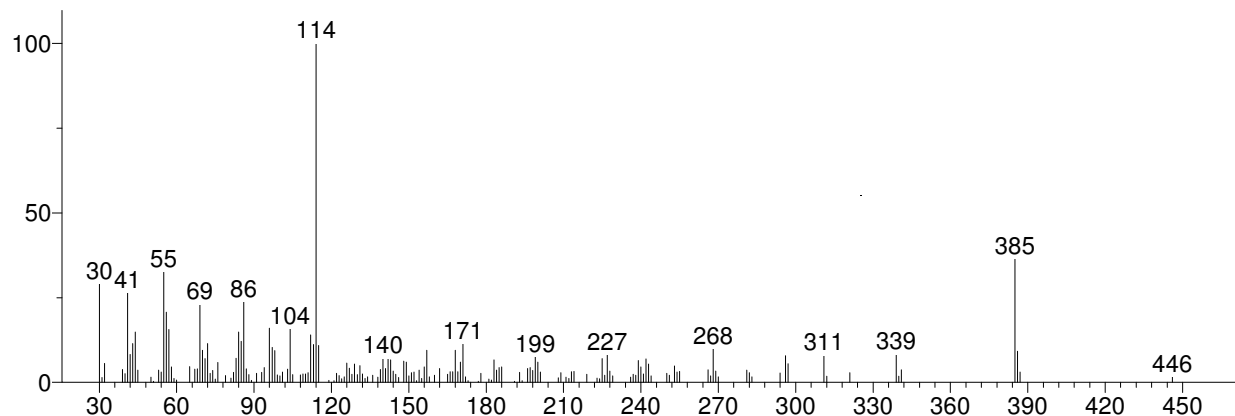


Hit 2 : Nonadecane
C₁₉H₄₀; MF: 771; RMF: 875; Prob 3.11%; CAS: 629-92-5; Lib: replib; ID: 5533.

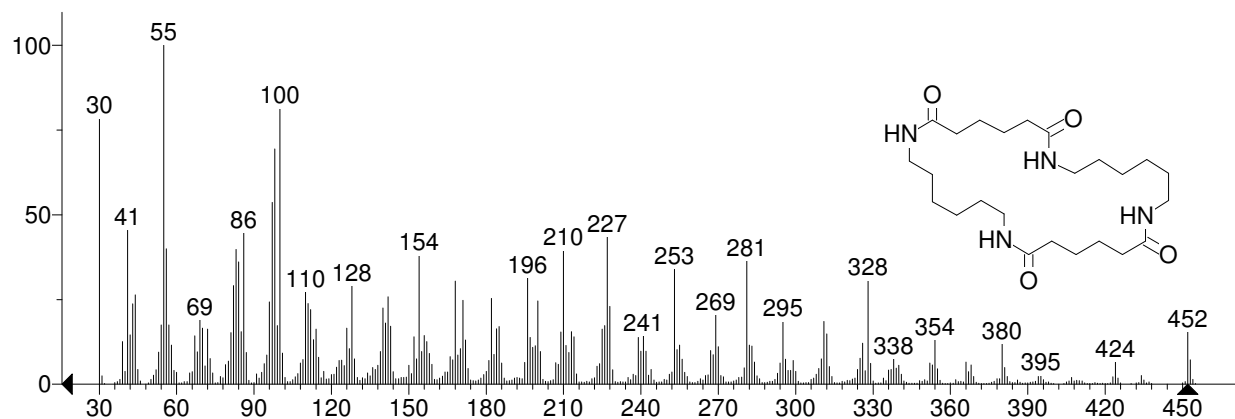


** Search Report Page 1 of 1 **

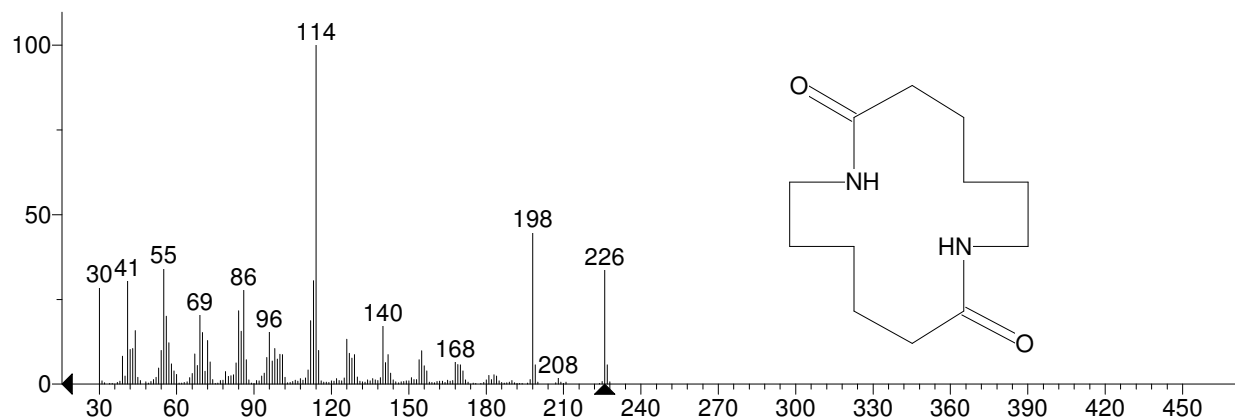
Unknown: Scan 1476 (11.210 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1491)
Compound in Library Factor = -1449



Hit 1 : 1,8,15,22-Tetraaza-2,7,16,21-cyclooctacosanetetron
C24H44N4O4; MF: 559; RMF: 561; Prob 25.0%; CAS: 4238-35-1; Lib: mainlib; ID: 19231.

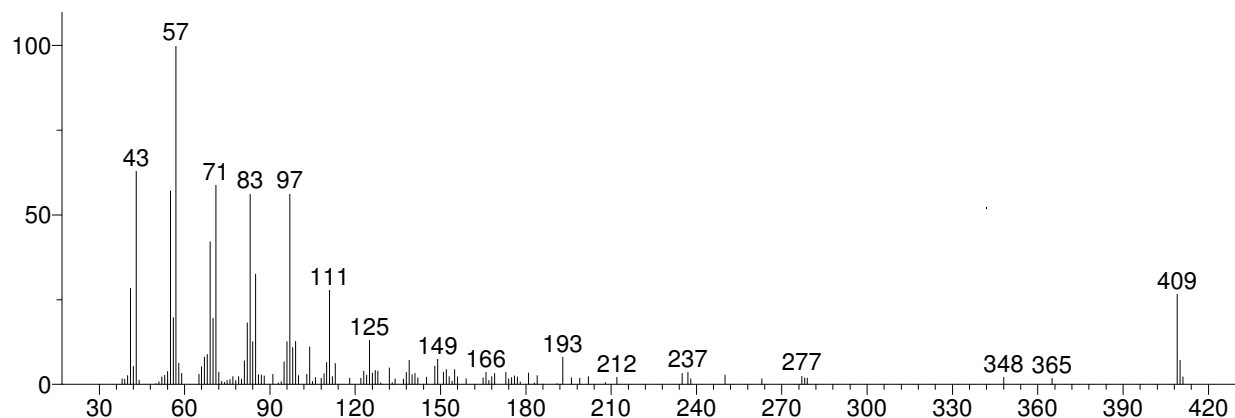


Hit 2 : 1,8-Diazacyclotetradecane-2,9-dione
C12H22N2O2; MF: 537; RMF: 700; Prob 9.86%; CAS: 5776-79-4; Lib: mainlib; ID: 77439.

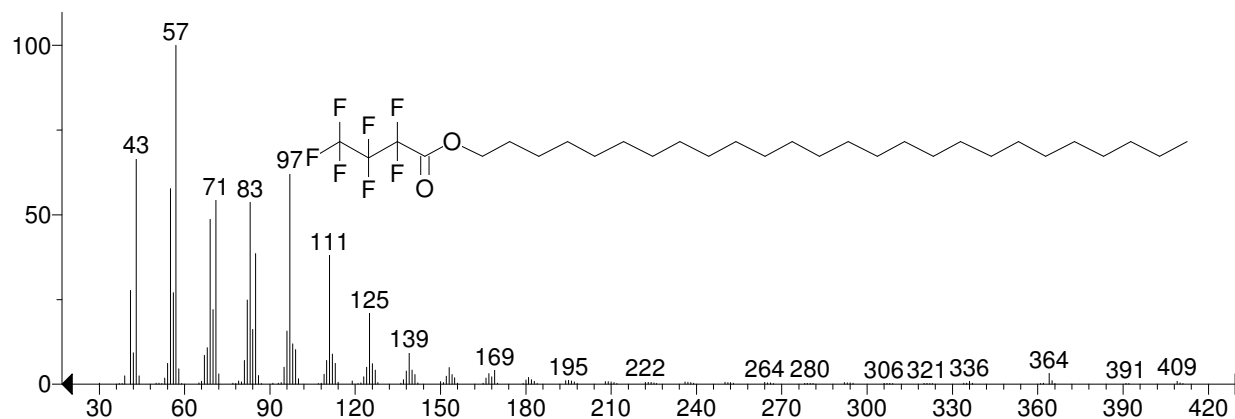


** Search Report Page 1 of 1 **

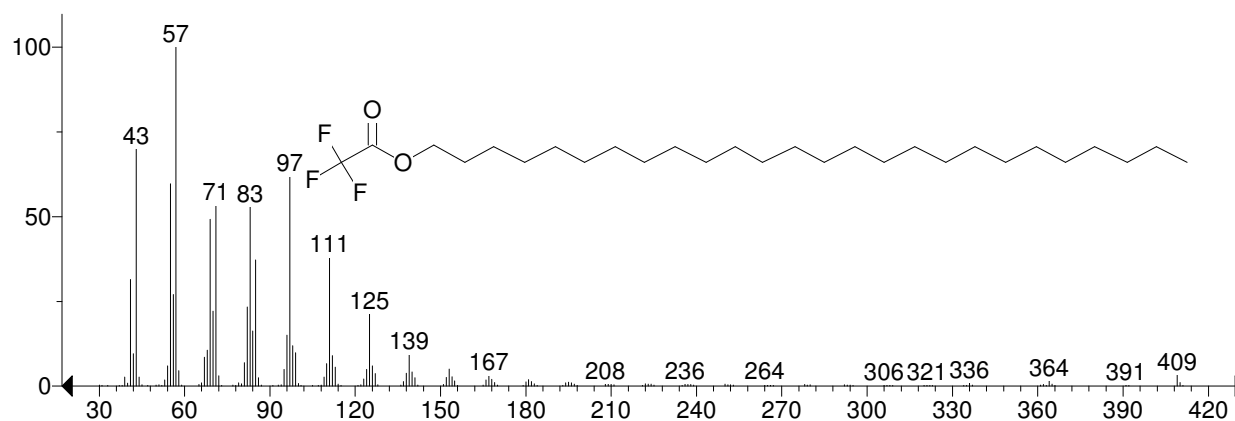
Unknown: Scan 1504 (11.421 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1494)
Compound in Library Factor = -1032



Hit 1 : Hexacosyl heptafluorobutyrate
C₃₀H₅₃F₇O₂; MF: 684; RMF: 741; Prob 8.28%; Lib: mainlib; ID: 22108.

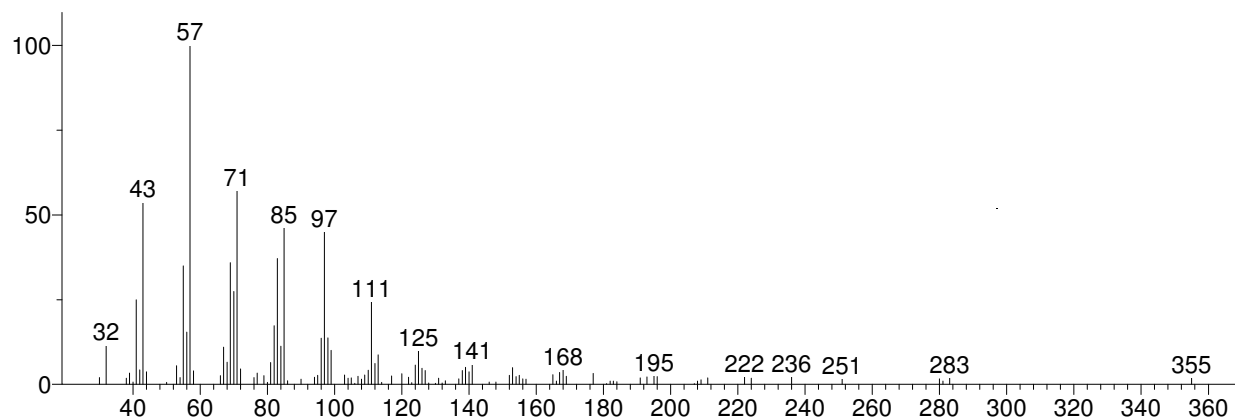


Hit 2 : Hexacosyl trifluoroacetate
C₂₈H₅₃F₃O₂; MF: 680; RMF: 729; Prob 6.99%; Lib: mainlib; ID: 22100.



** Search Report Page 1 of 1 **

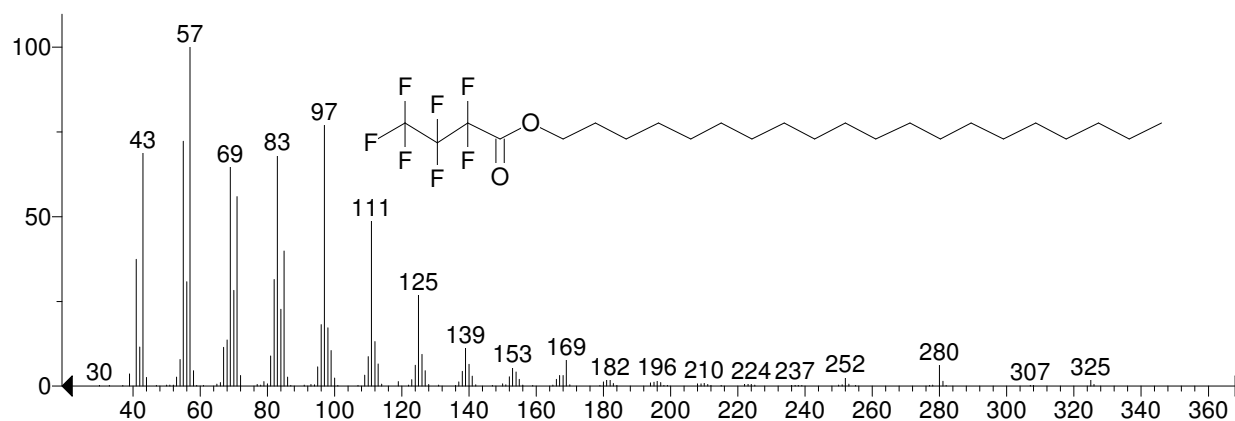
Unknown: Scan 1542 (11.707 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1551)
Compound in Library Factor = -811



Hit 1 : 1-Decanol, 2-hexyl-
C₁₆H₃₄O; MF: 775; RMF: 846; Prob 3.15%; CAS: 2425-77-6; Lib: replib; ID: 5418.

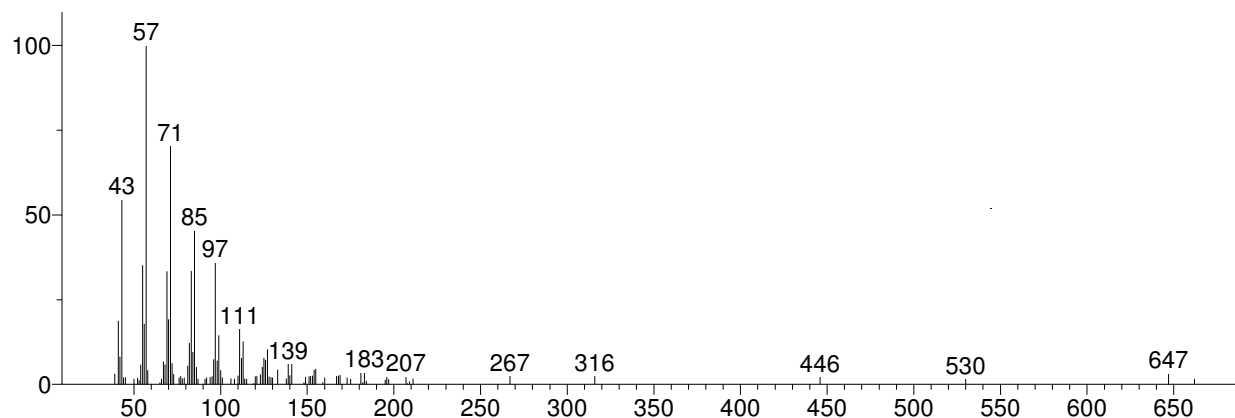


Hit 2 : Eicosyl heptafluorobutyrate
C₂₄H₄₁F₇O₂; MF: 768; RMF: 807; Prob 2.41%; Lib: mainlib; ID: 23347.

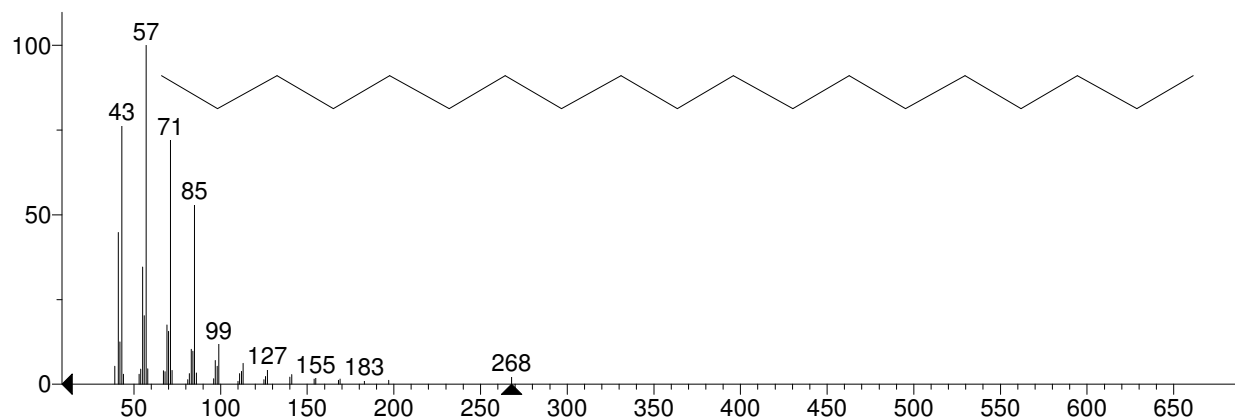


** Search Report Page 1 of 1 **

Unknown: Scan 1615 (12.257 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1639)
Compound in Library Factor = -1131



Hit 1 : Nonadecane
C₁₉H₄₀; MF: 730; RMF: 872; Prob 3.36%; CAS: 629-92-5; Lib: replib; ID: 5533.

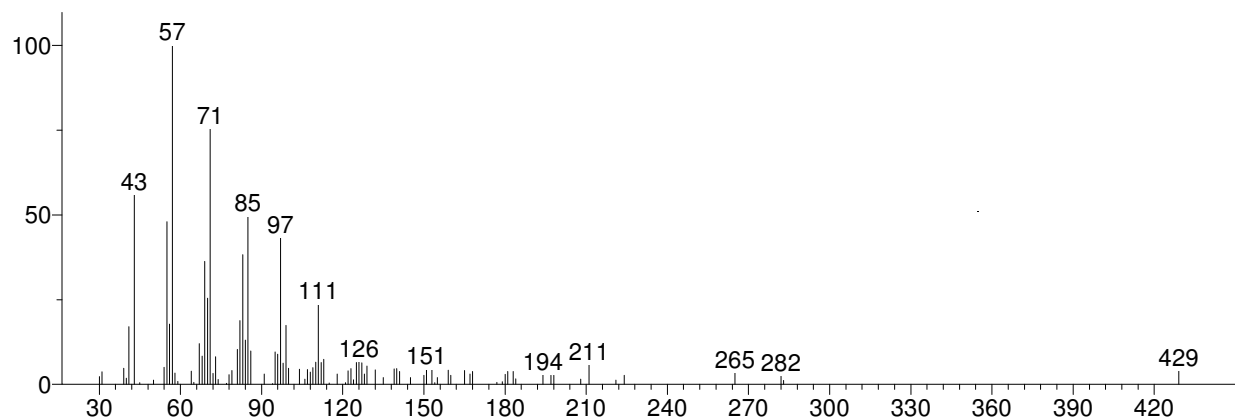


Hit 2 : 1-Decanol, 2-hexyl-
C₁₆H₃₄O; MF: 729; RMF: 846; Prob 3.23%; CAS: 2425-77-6; Lib: mainlib; ID: 22297.

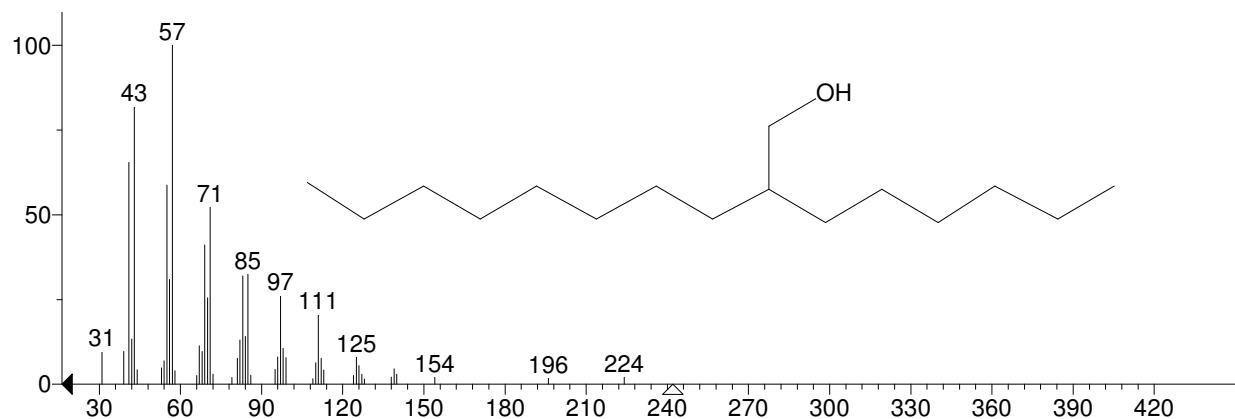


** Search Report Page 1 of 1 **

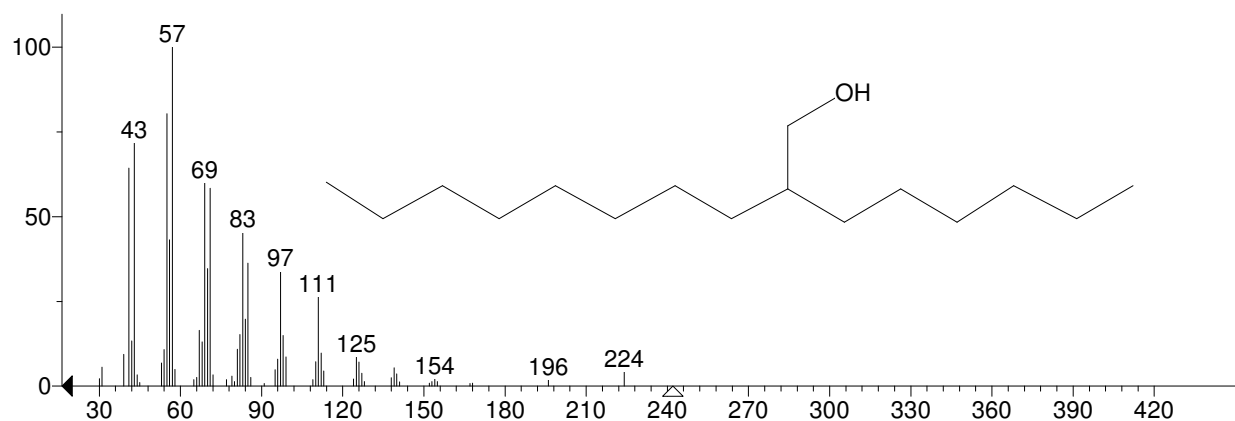
Unknown: Scan 1715 (13.011 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py1.D\data.ms (-1738)
Compound in Library Factor = -1131



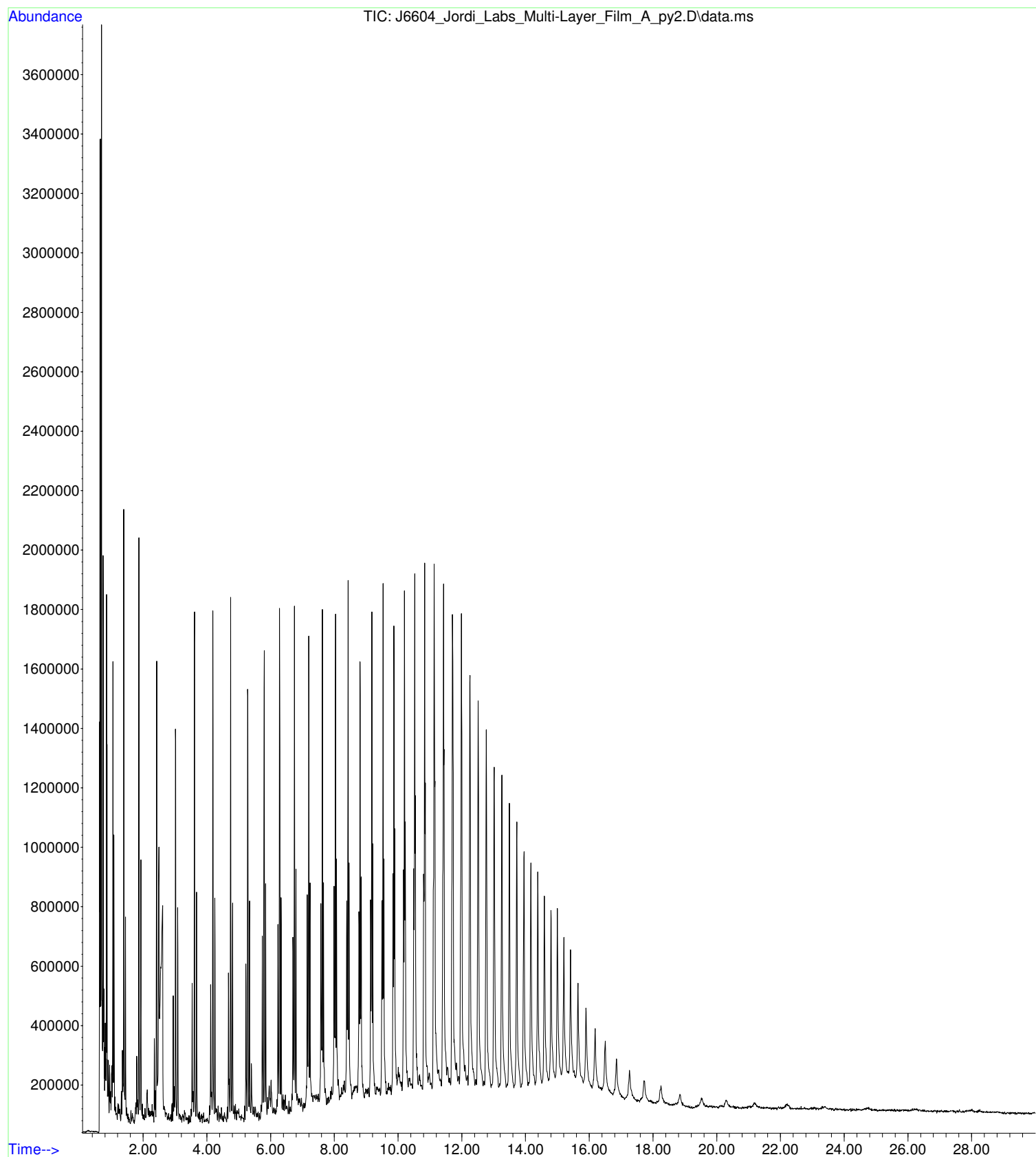
Hit 1 : 1-Decanol, 2-hexyl-
C₁₆H₃₄O; MF: 721; RMF: 872; Prob 5.44%; CAS: 2425-77-6; Lib: replib; ID: 5417.



Hit 2 : 1-Decanol, 2-hexyl-
C₁₆H₃₄O; MF: 715; RMF: 845; Prob 5.44%; CAS: 2425-77-6; Lib: mainlib; ID: 22297.

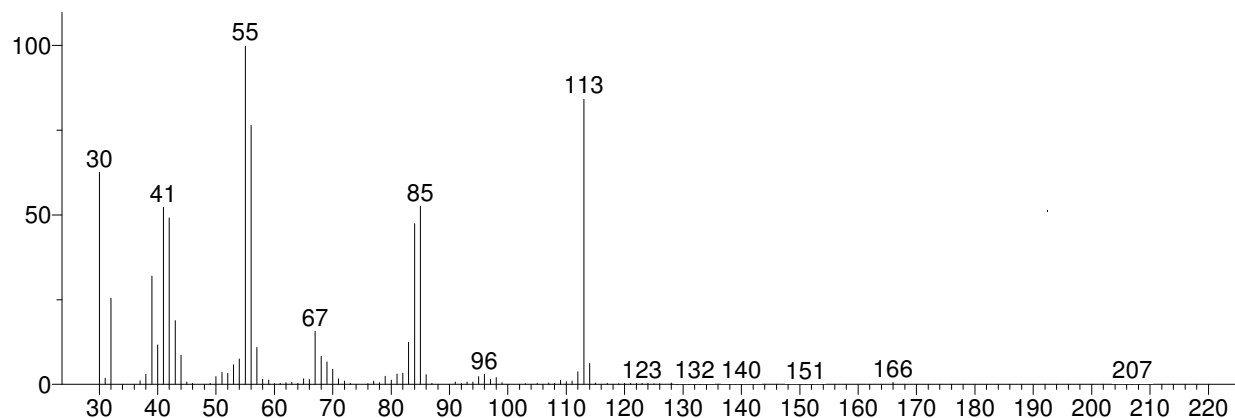


File :C:\msdchem\1\DATA\2012\Temp\040512\J6604_Jordi_Labs_Multi-La
... yer_Film_A_py2.D
Operator : Mark Jordi
Instrument : Instrument #1
Acquired : 9 Apr 2012 9:57 using AcqMethod PYMS.M
Sample Name: J6604 Jordi Labs Multi-Layer Film
Misc Info : J6604 Jordi Labs Multi-Layer Film

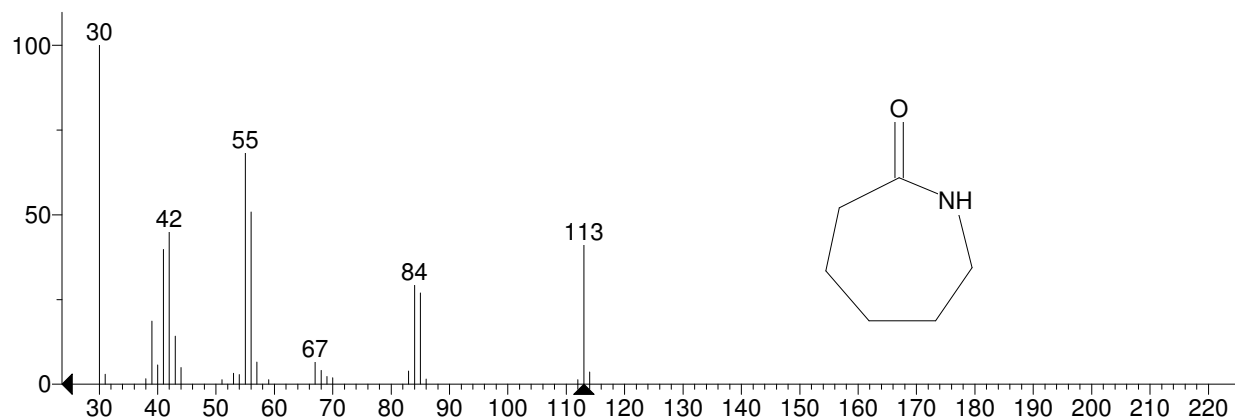


** Search Report Page 1 of 1 **

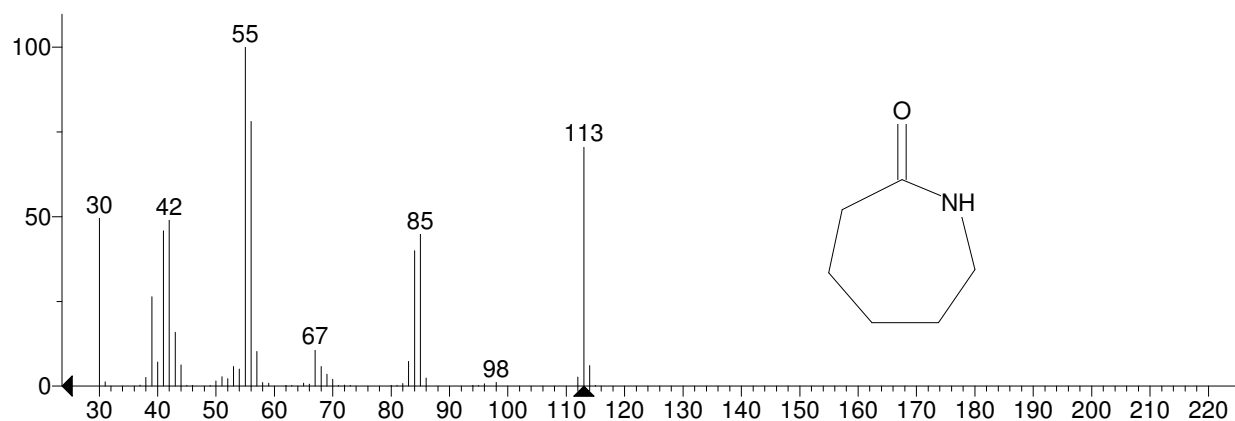
Unknown: Scan 331 (2.582 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = 191



Hit 1 : Caprolactam
C₆H₁₁NO; MF: 881; RMF: 935; Prob 79.3%; CAS: 105-60-2; Lib: replib; ID: 413.

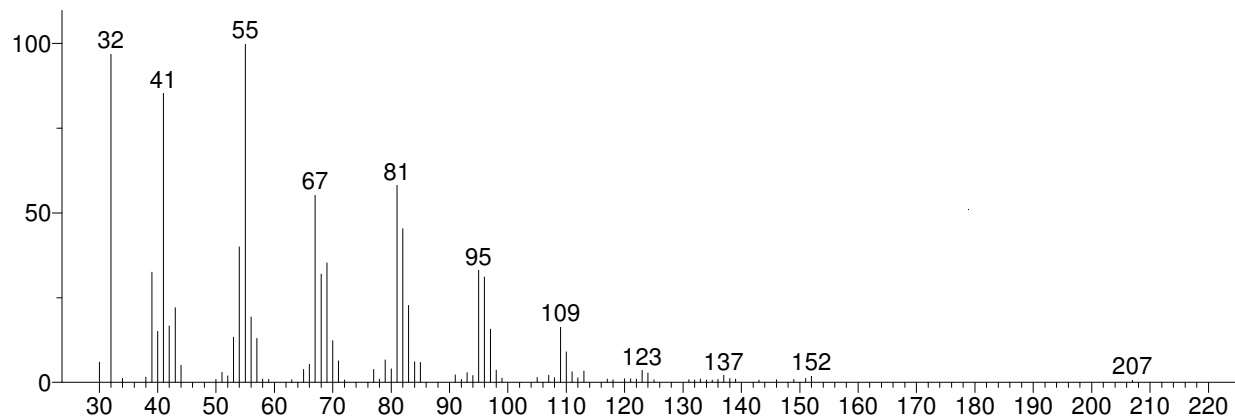


Hit 2 : Caprolactam
C₆H₁₁NO; MF: 864; RMF: 889; Prob 79.3%; CAS: 105-60-2; Lib: replib; ID: 4436.

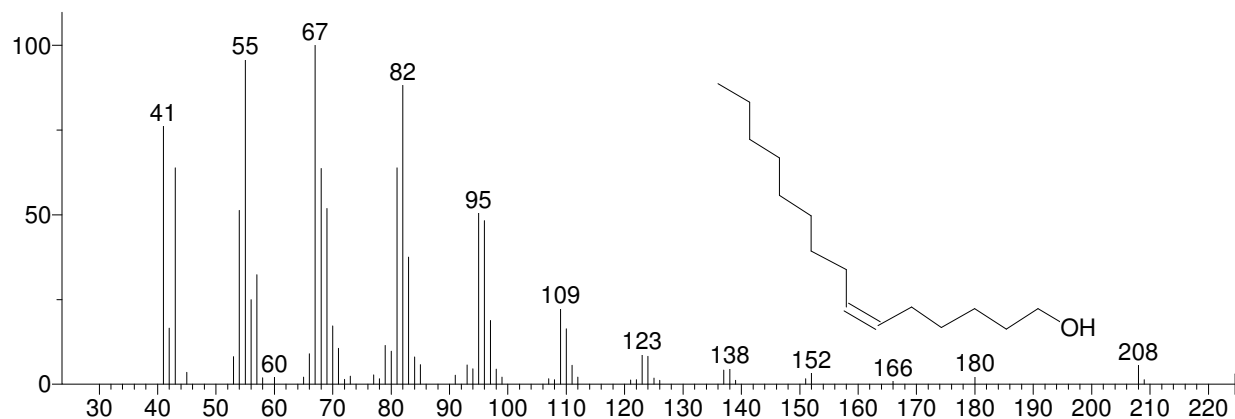


** Search Report Page 1 of 1 **

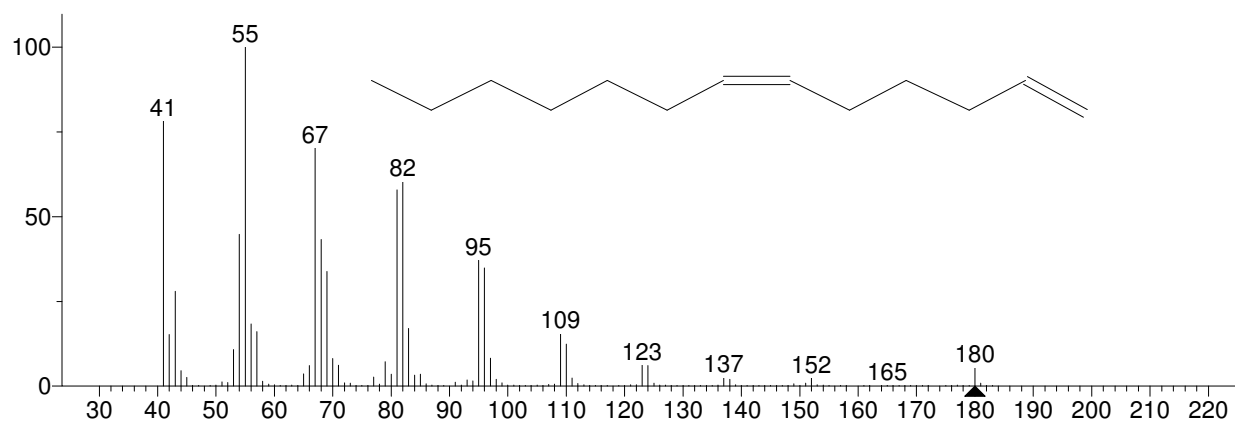
Unknown: Scan 378 (2.936 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -217



Hit 1 : (Z)6-Pentadecen-1-ol
C₁₅H₃₀O; MF: 875; RMF: 899; Prob 6.80%; CAS: 68797-95-5; Lib: mainlib; ID: 28658.

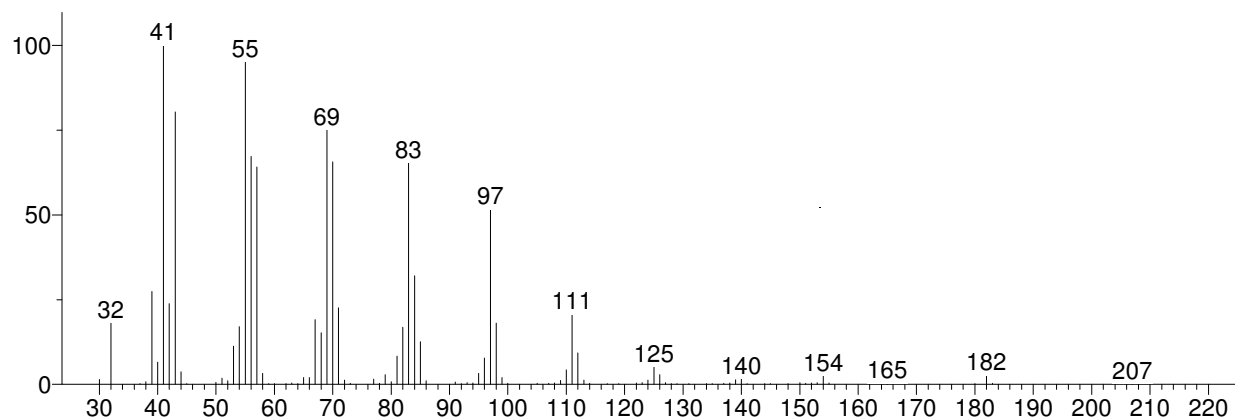


Hit 2 : Z-1,6-Tridecadiene
C₁₃H₂₄; MF: 864; RMF: 873; Prob 4.66%; Lib: mainlib; ID: 17368.

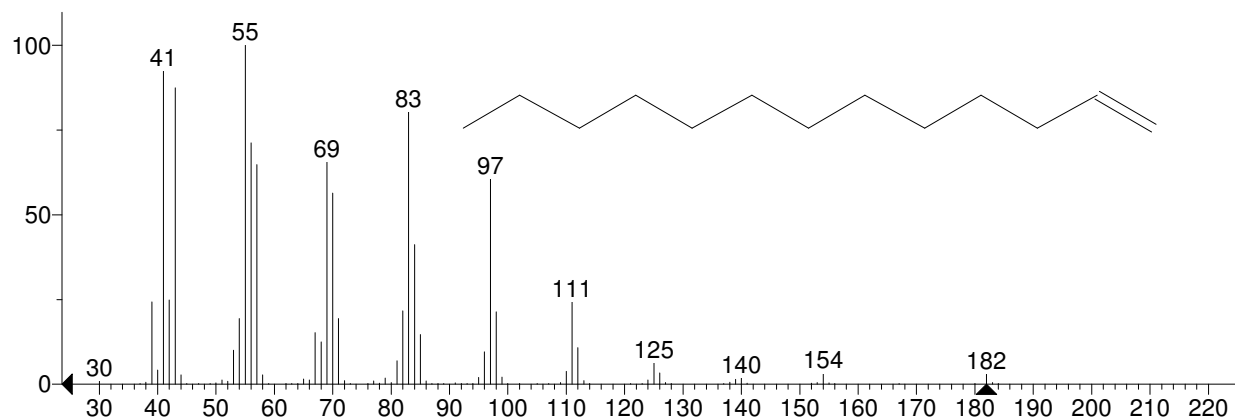


** Search Report Page 1 of 1 **

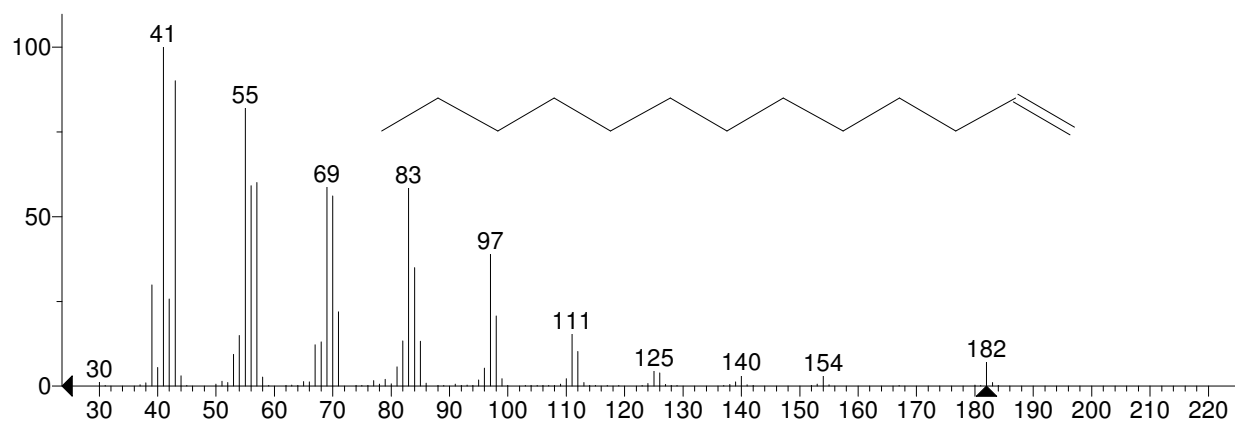
Unknown: Scan 388 (3.011 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -117



Hit 1 : 1-Tridecene
C₁₃H₂₆; MF: 927; RMF: 935; Prob 7.75%; CAS: 2437-56-1; Lib: replib; ID: 4180.

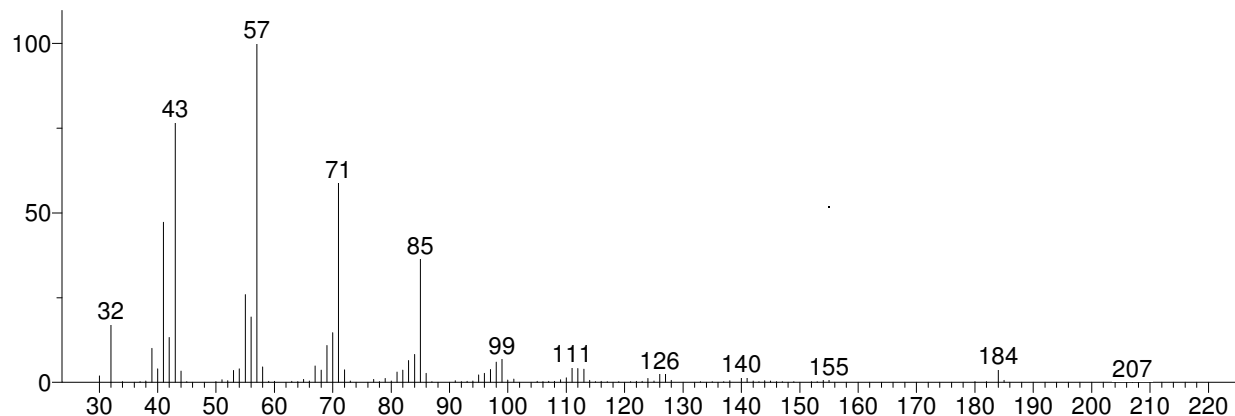


Hit 2 : 1-Tridecene
C₁₃H₂₆; MF: 918; RMF: 925; Prob 7.75%; CAS: 2437-56-1; Lib: replib; ID: 823.

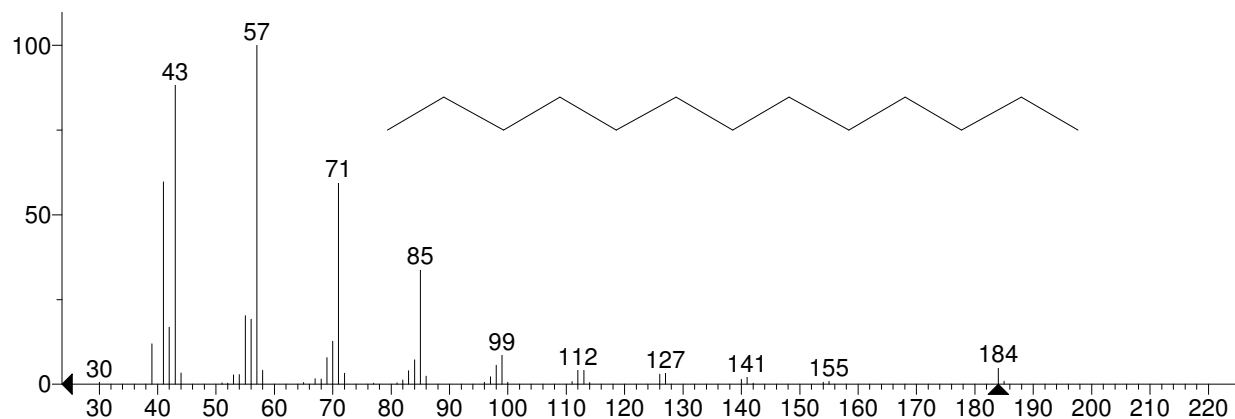


** Search Report Page 1 of 1 **

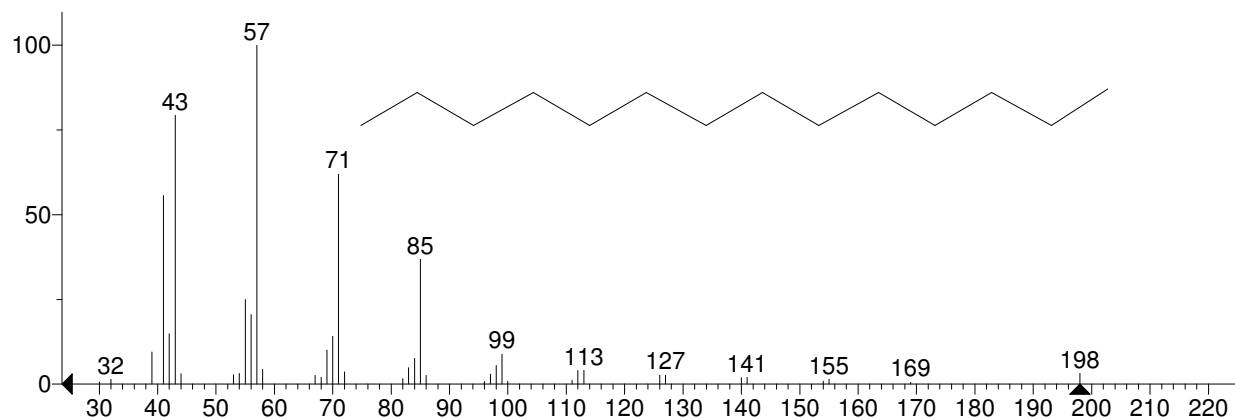
Unknown: Scan 397 (3.079 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -168



Hit 1 : Tridecane
C₁₃H₂₈; MF: 888; RMF: 921; Prob 23.3%; CAS: 629-50-5; Lib: replib; ID: 5380.

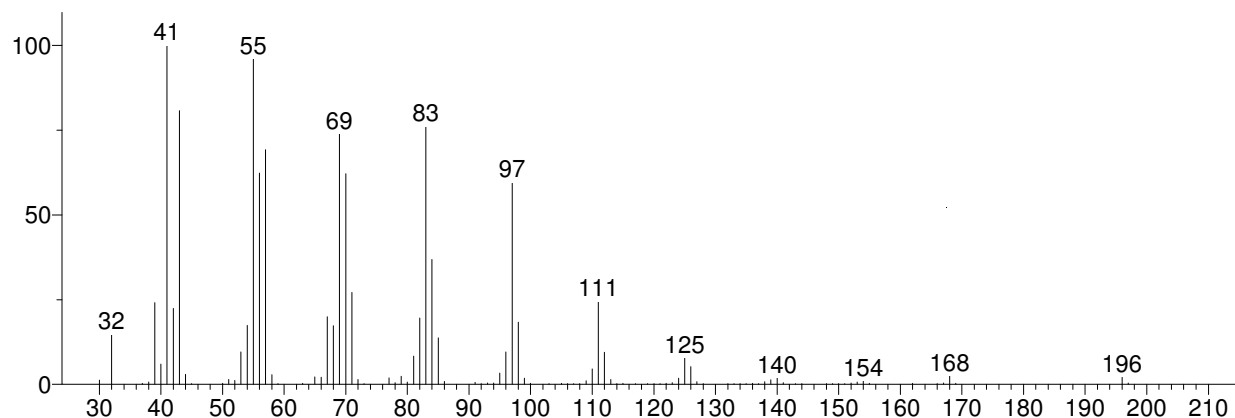


Hit 2 : Tetradecane
C₁₄H₃₀; MF: 882; RMF: 927; Prob 18.3%; CAS: 629-59-4; Lib: replib; ID: 5511.

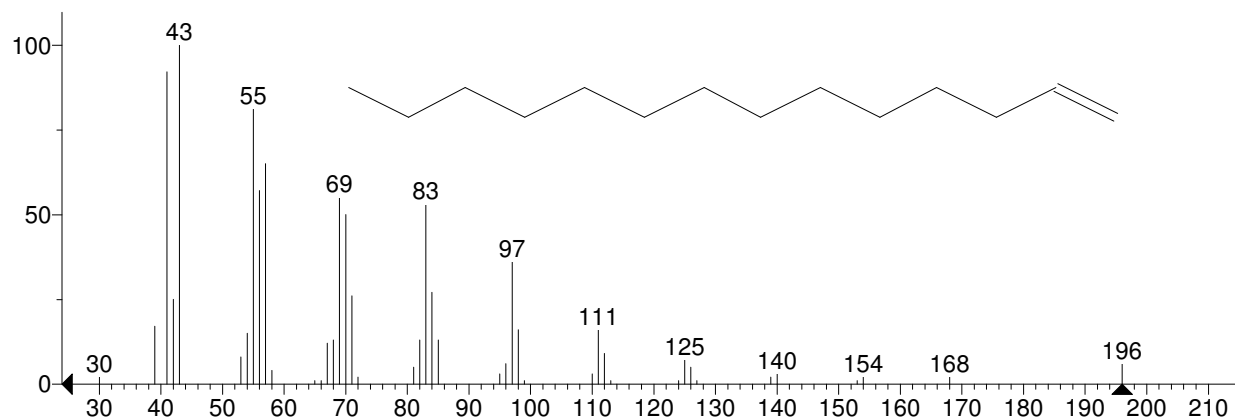


** Search Report Page 1 of 1 **

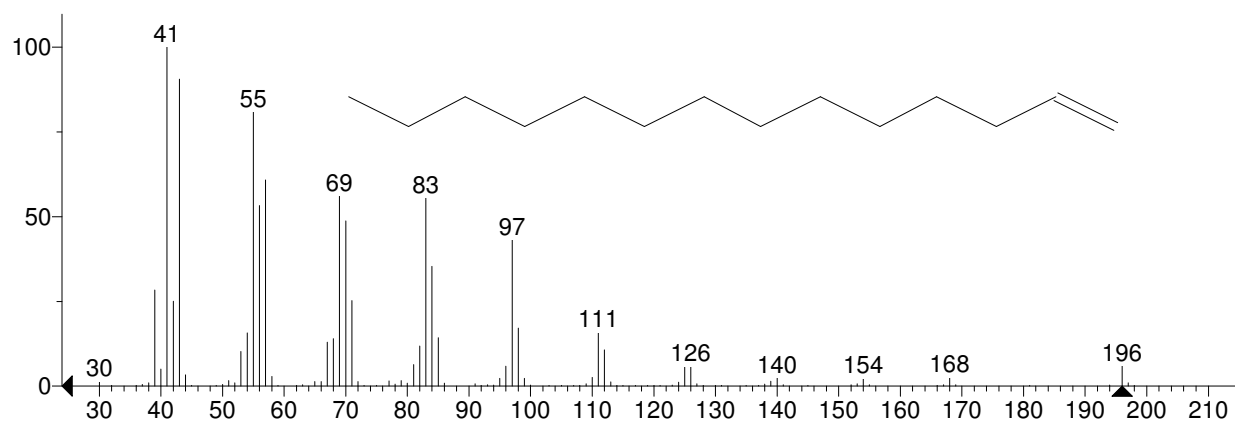
Unknown: Scan 467 (3.607 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -113



Hit 1 : 1-Tetradecene
C₁₄H₂₈; MF: 933; RMF: 951; Prob 8.16%; CAS: 1120-36-1; Lib: replib; ID: 1681.

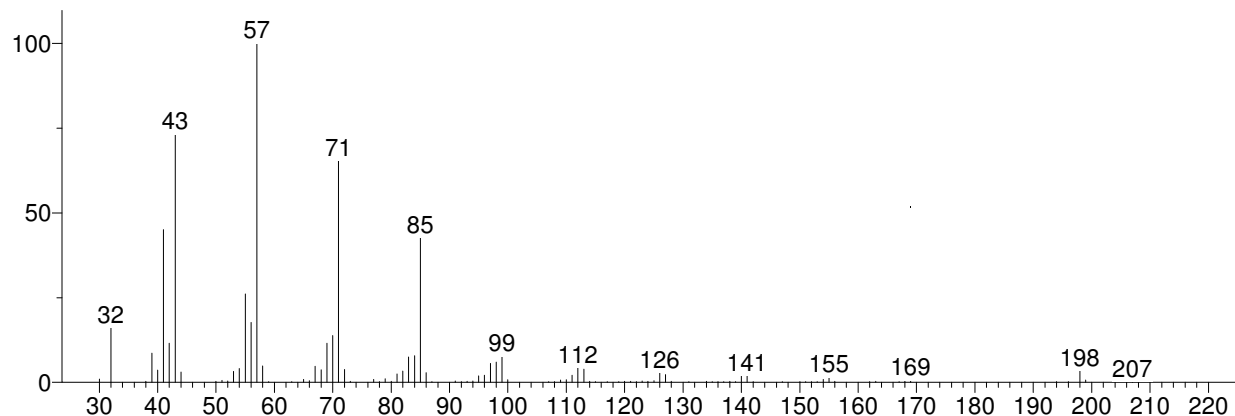


Hit 2 : 1-Tetradecene
C₁₄H₂₈; MF: 930; RMF: 934; Prob 8.16%; CAS: 1120-36-1; Lib: replib; ID: 817.

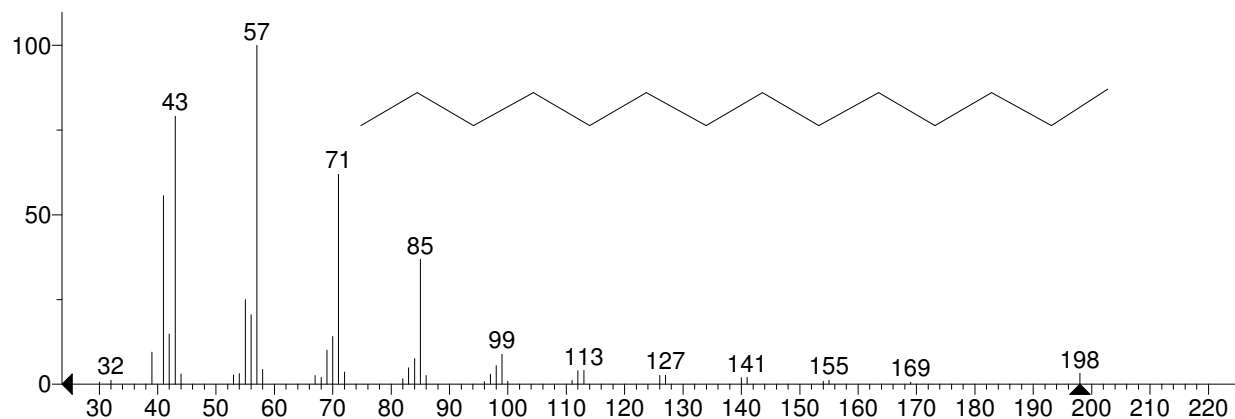


** Search Report Page 1 of 1 **

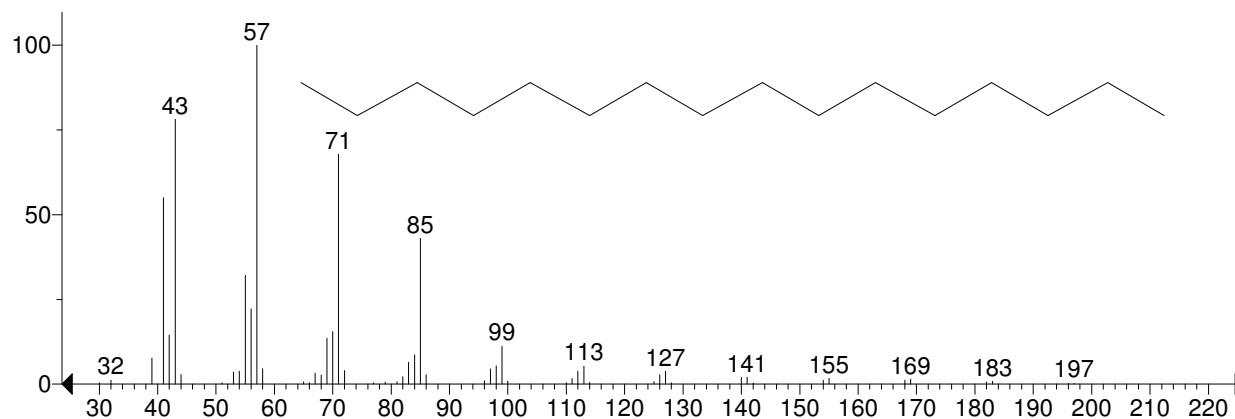
Unknown: Scan 476 (3.674 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -107



Hit 1 : Tetradecane
C₁₄H₃₀; MF: 923; RMF: 949; Prob 37.5%; CAS: 629-59-4; Lib: replib; ID: 5511.

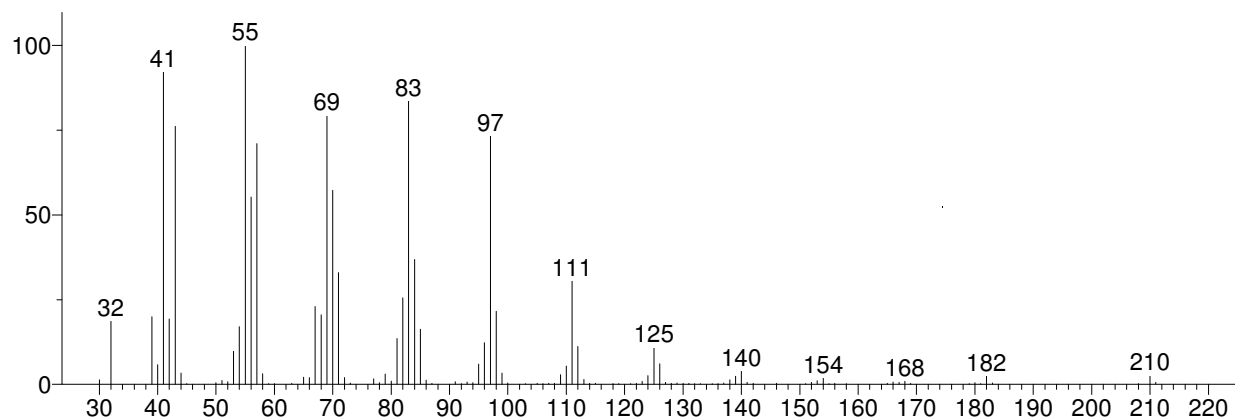


Hit 2 : Hexadecane
C₁₆H₃₄; MF: 894; RMF: 917; Prob 10.6%; CAS: 544-76-3; Lib: replib; ID: 5556.

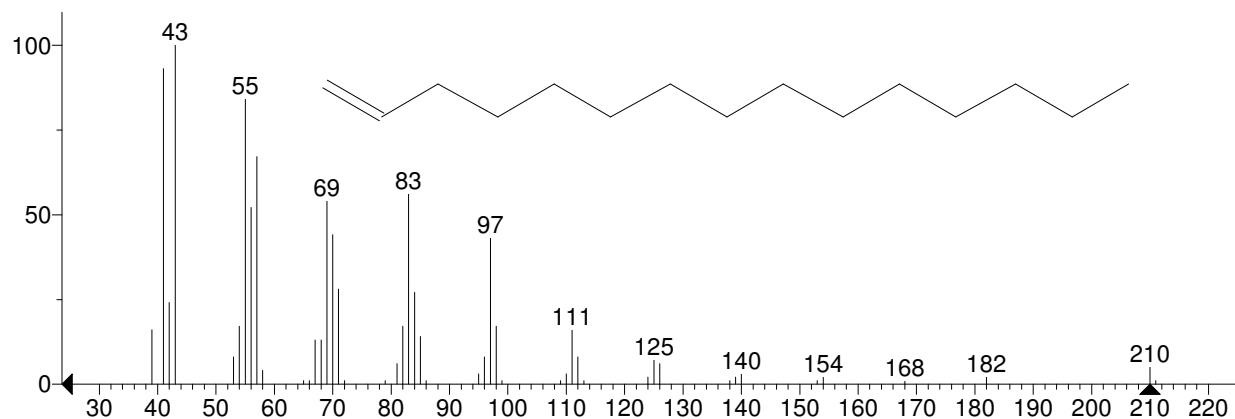


** Search Report Page 1 of 1 **

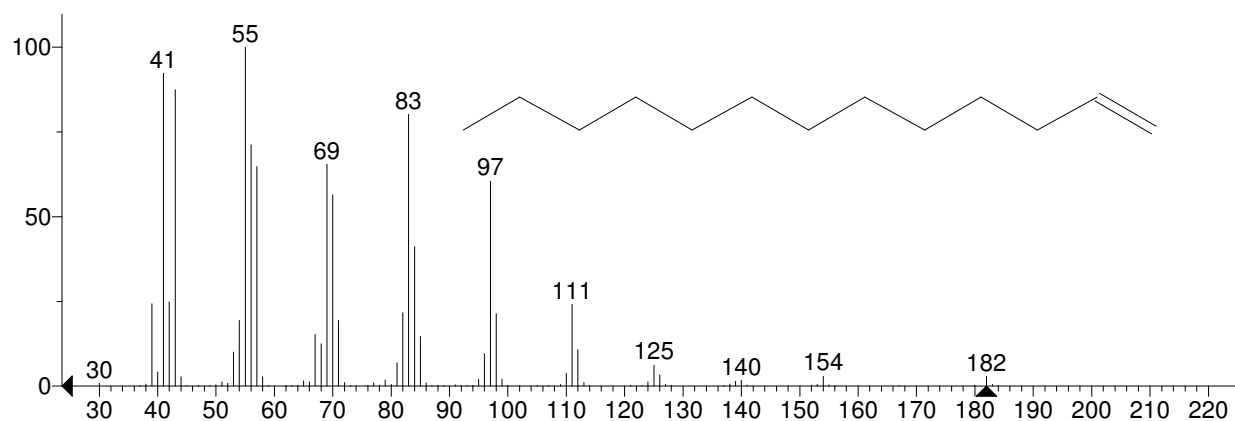
Unknown: Scan 545 (4.194 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -103



Hit 1 : 1-Pentadecene
C₁₅H₃₀; MF: 932; RMF: 952; Prob 12.9%; CAS: 13360-61-7; Lib: replib; ID: 1695.

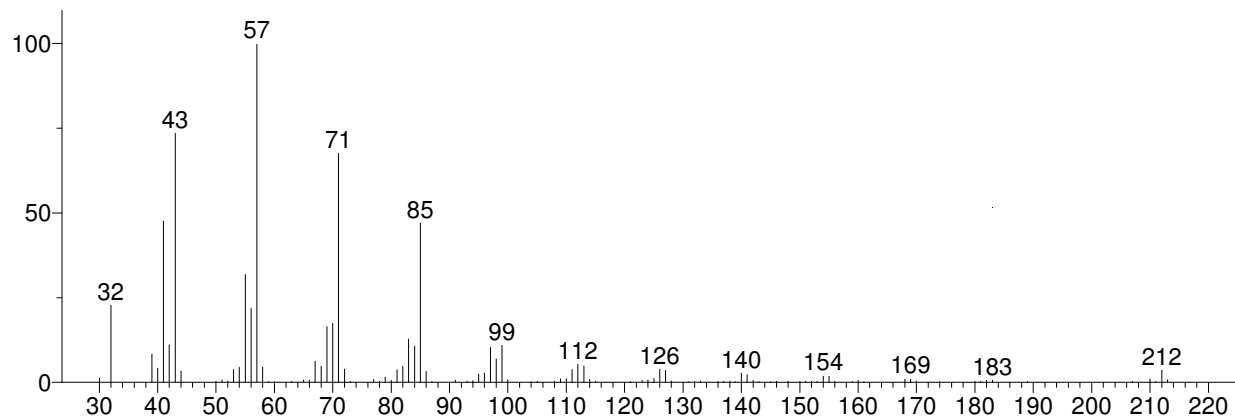


Hit 2 : 1-Tridecene
C₁₃H₂₆; MF: 909; RMF: 925; Prob 4.71%; CAS: 2437-56-1; Lib: replib; ID: 4180.

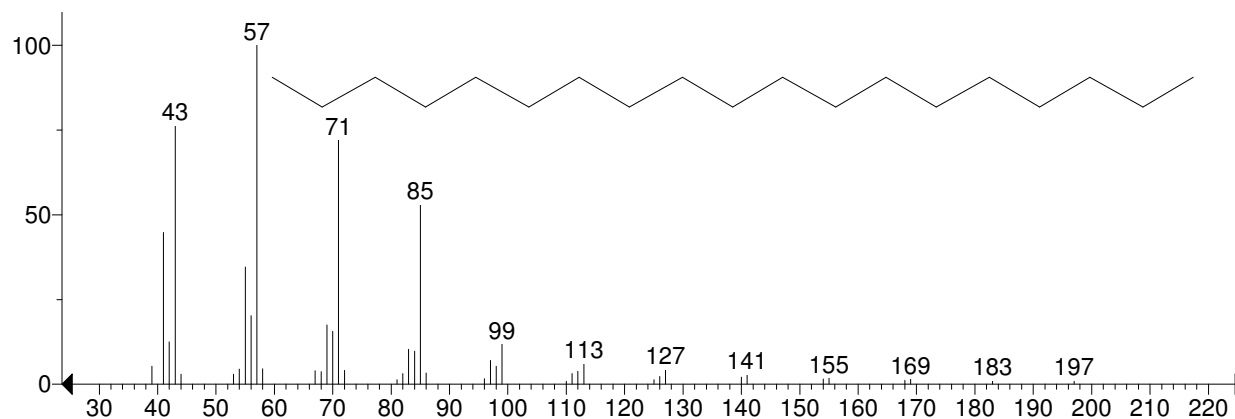


** Search Report Page 1 of 1 **

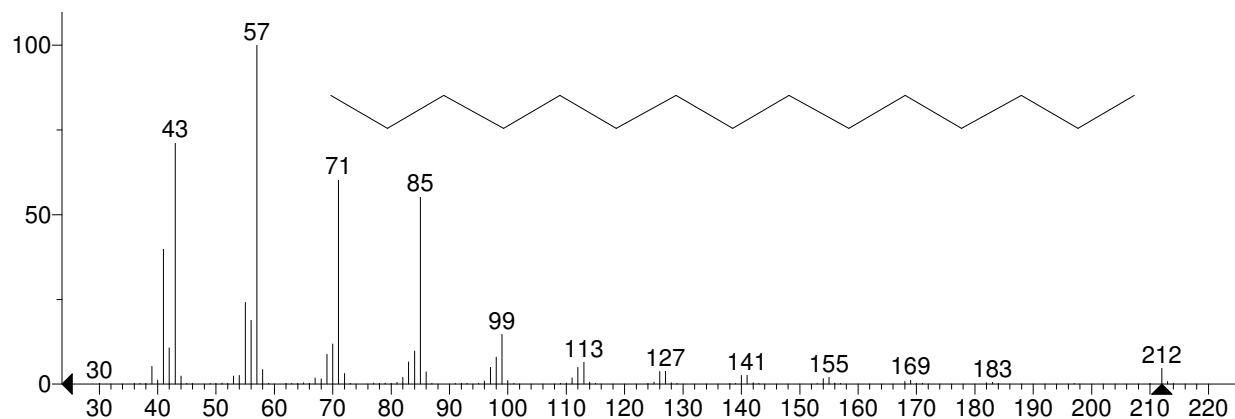
Unknown: Scan 553 (4.255 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -217



Hit 1 : Nonadecane
C₁₉H₄₀; MF: 876; RMF: 931; Prob 12.0%; CAS: 629-92-5; Lib: replib; ID: 5533.

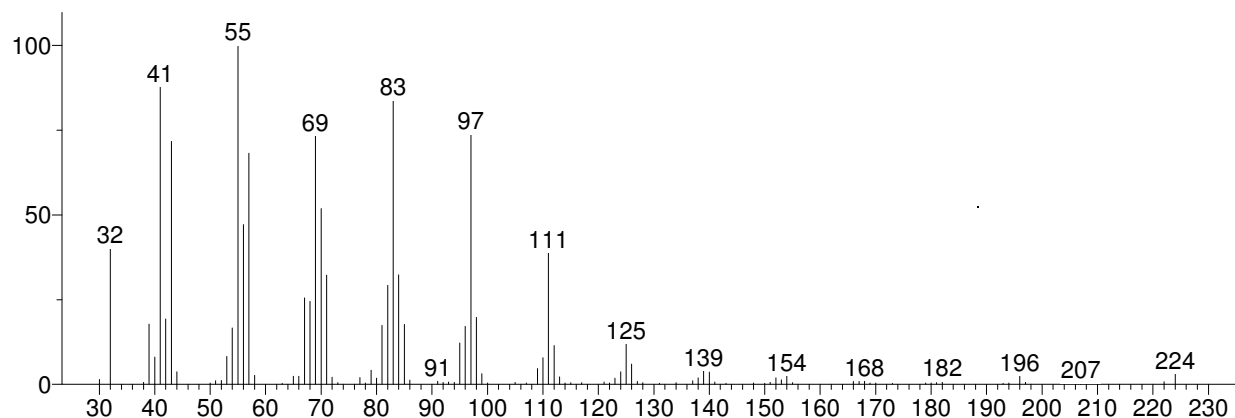


Hit 2 : Pentadecane
C₁₅H₃₂; MF: 872; RMF: 898; Prob 10.1%; CAS: 629-62-9; Lib: replib; ID: 5525.

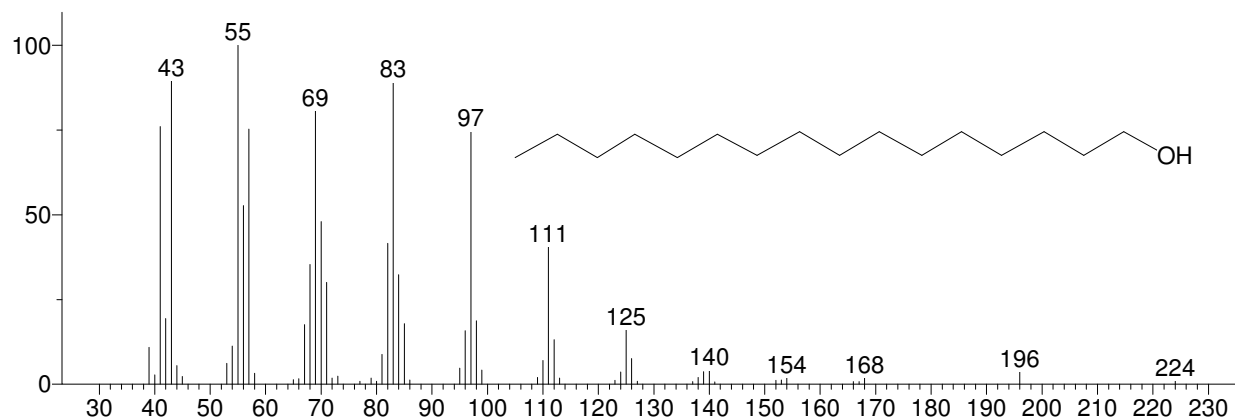


** Search Report Page 1 of 1 **

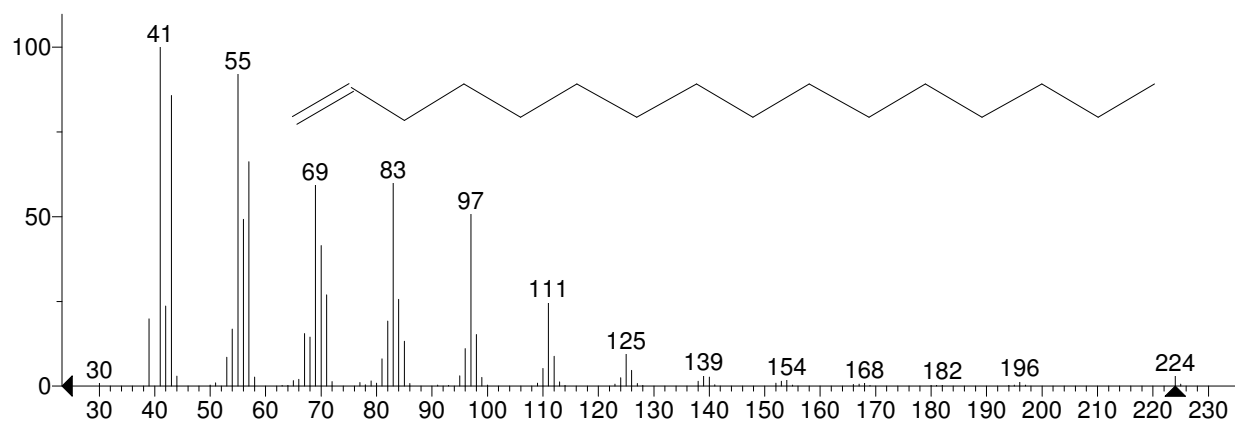
Unknown: Scan 619 (4.752 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -170



Hit 1 : 1-Hexadecanol
C₁₆H₃₄O; MF: 915; RMF: 928; Prob 8.72%; CAS: 36653-82-4; Lib: replib; ID: 4395.

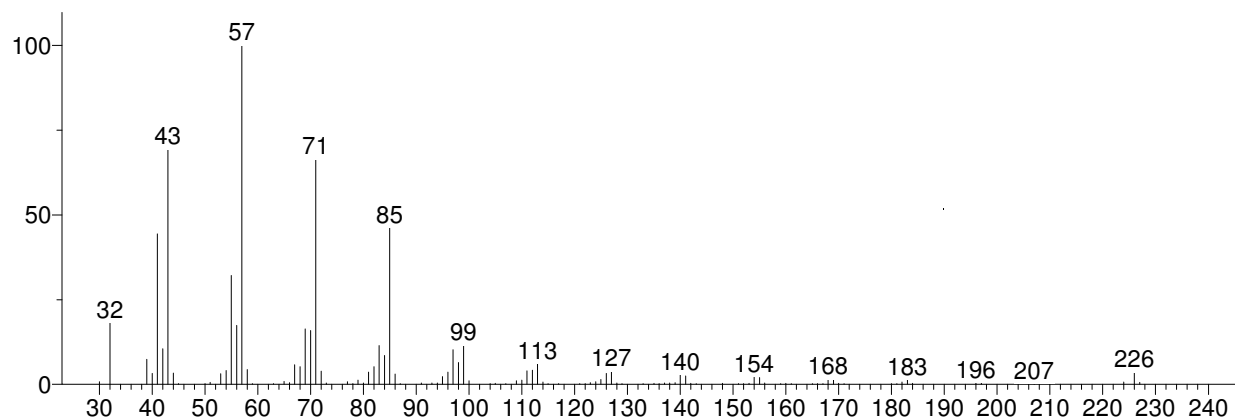


Hit 2 : 1-Hexadecene
C₁₆H₃₂; MF: 909; RMF: 928; Prob 6.85%; CAS: 629-73-2; Lib: replib; ID: 885.

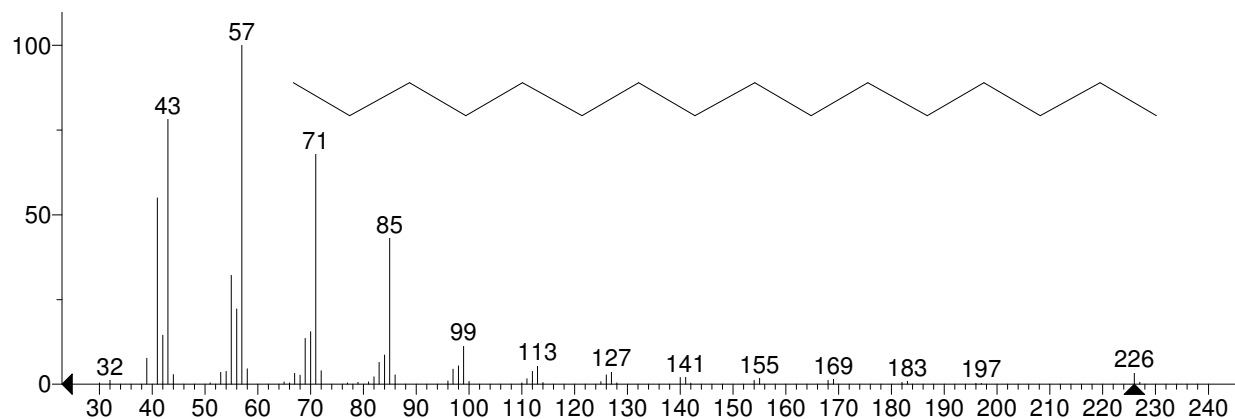


** Search Report Page 1 of 1 **

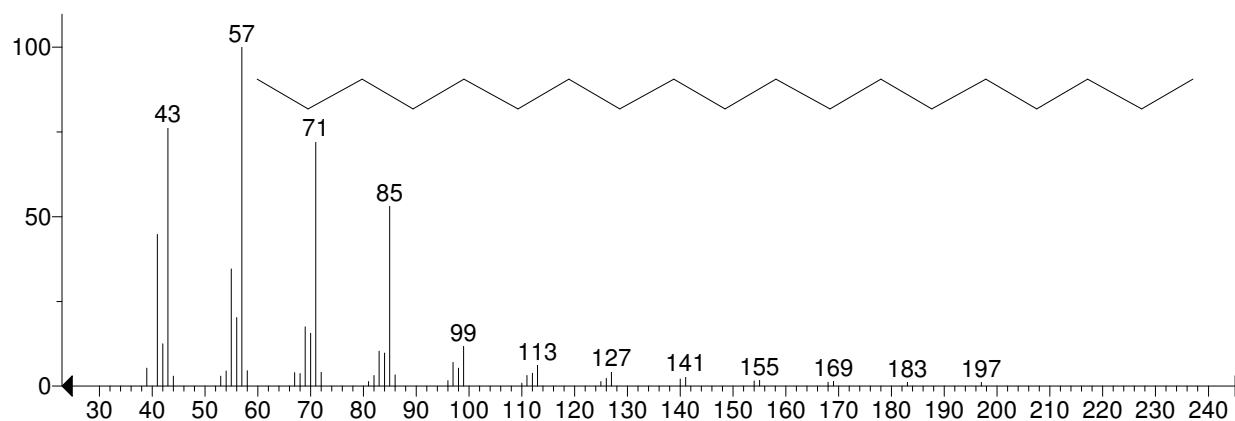
Unknown: Scan 626 (4.805 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -104



Hit 1 : Hexadecane
C₁₆H₃₄; MF: 907; RMF: 924; Prob 23.4%; CAS: 544-76-3; Lib: replib; ID: 5556.

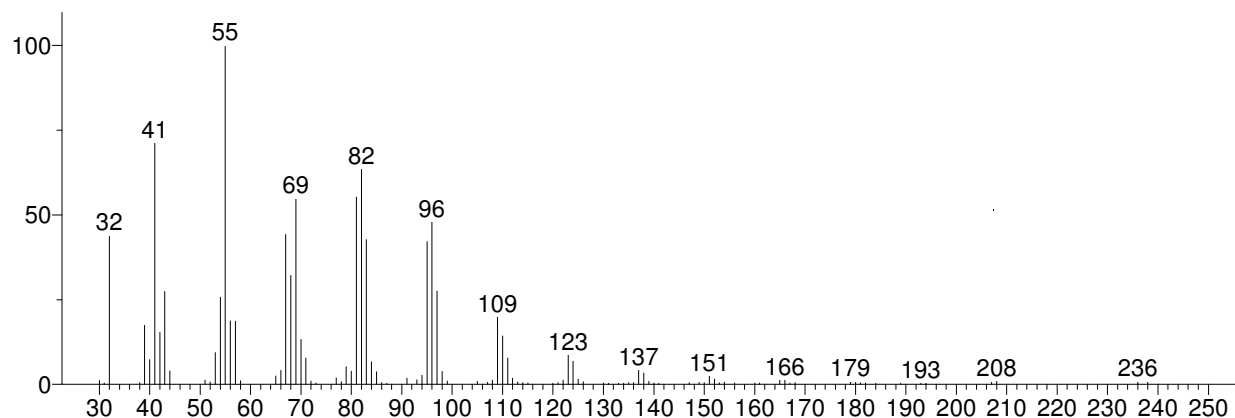


Hit 2 : Nonadecane
C₁₉H₄₀; MF: 894; RMF: 943; Prob 15.1%; CAS: 629-92-5; Lib: replib; ID: 5533.

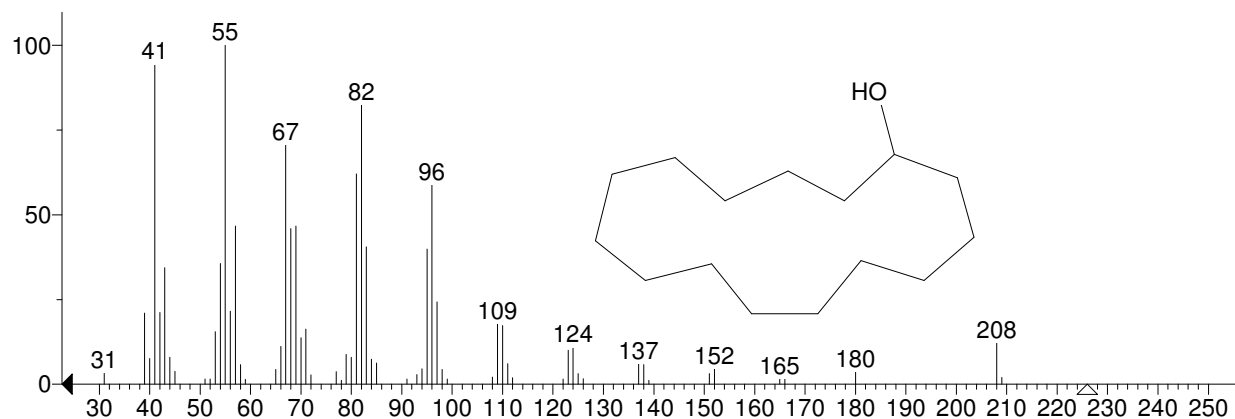


** Search Report Page 1 of 1 **

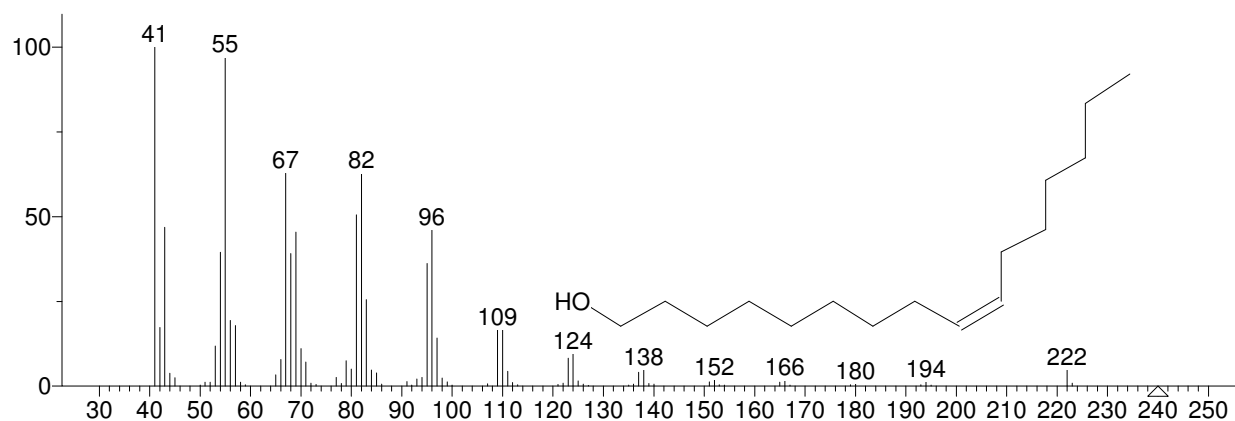
Unknown: Scan 682 (5.227 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -297



Hit 1 : Cyclopentadecanol
C₁₅H₃₀O; MF: 878; RMF: 908; Prob 4.52%; CAS: 4727-17-7; Lib: mainlib; ID: 17592.

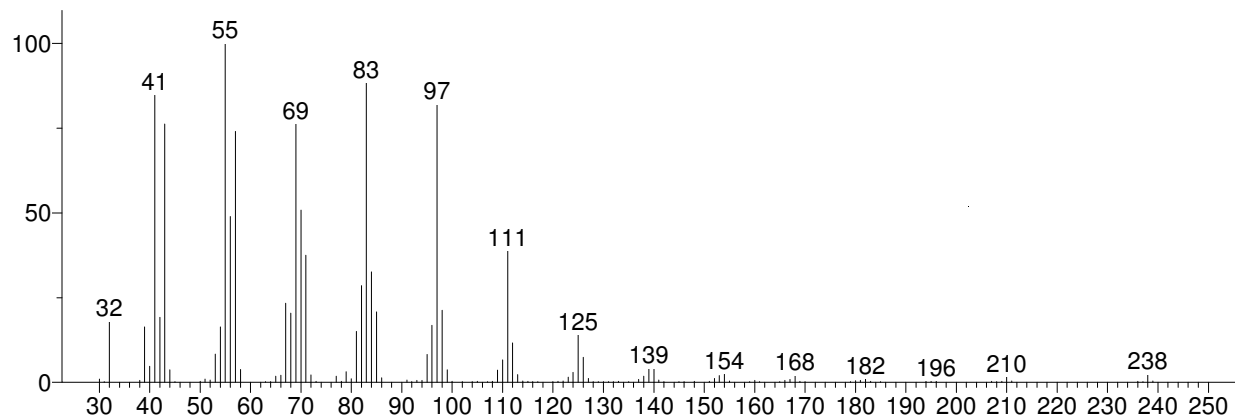


Hit 2 : 9-Hexadecen-1-ol, (Z)-
C₁₆H₃₂O; MF: 878; RMF: 893; Prob 4.52%; CAS: 10378-01-5; Lib: replib; ID: 908.

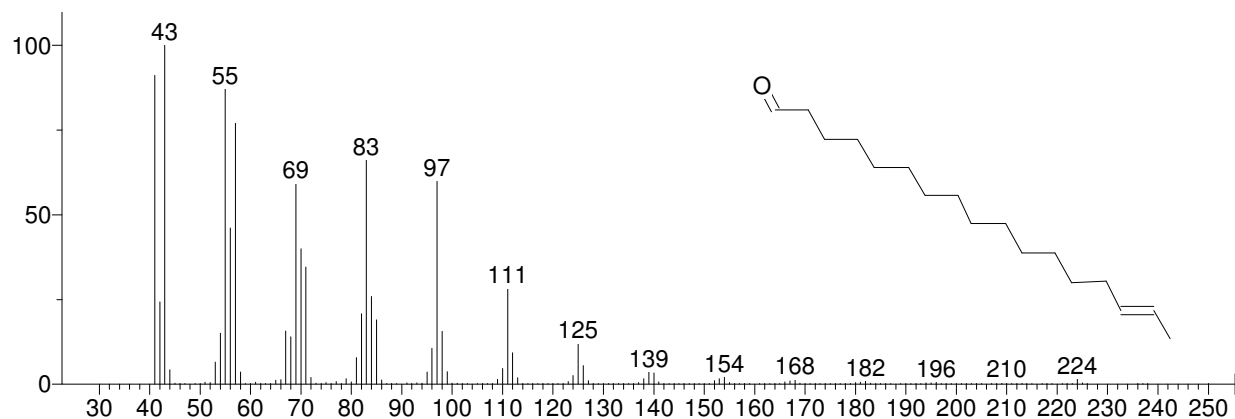


** Search Report Page 1 of 1 **

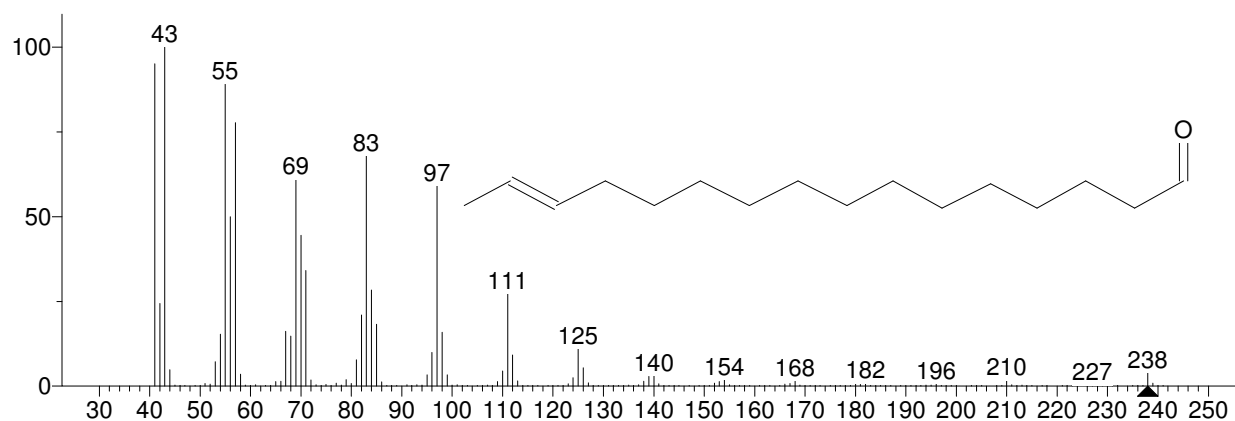
Unknown: Scan 690 (5.287 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -117



Hit 1 : E-15-Heptadecenal
C₁₇H₃₂O; MF: 929; RMF: 934; Prob 7.89%; Lib: mainlib; ID: 5518.

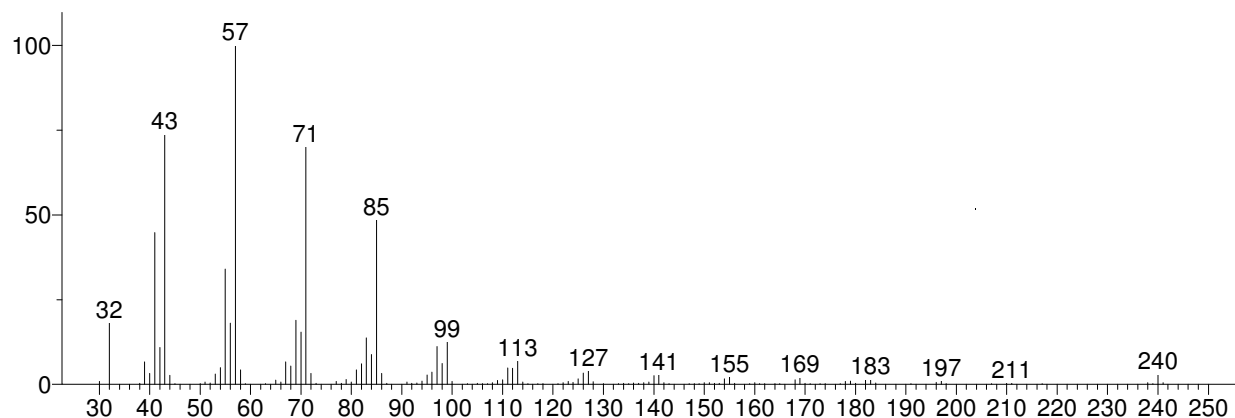


Hit 2 : E-14-Hexadecenal
C₁₆H₃₀O; MF: 924; RMF: 925; Prob 6.36%; CAS: 330207-53-9; Lib: mainlib; ID: 5588.

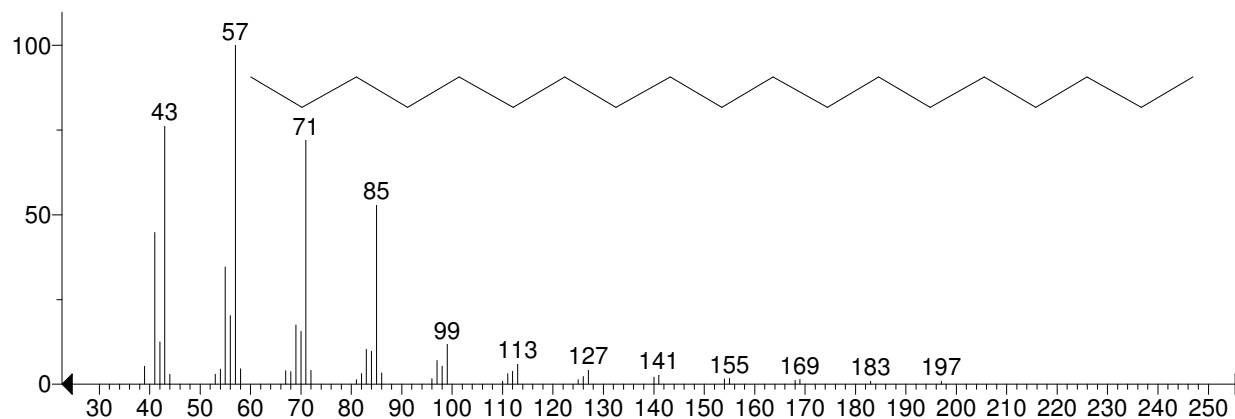


** Search Report Page 1 of 1 **

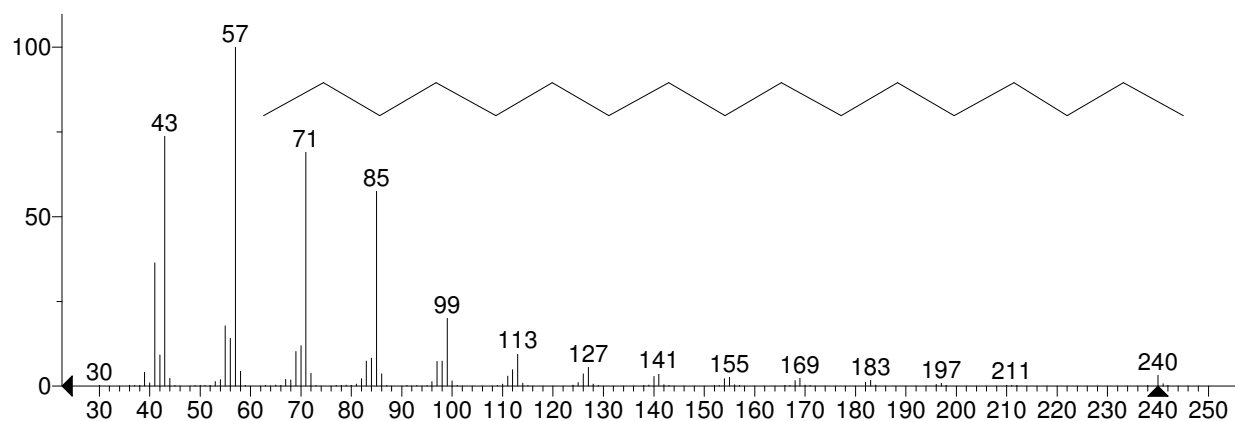
Unknown: Scan 697 (5.340 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -185



Hit 1 : Nonadecane
C₁₉H₄₀; MF: 890; RMF: 950; Prob 16.0%; CAS: 629-92-5; Lib: replib; ID: 5533.

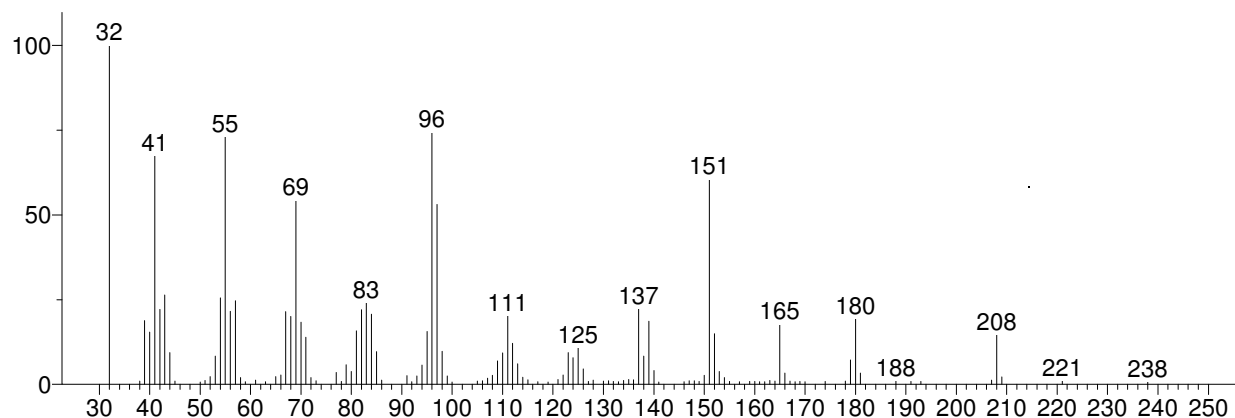


Hit 2 : Heptadecane
C₁₇H₃₆; MF: 876; RMF: 900; Prob 10.0%; CAS: 629-78-7; Lib: replib; ID: 5484.

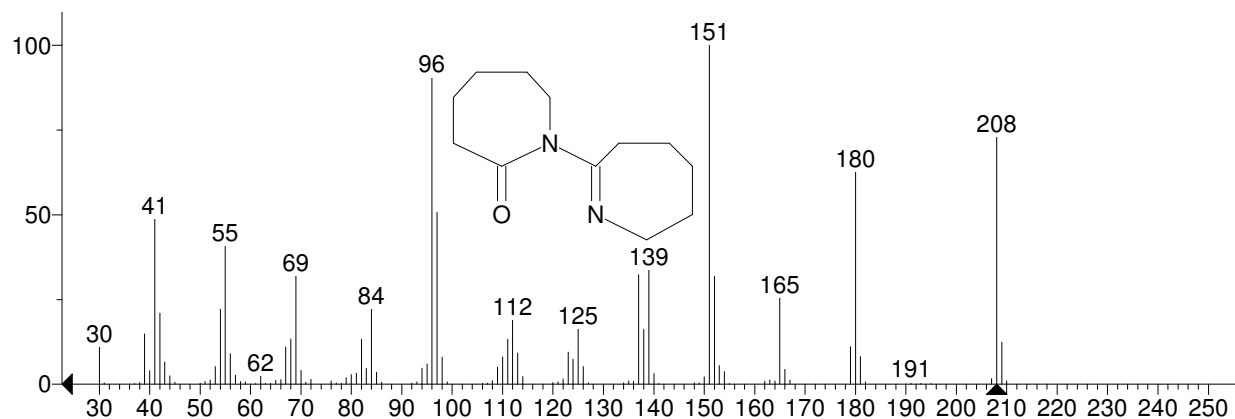


** Search Report Page 1 of 1 **

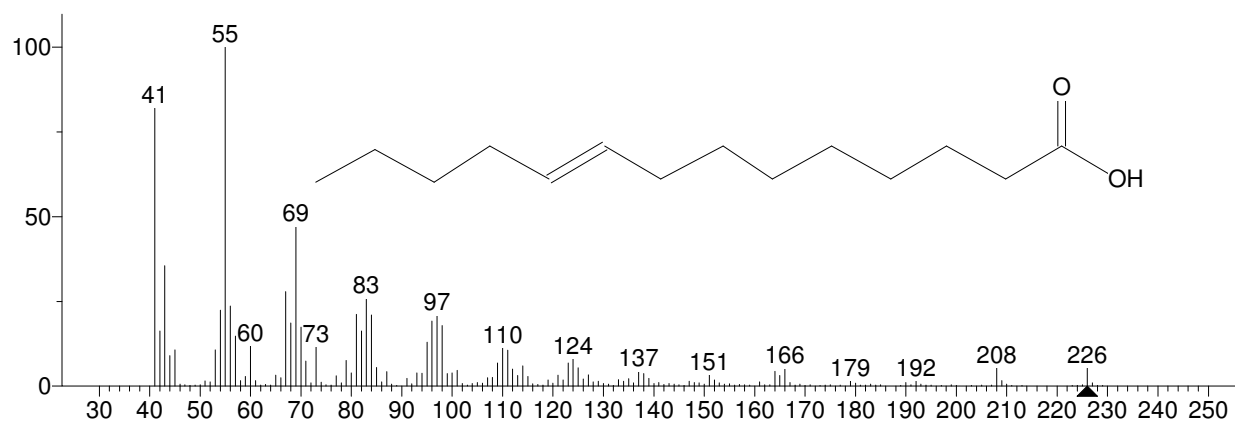
Unknown: Scan 704 (5.392 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -248



Hit 1 : 2H-Azepin-2-one, hexahydro-1-(3,4,5,6-tetrahydro-2H-azepin-7-yl)-
C₁₂H₂₀N₂O; MF: 784; RMF: 814; Prob 27.9%; CAS: 22993-71-1; Lib: mainlib; ID: 112495.

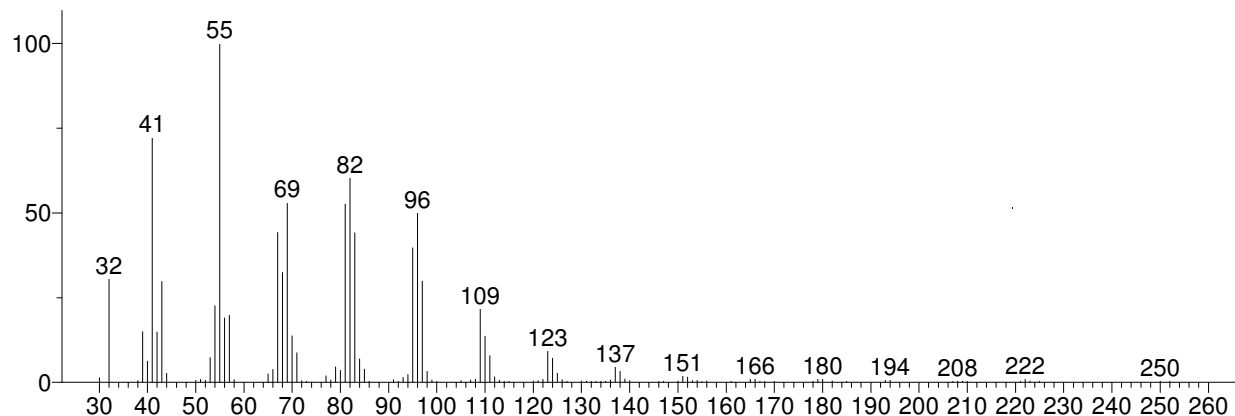


Hit 2 : E-9-Tetradecenoic acid
C₁₄H₂₆O₂; MF: 717; RMF: 722; Prob 4.31%; Lib: mainlib; ID: 17424.

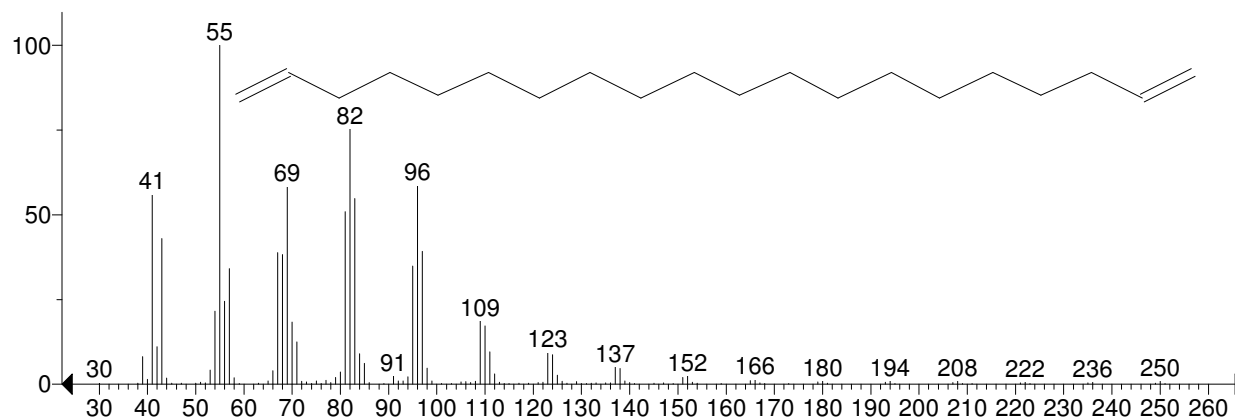


** Search Report Page 1 of 1 **

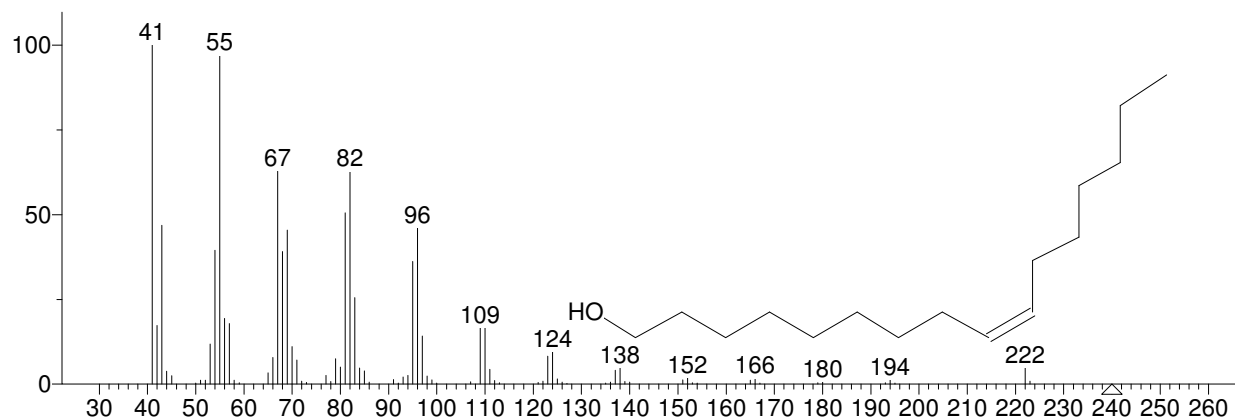
Unknown: Scan 750 (5.739 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -207



Hit 1 : 1,19-Eicosadiene
C₂₀H₃₈; MF: 892; RMF: 904; Prob 6.15%; CAS: 14811-95-1; Lib: mainlib; ID: 18670.

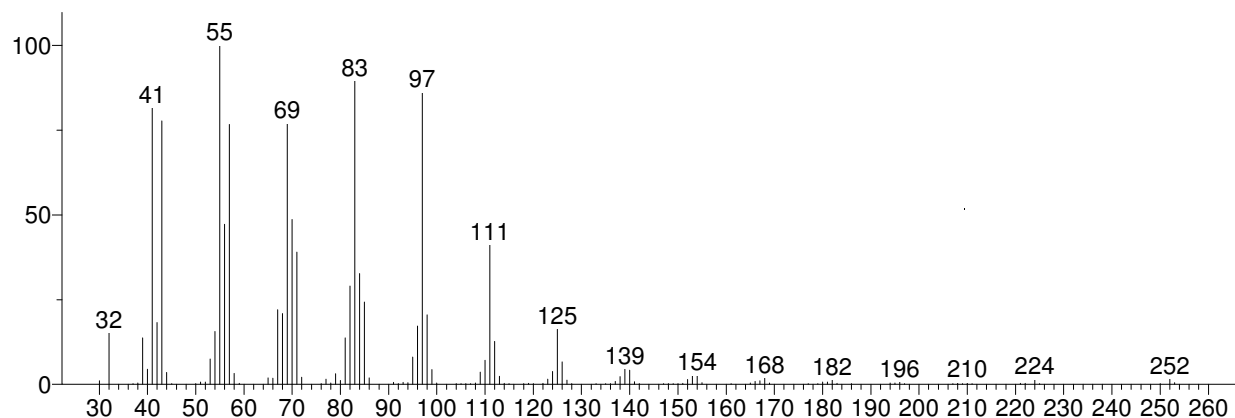


Hit 2 : 9-Hexadecen-1-ol, (Z)-
C₁₆H₃₂O; MF: 890; RMF: 900; Prob 5.67%; CAS: 10378-01-5; Lib: replib; ID: 908.

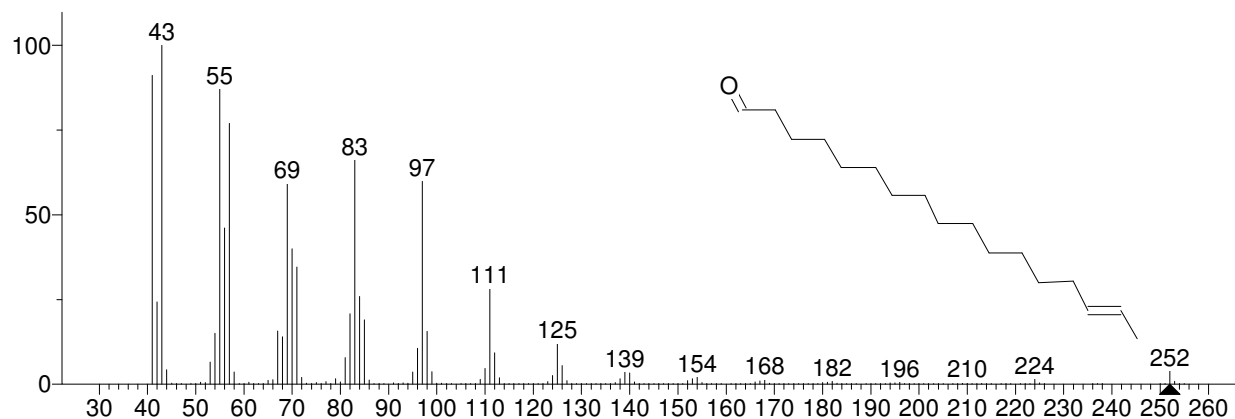


** Search Report Page 1 of 1 **

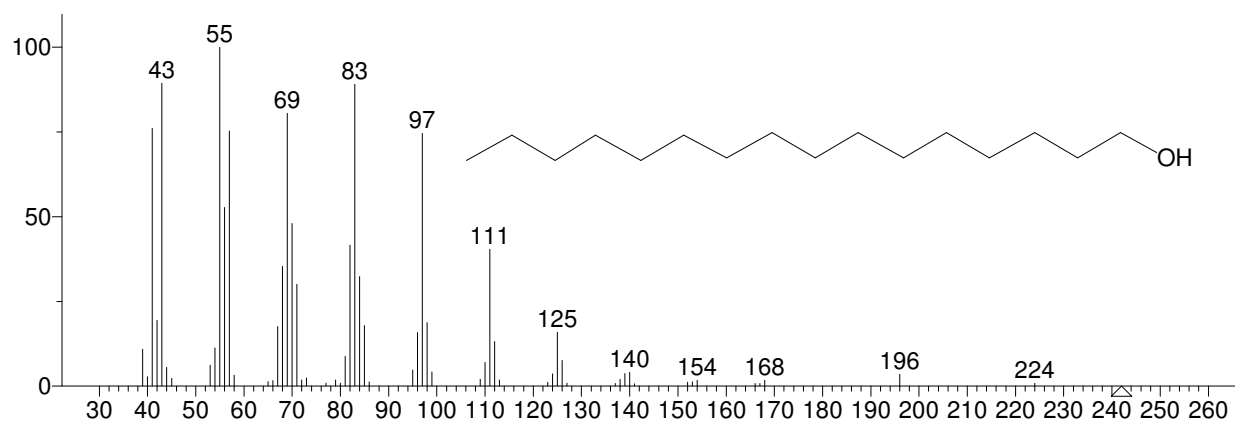
Unknown: Scan 758 (5.799 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -161



Hit 1 : E-15-Heptadecenal
C₁₇H₃₂O; MF: 929; RMF: 929; Prob 7.07%; Lib: mainlib; ID: 5518.

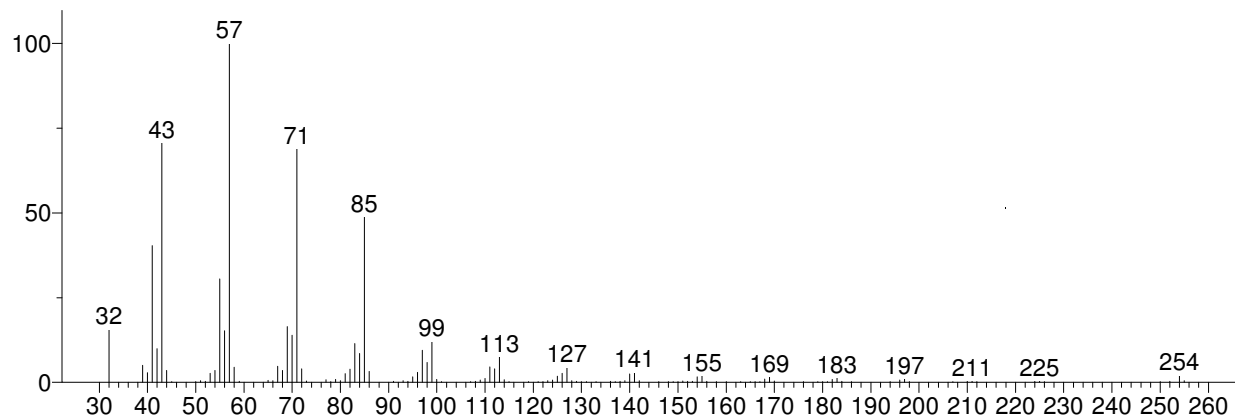


Hit 2 : 1-Hexadecanol
C₁₆H₃₄O; MF: 928; RMF: 941; Prob 6.79%; CAS: 36653-82-4; Lib: replib; ID: 4395.

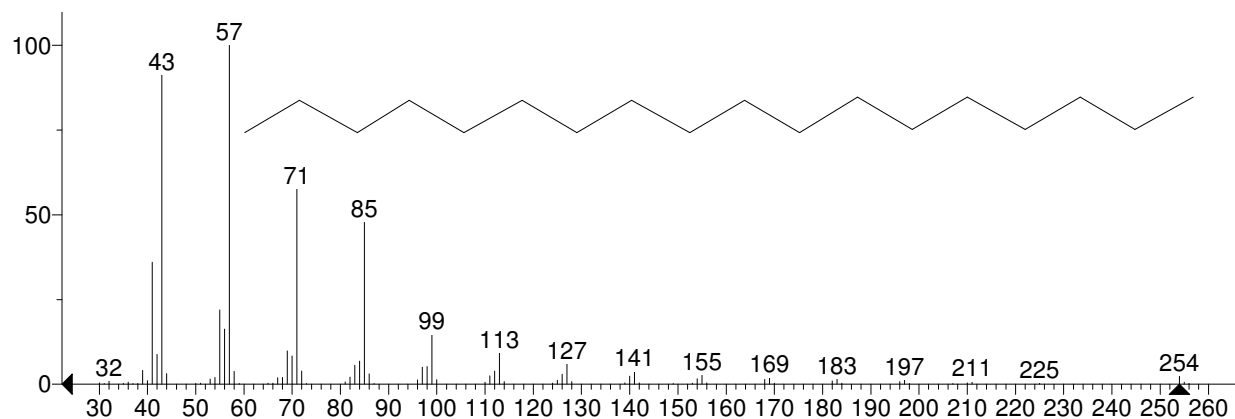


** Search Report Page 1 of 1 **

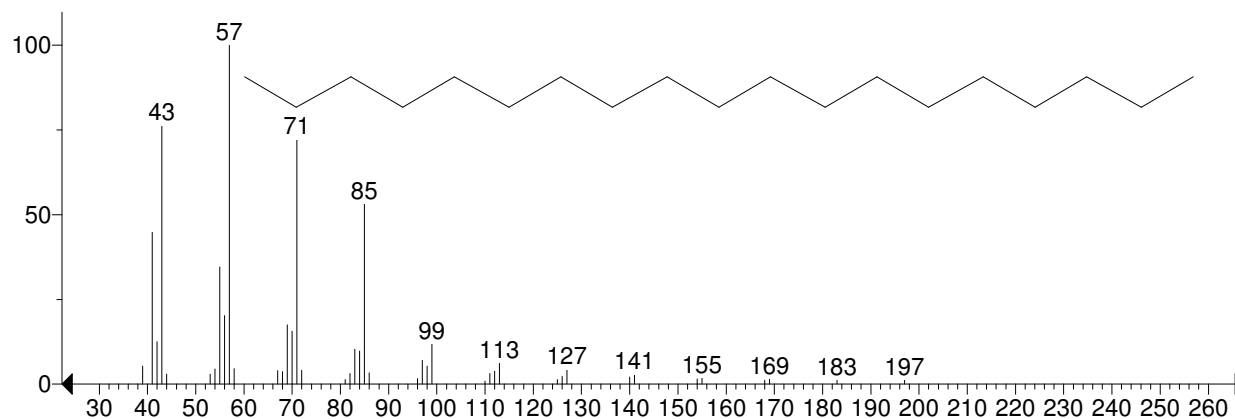
Unknown: Scan 764 (5.844 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -113



Hit 1 : Octadecane
C₁₈H₃₈; MF: 919; RMF: 929; Prob 18.3%; CAS: 593-45-3; Lib: replib; ID: 5495.

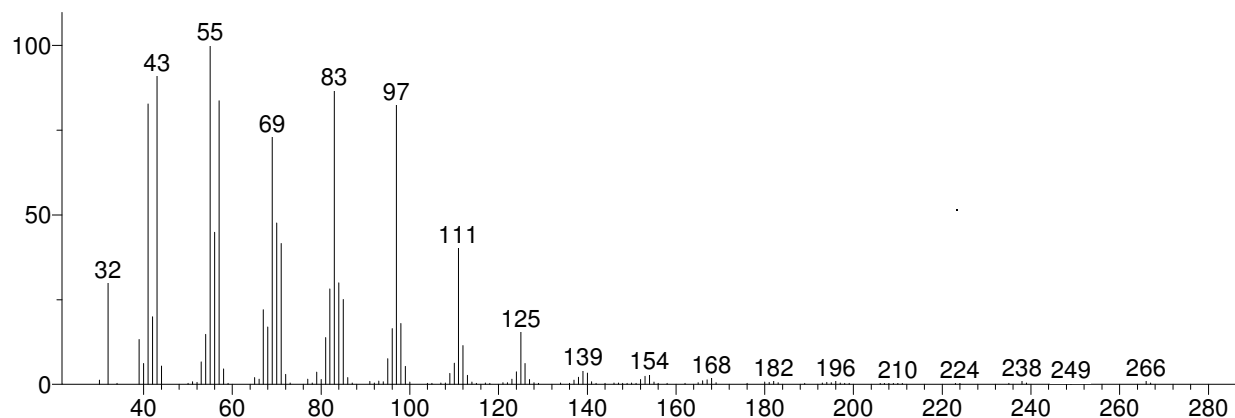


Hit 2 : Nonadecane
C₁₉H₄₀; MF: 914; RMF: 959; Prob 14.7%; CAS: 629-92-5; Lib: replib; ID: 5533.

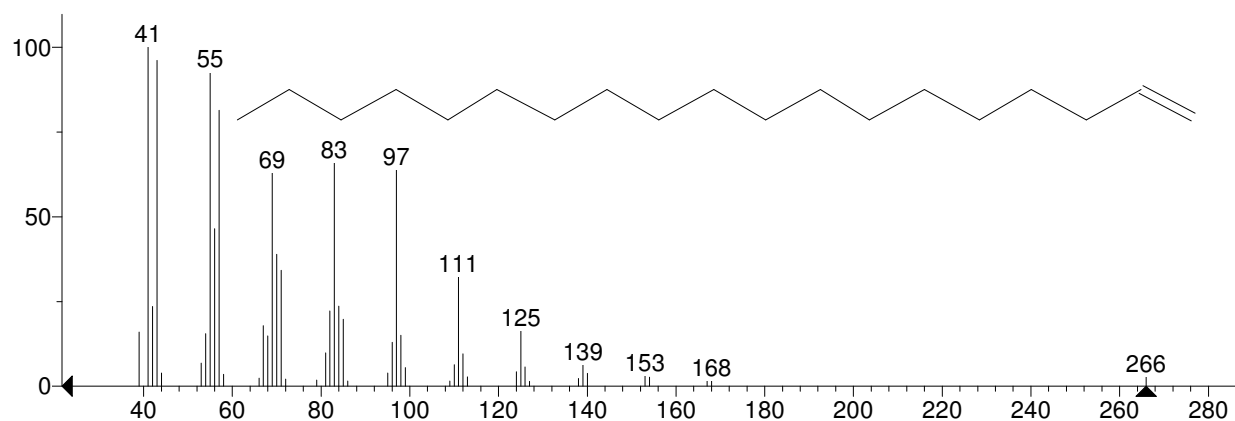


** Search Report Page 1 of 1 **

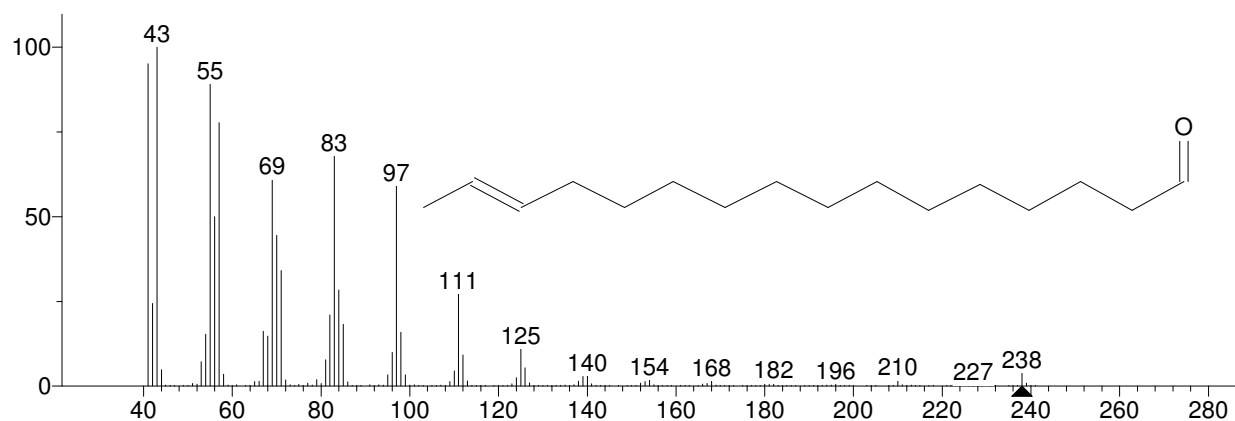
Unknown: Scan 821 (6.274 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -170



Hit 1 : 1-Nonadecene
C₁₉H₃₈; MF: 917; RMF: 957; Prob 6.25%; CAS: 18435-45-5; Lib: replib; ID: 818.

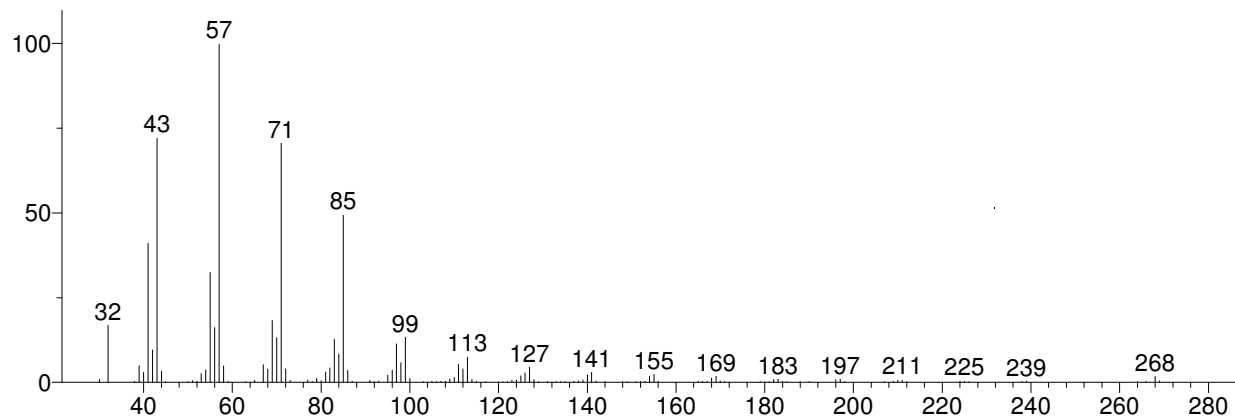


Hit 2 : E-14-Hexadecenal
C₁₆H₃₀O; MF: 910; RMF: 917; Prob 4.79%; CAS: 330207-53-9; Lib: mainlib; ID: 5588.

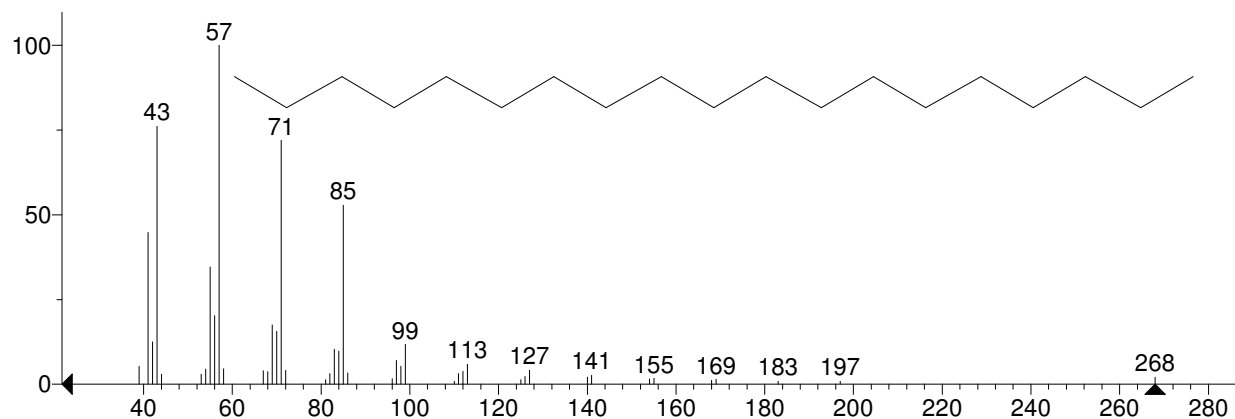


** Search Report Page 1 of 1 **

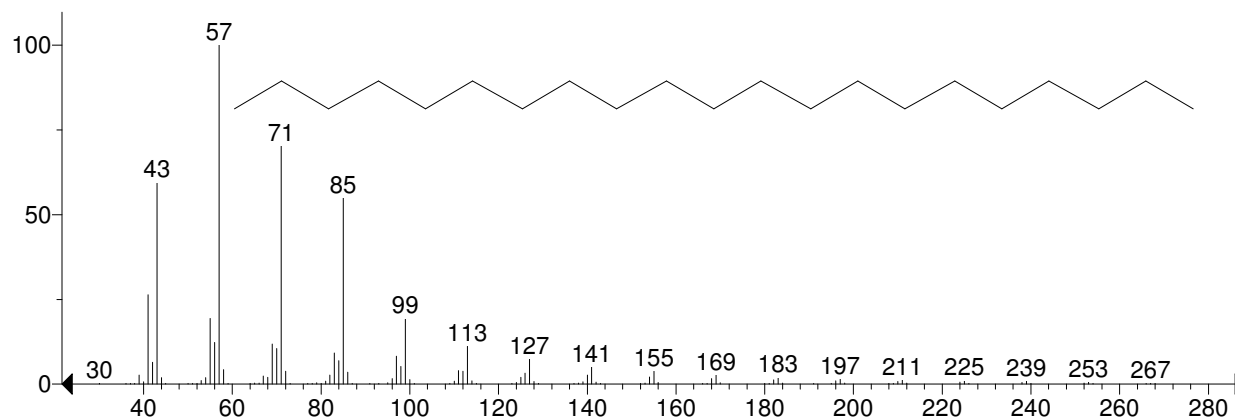
Unknown: Scan 828 (6.327 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = 103



Hit 1 : Nonadecane
C₁₉H₄₀; MF: 917; RMF: 965; Prob 24.1%; CAS: 629-92-5; Lib: replib; ID: 5533.

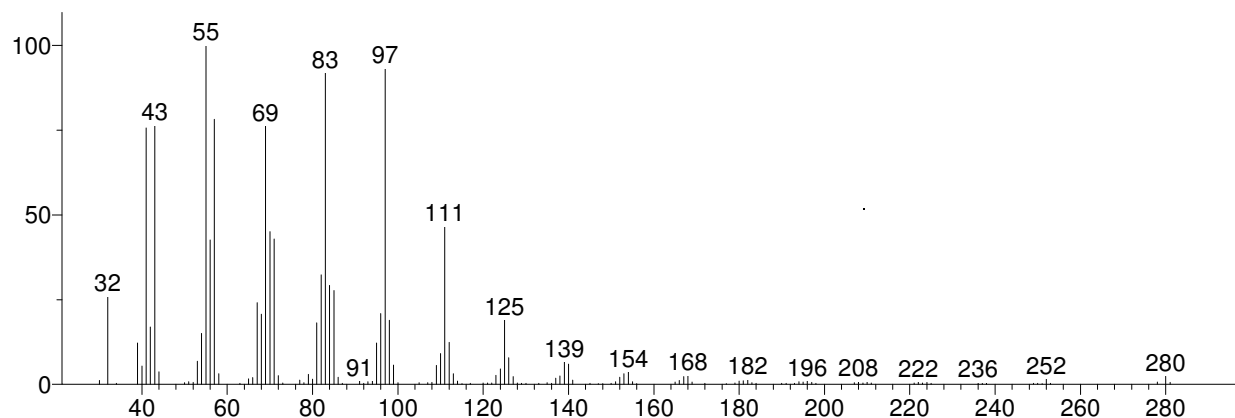


Hit 2 : Heneicosane
C₂₁H₄₄; MF: 885; RMF: 903; Prob 6.43%; CAS: 629-94-7; Lib: replib; ID: 5753.

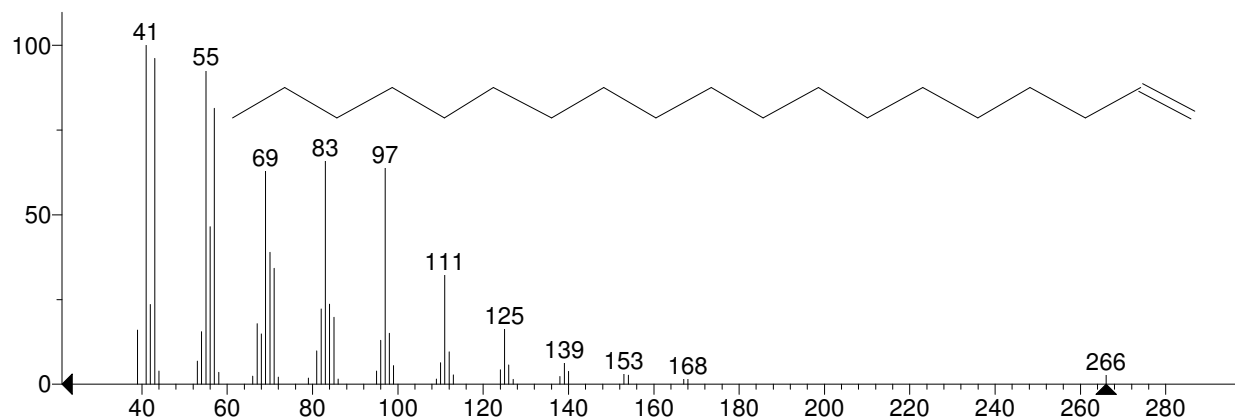


** Search Report Page 1 of 1 **

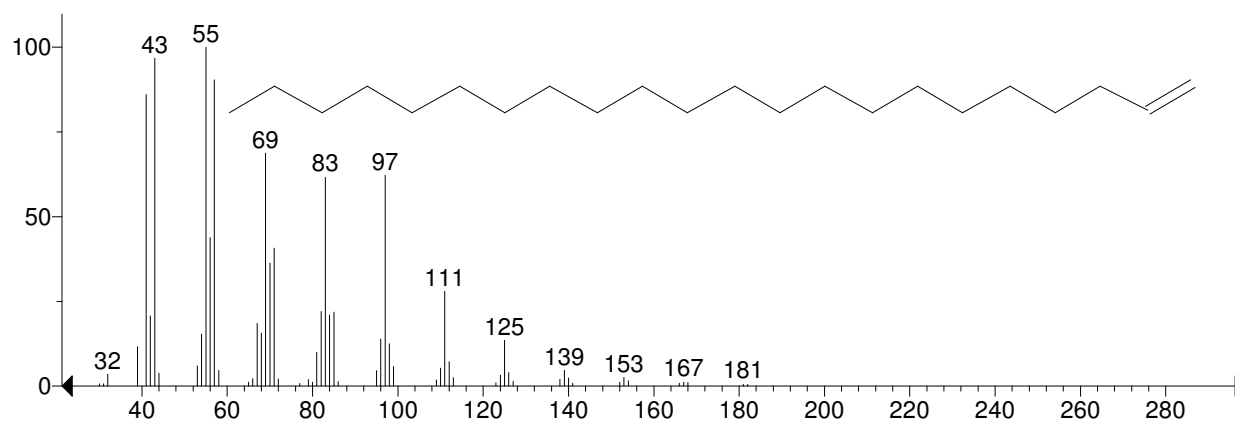
Unknown: Scan 885 (6.756 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -207



Hit 1 : 1-Nonadecene
C₁₉H₃₈; MF: 900; RMF: 950; Prob 4.66%; CAS: 18435-45-5; Lib: replib; ID: 818.

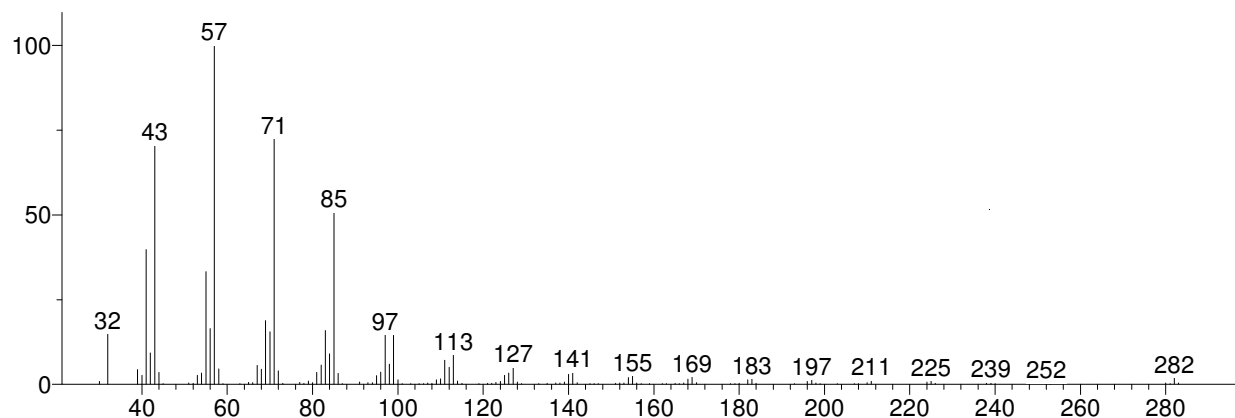


Hit 2 : 1-Docosene
C₂₂H₄₄; MF: 897; RMF: 931; Prob 4.12%; CAS: 1599-67-3; Lib: replib; ID: 4382.

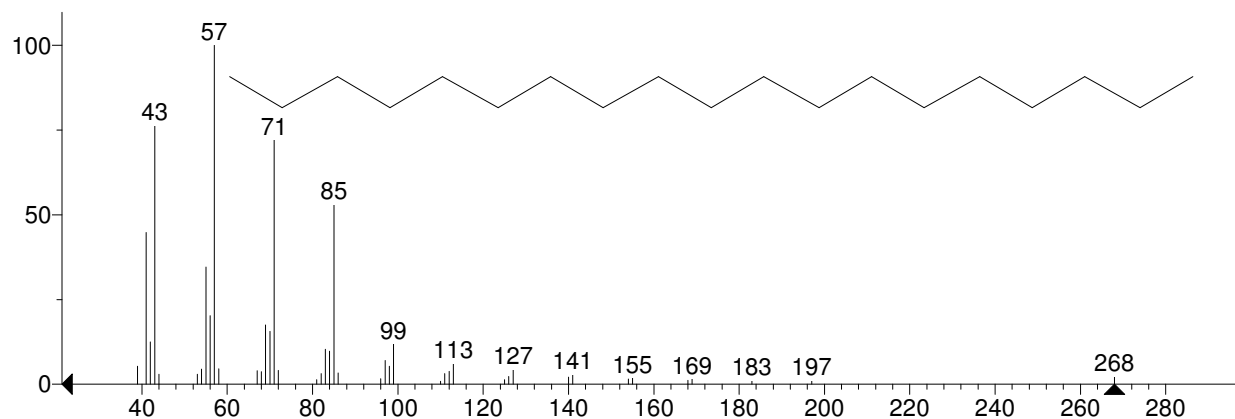


** Search Report Page 1 of 1 **

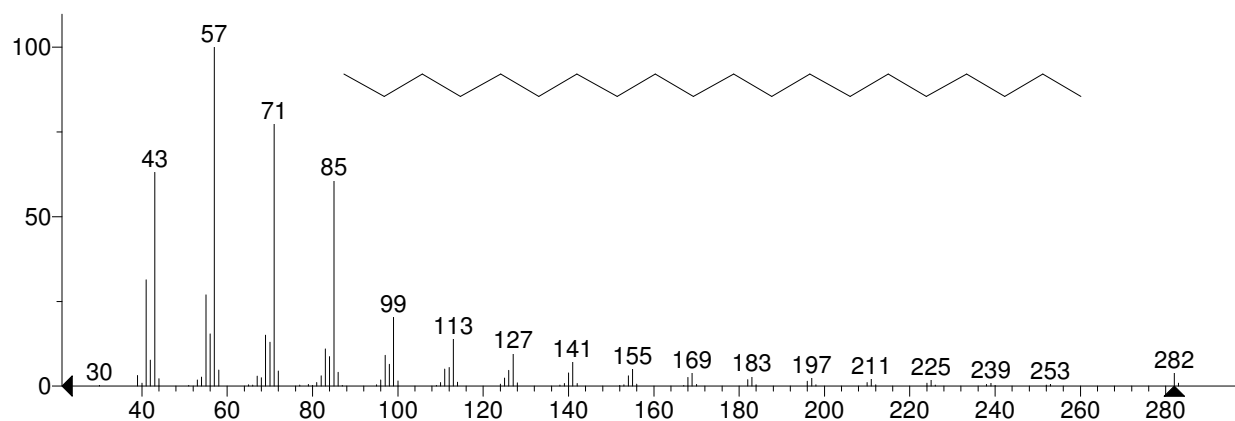
Unknown: Scan 890 (6.794 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -185



Hit 1 : Nonadecane
C₁₉H₄₀; MF: 890; RMF: 950; Prob 10.8%; CAS: 629-92-5; Lib: replib; ID: 5533.

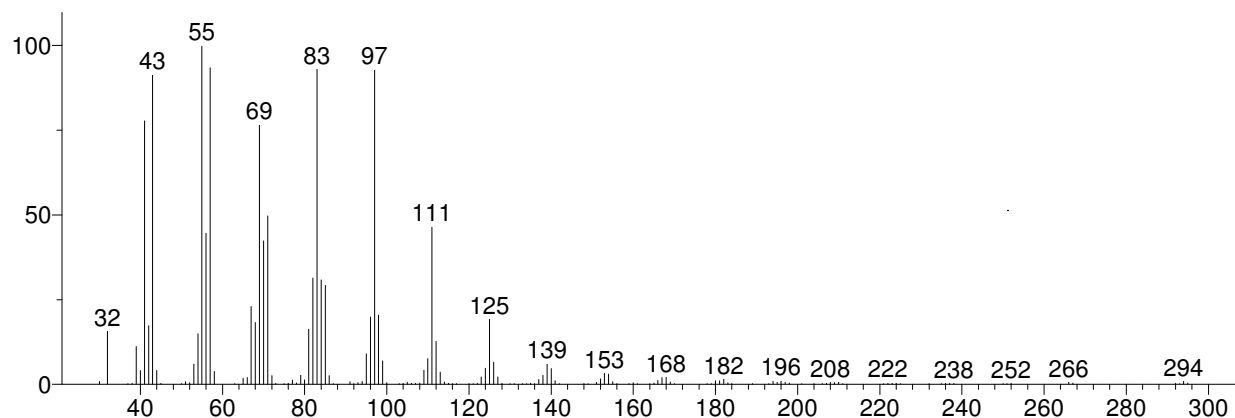


Hit 2 : Eicosane
C₂₀H₄₂; MF: 887; RMF: 899; Prob 9.53%; CAS: 112-95-8; Lib: mainlib; ID: 22772.

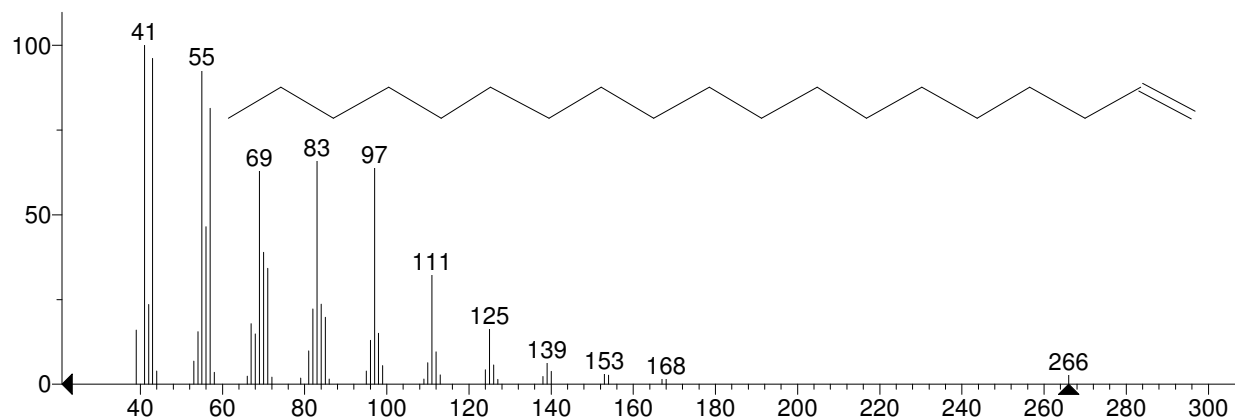


** Search Report Page 1 of 1 **

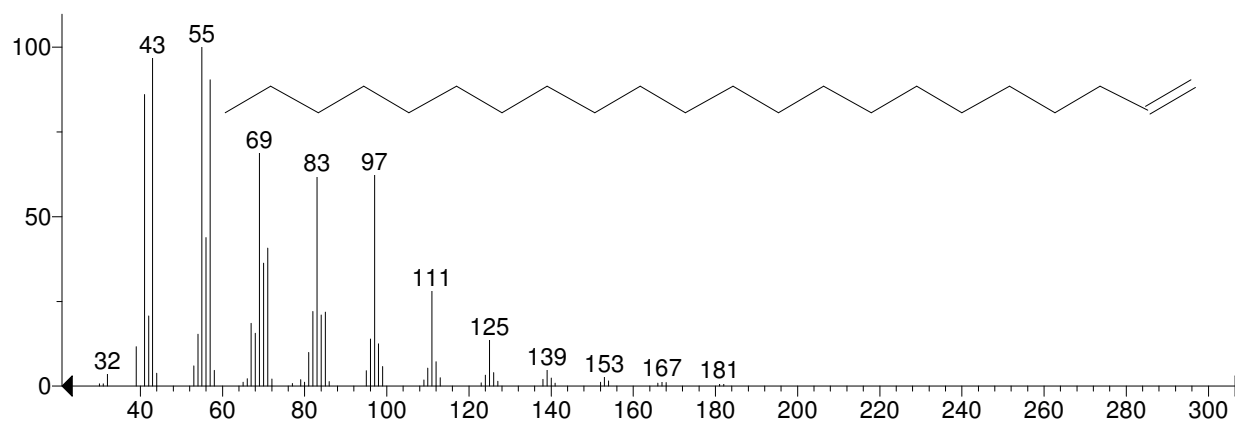
Unknown: Scan 943 (7.193 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -161



Hit 1 : 1-Nonadecene
C₁₉H₃₈; MF: 926; RMF: 962; Prob 7.64%; CAS: 18435-45-5; Lib: replib; ID: 818.

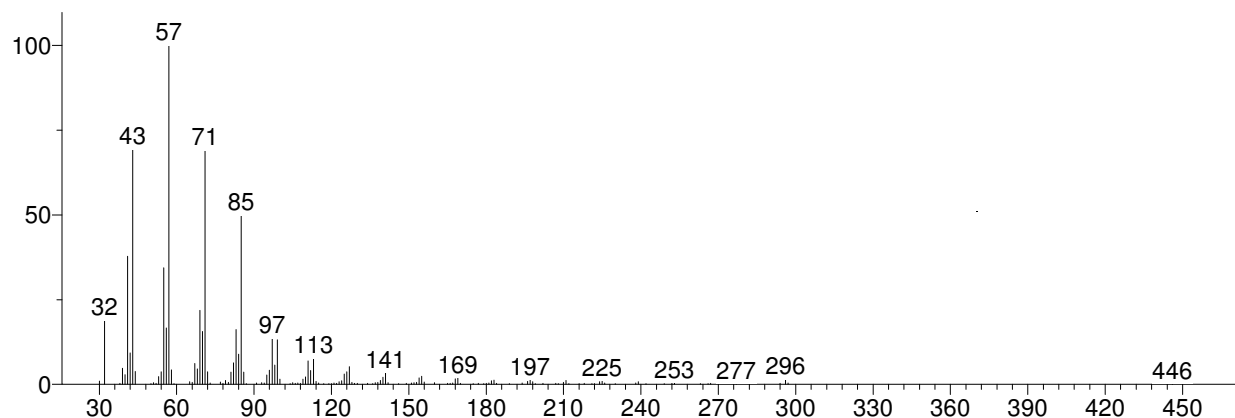


Hit 2 : 1-Docosene
C₂₂H₄₄; MF: 922; RMF: 946; Prob 6.45%; CAS: 1599-67-3; Lib: replib; ID: 4382.

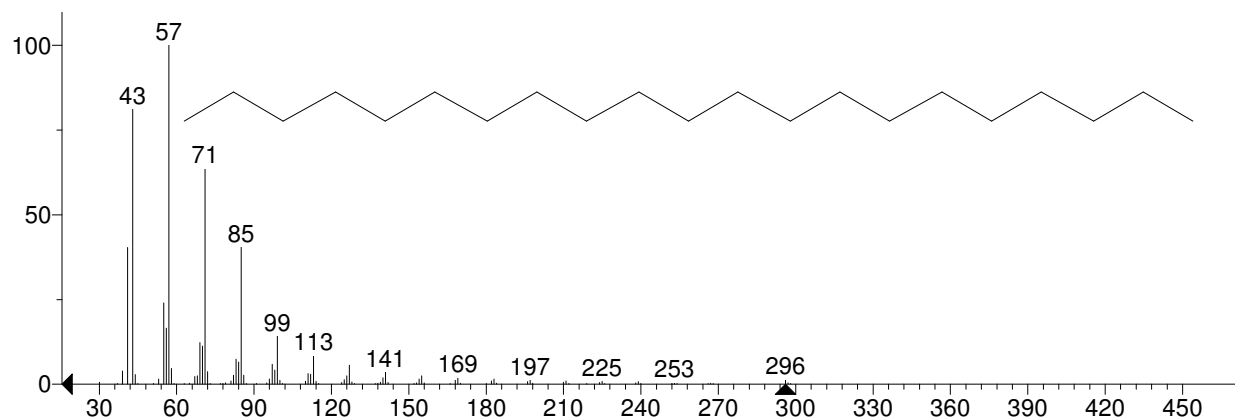


** Search Report Page 1 of 1 **

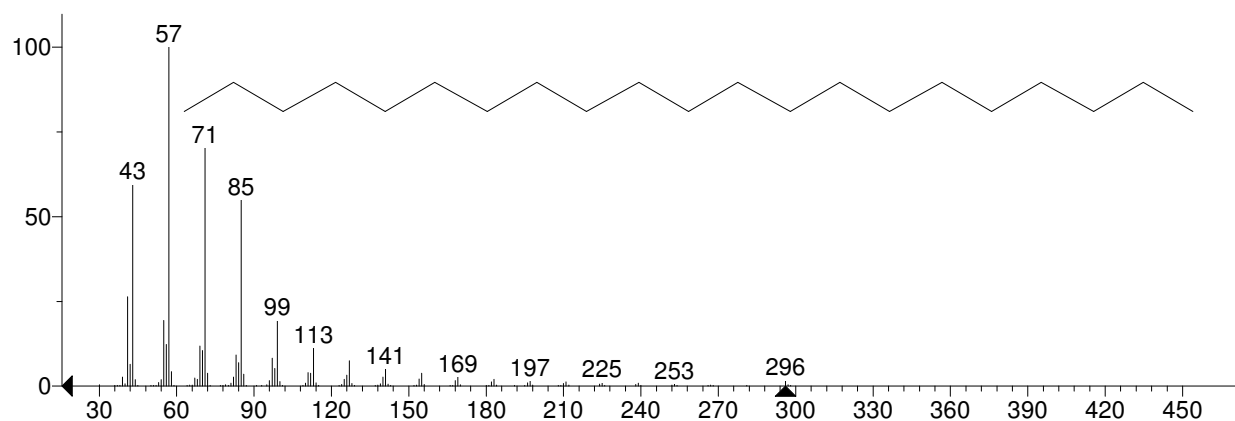
Unknown: Scan 948 (7.231 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -185



Hit 1 : Heneicosane
C₂₁H₄₄; MF: 883; RMF: 915; Prob 11.5%; CAS: 629-94-7; Lib: replib; ID: 5540.

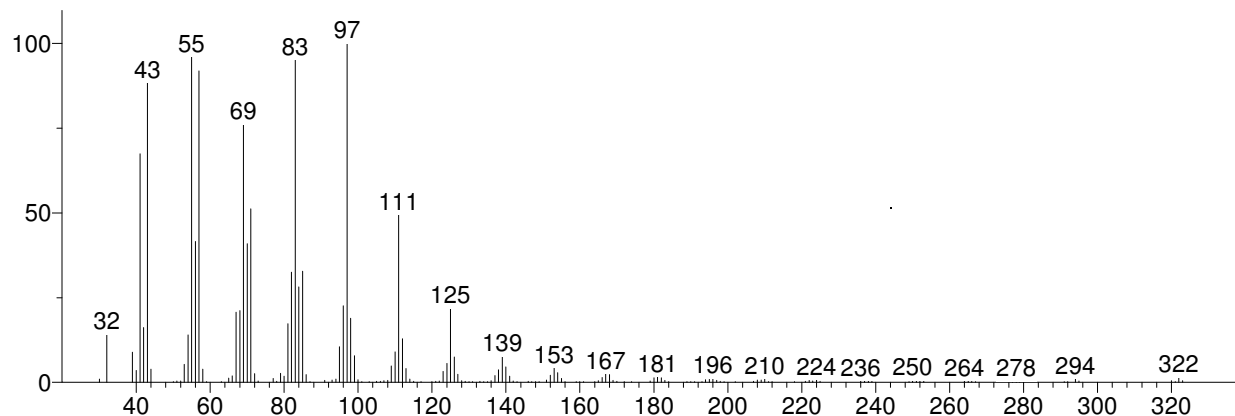


Hit 2 : Heneicosane
C₂₁H₄₄; MF: 872; RMF: 892; Prob 11.5%; CAS: 629-94-7; Lib: replib; ID: 5753.

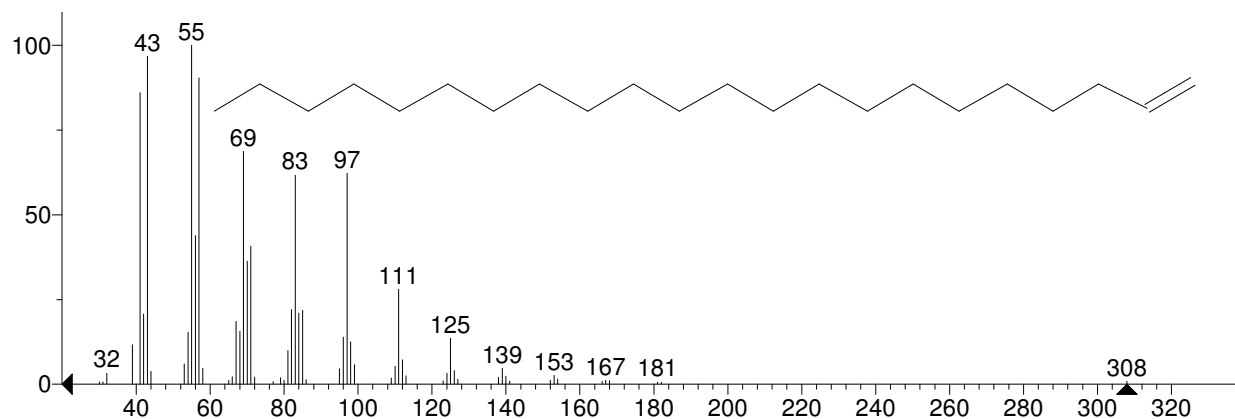


** Search Report Page 1 of 1 **

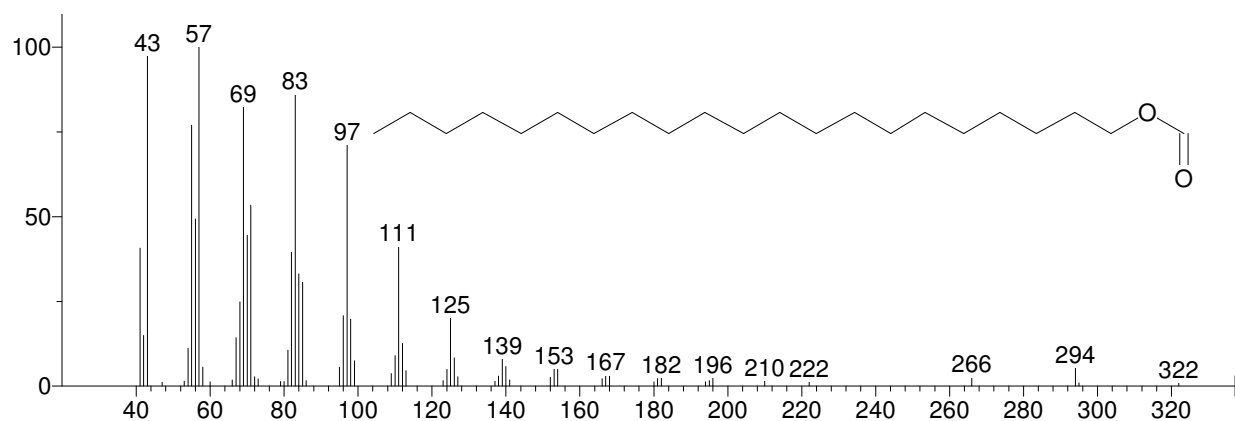
Unknown: Scan 1055 (8.037 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -170



Hit 1 : 1-Docosene
C₂₂H₄₄; MF: 919; RMF: 952; Prob 7.11%; CAS: 1599-67-3; Lib: replib; ID: 4382.

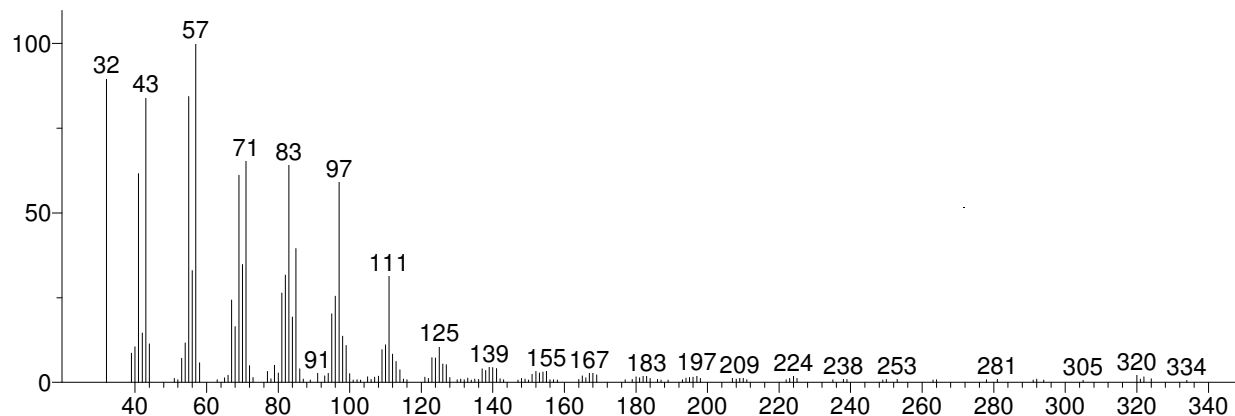


Hit 2 : 1-Heneicosyl formate
C₂₂H₄₄O₂; MF: 912; RMF: 934; Prob 5.45%; CAS: 77899-03-7; Lib: mainlib; ID: 22067.

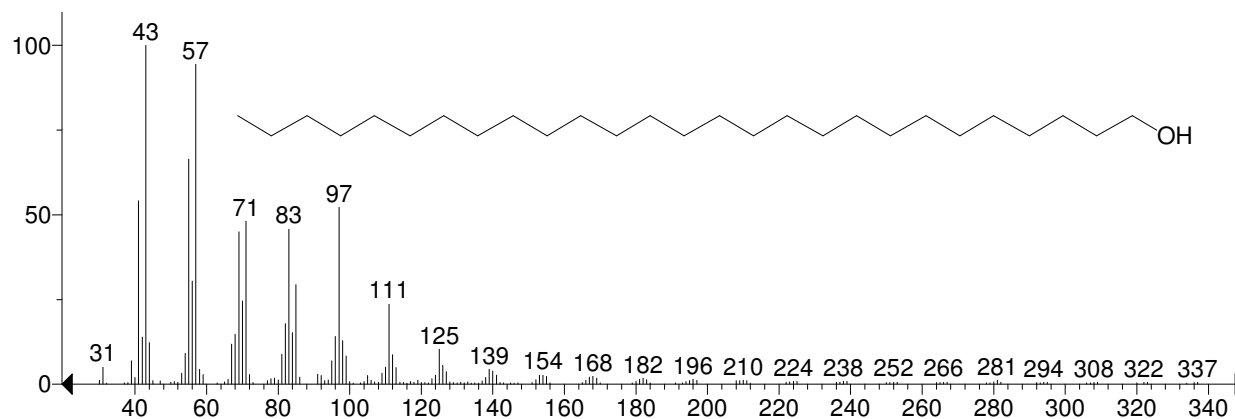


** Search Report Page 1 of 1 **

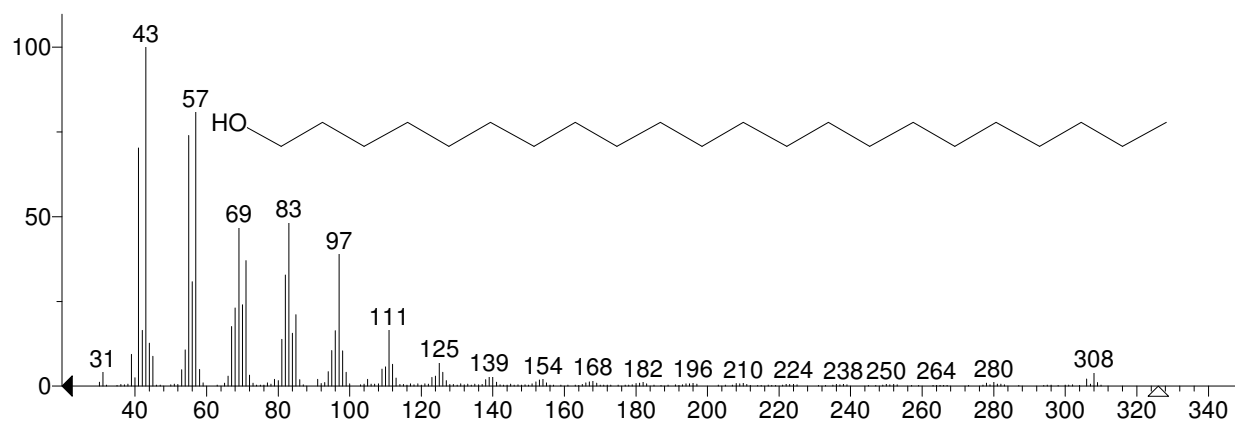
Unknown: Scan 1057 (8.052 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -503



Hit 1 : 1-Heptacosanol
C₂₇H₅₆O; MF: 826; RMF: 842; Prob 5.67%; CAS: 2004-39-9; Lib: replib; ID: 2100.

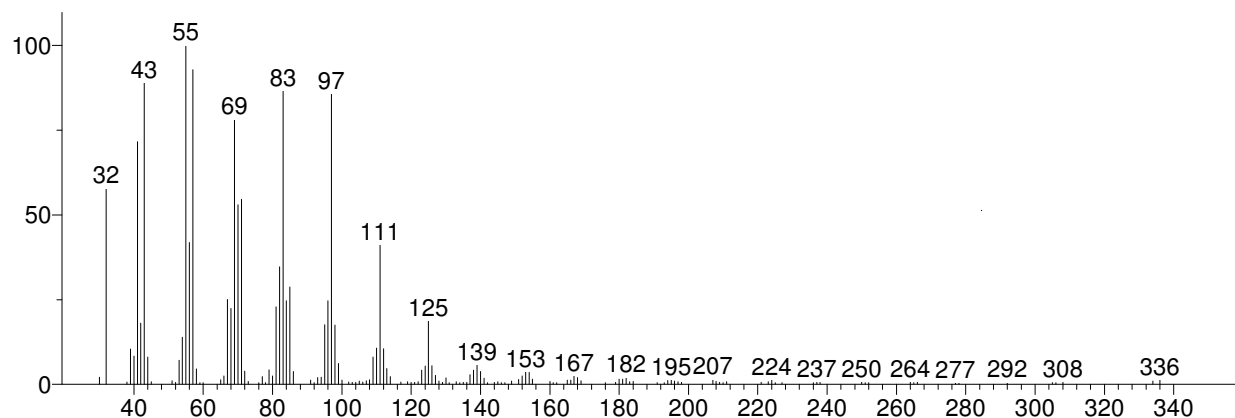


Hit 2 : Behenic alcohol
C₂₂H₄₆O; MF: 826; RMF: 842; Prob 5.67%; CAS: 661-19-8; Lib: replib; ID: 2104.

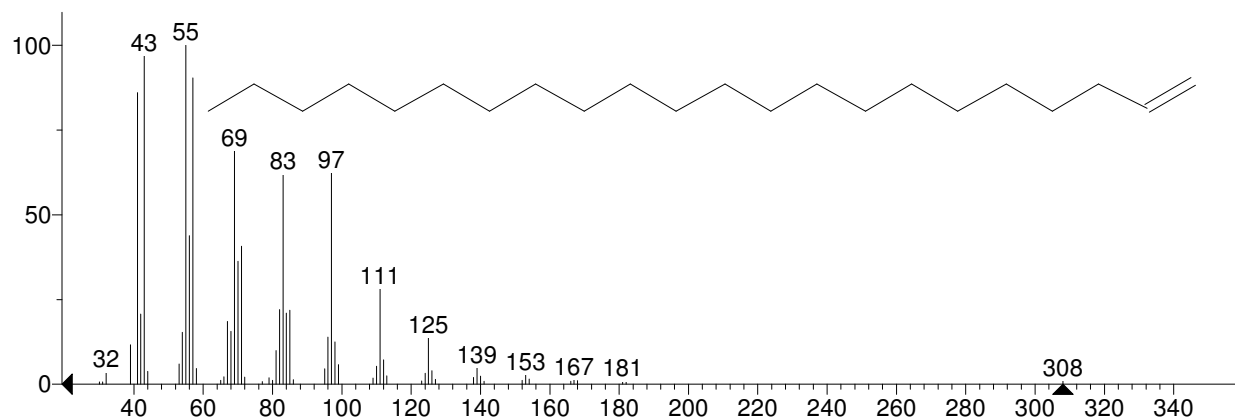


** Search Report Page 1 of 1 **

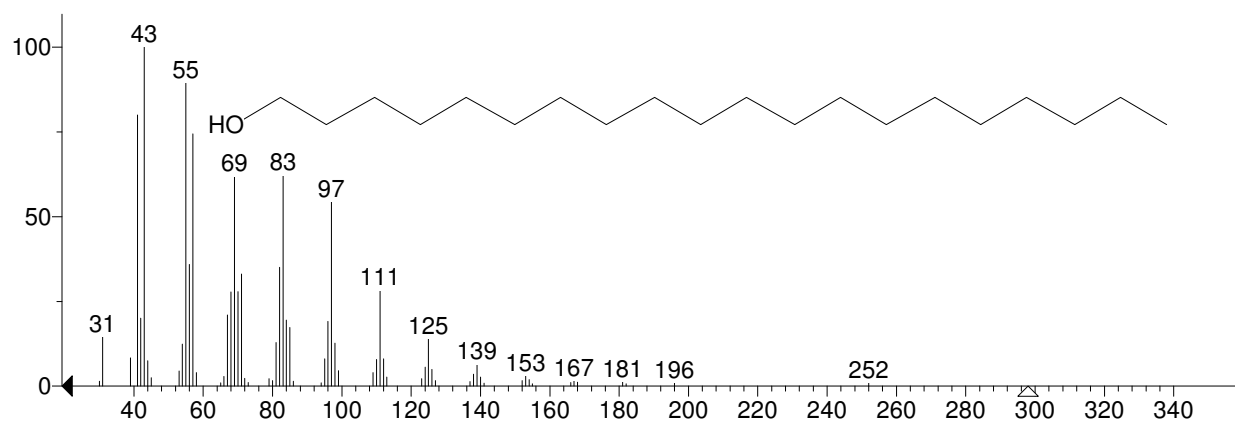
Unknown: Scan 1105 (8.414 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -338



Hit 1 : 1-Docosene
C₂₂H₄₄; MF: 867; RMF: 927; Prob 5.52%; CAS: 1599-67-3; Lib: replib; ID: 4382.

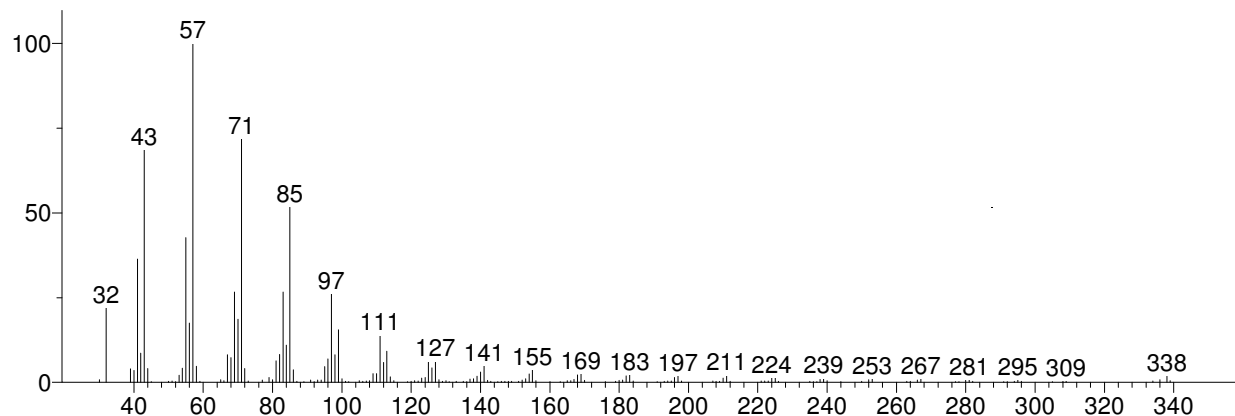


Hit 2 : 1-Eicosanol
C₂₀H₄₂O; MF: 860; RMF: 925; Prob 4.22%; CAS: 629-96-9; Lib: replib; ID: 1938.

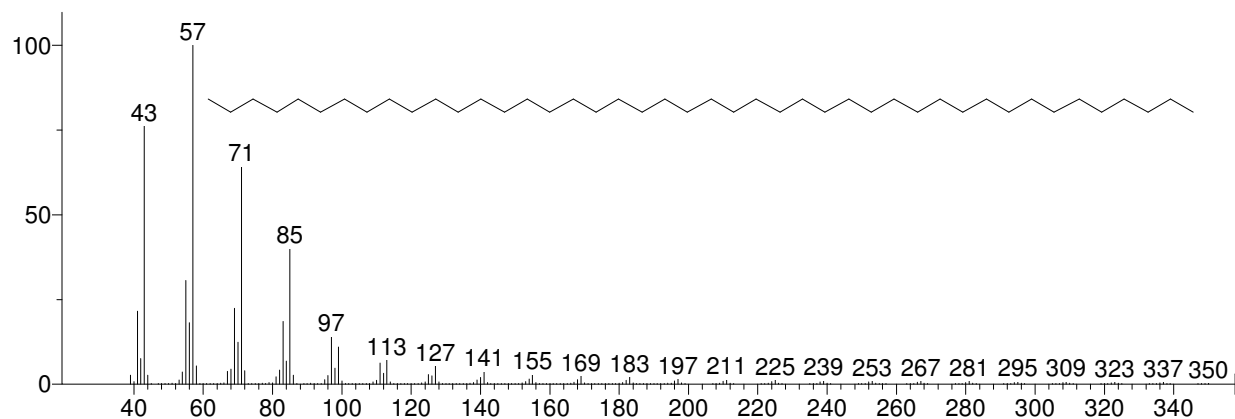


** Search Report Page 1 of 1 **

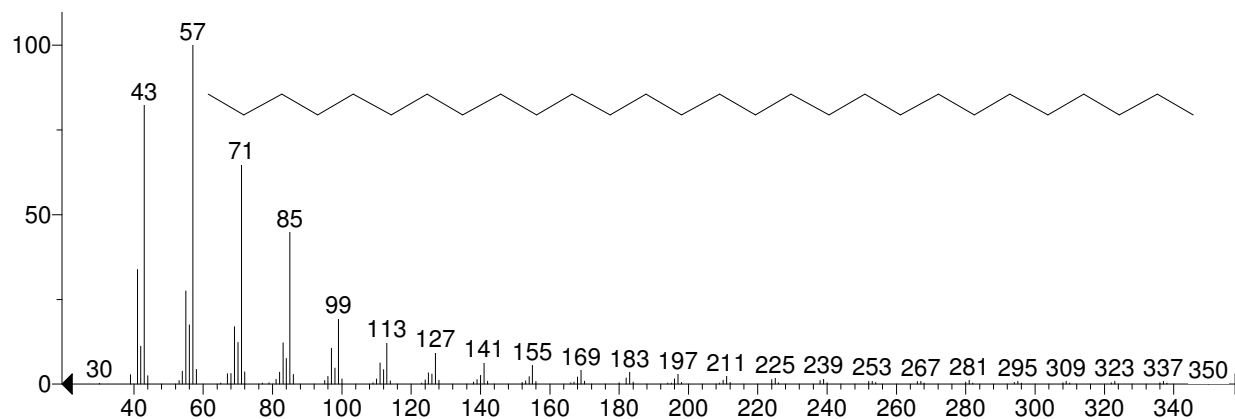
Unknown: Scan 1112 (8.467 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -338



Hit 1 : Tetratetracontane
C₄₄H₉₀; MF: 861; RMF: 861; Prob 9.67%; CAS: 7098-22-8; Lib: replib; ID: 5519.

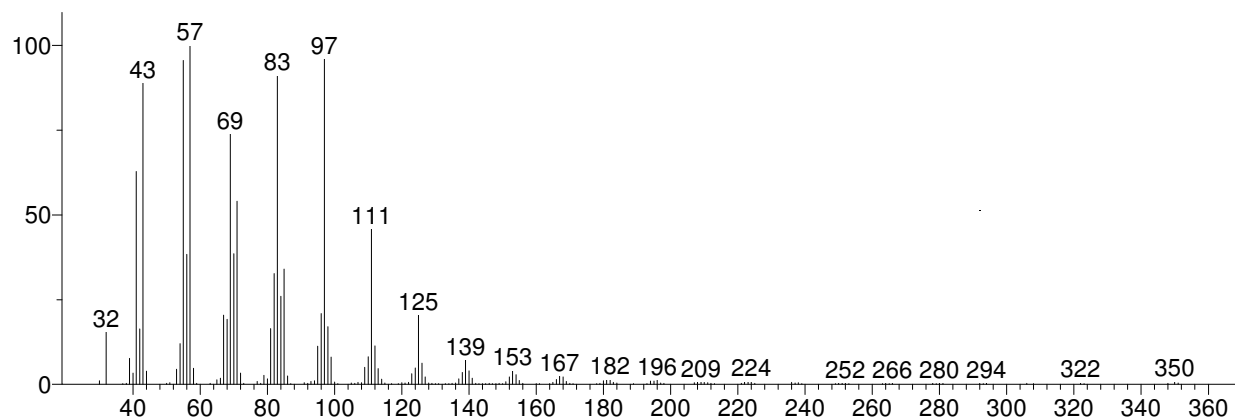


Hit 2 : Octacosane
C₂₈H₅₈; MF: 859; RMF: 885; Prob 8.92%; CAS: 630-02-4; Lib: replib; ID: 5471.

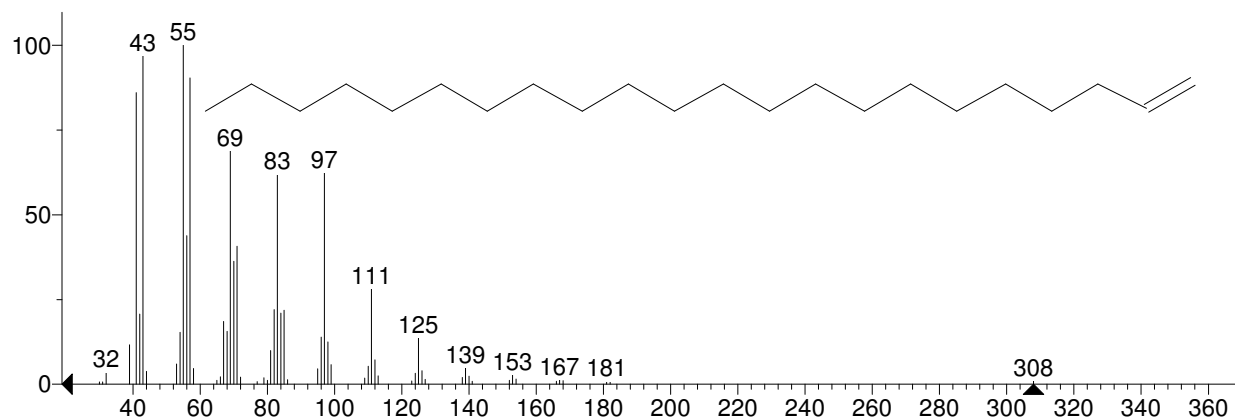


** Search Report Page 1 of 1 **

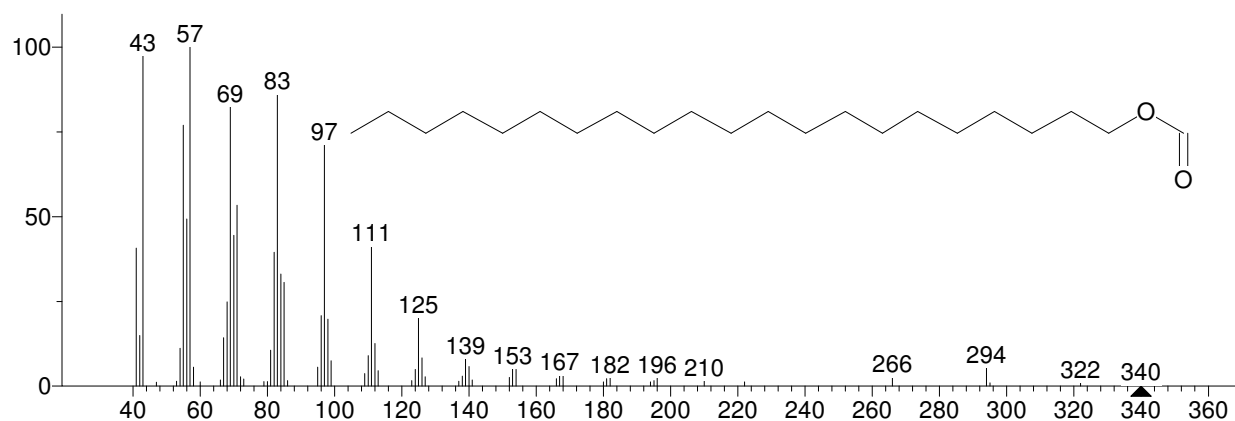
Unknown: Scan 1157 (8.806 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -124



Hit 1 : 1-Docosene
C₂₂H₄₄; MF: 918; RMF: 954; Prob 7.50%; CAS: 1599-67-3; Lib: replib; ID: 4382.

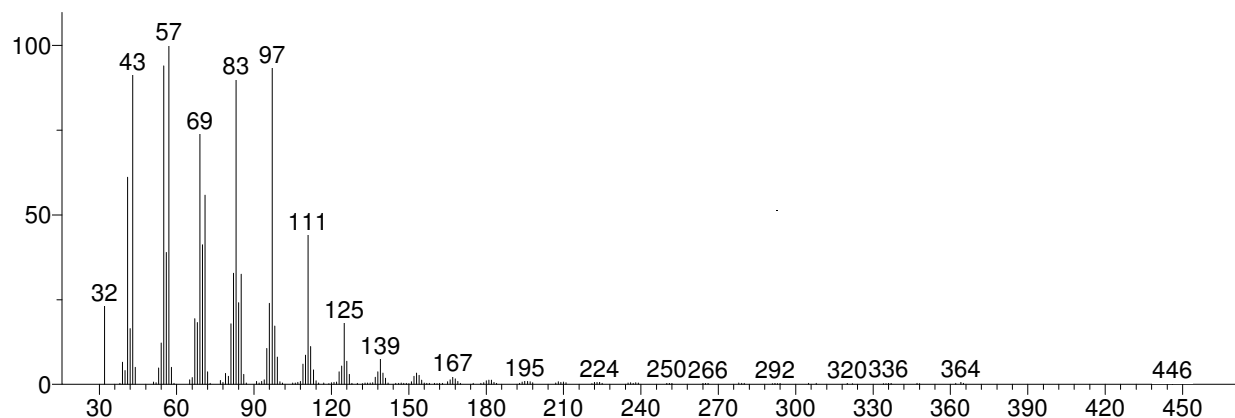


Hit 2 : 1-Heneicosyl formate
C₂₂H₄₄O₂; MF: 900; RMF: 928; Prob 3.87%; CAS: 77899-03-7; Lib: mainlib; ID: 22067.

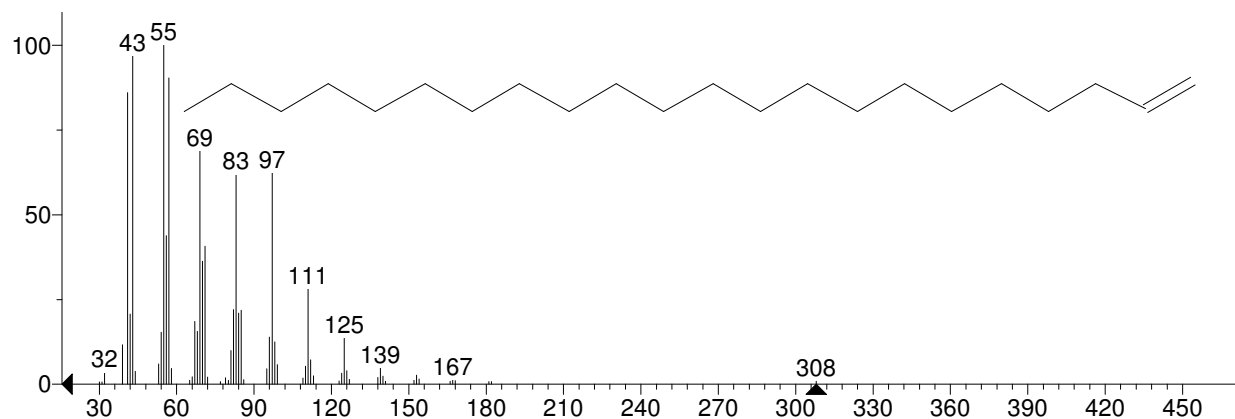


** Search Report Page 1 of 1 **

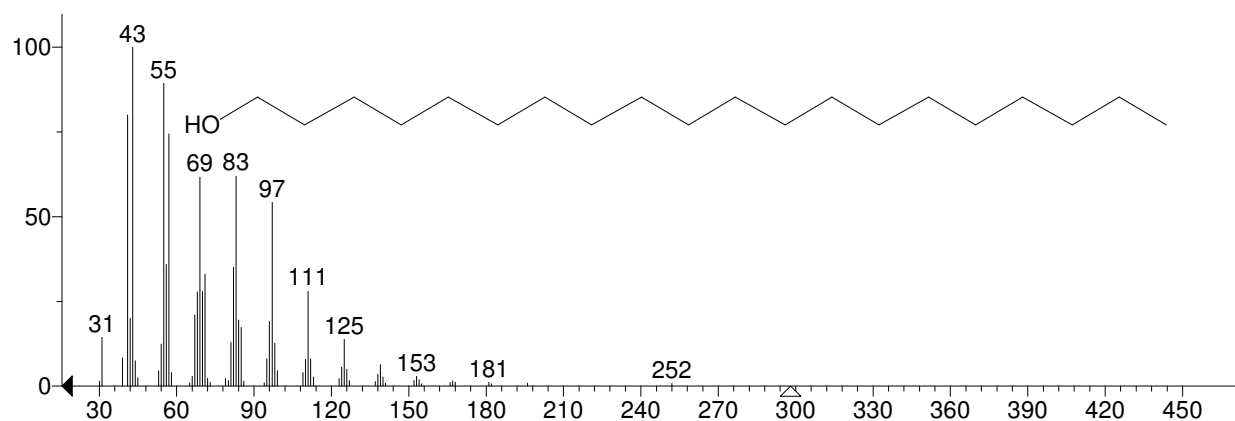
Unknown: Scan 1205 (9.168 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -134



Hit 1 : 1-Docosene
C₂₂H₄₄; MF: 904; RMF: 947; Prob 6.60%; CAS: 1599-67-3; Lib: replib; ID: 4382.

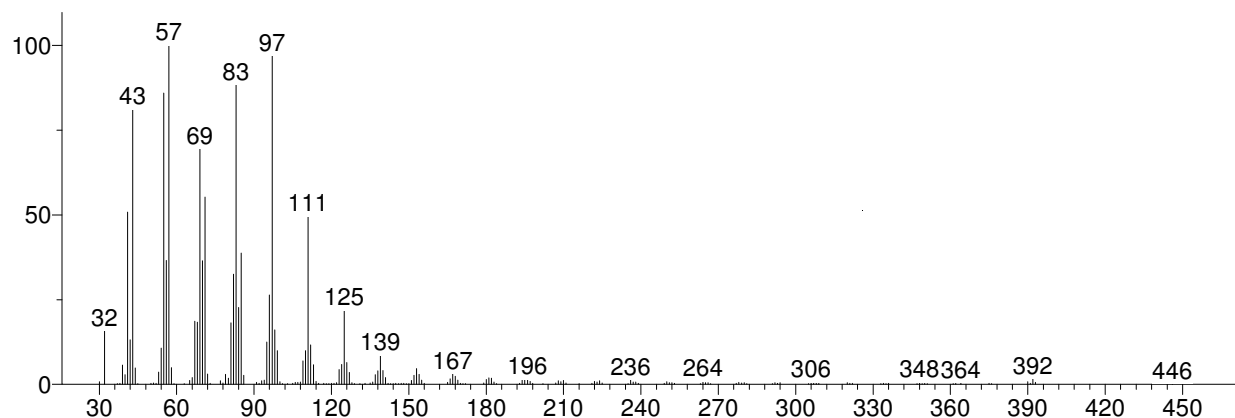


Hit 2 : 1-Eicosanol
C₂₀H₄₂O; MF: 894; RMF: 936; Prob 4.66%; CAS: 629-96-9; Lib: replib; ID: 1938.

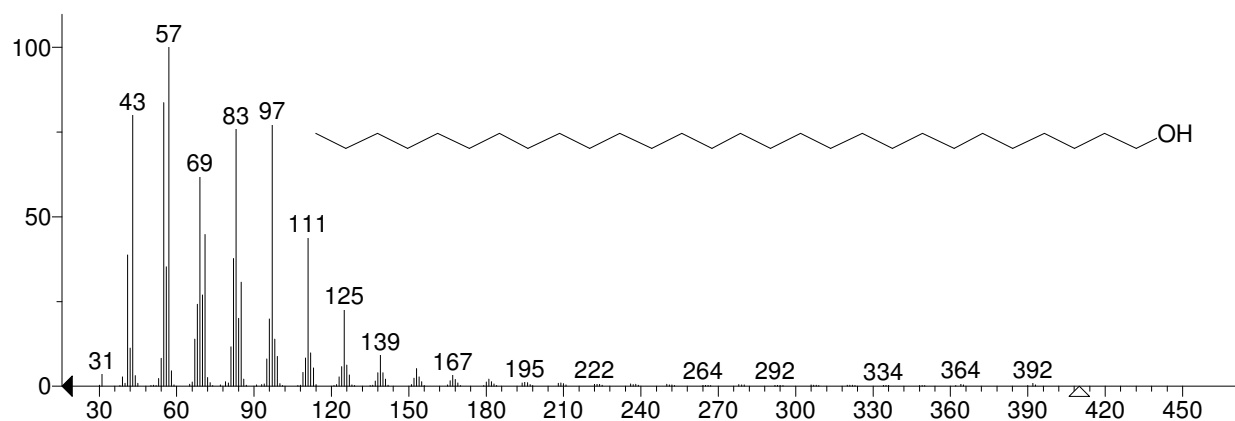


** Search Report Page 1 of 1 **

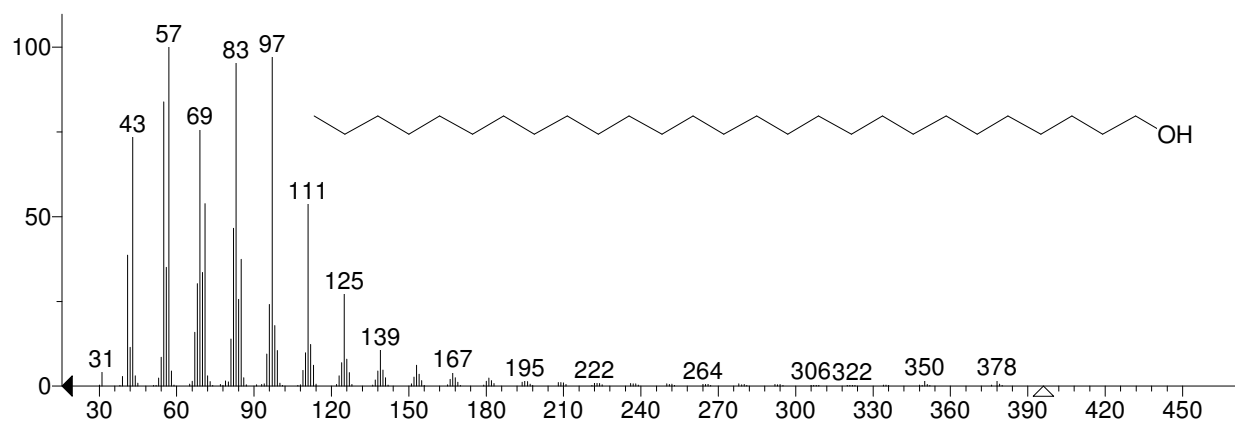
Unknown: Scan 1299 (9.876 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -124



Hit 1 : 1-Octacosanol
C₂₈H₅₈O; MF: 915; RMF: 921; Prob 8.86%; Lib: mainlib; ID: 22288.

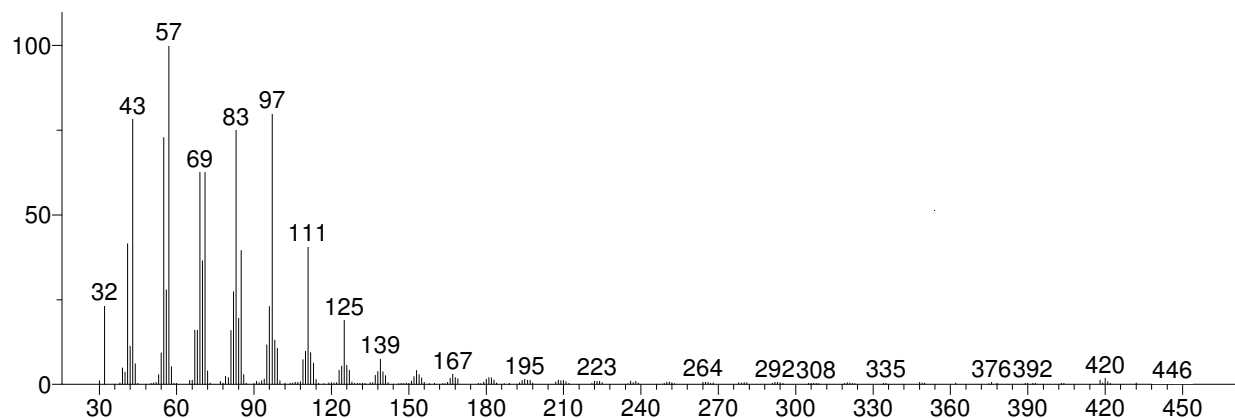


Hit 2 : 1-Heptacosanol
C₂₇H₅₆O; MF: 896; RMF: 910; Prob 4.30%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.

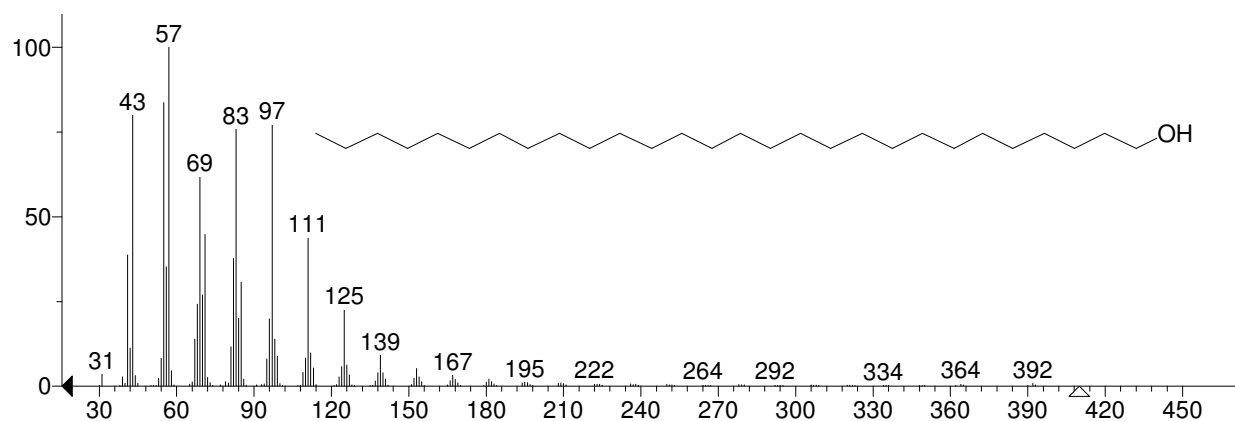


** Search Report Page 1 of 1 **

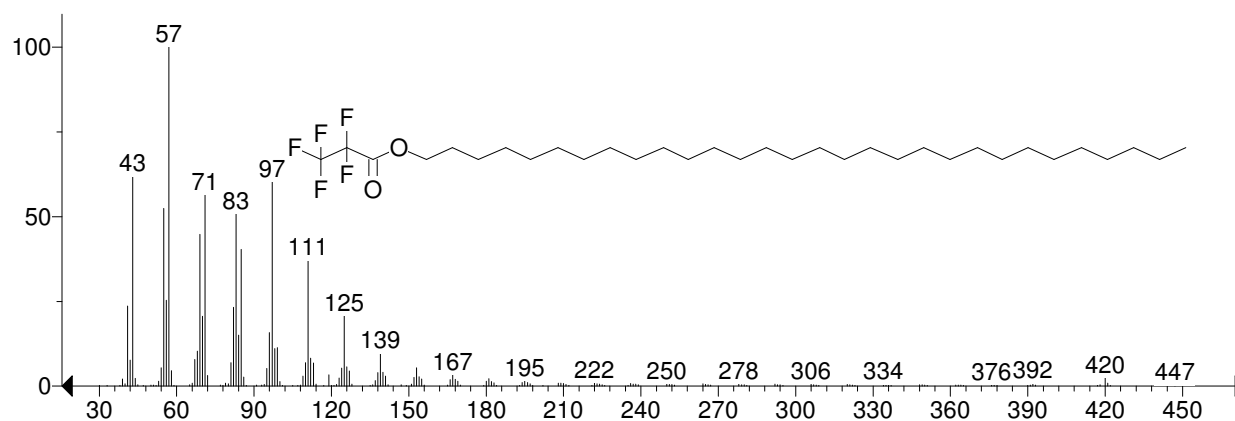
Unknown: Scan 1386 (10.531 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -185



Hit 1 : 1-Octacosanol
C₂₈H₅₈O; MF: 886; RMF: 912; Prob 5.58%; Lib: mainlib; ID: 22288.

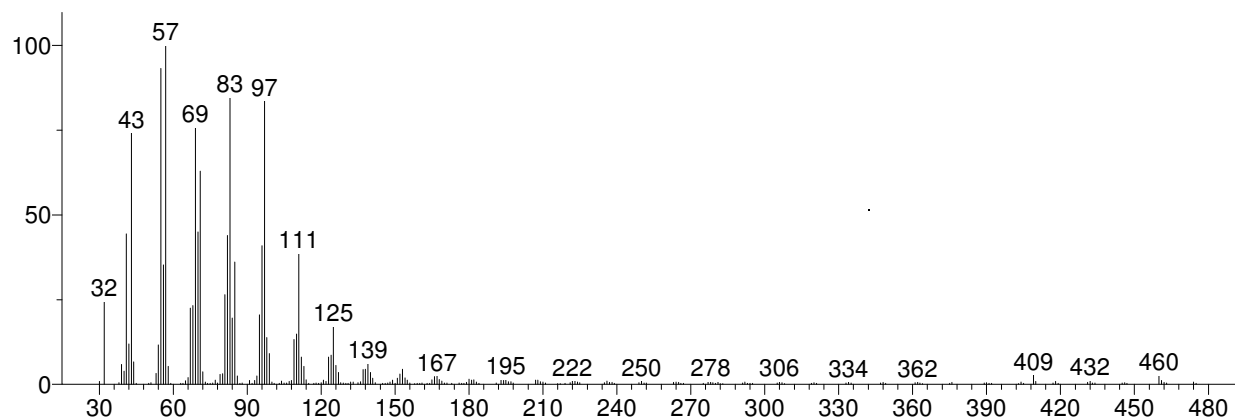


Hit 2 : Triacontyl pentafluoropropionate
C₃₃H₆₁F₅O₂; MF: 875; RMF: 887; Prob 3.83%; Lib: mainlib; ID: 22105.

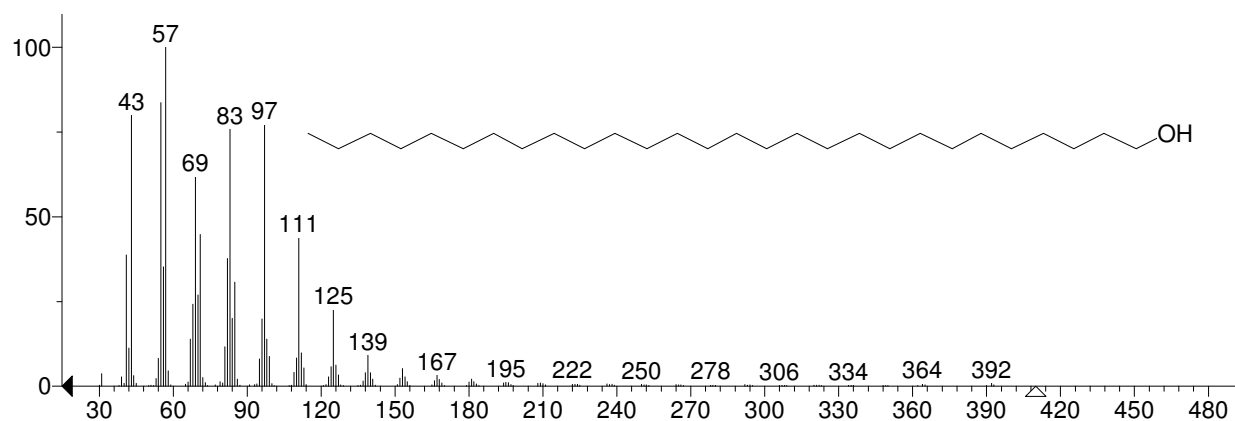


** Search Report Page 1 of 1 **

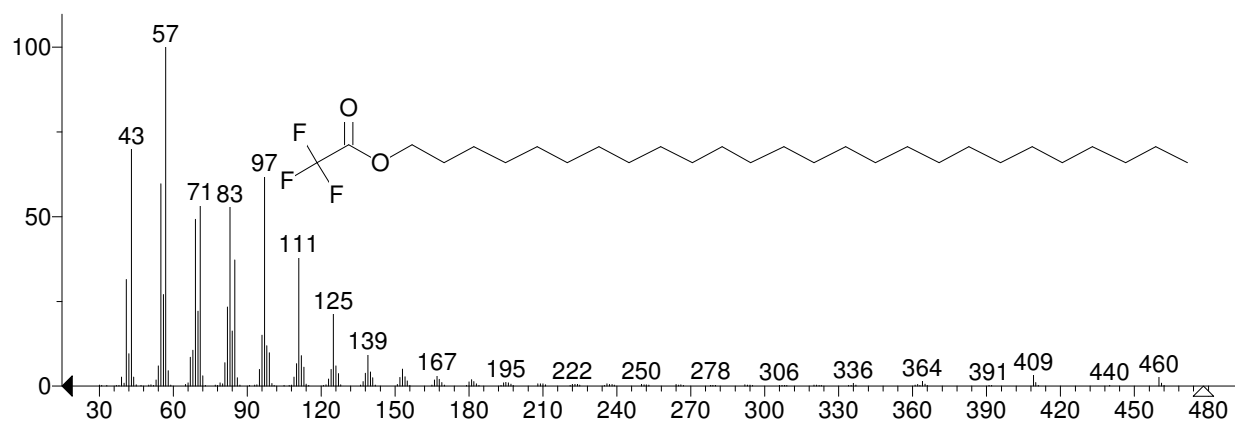
Unknown: Scan 1503 (11.413 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -493



Hit 1 : 1-Octacosanol
C₂₈H₅₈O; MF: 831; RMF: 885; Prob 5.24%; Lib: mainlib; ID: 22288.

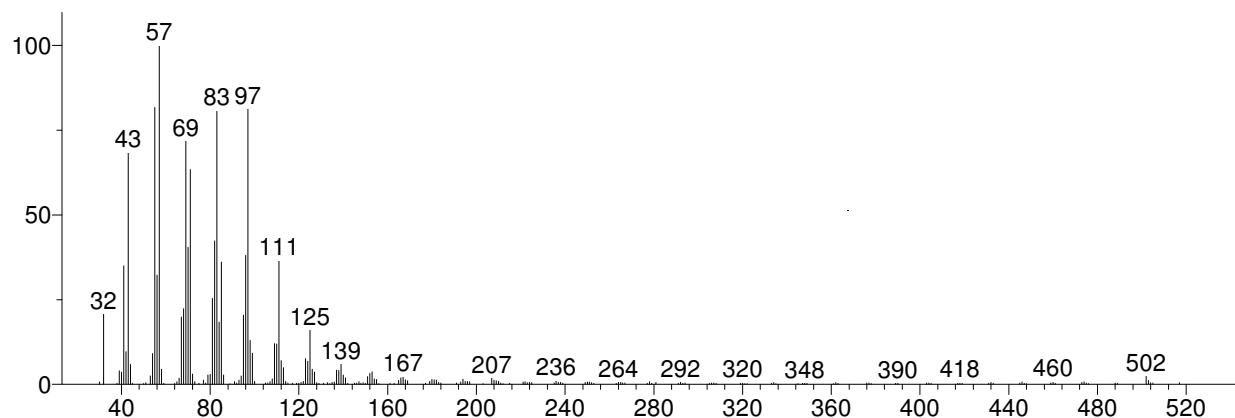


Hit 2 : Hexacosyl trifluoroacetate
C₂₈H₅₃F₃O₂; MF: 828; RMF: 862; Prob 4.63%; Lib: mainlib; ID: 22100.

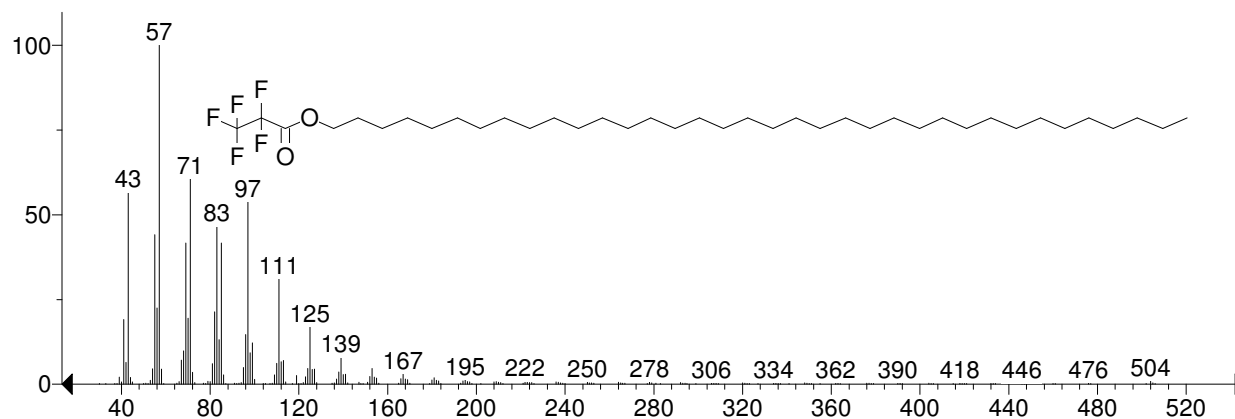


** Search Report Page 1 of 1 **

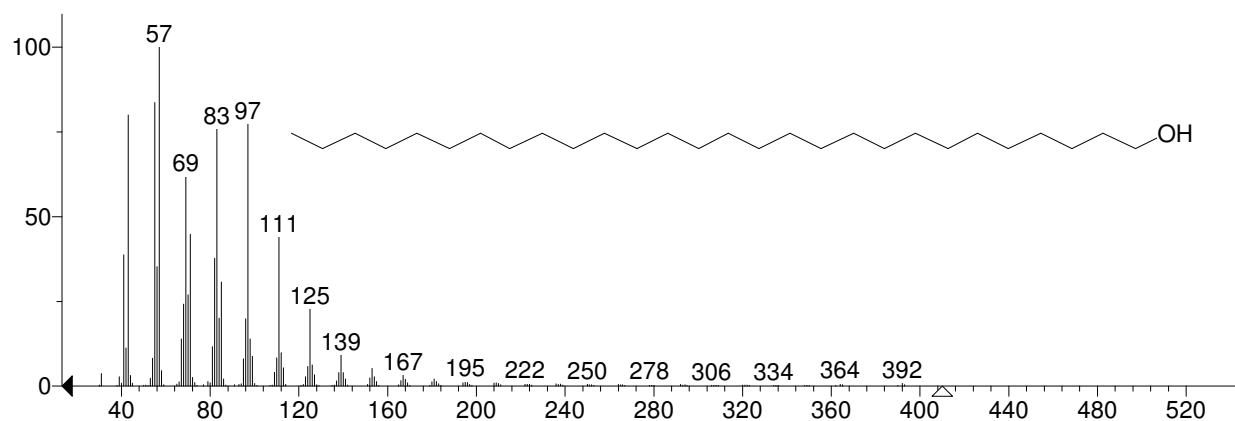
Unknown: Scan 1613 (12.242 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -493



Hit 1 : Hexatriacontyl pentafluoropropionate
C₃₉H₇₃F₅O₂; MF: 835; RMF: 858; Prob 4.24%; Lib: mainlib; ID: 22752.

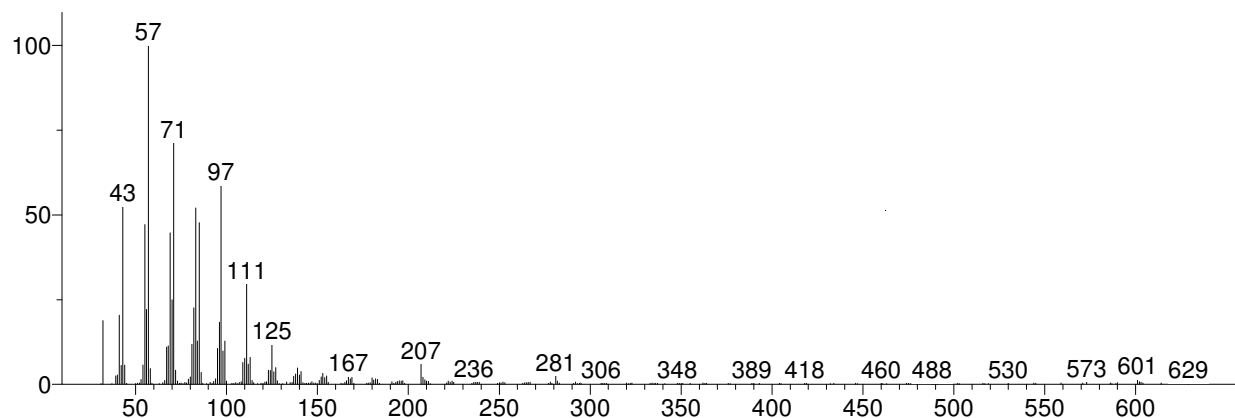


Hit 2 : 1-Octacosanol
C₂₈H₅₈O; MF: 834; RMF: 881; Prob 4.07%; Lib: mainlib; ID: 22288.

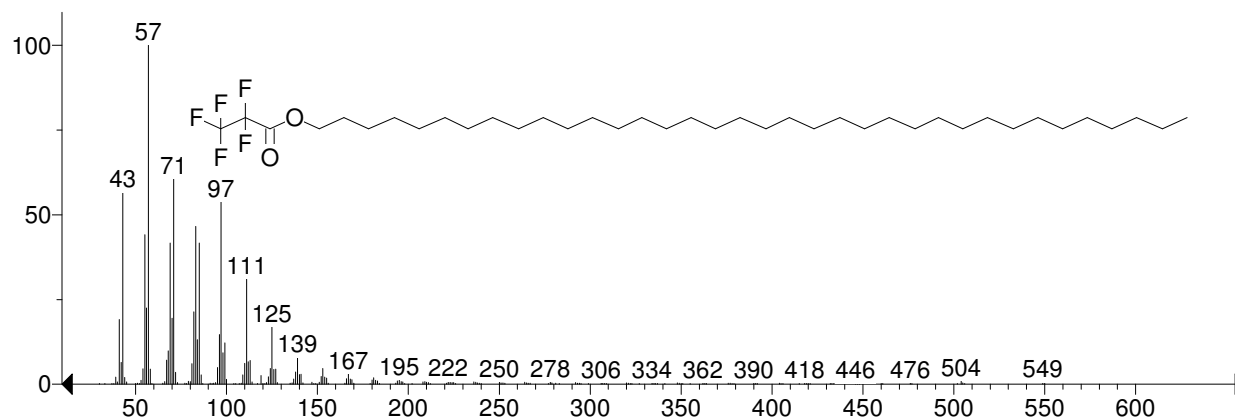


** Search Report Page 1 of 1 **

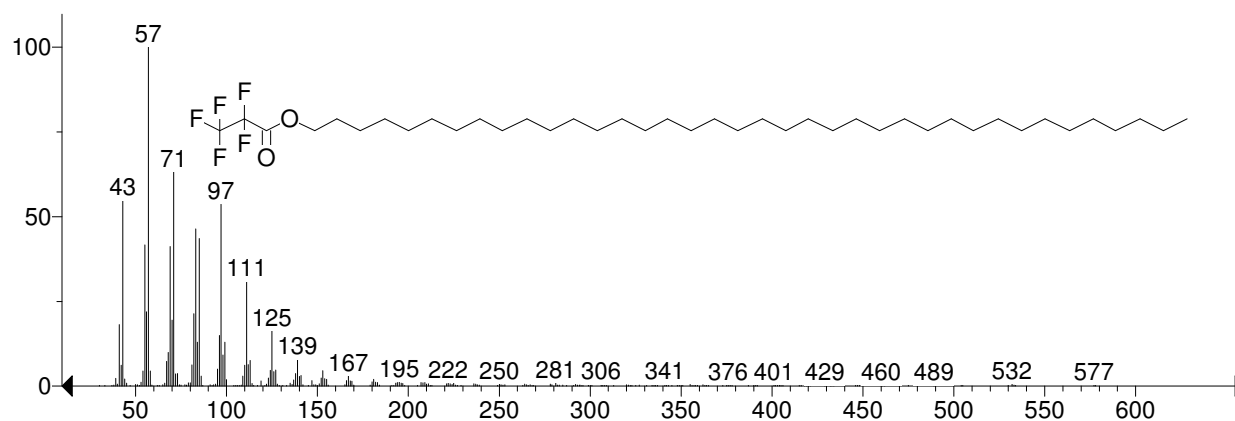
Unknown: Scan 1840 (13.952 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -493



Hit 1 : Hexatriacontyl pentafluoropropionate
C₃₉H₇₃F₅O₂; MF: 837; RMF: 882; Prob 7.50%; Lib: mainlib; ID: 22752.

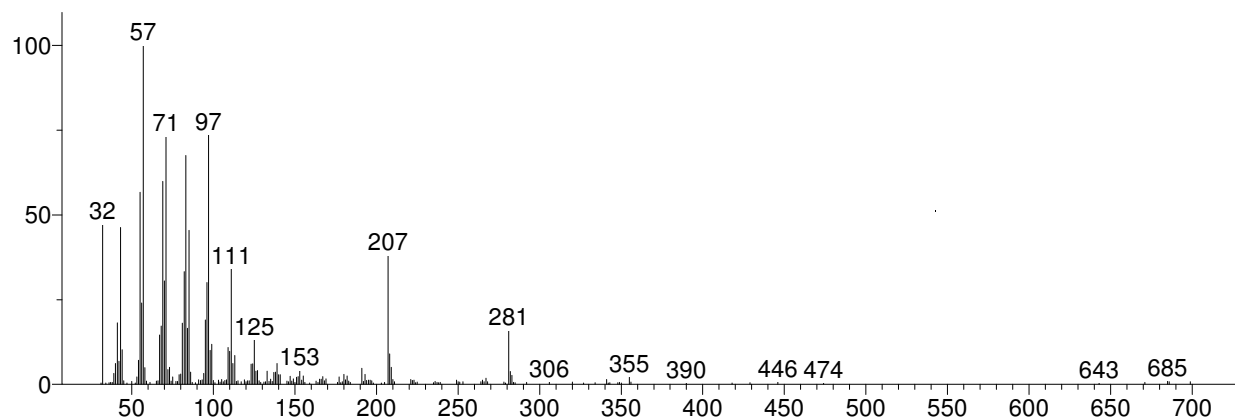


Hit 2 : Octatriacontyl pentafluoropropionate
C₄₁H₇₇F₅O₂; MF: 832; RMF: 863; Prob 6.04%; Lib: mainlib; ID: 22753.

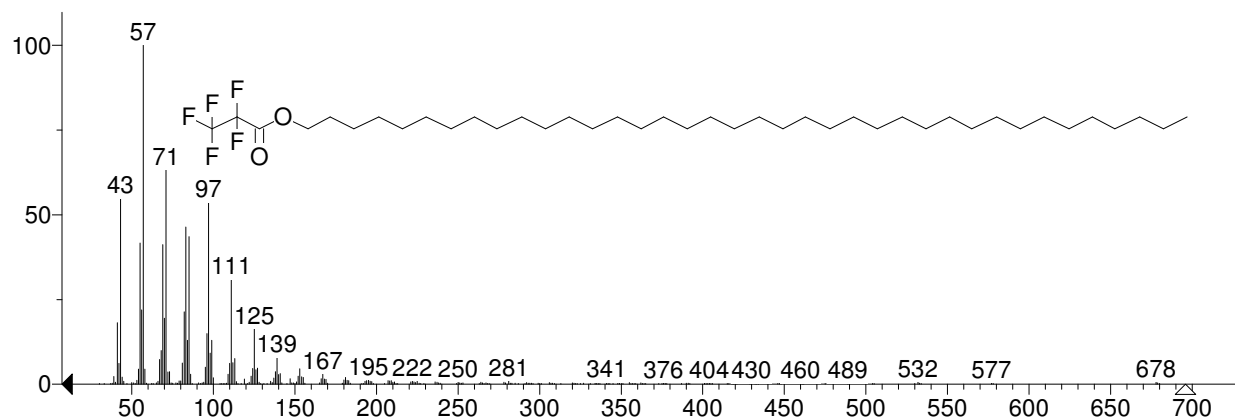


** Search Report Page 1 of 1 **

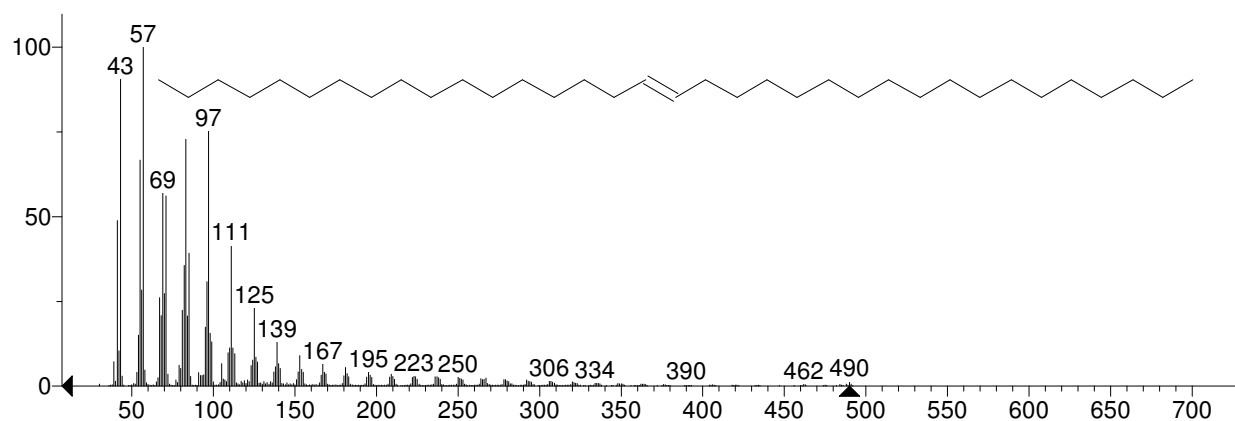
Unknown: Scan 2004 (15.188 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -458



Hit 1 : Octatriacontyl pentafluoropropionate
C₄₁H₇₇F₅O₂; MF: 775; RMF: 797; Prob 17.1%; Lib: mainlib; ID: 22753.

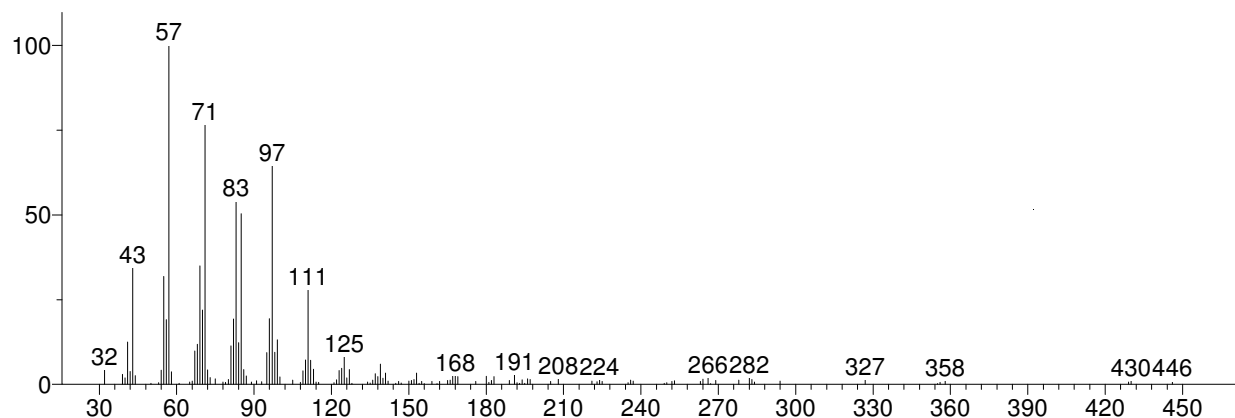


Hit 2 : 17-Pentatriacontene
C₃₅H₇₀; MF: 740; RMF: 759; Prob 4.30%; CAS: 6971-40-0; Lib: mainlib; ID: 22111.

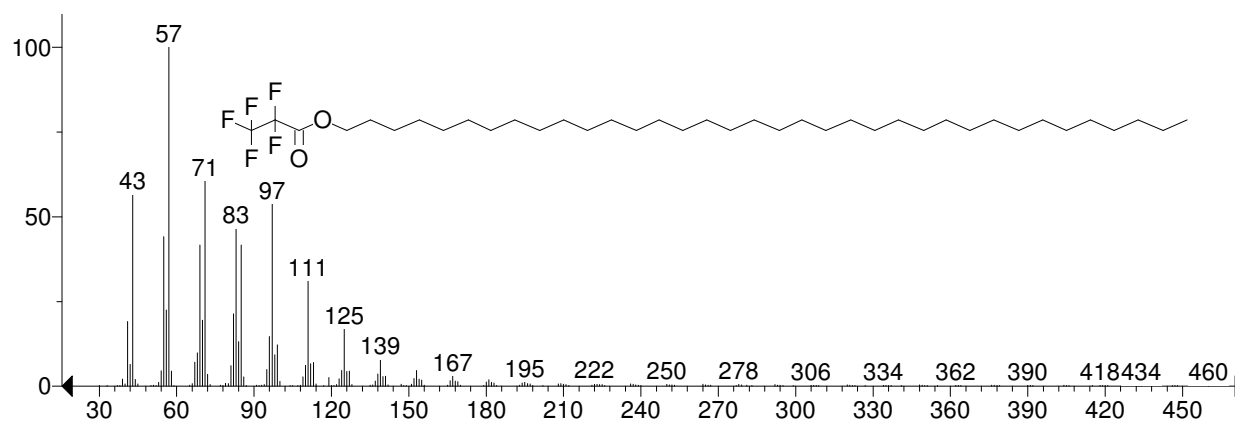


** Search Report Page 1 of 1 **

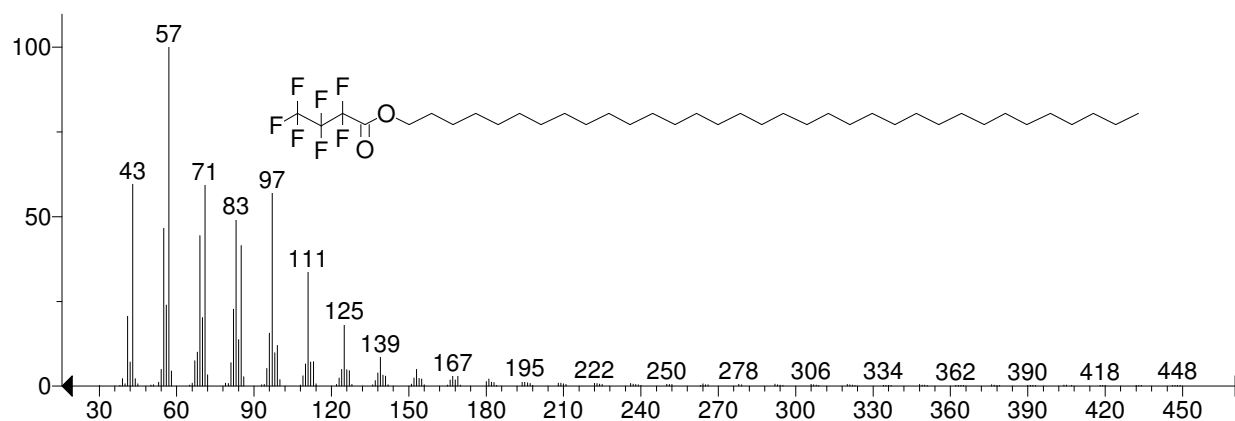
Unknown: Scan 2178 (16.499 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms (-2168)
Compound in Library Factor = -811



Hit 1 : Hexatriacontyl pentafluoropropionate
C₃₉H₇₃F₅O₂; MF: 780; RMF: 813; Prob 4.40%; Lib: mainlib; ID: 22752.

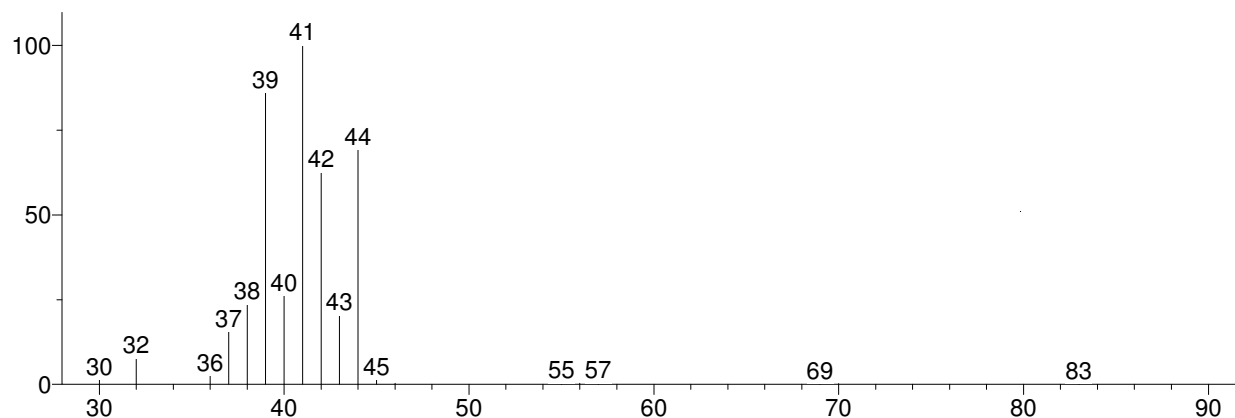


Hit 2 : Tetratriacontyl heptafluorobutyrate
C₃₈H₆₉F₇O₂; MF: 773; RMF: 817; Prob 3.37%; Lib: mainlib; ID: 21855.



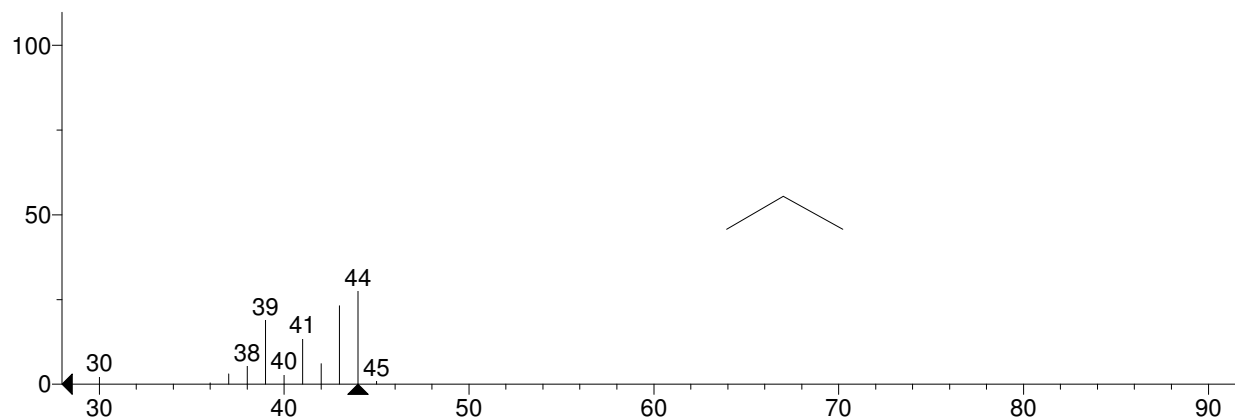
** Search Report Page 1 of 1 **

Unknown: Scan 72 (0.630 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -388



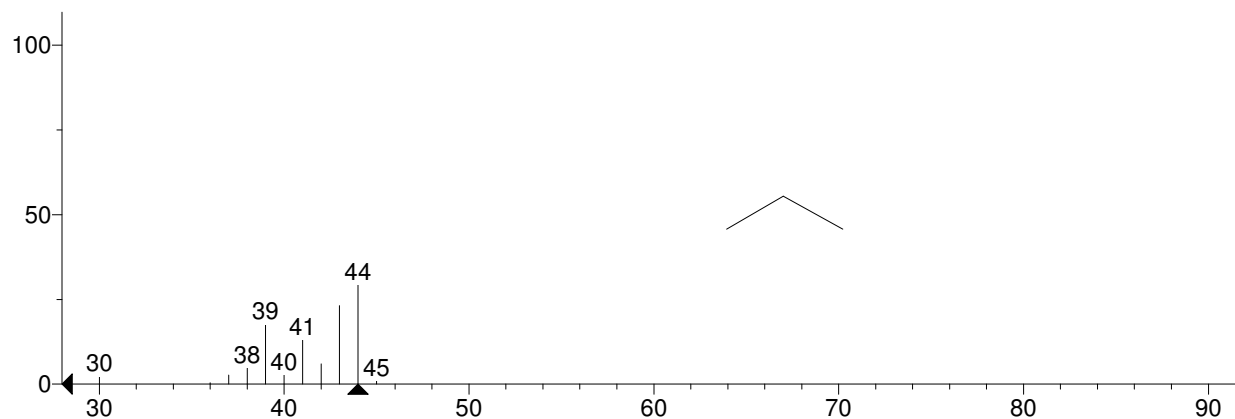
Hit 1 : Propane

C3H8; MF: 804; RMF: 812; Prob 61.0%; CAS: 74-98-6; Lib: mainlib; ID: 399.



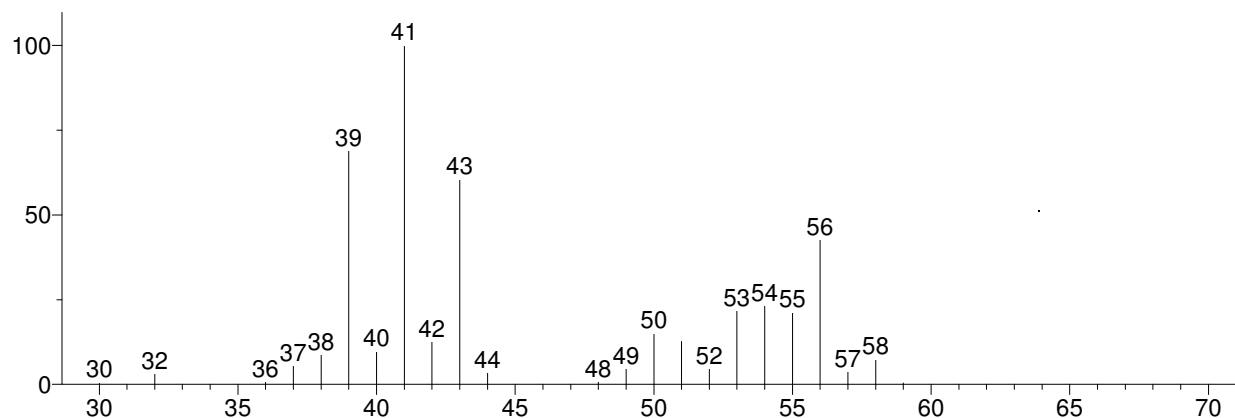
Hit 2 : Propane

C3H8; MF: 803; RMF: 811; Prob 61.0%; CAS: 74-98-6; Lib: replib; ID: 139.

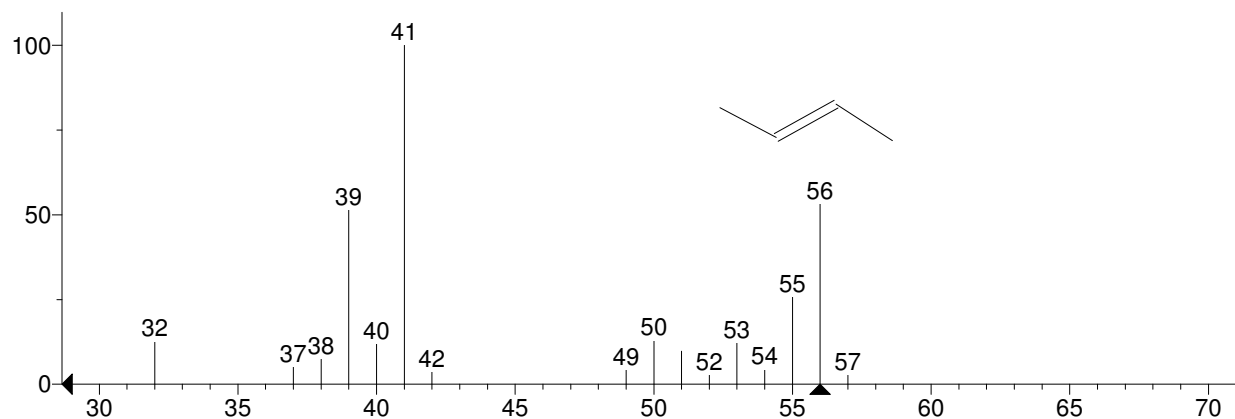


** Search Report Page 1 of 1 **

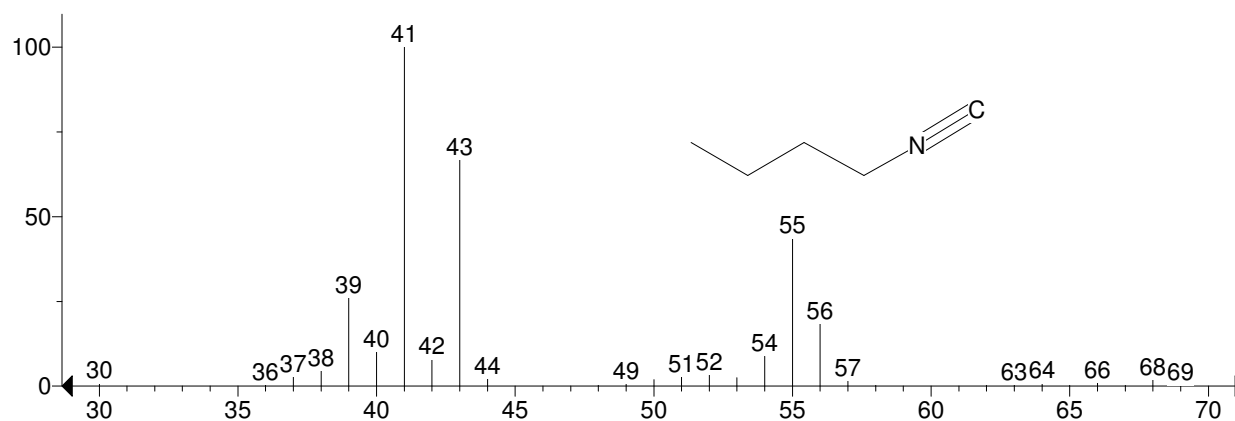
Unknown: Scan 74 (0.645 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -464



Hit 1 : 2-Butene
C₄H₈; MF: 800; RMF: 887; Prob 30.0%; CAS: 107-01-7; Lib: mainlib; ID: 1863.

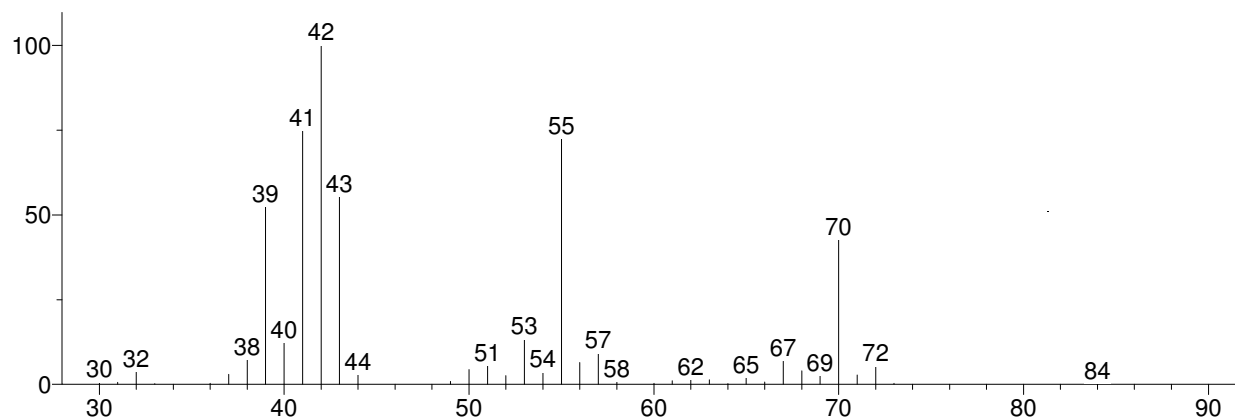


Hit 2 : Butane, 1-isocyano-
C₅H₉N; MF: 777; RMF: 790; Prob 11.0%; CAS: 2769-64-4; Lib: replib; ID: 802.

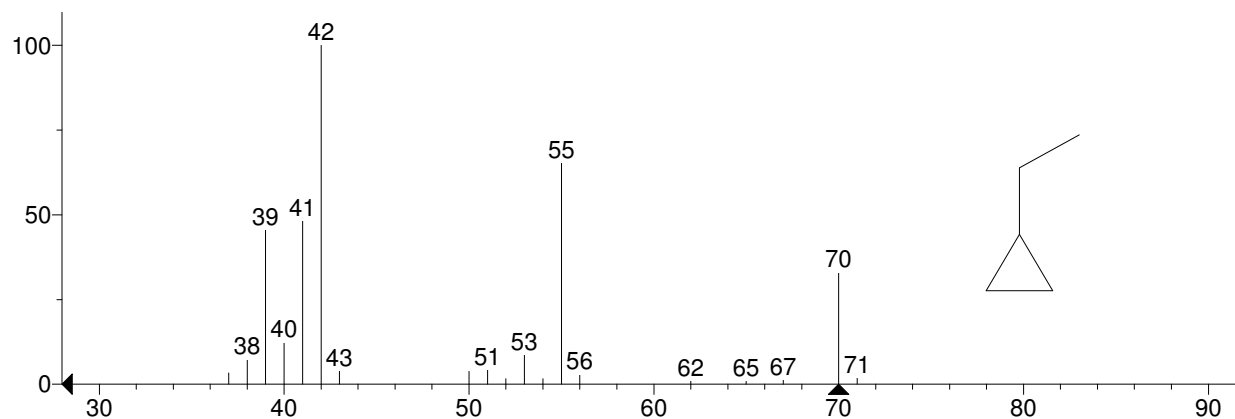


** Search Report Page 1 of 1 **

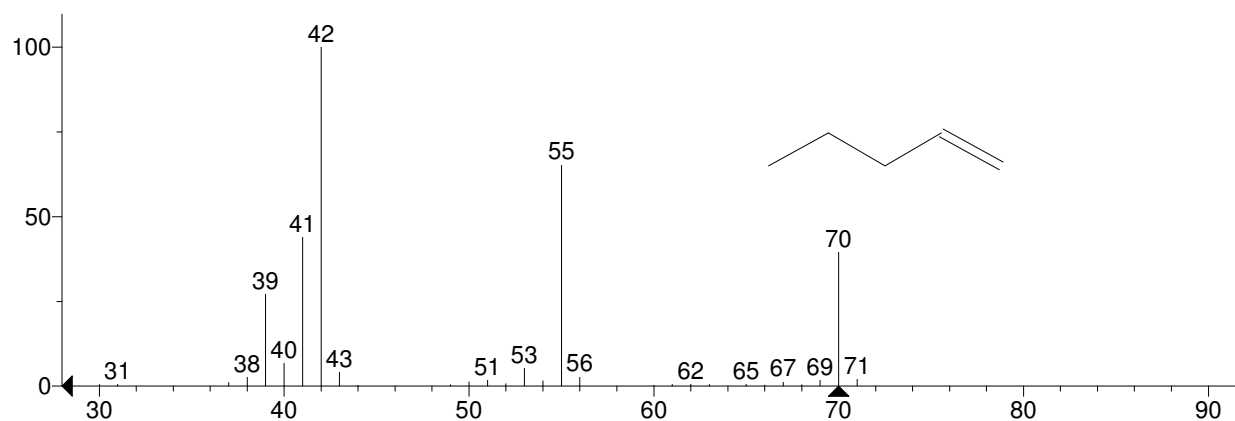
Unknown: Scan 76 (0.660 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -331



Hit 1 : Cyclopropane, ethyl-
C₅H₁₀; MF: 845; RMF: 889; Prob 16.1%; CAS: 1191-96-4; Lib: replib; ID: 1385.

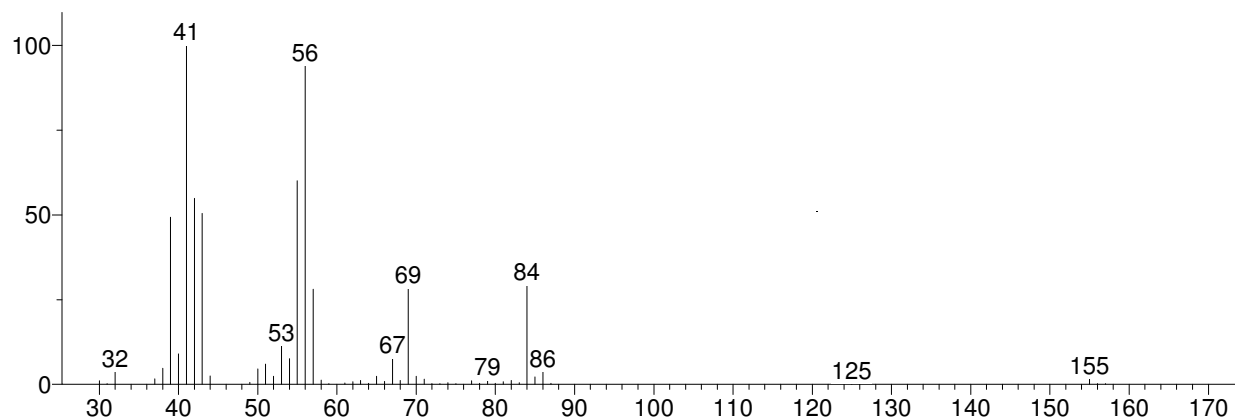


Hit 2 : 1-Pentene
C₅H₁₀; MF: 838; RMF: 859; Prob 12.3%; CAS: 109-67-1; Lib: mainlib; ID: 4375.

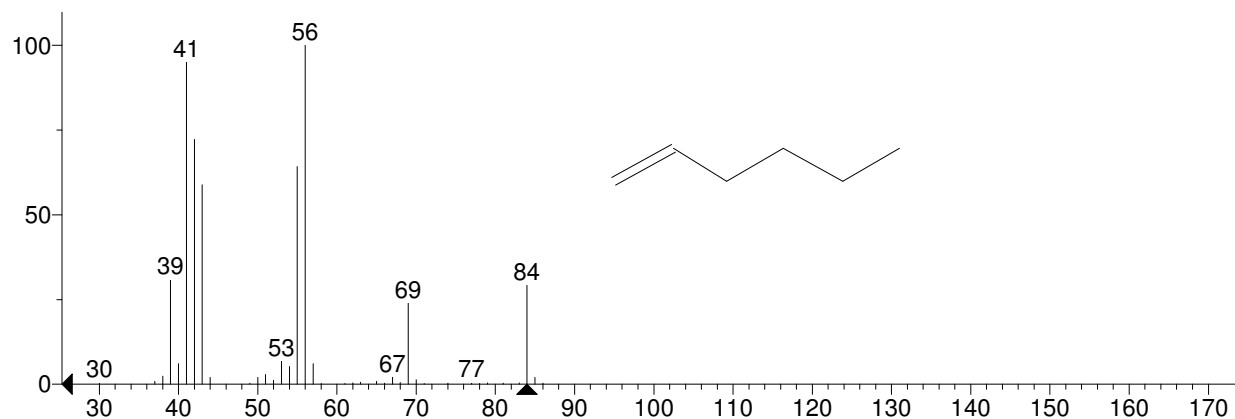


** Search Report Page 1 of 1 **

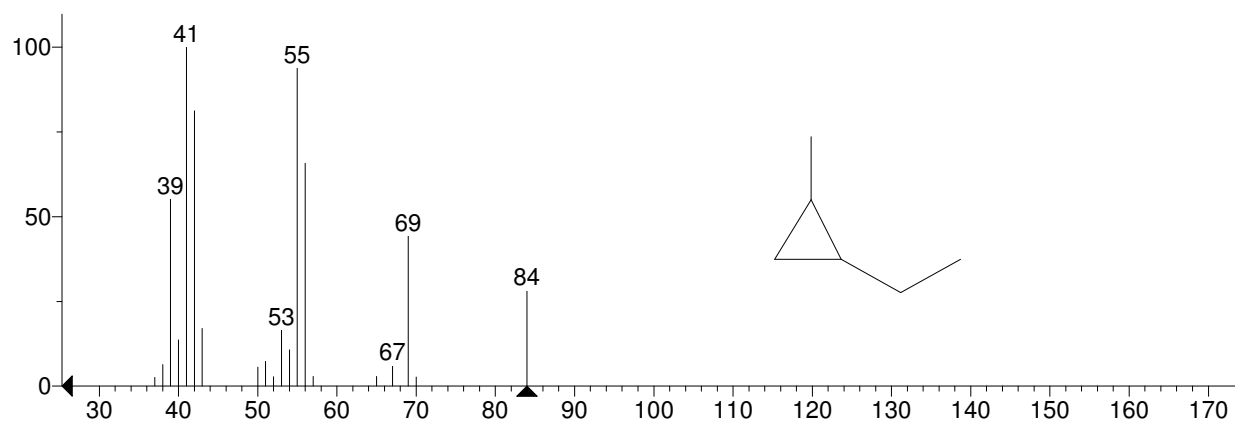
Unknown: Scan 80 (0.690 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -246



Hit 1 : 1-Hexene
C₆H₁₂; MF: 867; RMF: 876; Prob 14.3%; CAS: 592-41-6; Lib: mainlib; ID: 19842.

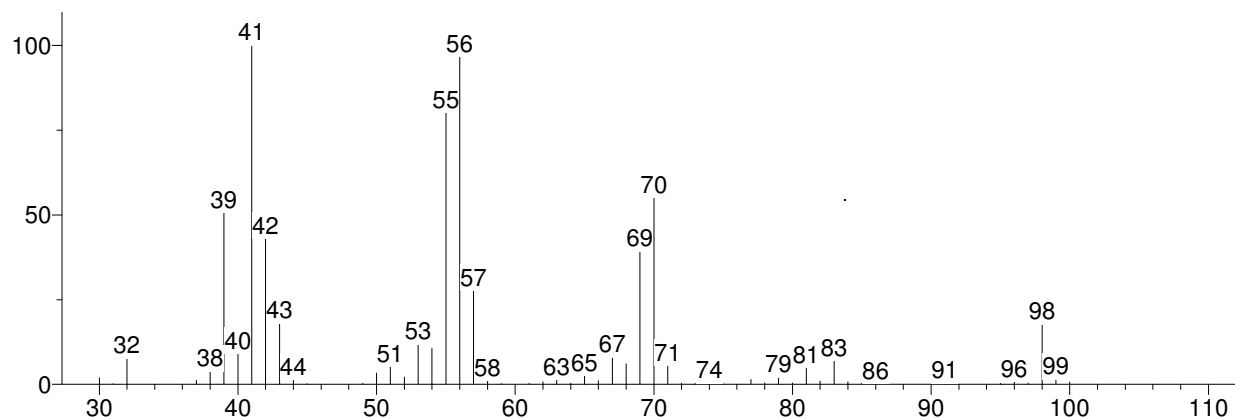


Hit 2 : Cyclopropane, 1-ethyl-2-methyl-, cis-
C₆H₁₂; MF: 855; RMF: 889; Prob 9.49%; CAS: 19781-68-1; Lib: mainlib; ID: 2449.

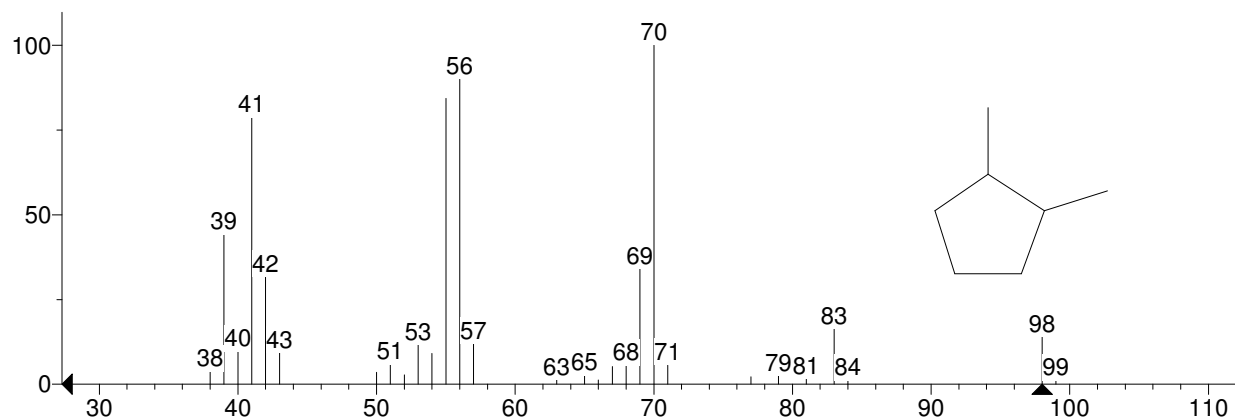


** Search Report Page 1 of 1 **

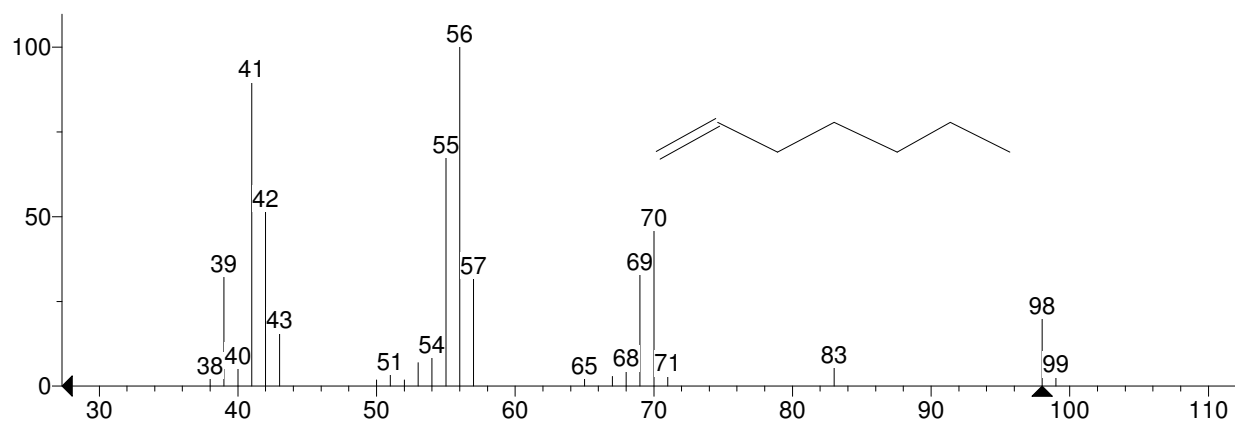
Unknown: Scan 87 (0.743 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -134



Hit 1 : Cyclopentane, 1,2-dimethyl-, cis-
C₇H₁₄; MF: 910; RMF: 925; Prob 13.6%; CAS: 1192-18-3; Lib: mainlib; ID: 32333.

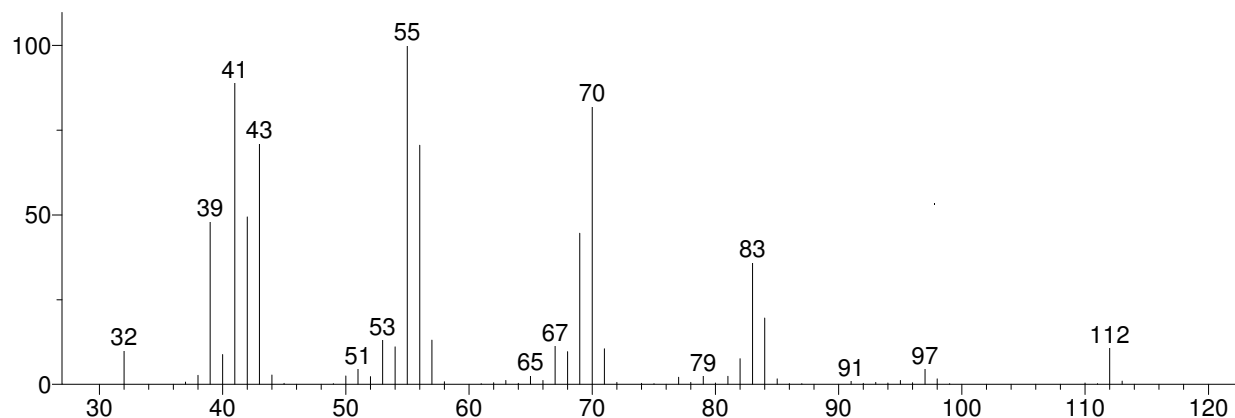


Hit 2 : 1-Heptene
C₇H₁₄; MF: 909; RMF: 937; Prob 13.1%; CAS: 592-76-7; Lib: replib; ID: 4878.

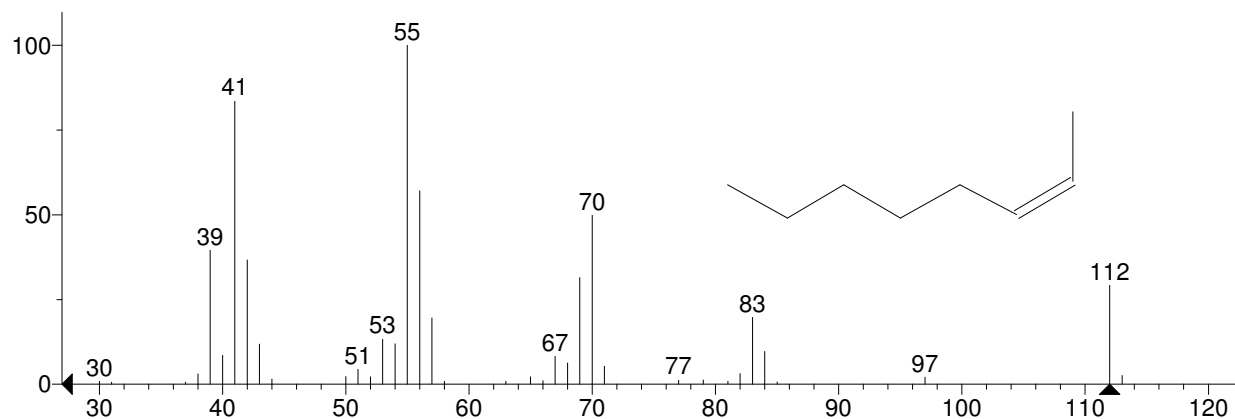


** Search Report Page 1 of 1 **

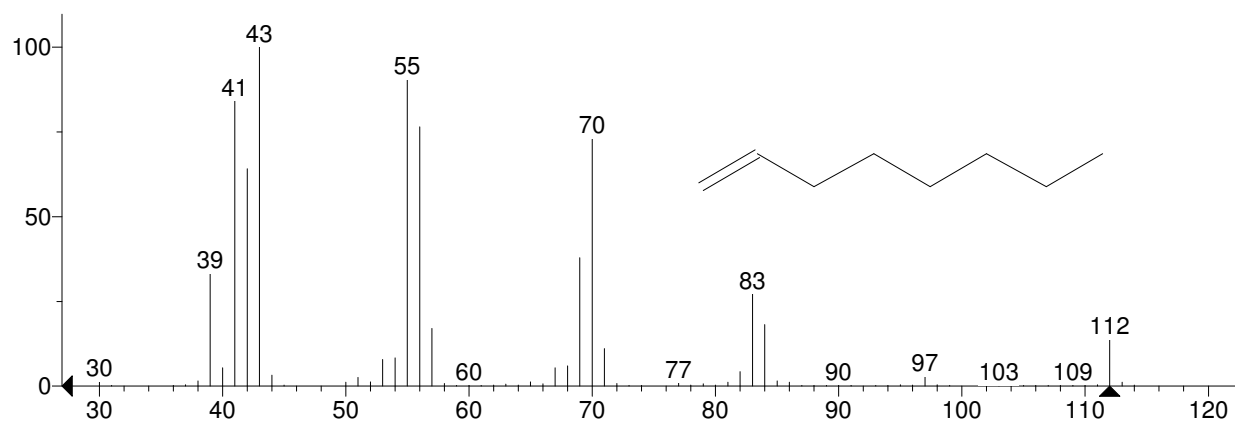
Unknown: Scan 101 (0.849 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -134



Hit 1 : 2-Octene, (Z)-
C₈H₁₆; MF: 909; RMF: 921; Prob 12.8%; CAS: 7642-04-8; Lib: replib; ID: 4208.

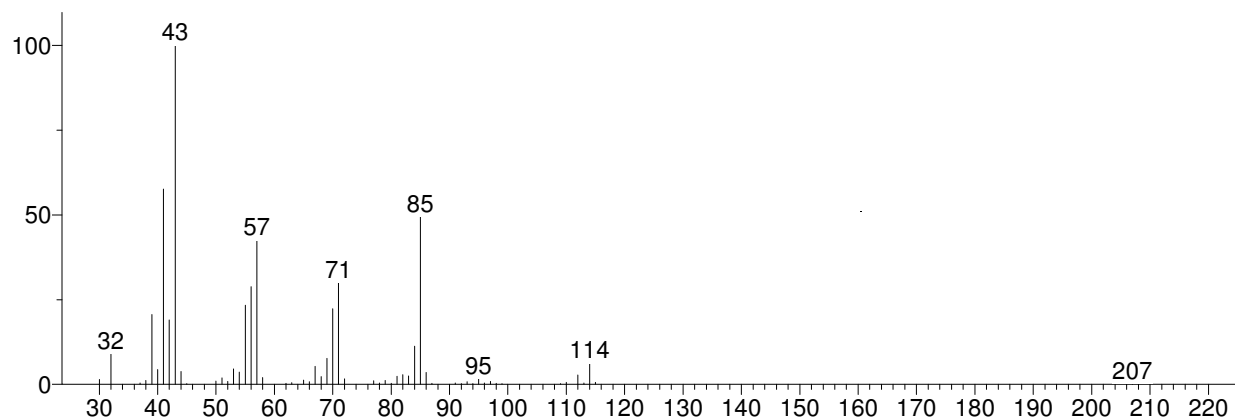


Hit 2 : 1-Octene
C₈H₁₆; MF: 900; RMF: 904; Prob 9.25%; CAS: 111-66-0; Lib: replib; ID: 1923.

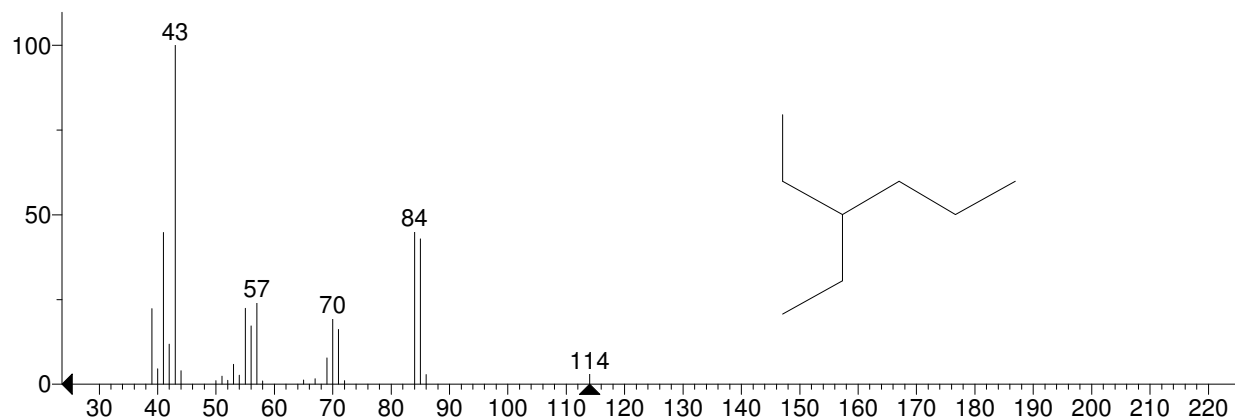


** Search Report Page 1 of 1 **

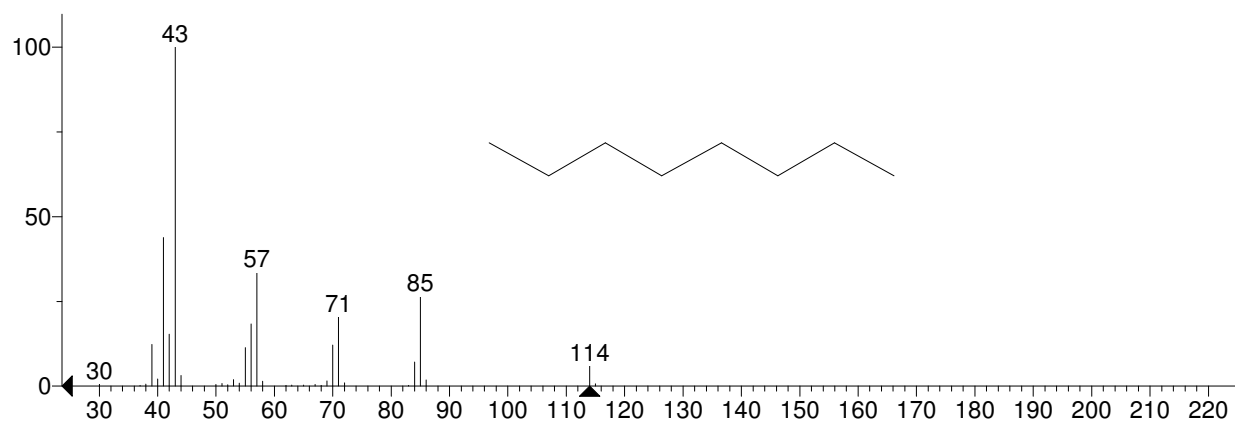
Unknown: Scan 103 (0.864 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -190



Hit 1 : Hexane, 3-ethyl-
C₈H₁₈; MF: 864; RMF: 908; Prob 24.1%; CAS: 619-99-8; Lib: replib; ID: 2636.

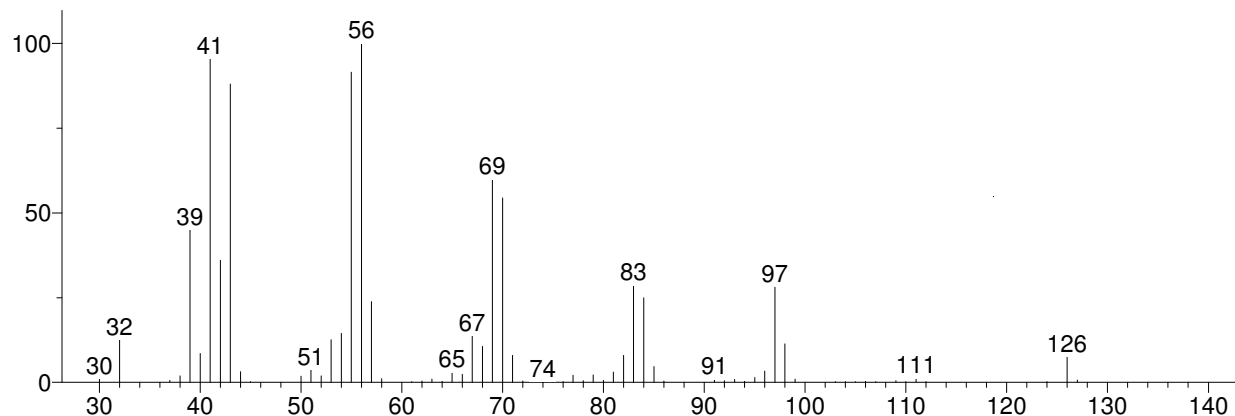


Hit 2 : Octane
C₈H₁₈; MF: 863; RMF: 895; Prob 23.2%; CAS: 111-65-9; Lib: mainlib; ID: 5692.

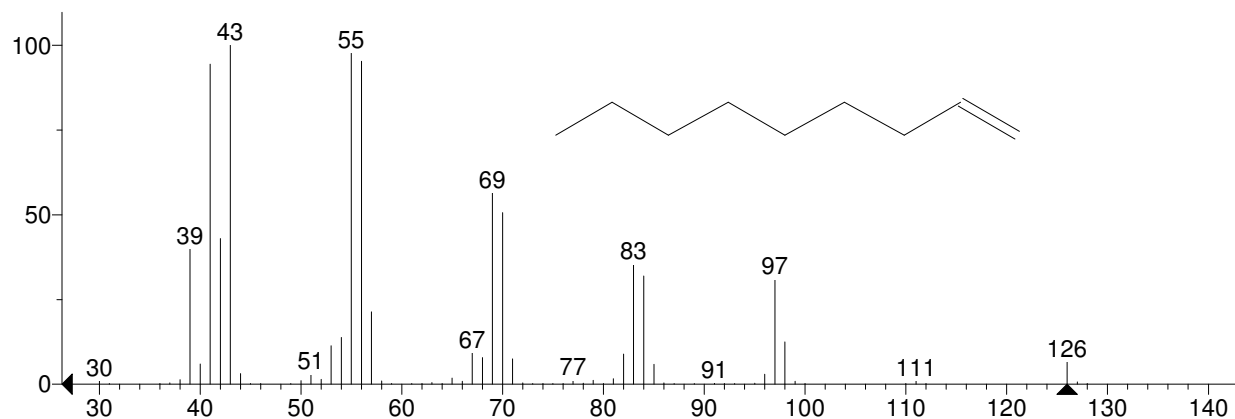


** Search Report Page 1 of 1 **

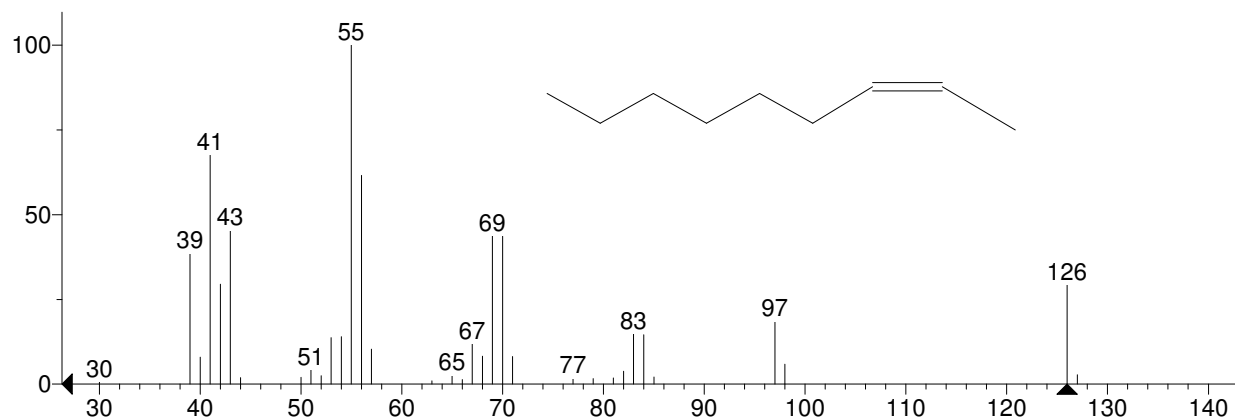
Unknown: Scan 128 (1.052 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -117



Hit 1 : 1-Nonene
C₉H₁₈; MF: 925; RMF: 931; Prob 12.2%; CAS: 124-11-8; Lib: replib; ID: 1943.

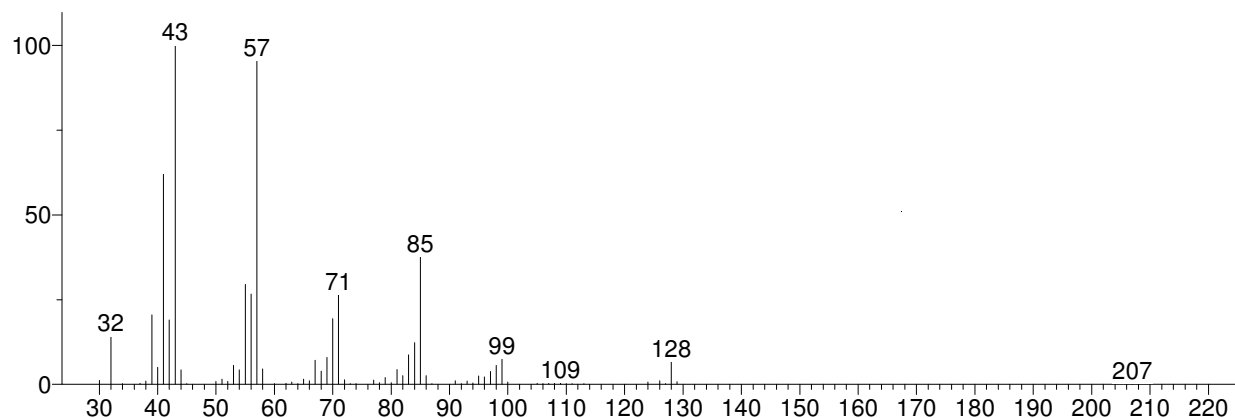


Hit 2 : cis-2-Nonene
C₉H₁₈; MF: 909; RMF: 927; Prob 7.04%; CAS: 6434-77-1; Lib: mainlib; ID: 17345.

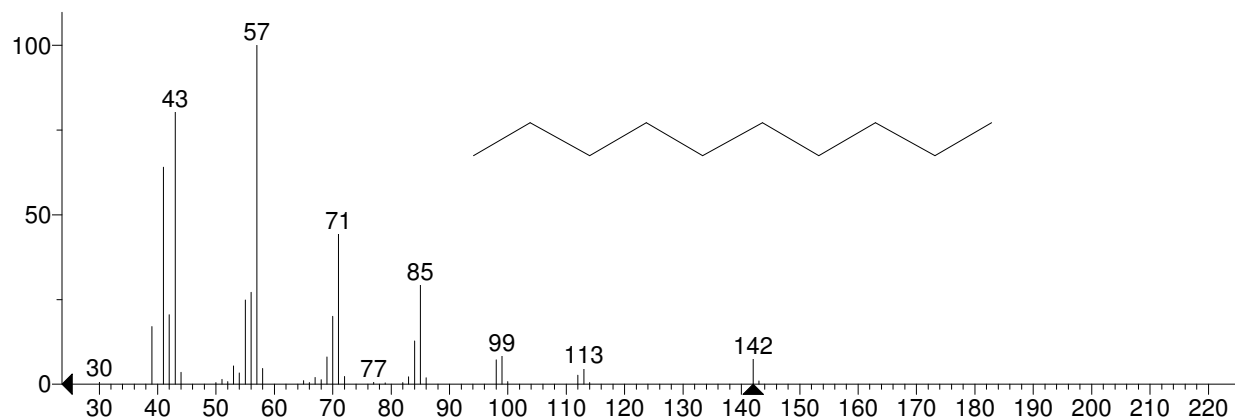


** Search Report Page 1 of 1 **

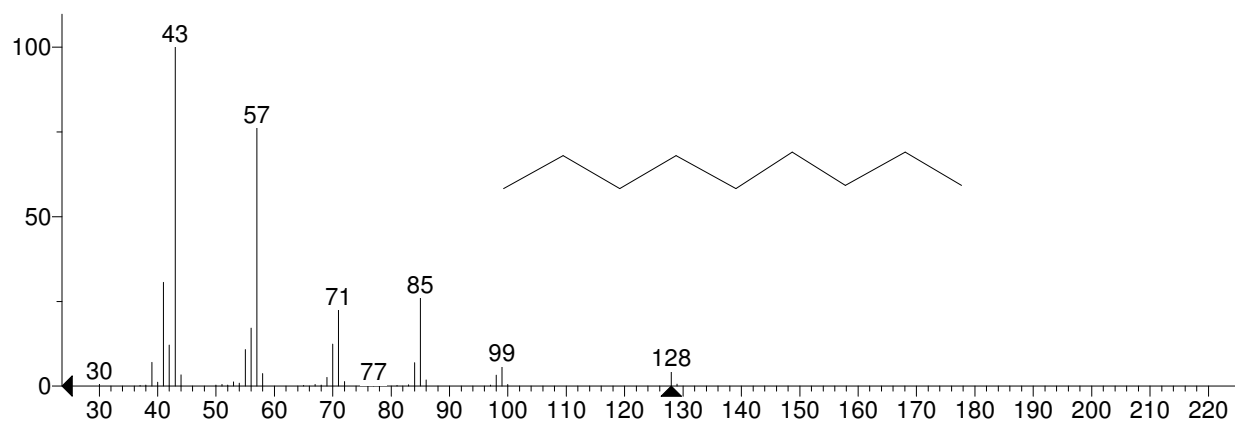
Unknown: Scan 132 (1.082 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -359



Hit 1 : Decane
C₁₀H₂₂; MF: 834; RMF: 887; Prob 9.61%; CAS: 124-18-5; Lib: mainlib; ID: 21679.

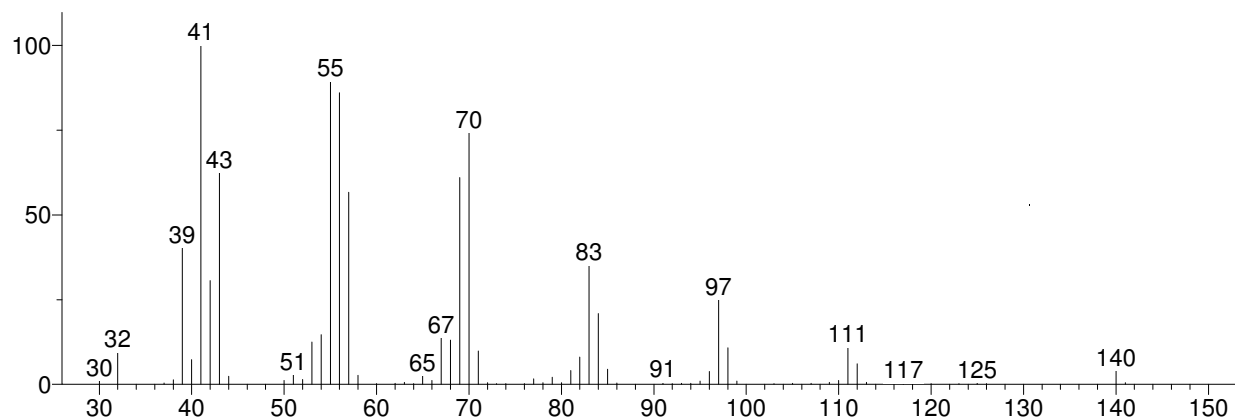


Hit 2 : Nonane
C₉H₂₀; MF: 832; RMF: 863; Prob 8.86%; CAS: 111-84-2; Lib: mainlib; ID: 7170.

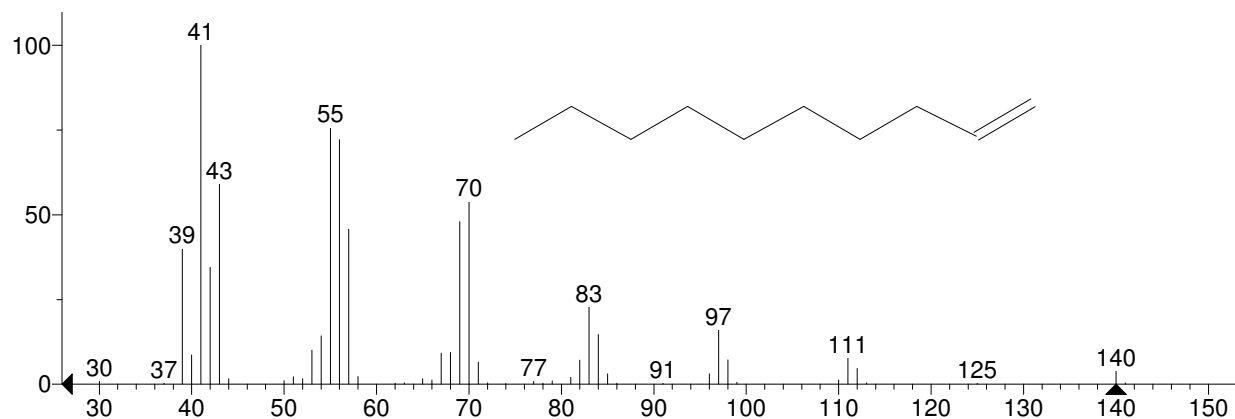


** Search Report Page 1 of 1 **

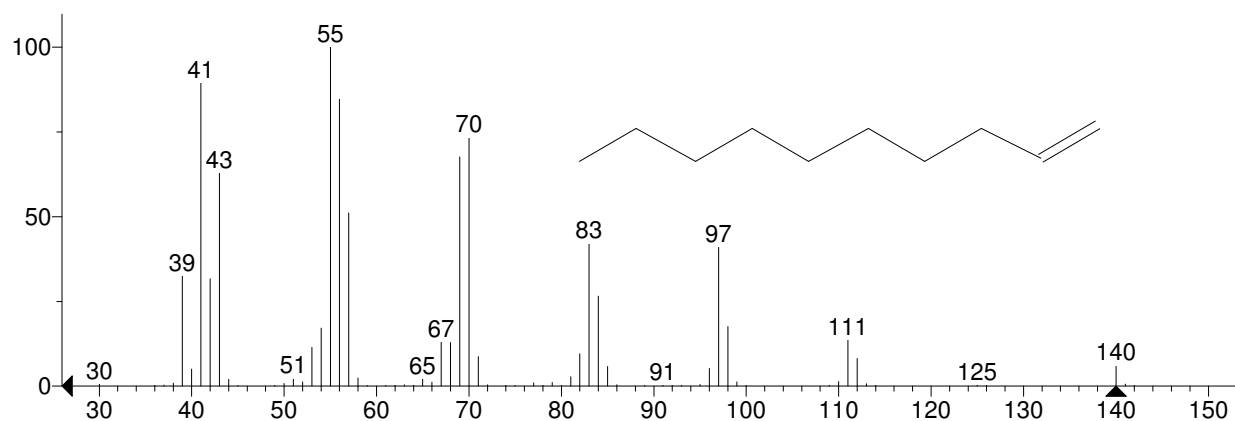
Unknown: Scan 173 (1.391 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = 116



Hit 1 : 1-Decene
C₁₀H₂₀; MF: 943; RMF: 950; Prob 15.2%; CAS: 872-05-9; Lib: replib; ID: 896.

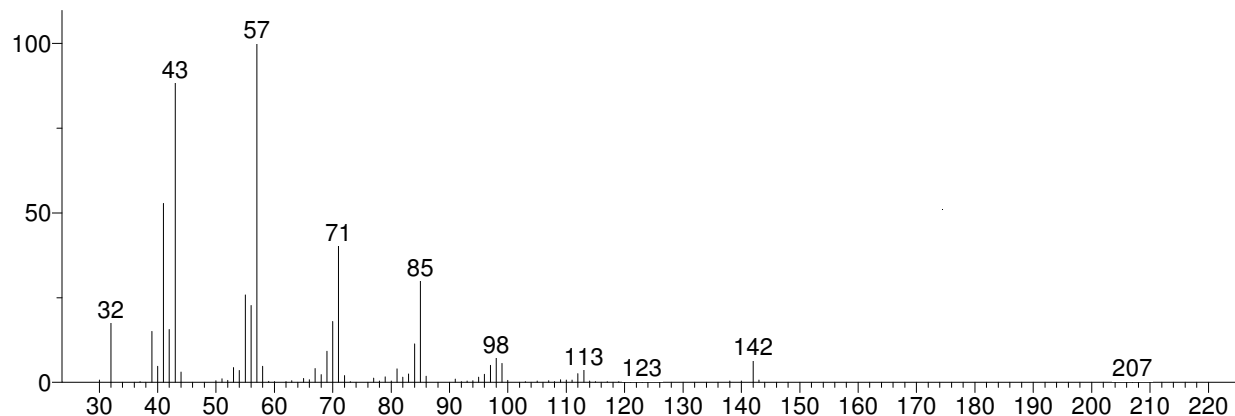


Hit 2 : 1-Decene
C₁₀H₂₀; MF: 932; RMF: 937; Prob 15.2%; CAS: 872-05-9; Lib: replib; ID: 4200.

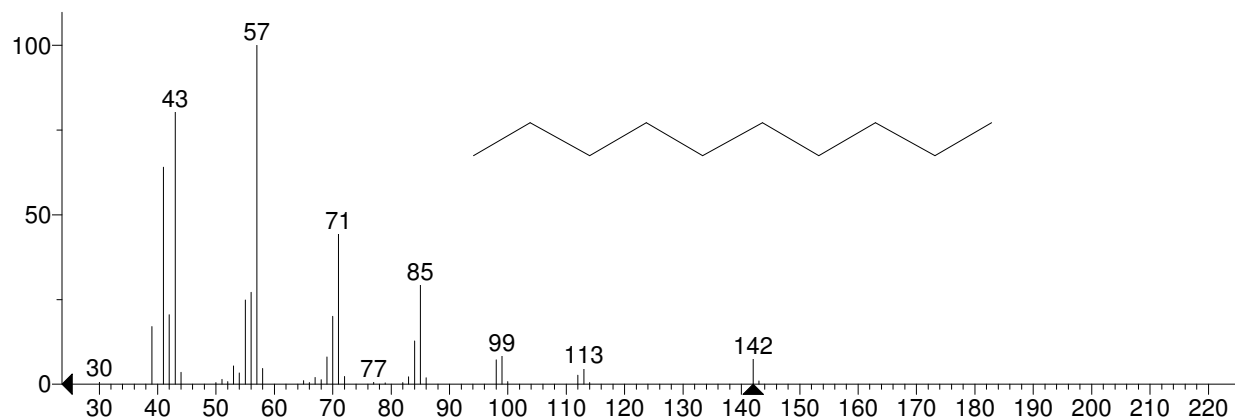


**** Search Report Page 1 of 1 ****

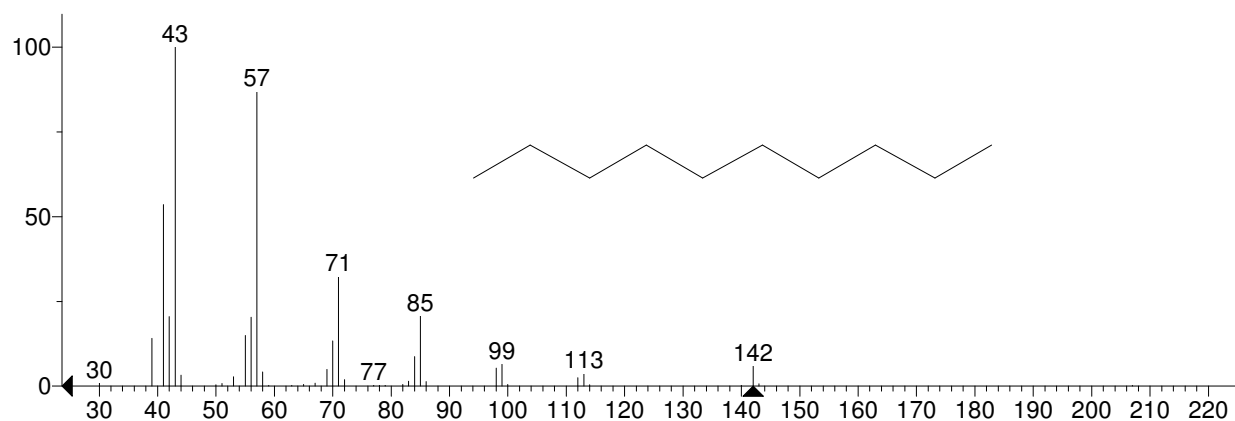
Unknown: Scan 180 (1.444 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = 120



Hit 1 : Decane
C₁₀H₂₂; MF: 900; RMF: 946; Prob 29.5%; CAS: 124-18-5; Lib: mainlib; ID: 21679.

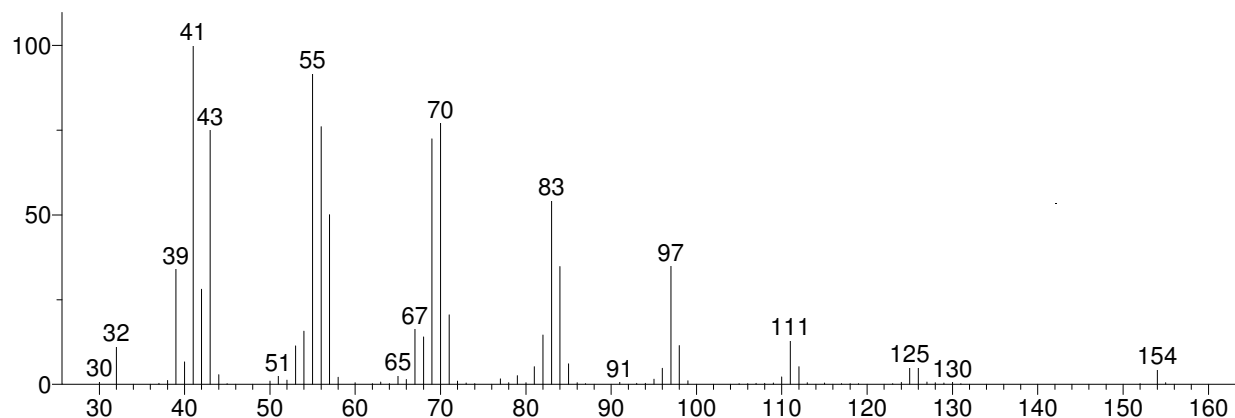


Hit 2 : Decane
C₁₀H₂₂; MF: 869; RMF: 921; Prob 29.5%; CAS: 124-18-5; Lib: replib; ID: 2052.

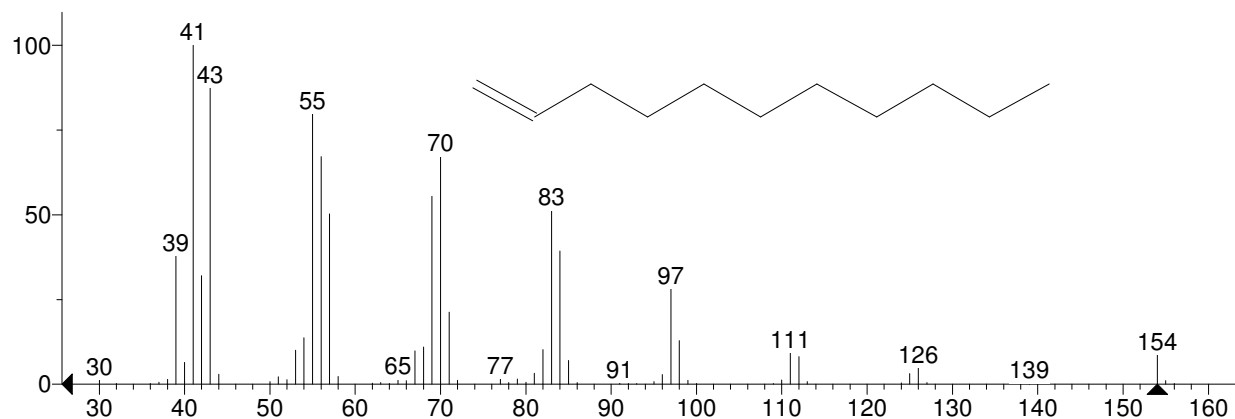


** Search Report Page 1 of 1 **

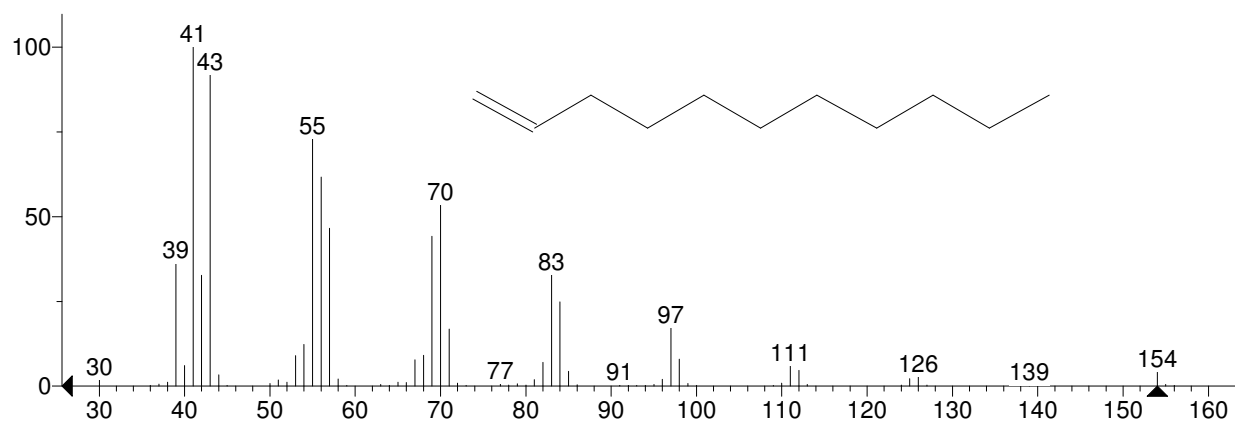
Unknown: Scan 236 (1.866 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -161



Hit 1 : 1-Undecene
C₁₁H₂₂; MF: 926; RMF: 929; Prob 6.85%; CAS: 821-95-4; Lib: replib; ID: 825.

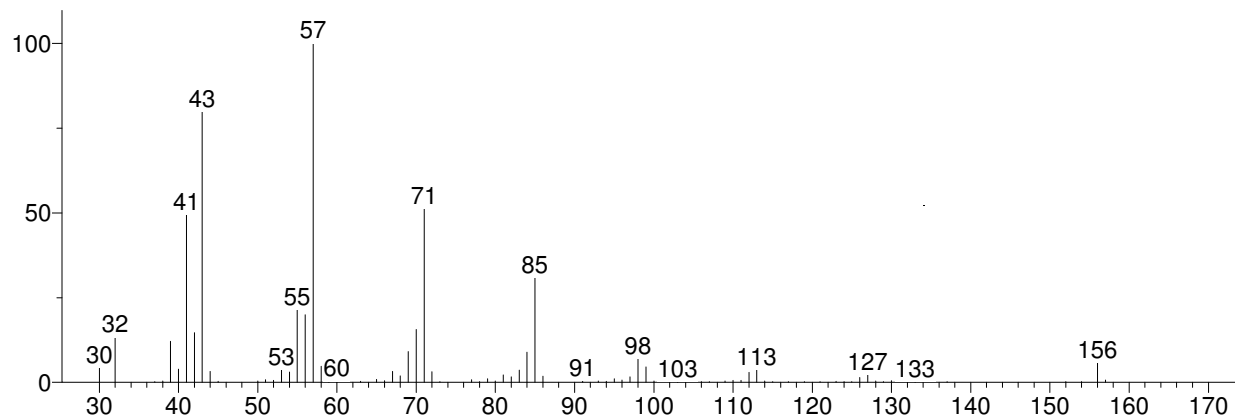


Hit 2 : 1-Undecene
C₁₁H₂₂; MF: 925; RMF: 931; Prob 6.85%; CAS: 821-95-4; Lib: replib; ID: 824.

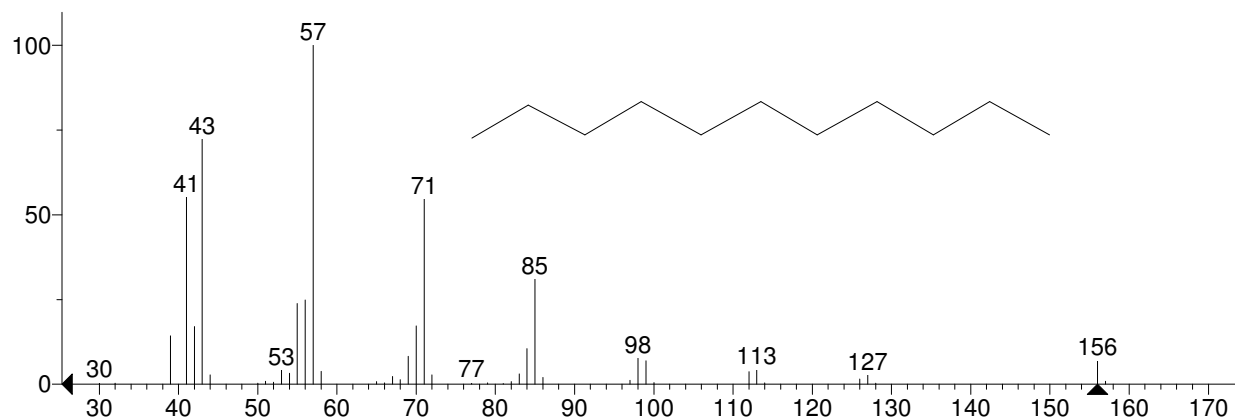


** Search Report Page 1 of 1 **

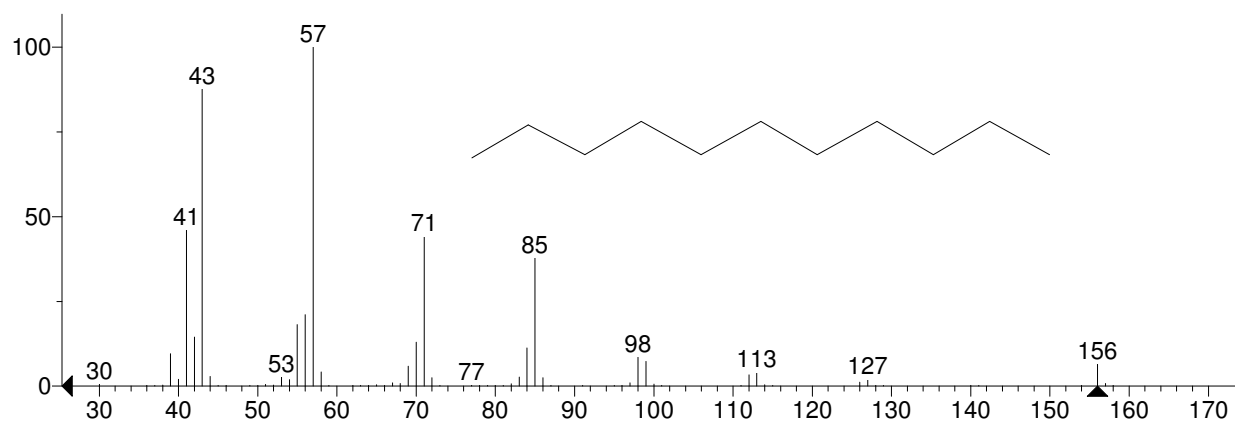
Unknown: Scan 244 (1.926 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = 146



Hit 1 : Undecane
C₁₁H₂₄; MF: 918; RMF: 930; Prob 29.8%; CAS: 1120-21-4; Lib: replib; ID: 5429.

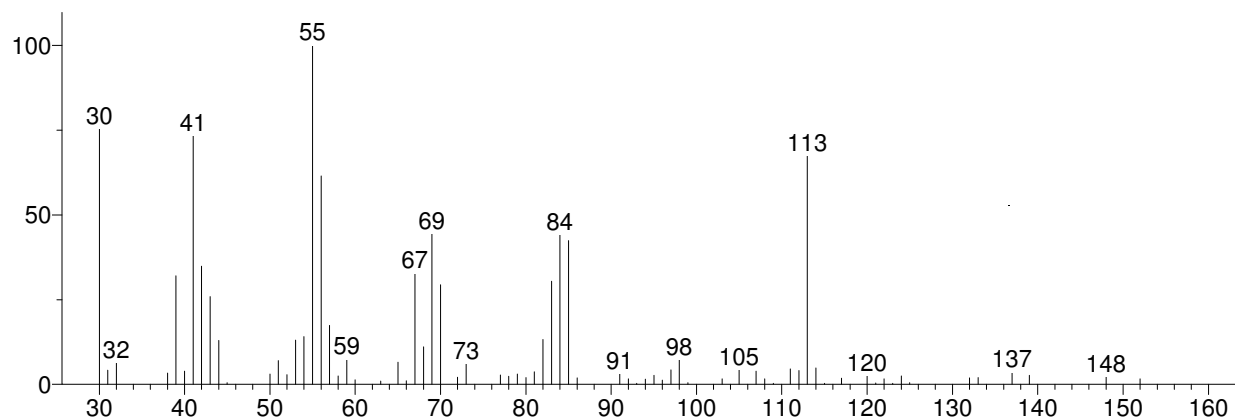


Hit 2 : Undecane
C₁₁H₂₄; MF: 898; RMF: 914; Prob 29.8%; CAS: 1120-21-4; Lib: replib; ID: 5428.

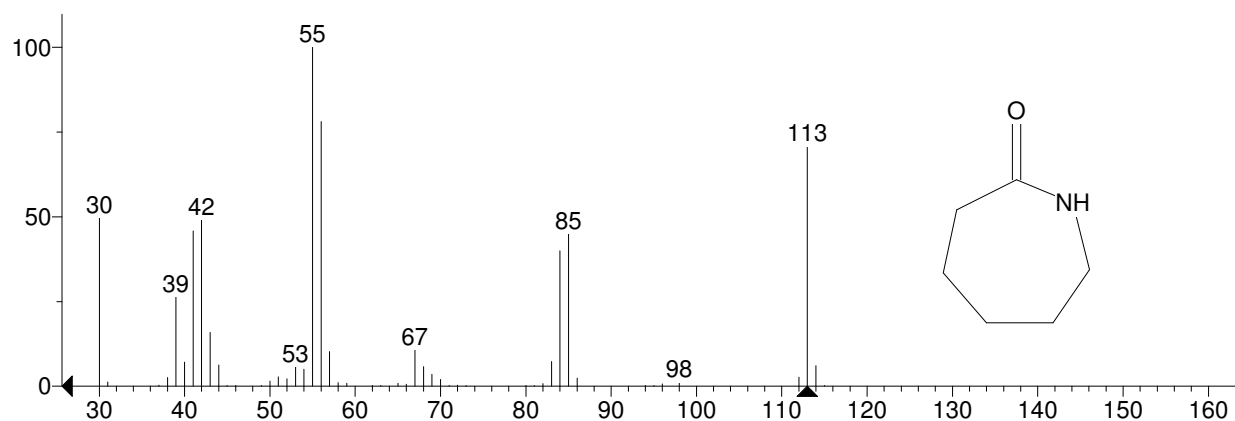


** Search Report Page 1 of 1 **

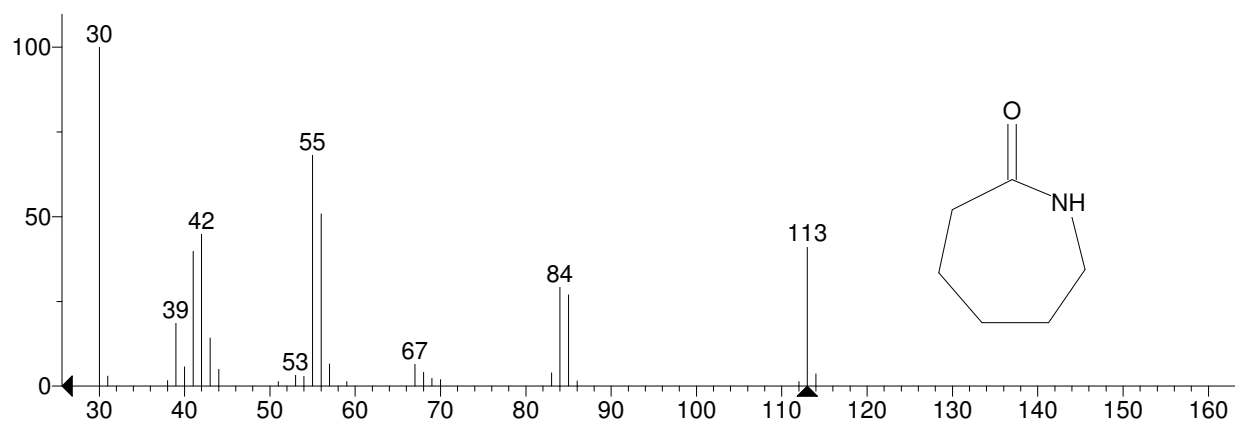
Unknown: Scan 271 (2.130 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms (-279)
Compound in Library Factor = -513



Hit 1 : Caprolactam
C₆H₁₁NO; MF: 749; RMF: 801; Prob 28.4%; CAS: 105-60-2; Lib: replib; ID: 4436.

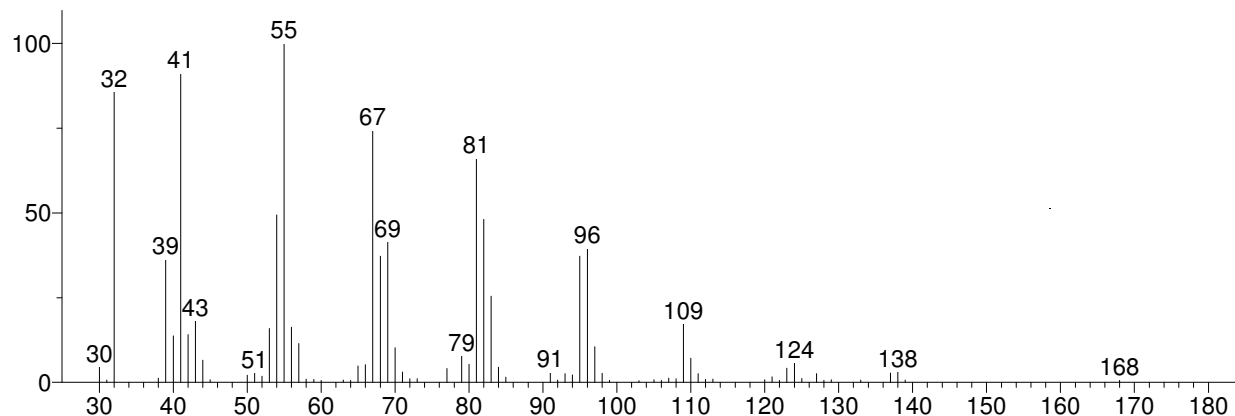


Hit 2 : Caprolactam
C₆H₁₁NO; MF: 737; RMF: 832; Prob 28.4%; CAS: 105-60-2; Lib: replib; ID: 413.

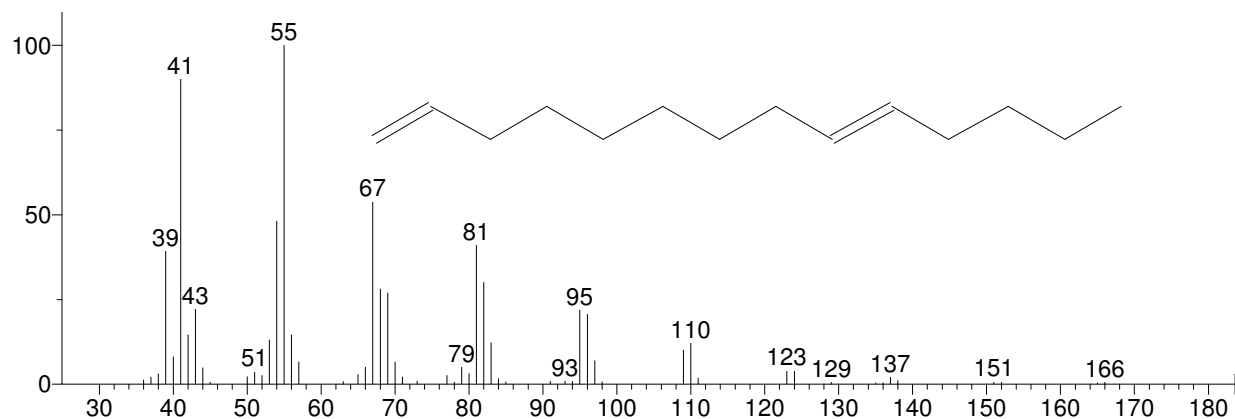


** Search Report Page 1 of 1 **

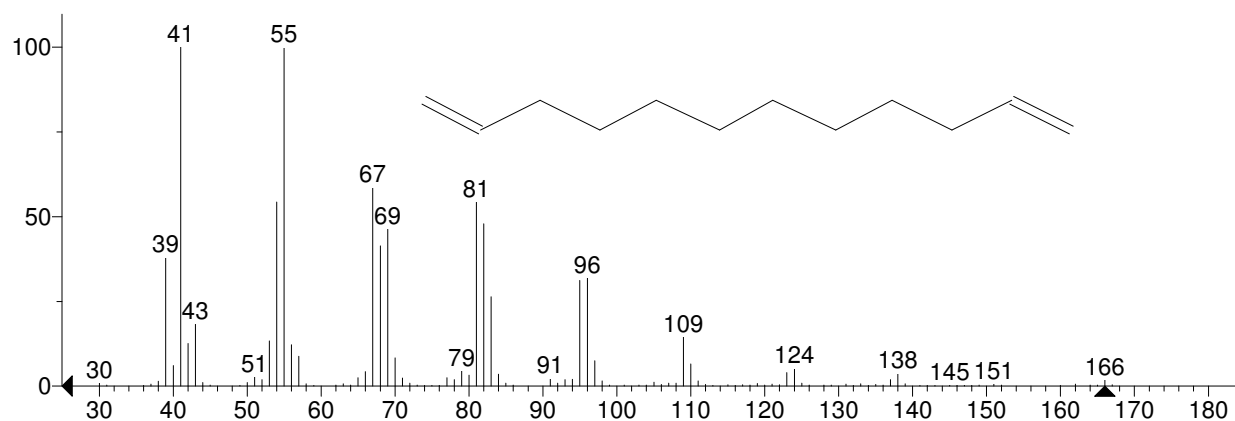
Unknown: Scan 301 (2.356 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -253



Hit 1 : E-1,9-Tetradecadiene
C₁₄H₂₆; MF: 883; RMF: 901; Prob 6.27%; Lib: mainlib; ID: 17378.

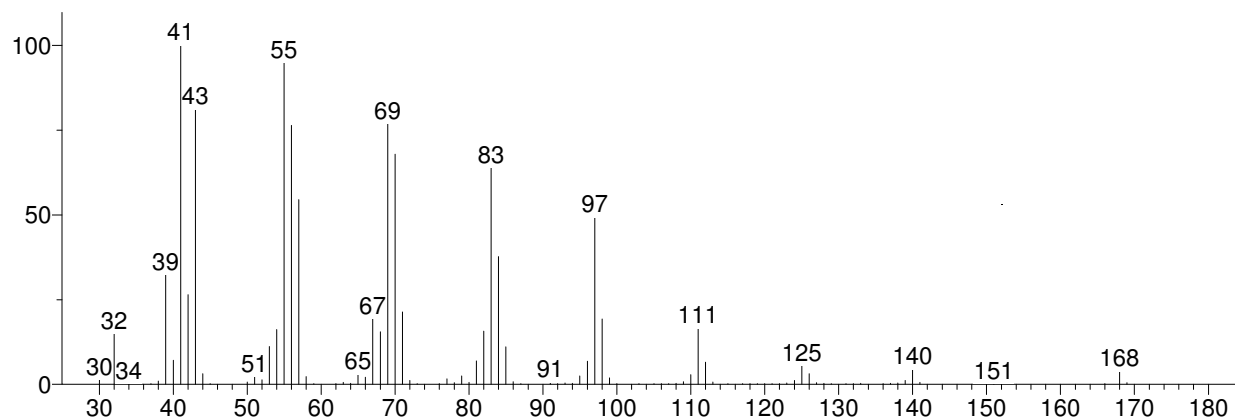


Hit 2 : 1,11-Dodecadiene
C₁₂H₂₂; MF: 881; RMF: 908; Prob 5.79%; CAS: 5876-87-9; Lib: mainlib; ID: 2567.

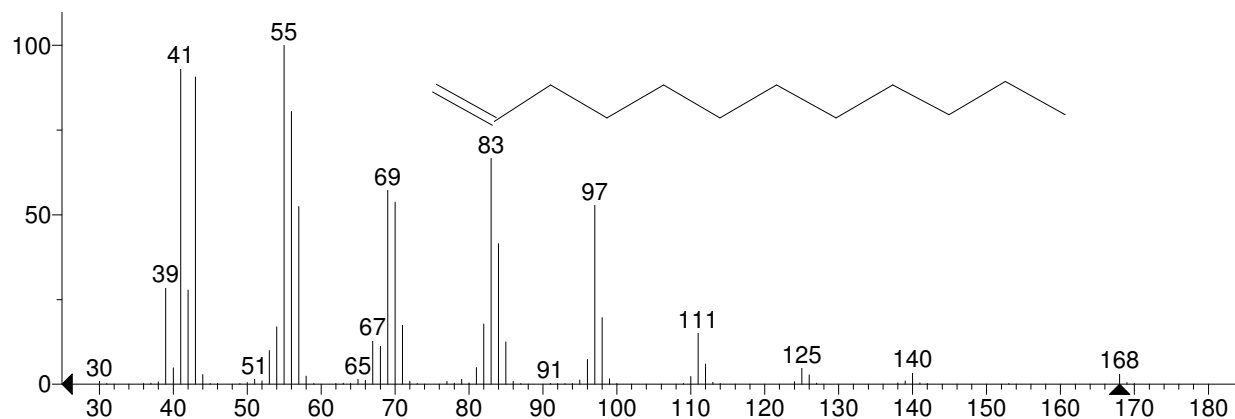


** Search Report Page 1 of 1 **

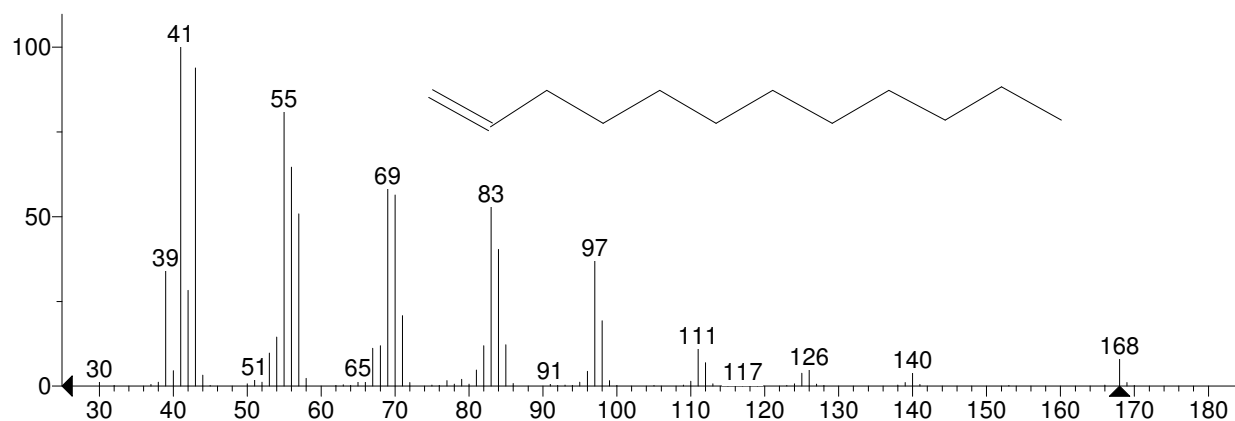
Unknown: Scan 310 (2.423 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -110



Hit 1 : 1-Dodecene
C₁₂H₂₄; MF: 942; RMF: 947; Prob 9.60%; CAS: 112-41-4; Lib: replib; ID: 4170.

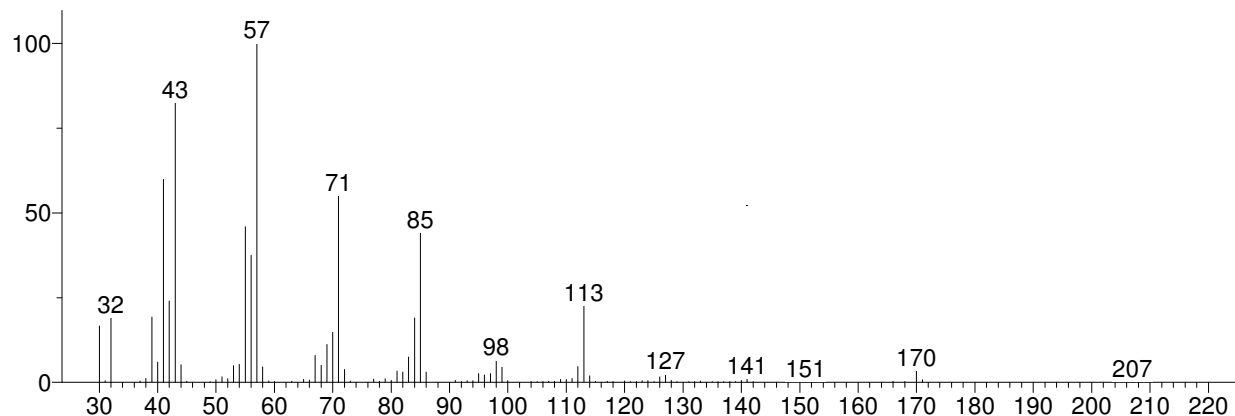


Hit 2 : 1-Dodecene
C₁₂H₂₄; MF: 927; RMF: 928; Prob 9.60%; CAS: 112-41-4; Lib: mainlib; ID: 2198.

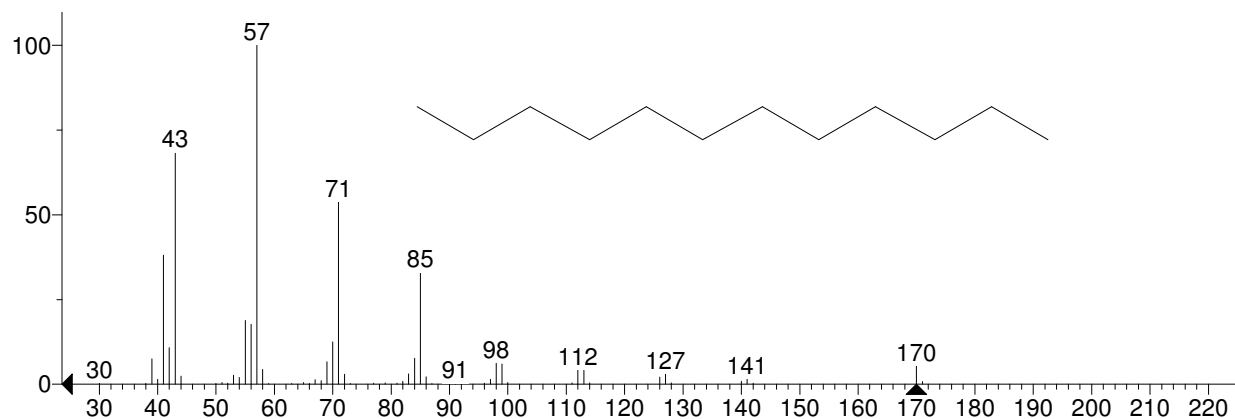


** Search Report Page 1 of 1 **

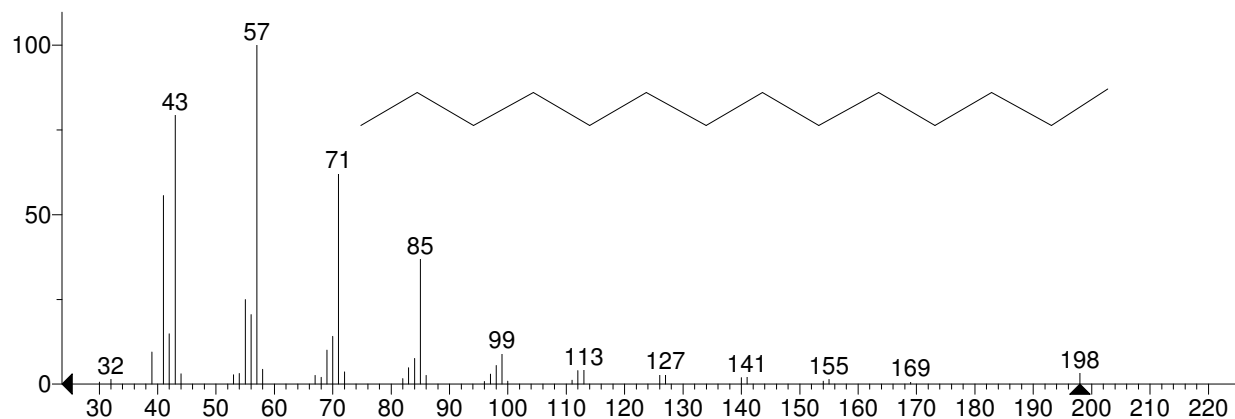
Unknown: Scan 318 (2.484 min): J6604_Jordi_Labs_Multi-Layer_Film_A_py2.D\data.ms
Compound in Library Factor = -454



Hit 1 : Dodecane
C₁₂H₂₆; MF: 843; RMF: 861; Prob 9.89%; CAS: 112-40-3; Lib: mainlib; ID: 21869.



Hit 2 : Tetradecane
C₁₄H₃₀; MF: 834; RMF: 871; Prob 7.18%; CAS: 629-59-4; Lib: replib; ID: 5511.

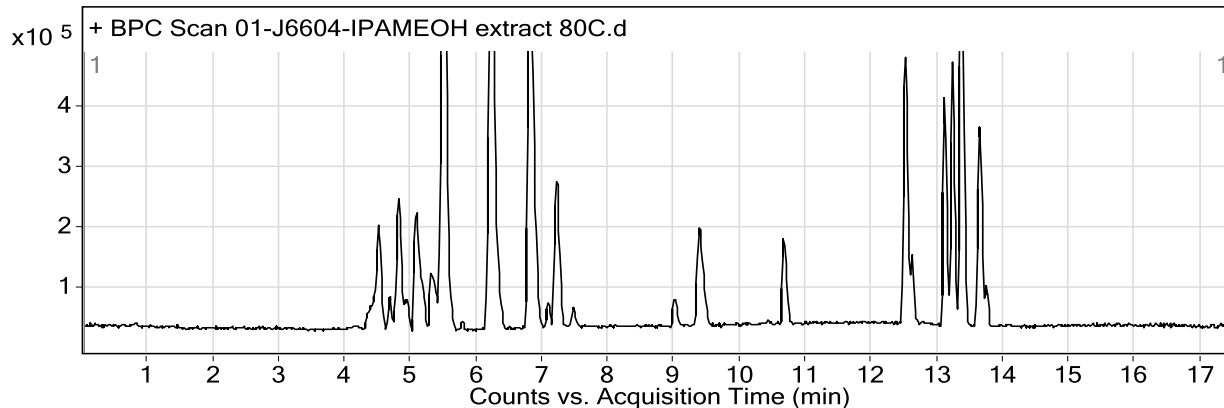


LCMS Data

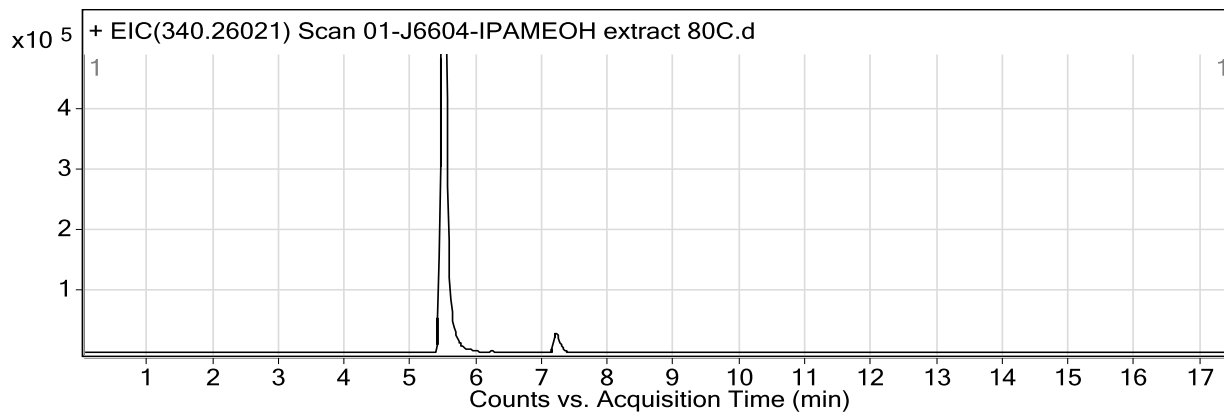
Qualitative Analysis Report

Data Filename	01-J6604-IPAMEOH extract 80C.d	Sample Name	Sample
Sample Type	Sample	Position	Vial 22
Instrument Name	Instrument 1	User Name	
Acq Method	J6604 Pos C8 MM.m	Acquired Time	4/5/2012 4:43:29 PM
IRM Calibration Status	Success	DA Method	proc-meth2.m
Comment			
User Chromatograms			

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Mixed

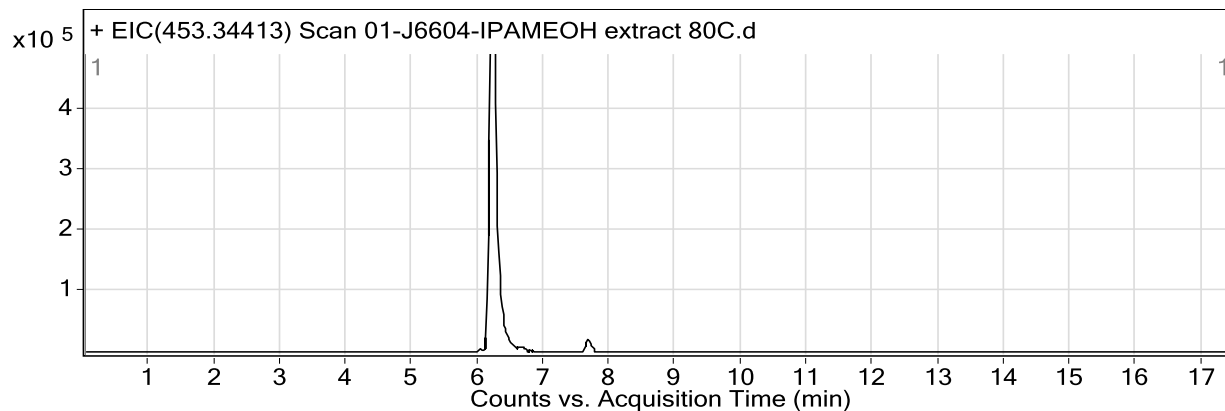


Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Mixed

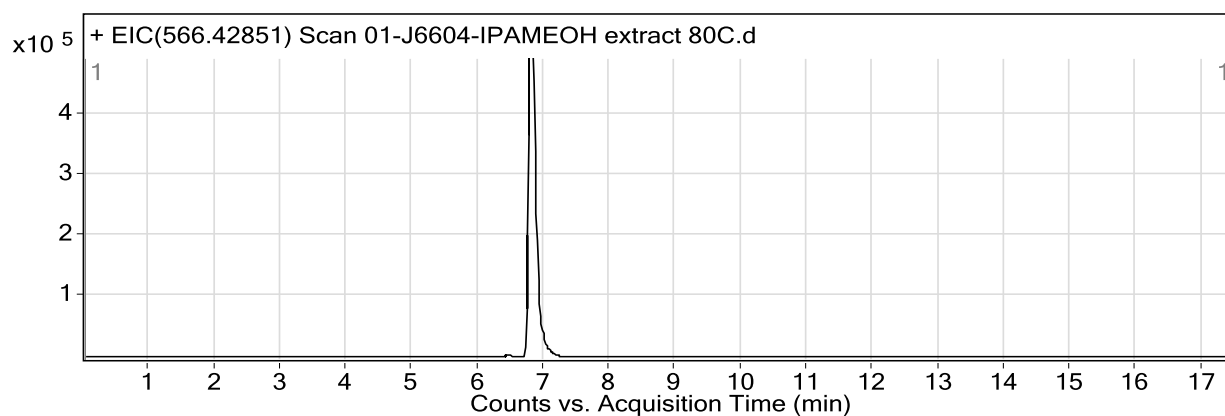


Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Mixed

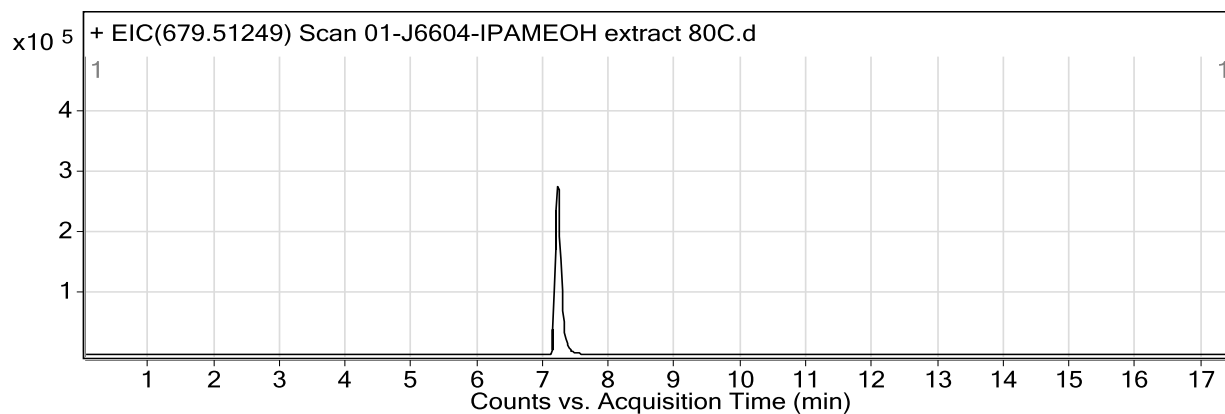
Qualitative Analysis Report



Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

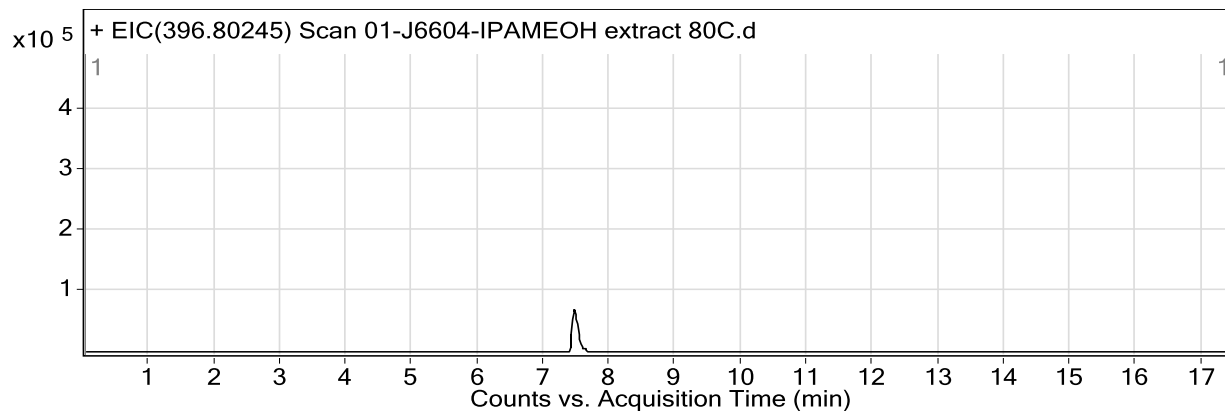


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

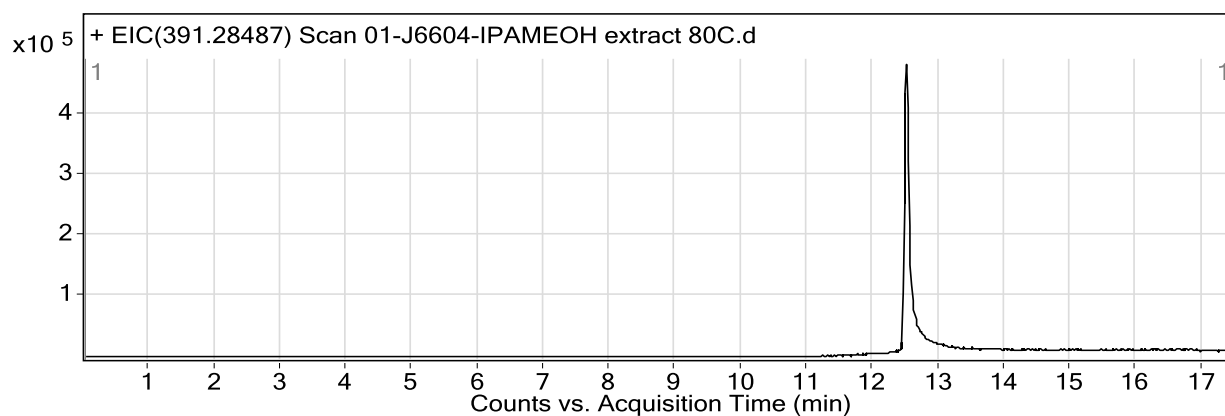


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

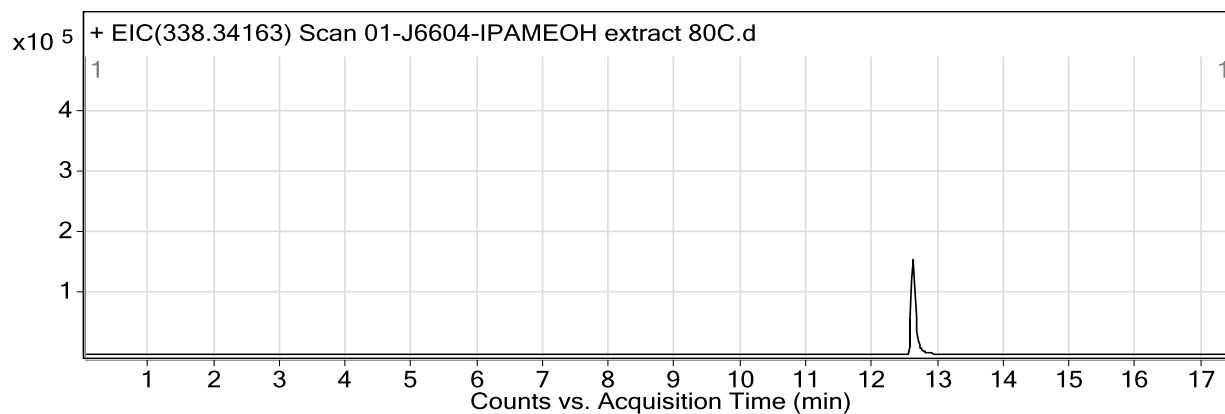
Qualitative Analysis Report



Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

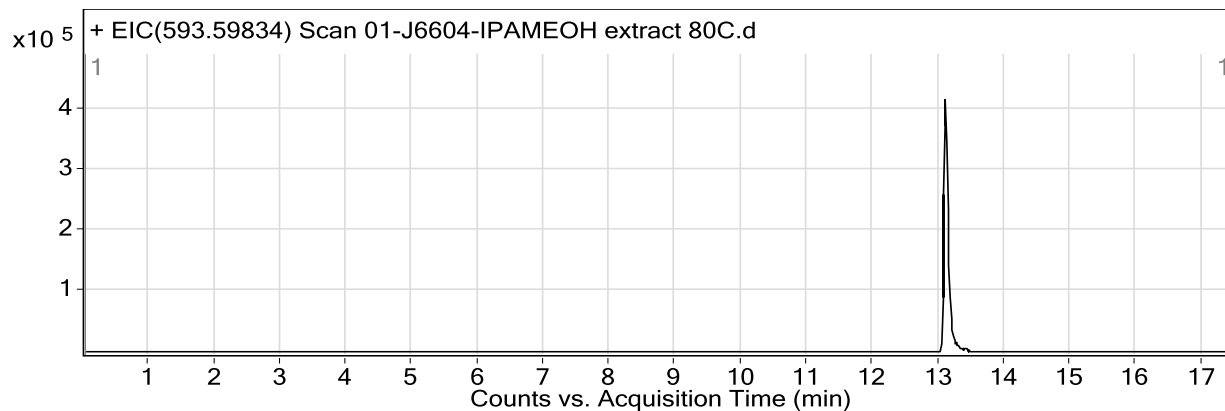


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

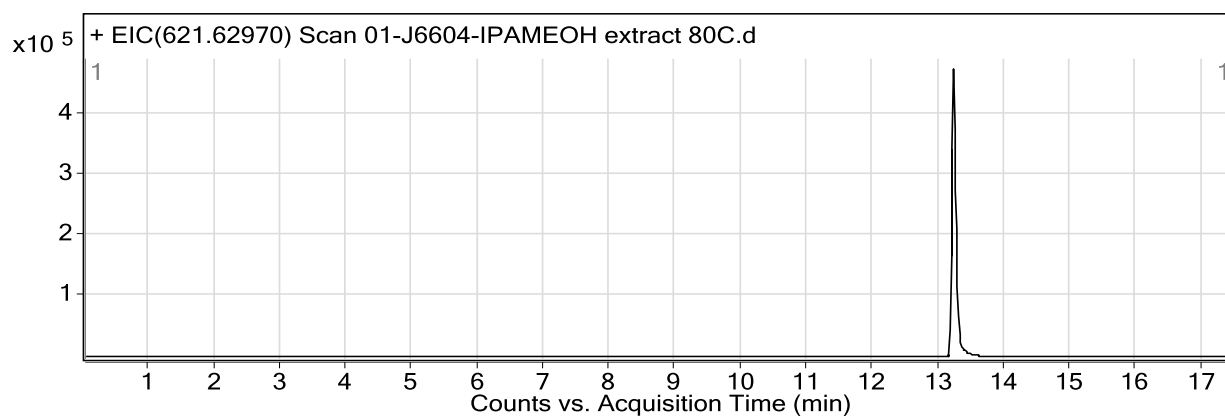


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

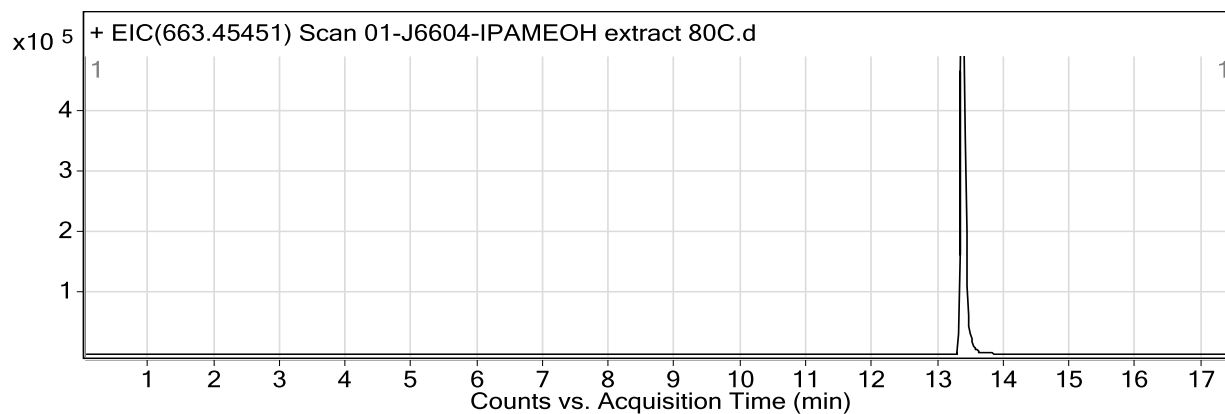
Qualitative Analysis Report



Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

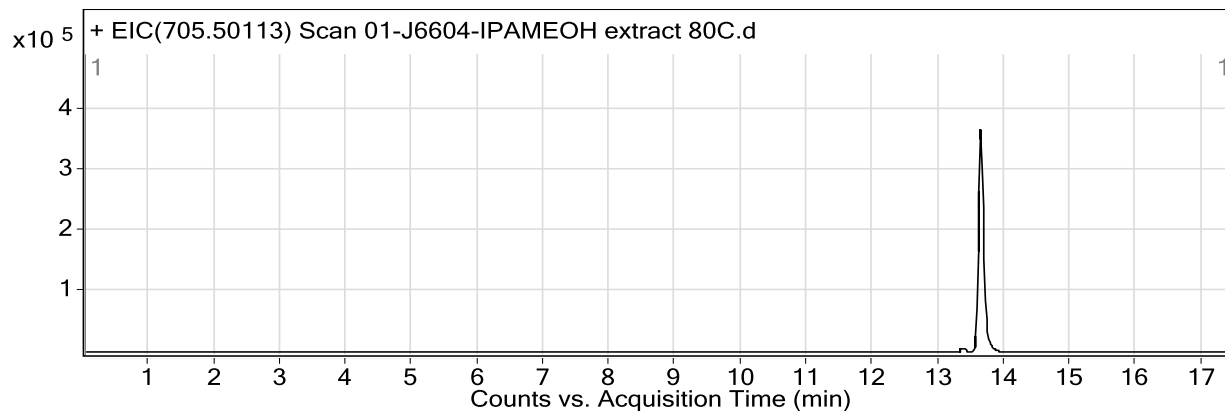


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

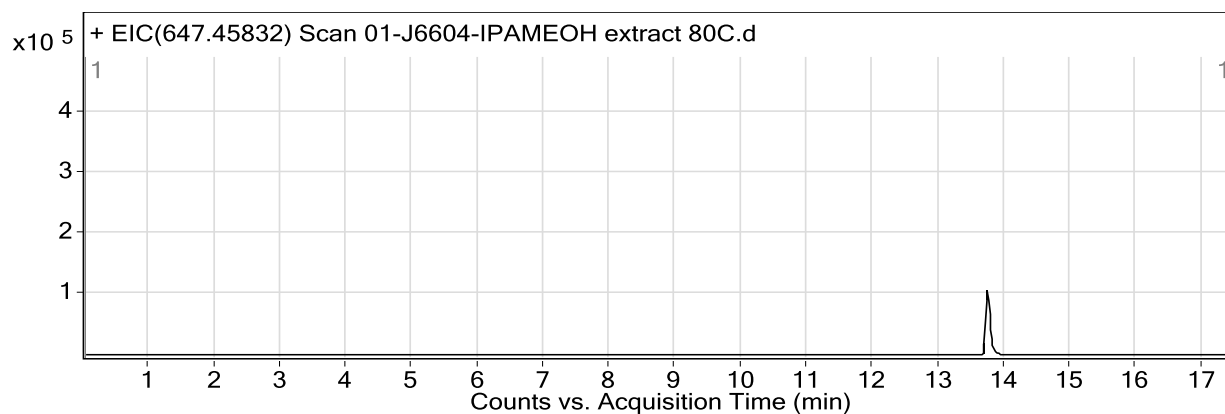


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

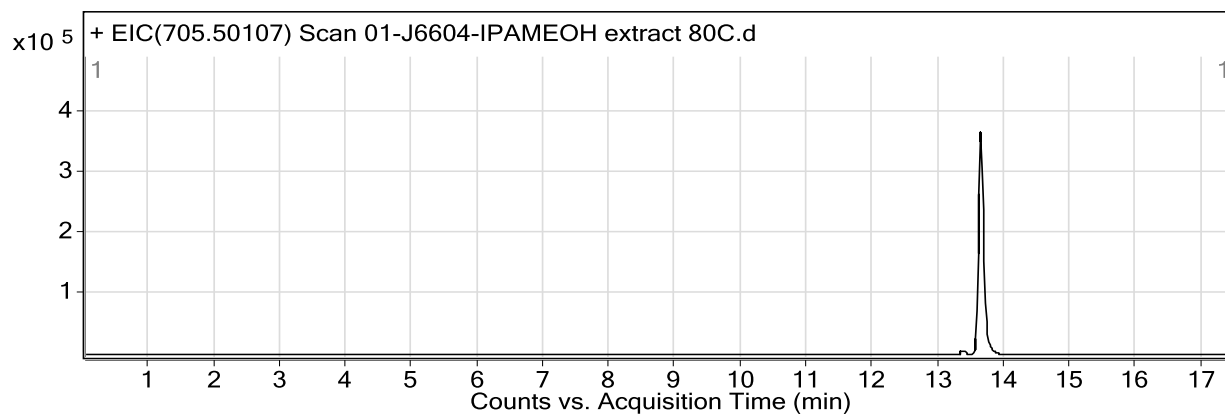
Qualitative Analysis Report



Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Mixed

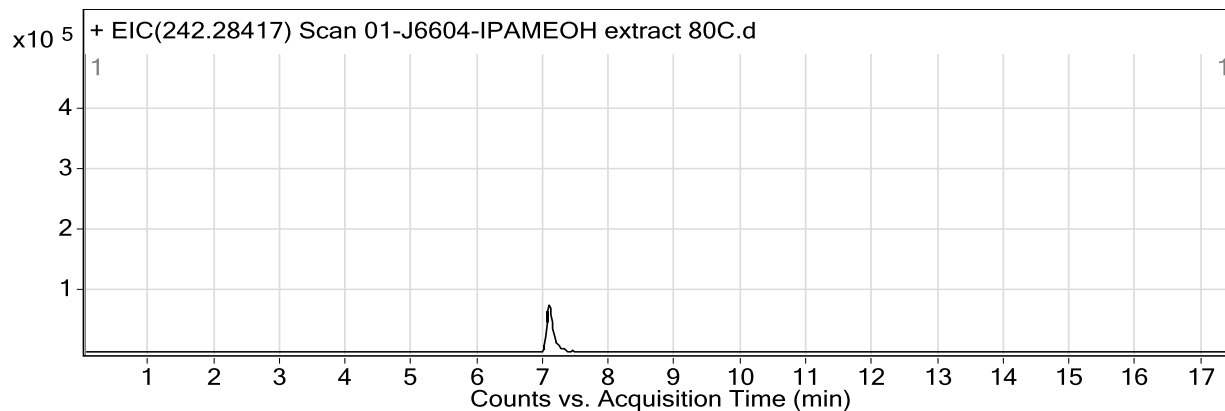


Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Mixed

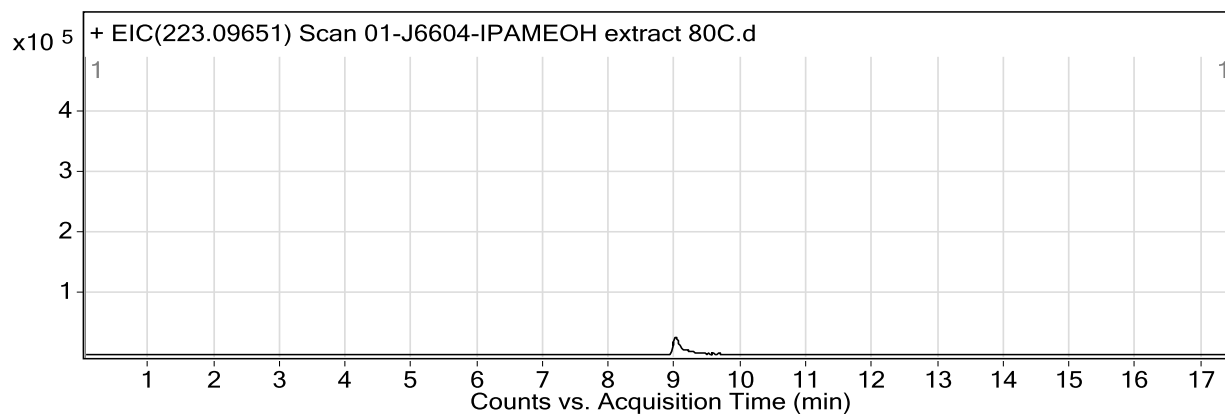


Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** Mixed

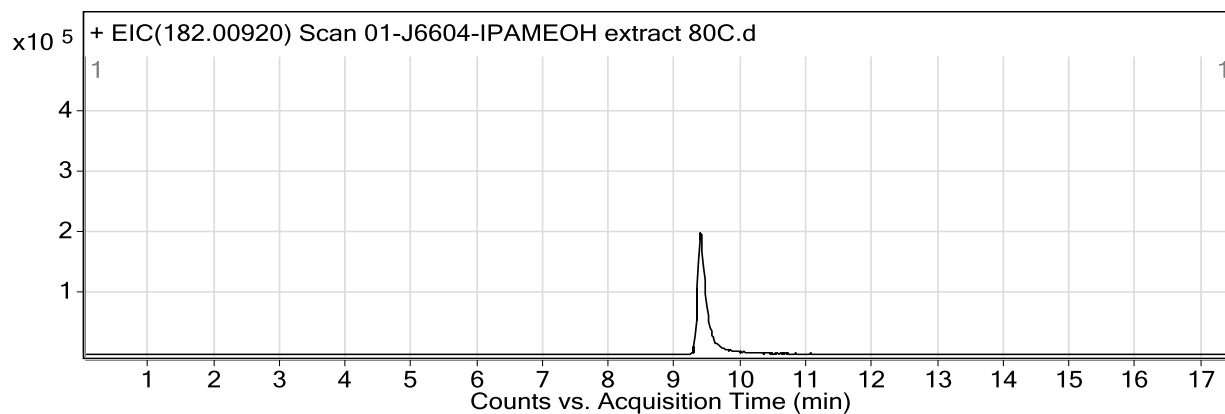
Qualitative Analysis Report



Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

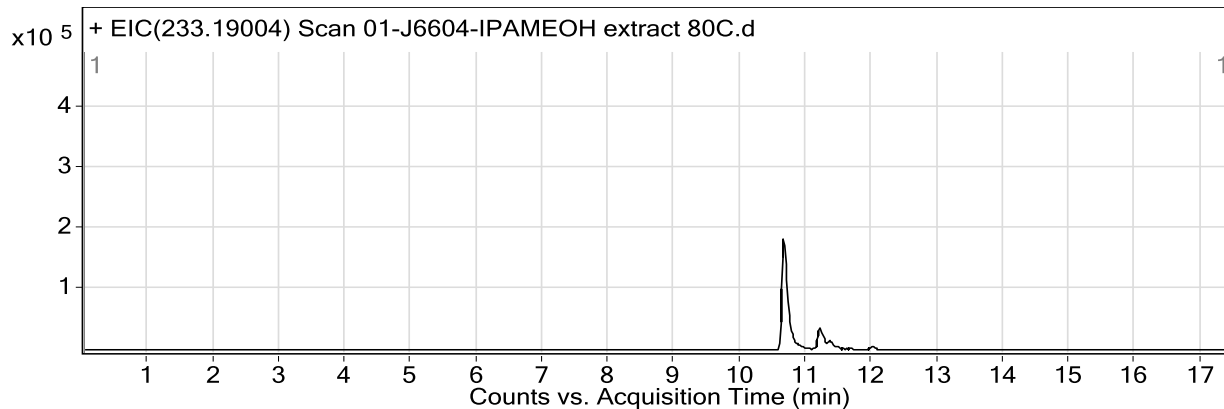


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

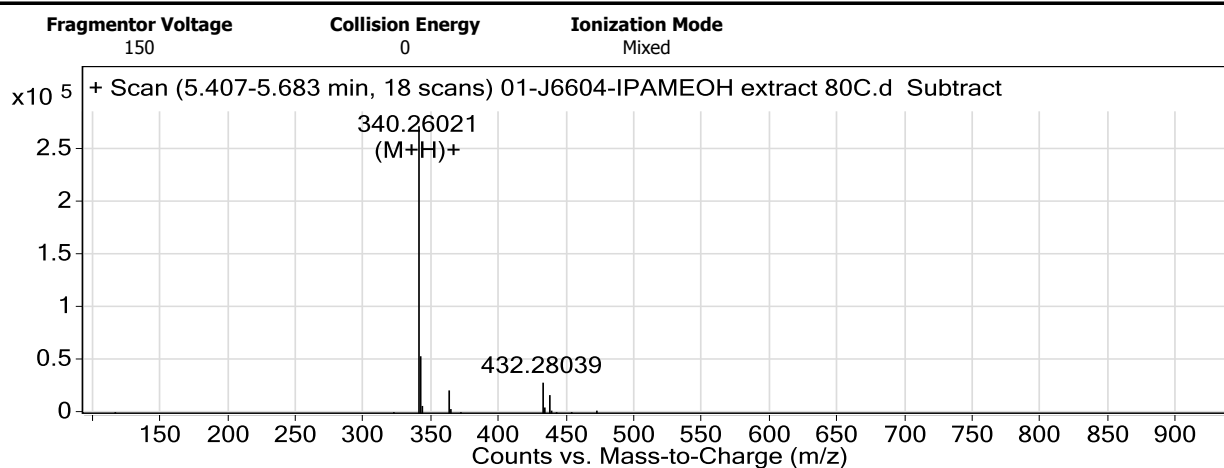


Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

Qualitative Analysis Report

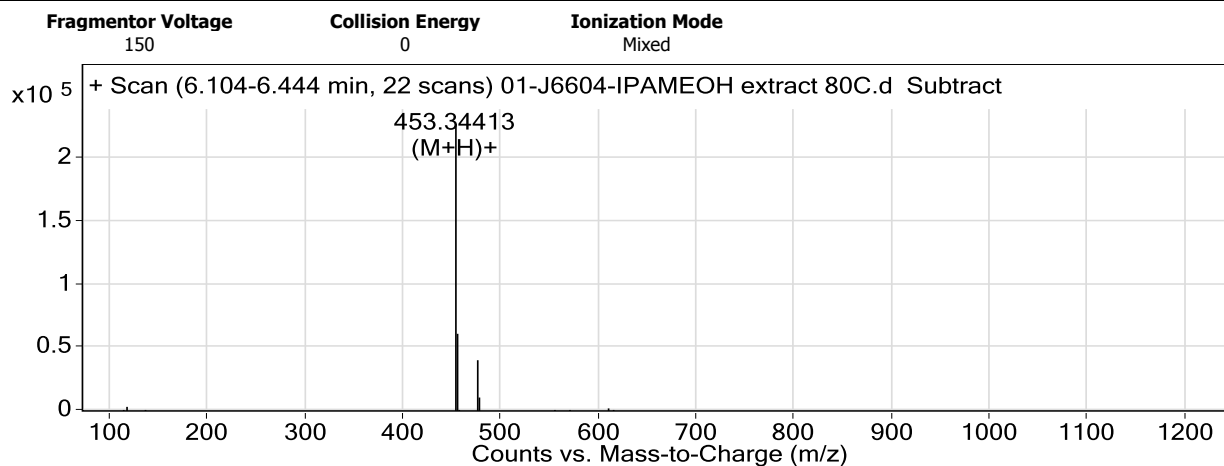


User Spectra



Peak List

m/z	z	Abund	Formula	Ion
340.26021	1	272232	C18 H34 N3 O3	(M+H)+
341.26291	1	54988	C18 H34 N3 O3	(M+H)+
362.24169		21515		
432.28039		29700		
437.23583		17546		



Qualitative Analysis Report

Peak List

<i>m/z</i>	<i>z</i>	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
453.34413	1	227204	Dow Ecosurf 2A1 Component C4-PPG5-PEG2-OH surfactant	C23 H49 O8	(M+H)+	91.17	1
454.34688	1	61497		C24 H45 N4 O4	(M+H)+		
475.32557		40953					

Fragmentor Voltage

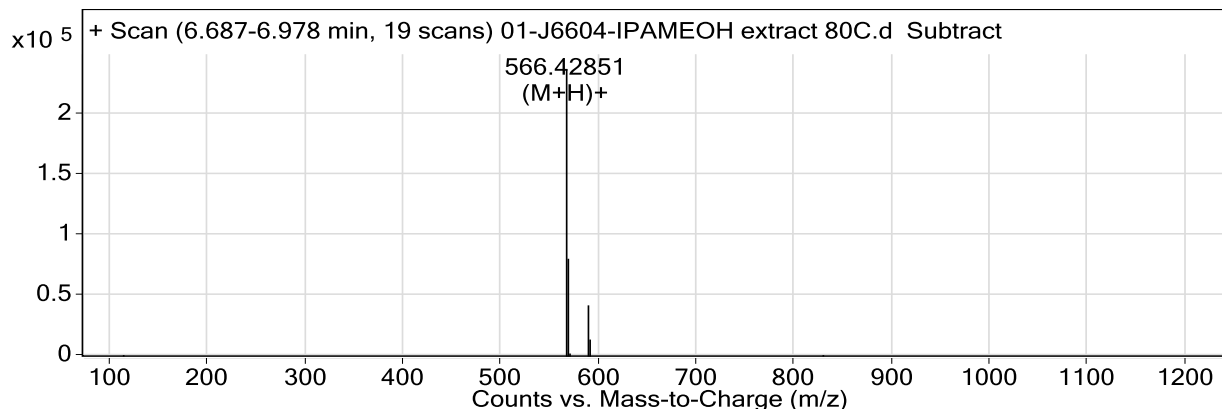
150

Collision Energy

0

Ionization Mode

Mixed



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
566.42851	1	236143	C30 H56 N5 O5	(M+H)+
567.43104	1	80408	C30 H56 N5 O5	(M+H)+
568.4336	1	15403	C30 H56 N5 O5	(M+H)+
588.40966	1	42356		
589.41267	1	14629		

Fragmentor Voltage

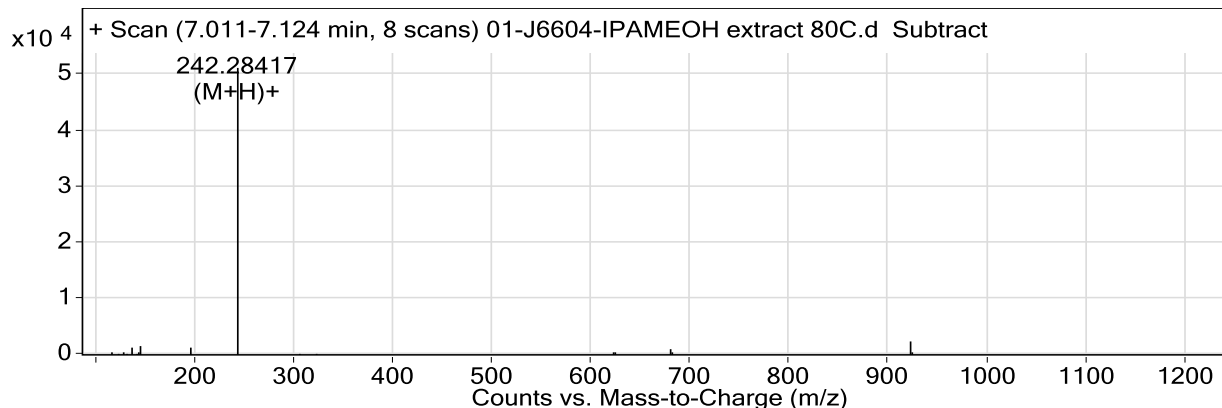
150

Collision Energy

0

Ionization Mode

Mixed



Peak List

<i>m/z</i>	<i>z</i>	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
242.28417	1	51166	Diocetylamine	C16 H36 N	(M+H)+	87.13	1
243.28732	1	9229		C16 H36 N	(M+H)+		

Fragmentor Voltage

150

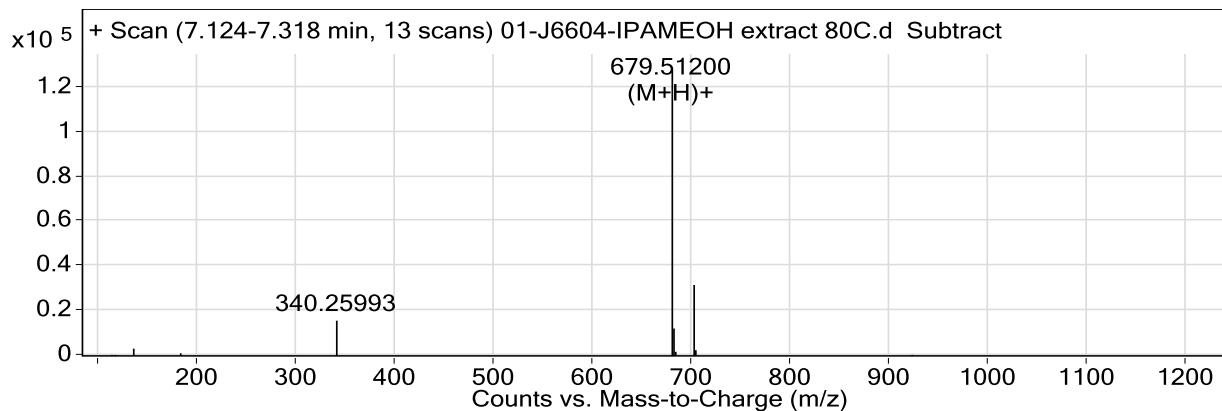
Collision Energy

0

Ionization Mode

Mixed

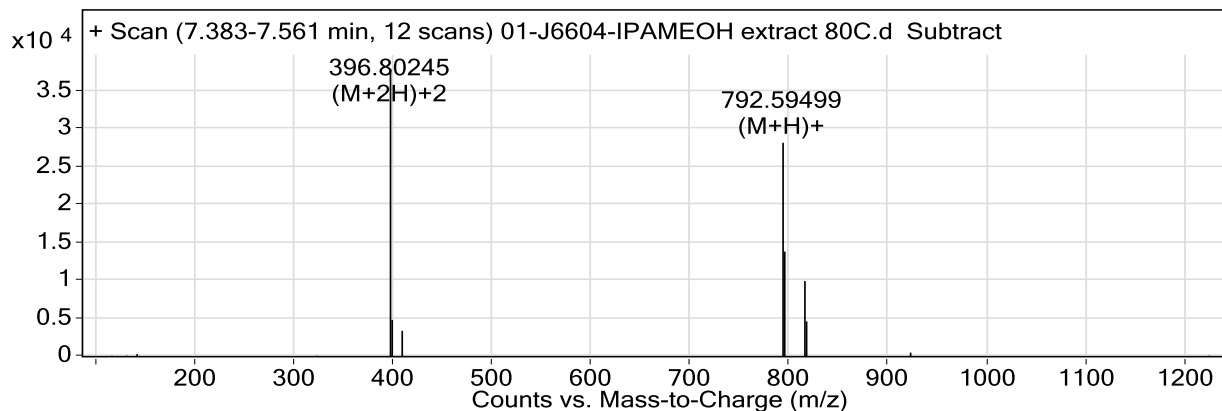
Qualitative Analysis Report



Peak List

m/z	z	Abund	Formula	Ion
340.25993	2	15901		
340.76173	2	6519		
679.512	1	128139	C ₃₆ H ₆₇ N ₆ O ₆	(M+H) ⁺
680.5146	1	52245	C ₃₆ H ₆₇ N ₆ O ₆	(M+H) ⁺
681.51686	1	12337	C ₃₆ H ₆₇ N ₆ O ₆	(M+H) ⁺
701.49345	1	31984		
702.49605	1	13285		

Fragmentor Voltage Collision Energy Ionization Mode
150 0 Mixed

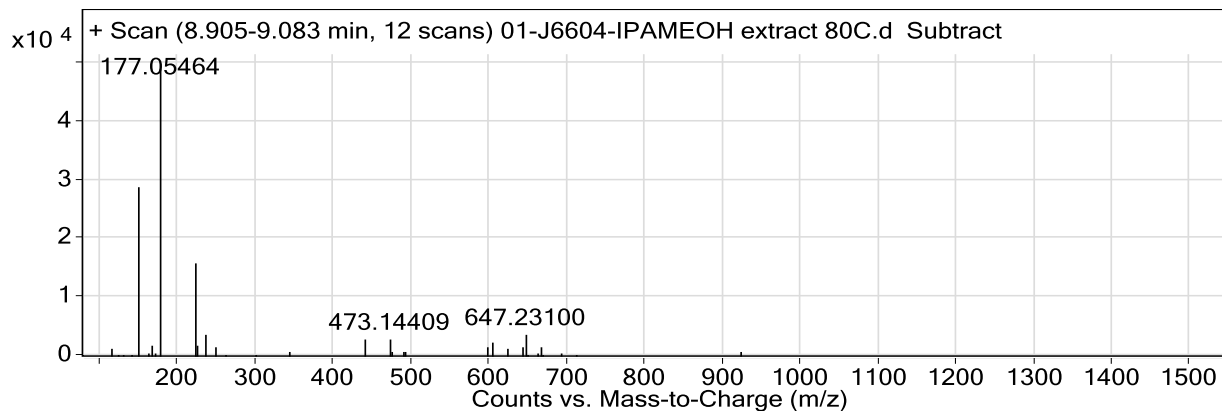


Peak List

m/z	z	Abund	Formula	Ion
396.80245	2	37707	C ₄₂ H ₇₉ N ₇ O ₇	(M+2H) ²⁺
397.30381	2	18155	C ₄₂ H ₇₉ N ₇ O ₇	(M+2H) ²⁺
397.8056	2	4991	C ₄₂ H ₇₉ N ₇ O ₇	(M+2H) ²⁺
407.79318		3538		
792.59499	1	28226	C ₄₂ H ₇₈ N ₇ O ₇	(M+H) ⁺
793.59823	1	13942	C ₄₂ H ₇₈ N ₇ O ₇	(M+H) ⁺
794.60087	1	3589	C ₄₂ H ₇₈ N ₇ O ₇	(M+H) ⁺
814.57722	1	9962		
815.5795	1	4769		

Fragmentor Voltage Collision Energy Ionization Mode
150 0 Mixed

Qualitative Analysis Report



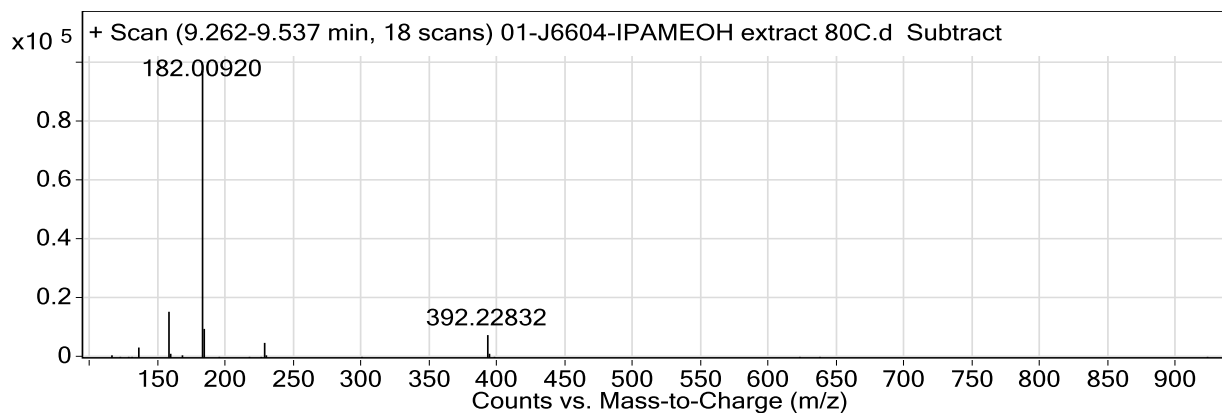
Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
149.02337		28820					
177.05464	1	48943					
178.05813	1	5151					
223.09651		15994	diethyl phthalate	C12 H15 O4	(M+H)+	86.21	1
235.13302		3710					
440.19149		2906					
473.14409		2930					
647.231		3608					

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
Mixed



Peak List

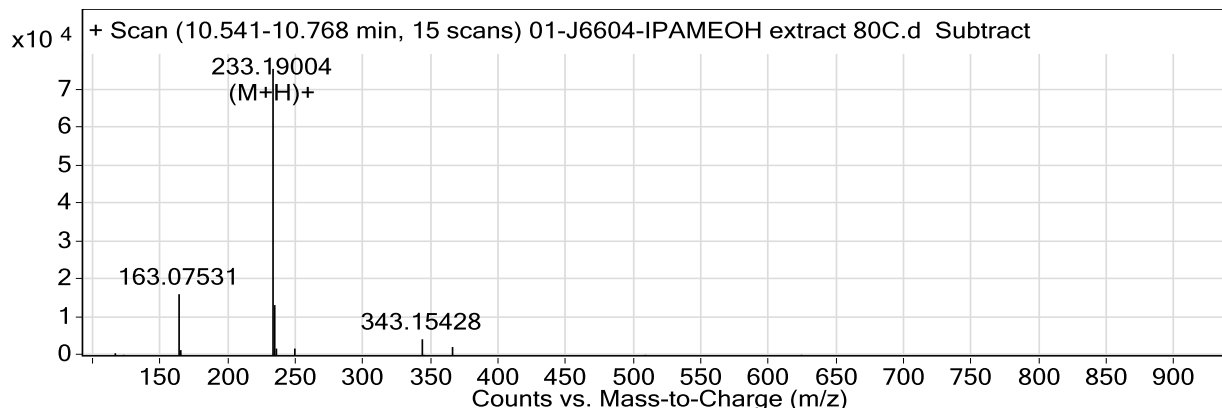
m/z	z	Abund
158.15375		15712
182.0092	1	97208
183.01182	1	10246
184.00519	1	8700
228.19573		5346
392.22832		7955

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
Mixed

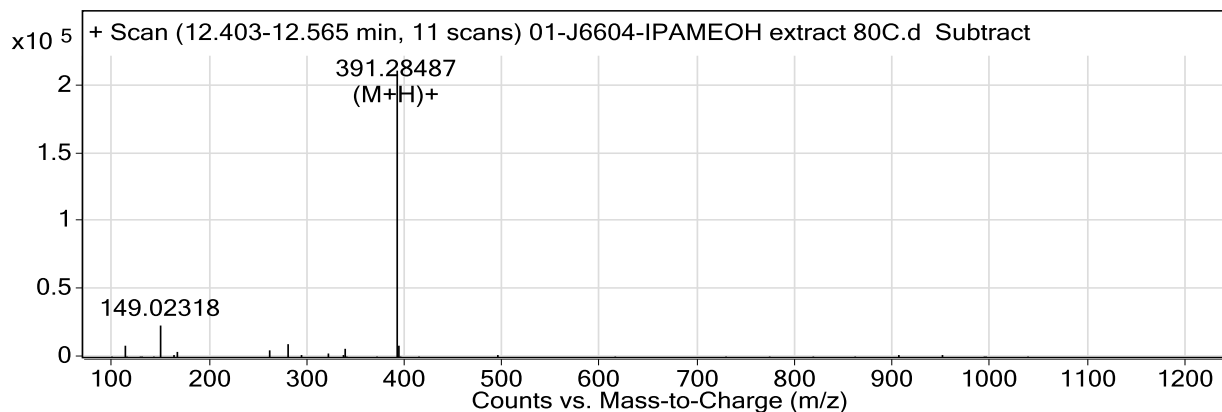
Qualitative Analysis Report



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
163.07531		16441					
233.19004	1	75547	Oxidized BHEB	C16 H25 O	(M+H)+	86.71	1
234.19315	1	13420		C16 H25 O	(M+H)+		
343.15428		4419					

Fragmentor Voltage Collision Energy Ionization Mode
150 0 Mixed

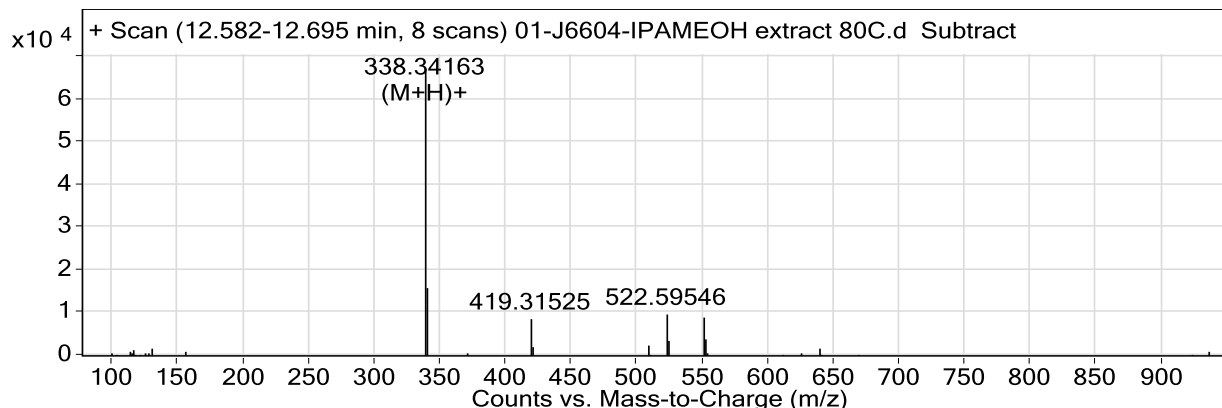


Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
149.02318		23482					
279.15901		10595					
391.28487	1	210855	heptyl nonyl phthalate	C24 H39 O4	(M+H)+	95.1	7
392.28696	1	52554		C24 H39 O4	(M+H)+		

Fragmentor Voltage Collision Energy Ionization Mode
150 0 Mixed

Qualitative Analysis Report



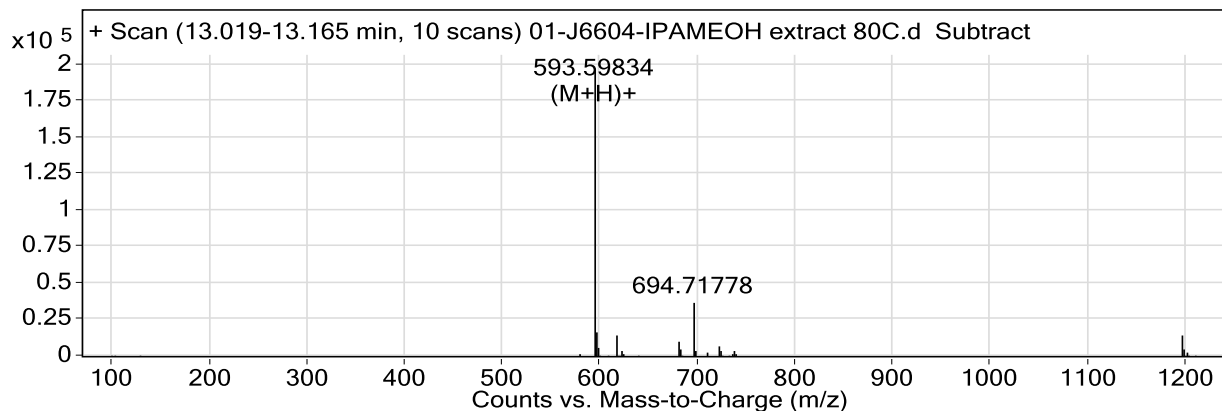
Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
338.34163	1	67003	Erucylamide	C22 H44 N O	(M+H)+	99.2	1
339.34455	1	16059		C22 H44 N O	(M+H)+		
419.31525		8689					
522.59546	1	9967					
523.59827	1	3654					
550.62783	1	9173					
551.63055	1	3817					

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
Mixed



Peak List

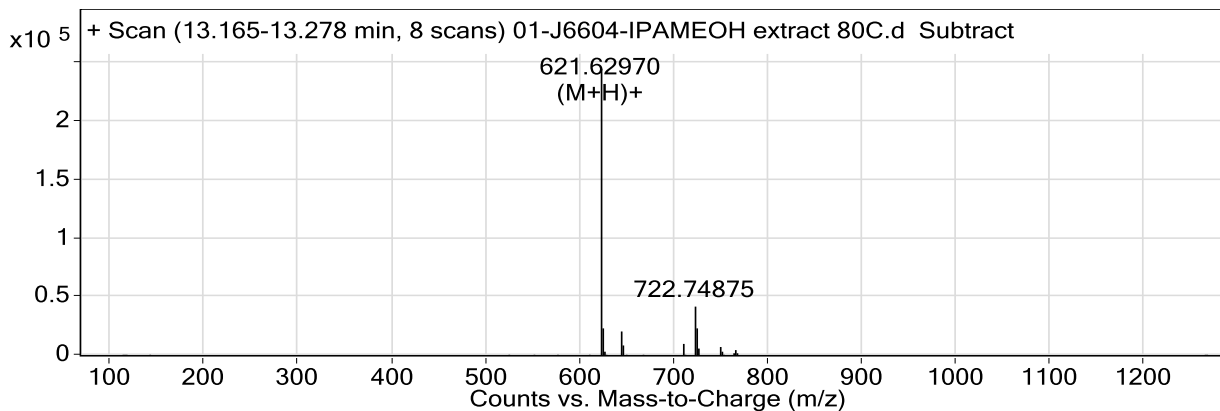
m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
593.59834	1	196313	Ethylendistearamide	C38 H77 N2 O2	(M+H)+	98.5	1
594.60119	1	81762		C38 H77 N2 O2	(M+H)+		
595.60373	1	17062		C38 H77 N2 O2	(M+H)+		
596.59839		17331					
615.57898		14834					
680.70137		10095					
694.71778	1	36756					
695.72073	1	18003					
1194.81762	1	14461					
1195.82096	1	12091					

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
Mixed

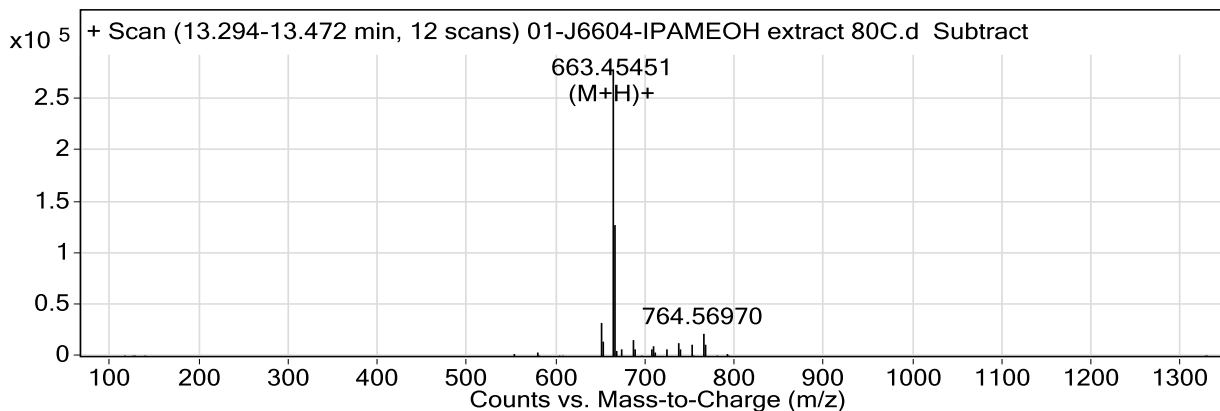
Qualitative Analysis Report



Peak List

m/z	z	Abund	Formula	Ion
621.6297	1	244992	C40 H81 N2 O2	(M+H)+
622.63252	1	106869	C40 H81 N2 O2	(M+H)+
623.63486	1	24201	C40 H81 N2 O2	(M+H)+
624.6311		12797		
643.61023		20924		
722.74875	1	42558		
723.75216	1	23535		

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

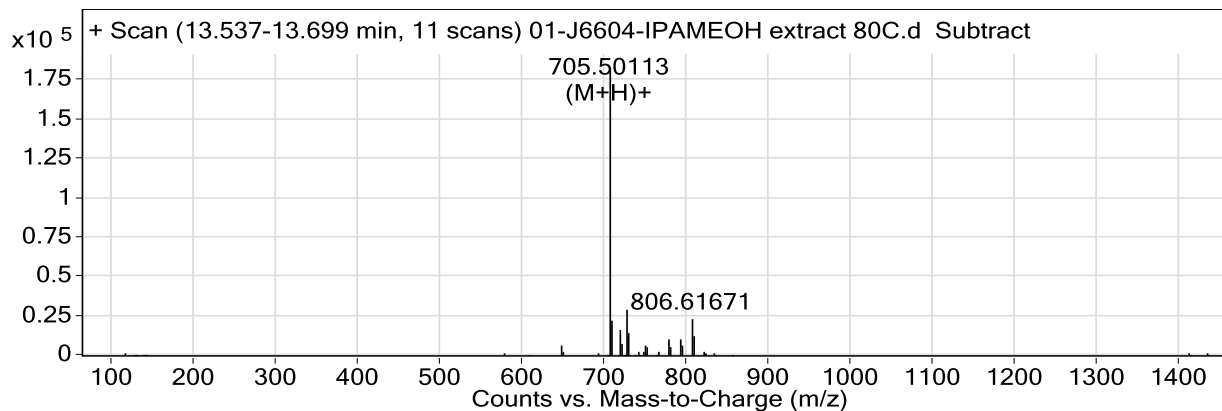


Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
649.6599	1	33306					
650.66318	1	15256					
663.45451	1	278652	Oxidized Irgafos 168	C42 H64 O4 P	(M+H)+	98.17	1
664.4574	1	128446		C33 H59 N8 O6	(M+H)+		
665.46026	1	30685		C33 H59 N8 O6	(M+H)+		
685.4349		16347					
736.51203		14109					
764.5697		23160					

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode Mixed

Qualitative Analysis Report



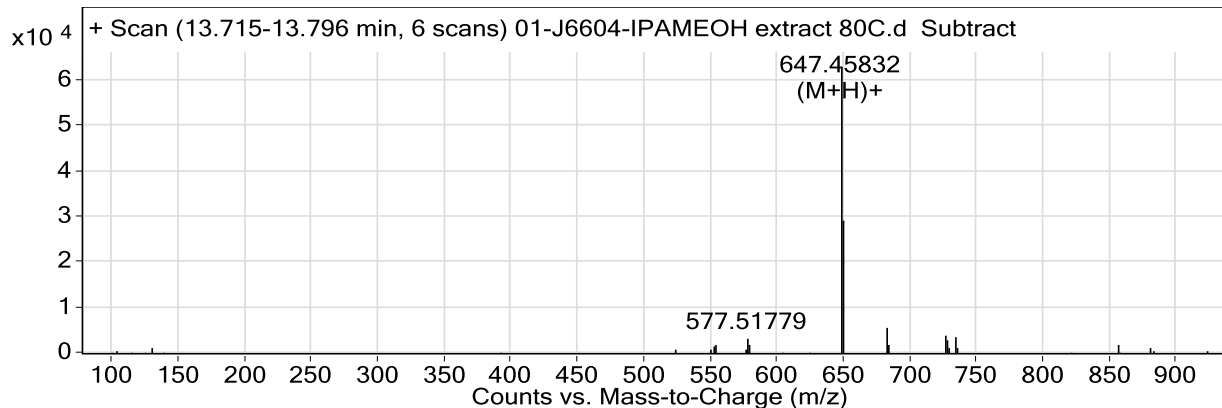
Peak List

m/z	z	Abund	Formula	Ion
705.50113	1	182089	C ₃₆ H ₆₅ N ₈ O ₆	(M+H) ⁺
706.50401	1	88742	C ₃₆ H ₆₅ N ₈ O ₆	(M+H) ⁺
707.50664	1	22685	C ₃₆ H ₆₅ N ₈ O ₆	(M+H) ⁺
719.51583		16948		
727.48163	1	29547		
728.48481	1	14482		
778.56013		11327		
792.60051		11328		
806.61671	1	23383		
807.61971	1	13104		

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
Mixed



Peak List

m/z	z	Abund	Name	Formula	Ion	Score (DB)	Hits (DB)
577.51779		3416					
647.45832	1	62970	Irgafos 168	C ₄₂ H ₆₄ O ₃ P	(M+H) ⁺	98.78	1
648.46155	1	29164		C ₄₄ H ₅₉ N ₂ O ₂	(M+H) ⁺		
649.46455	1	6960		C ₄₄ H ₅₉ N ₂ O ₂	(M+H) ⁺		
681.42007		5668					
725.36891		3970					
733.53152		3646					

--- End Of Report ---