

Client Name  
Contact Name

Released by:

Mark Jordi, Ph.D.  
President

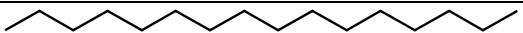
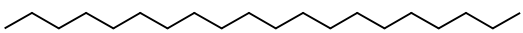

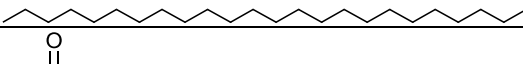
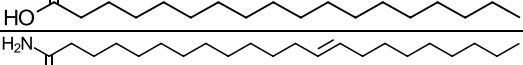
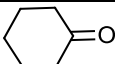
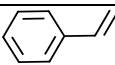
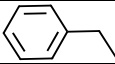
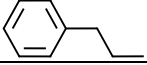
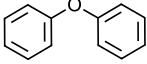
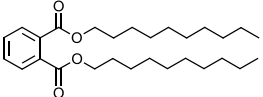
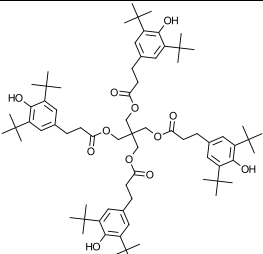
Job Number: J8674\_Phase 1

**CONFIDENTIAL**

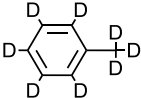
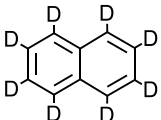
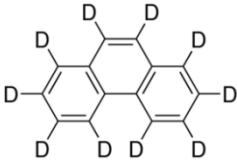
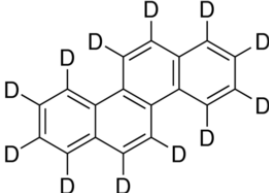
August 21, 2015

Dear Valued Customer,

A study was conducted utilizing the following standards to assess the accuracy of relative and formal quantitation methods:

1. Hexadecane	
2. Eicosane	
3. Tetracosane	
4. Stearic acid	
5. Erucamide	
6. Cyclohexanone	
7. Styrene	
8. Ethylbenzene	
9. Propylbenzene	
10. Diphenyl ether	
11. Didecylphthalate	
12. Irganox 1010	

The following deuterated compounds were utilized as internal standards.

1. Toluene-d8	
2. Naphthalene-d8	
3. Phenanthrene-d10	
4. Chrysene-d12	

The following test was performed:

1. Quadrupole Time-of-Flight Gas Chromatography Mass Spectrometry (QTOF-GCMS)

## Objective

The goal of this analysis was to demonstrate the accuracy of both relative and formal quantitation methods for various compounds by QTOF-GCMS, and to show the importance of proper method selection when performing quantitation.

For the purpose of this study, twelve compounds with different volatility were selected as target analytes and four deuterated compounds (toluene-d8, naphthalene-d8, phenanthrene-d10 and chrysene-d12) were selected as internal standards. Solutions of the twelve compounds with known concentrations were directly analyzed by QTOF-GCMS, in order to compare the accuracy of quantitative values obtained using formal quantitation as compared to relative quantitation. Formal quantitation involves comparing the observed signal for each compound against a calibration curve made using the same compound. Relative quantitation utilizes internal standards of different chemistry from the target analyte to estimate the concentration of the target molecule. This approach is often used when no standard is available for a compound, when there are a large number of target compounds, or when formal quantitation is not practical.

In this report relative quantitation was performed for the twelve compounds against the four deuterated internal standards. The formal quantitation method was performed using a calibration curve of the target compound of interest analyzed at five different concentrations (ranging from 1

ppm to 25 ppm), and using this to directly relate the peak areas from the target compound present in the solution to the concentration of the target compound present.

## **Summary of Results**

Twelve compounds of varying volatility and polarity have been quantitated by GCMS using both relative and formal quantitation techniques. As the concentration of these twelve compounds were known (8 ppm), it is possible to deduce the effectiveness of both methods. Formal quantitation was found to produce a high level of accuracy (7-9 ppm) and recovery values ranging from 88-111%.

In contrast, relative quantitation values varied strongly with the nature of the analyte and the standard used for quantitation. When toluene-d<sub>8</sub> was utilized as the internal standard quantitative values ranged from .5-19 ppm (actual value was 8 ppm, recovery values of 6-238%). Naphthalene-d<sub>8</sub> produced values ranging from .2-7 ppm (recovery values of 2-79%). Phenanthrene-d<sub>10</sub> resulted in values from .1-5 ppm (recovery values of 2-72%) and Chrysene-d<sub>12</sub> resulted in values from .05-2 ppm (recovery values of .6-24%). Lastly, if a structural homolog was used as the standard (linear alkane standard for a linear alkane target) accuracy improved to 7-10 ppm (recovery values of 86-121%). Similarly when a series of alkyl benzenes were quantitated against ethylbenzene accuracy was acceptable at 5-9 ppm (recovery values of 69-105%).

## **Discussion of Results**

The results of this study indicate that the quantitative values obtained by relative quantitation with GCMS are very dependent upon the nature of the standard utilized. In some instances compounds which have generally similar chemical structures show large errors in the calculated values (e.g. erucamide and steric acid as compared to linear alkanes). Only standards which were homologous with the target compound were found to produce acceptable accuracy levels. In contrast formal quantitation consistently produces accurate quantitative values. This study strongly demonstrates the advantage of using formal quantitation to obtain accurate and reliable quantitative values.

## **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.

## **Sample Preparation**

### ***Relative Quantitation***

If the compound under investigation is an unknown species, or if the compound is unavailable commercially, it is common for a relative quantitation to be performed. This involves attempting to quantitate the compound of interest relative to different compound. It is generally preferred that the compound utilized as the standard be as close in chemistry to that of the unknown as possible. For GCMS analysis, the reference standard can be an external standard that is analyzed in the same analytical sequence as the sample. It can also be an internal standard that is added to the sample matrix prior to analysis. Both approaches assume similar ionization efficiency (detector response) between the analyte and the corresponding standard. In some instances, more than a single standard is used to adjust for differences in sample volatility.

For this study, the internal standards were prepared at concentration of 5 ppm ( $5\ \mu\text{g mL}^{-1}$ ) in DCM. The compounds to be analyzed were prepared at a concentration of 8 ppm ( $8\ \mu\text{g mL}^{-1}$ ) in DCM. The solution was analyzed in triplicate by QTOF-GCMS.

### ***Formal Quantitation***

When the identity of the analytes/compound of interest is known and a standard is available, a formal quantitation can be performed. This entails preparing known concentration of the compounds of interest at several concentration levels. These are then analyzed to calibrate the GCMS (based on peak area).

For this study, standards were prepared containing the twelve compounds at five different concentration levels (1, 5, 10, 15 and 25 ppm), with each level also containing the four deuterated internal standards at known concentrations (5 ppm, as in the relative quantitation method). The sample solution from the relative quantitation was also used for the formal quantitation as the two methods of quantitation are to be compared. As in the relative quantitation, samples have been injected in triplicate, while the standards were injected in duplicate.

## **QTOF-GCMS Analysis**

QTOF-GCMS analysis was performed in electron impact mode. The spectra collected using electron impact (EI) ionization can be compared to the NIST mass spectral database for identification. In addition, fragments can be identified using the accurate mass data collected. This ionization mode is high energy and generally causes analyte fragmentation which aids in identification. Compounds were considered detectable provided a signal to noise ratio of at least 3:1 was observed.

### ***Relative Quantitation***

A relative quantitation of twelve compounds was performed using a selection of internal standards of varying boiling points (toluene-d<sub>8</sub>, naphthalene-d<sub>8</sub>, phenanthrene-d<sub>10</sub> and chrysene-d<sub>12</sub>). For relative quantitation using QTOF-GCMS it is common to select an internal

standard of a similar boiling point to the compound(s) of interest; for the purpose of this study, each target compound has been quantitated against each deuterated internal standard to highlight how the calculated concentration can vary depending upon the relative standard selected.

The equations used to calculate the relative concentration of each target compound (**Equation 1**) and the recovery calculation (**Equation 2**) are presented below.

**Equation 1: Calculation of target compound concentration from GCMS data**

Target Compound Concentration( $\mu\text{g/mL}$ ) =

$$\frac{\text{Target Compound Response}}{\text{Internal Standard Response}} \times \text{Internal Standard Concentration } (\mu\text{g/mL})$$

where

Internal Standard Concentration = 5  $\mu\text{g/mL}$

**Equation 2: Calculation of percent recovery from QTOF-GCMS data**

$$\text{Recovery } (\%) = \frac{\text{Calculated Concentration } (\mu\text{g/mL})}{\text{Actual Concentration } (\mu\text{g/mL})} \times 100$$

where

Actual concentration = 8  $\mu\text{g/mL}$

In order to determine the accuracy of this method, a solution of the twelve compounds with known concentration (8 ppm) was analyzed by QTOF-GCMS. The peak areas of the twelve compounds were quantitated using all four of the deuterated internal standards; the results (average of triplicate injections) are presented in **Table 1**.

**Table 1: Relative Quantitation using 4 Internal Standards (I.S.)**

Target Compound	RT (min)	Concentration Calculated Relative to Deuterated I.S.							
		Toluene-d <sub>8</sub> (RT 5.05)		Naphthalene-d <sub>8</sub> (RT 13.93)		Phenanthrene-d <sub>10</sub> (RT 19.84)		Chrysene-d <sub>12</sub> (RT 24.19)	
		Calculated Conc (ppm)	% Recovery	Calculated Conc (ppm)	% Recovery	Calculated Conc (ppm)	% Recovery	Calculated Conc (ppm)	% Recovery
Ethylbenzene	7.54	16.36	204.51*	5.98	74.69	4.96	61.99	1.72	21.53*
Styrene	8.26	11.32	141.50*	4.13	51.68*	3.43	42.89*	1.19	14.89*
Cyclohexanone	8.36	6.79	84.82	2.48	30.98*	2.06	25.71*	0.71	8.93*
Propylbenzene	9.72	17.27	215.90*	6.31	78.85	5.24	65.45	1.82	22.72*
Diphenyl ether	16.54	16.67	208.40*	6.09	76.11	5.05	63.16	1.75	21.93*
Hexadecane	18.18	9.58	119.73	3.50	43.72*	2.90	36.28*	1.01	12.60*
Eicosane	21.07	11.13	139.09*	4.06	50.78*	3.37	42.15*	1.17	14.63*
Steric acid	22.08	0.46	5.81*	0.17	2.12*	0.14	1.76*	0.05	0.61*
Tetracosane	23.46	13.41	167.62*	4.90	61.20	4.06	50.79*	1.41	17.64*
Erucamide	25.47	4.07	50.92*	1.49	18.58*	1.23	15.42*	0.43	5.35*
Didecylphthalate	25.47	18.98	237.22*	6.93	86.59	5.75	71.87	2.00	24.95*
Irganox 1010	ND	--	--	--	--	--	--	--	--

ND – Not Detected

\* Out of the acceptable range for %recovery (60-120%)

The quantitation of the target compounds using any of the four internal standards yielded poor results. This is due to differences in ionization efficiency, adsorption and volatility of the target compounds compared to the deuterated internal standards. The choice of internal standard significantly affected the recovery values. For example, the concentration value for propylbenzene varies between 1.82 and 17.27 ppm (recovery values of 22.7% and 215.9% respectively) depending upon which internal standard is used to perform the relative quantitation. In general the results for Naphthalene-d<sub>8</sub> showed the highest accuracy for the largest number of compounds (6 of 12 compounds did not meet the acceptance criteria). Chrysene-d<sub>12</sub> produced the poorest recovery values (all 12 compounds did not meet the acceptance criteria) and significantly underestimates the amount of the target compounds in the solution.

A homologous series of linear alkanes and a family of related alkyl benzenes were examined to further test the accuracy of relative quantitation when standards of very similar chemistry are used. The linear alkanes hexadecane and tetracosane were quantitated against eicosane. Styrene and propylbenzene were quantitated against ethylbenzene. Results for the two series are shown in **Table 2**. The values obtained were generally improved as compared to those for the deuterated standard but still showed significantly worse recovery values as compared to formal quantitation.

Table 2: Relative Quantitation Results					
Target Compound	RT (min)	Concentration Calculated			
		Eicosane (RT 21.07)		Ethylbenzene (RT 7.54)	
		Calculated Conc (ppm)	% Recovery	Calculated Conc (ppm)	% Recovery
Hexadecane	18.18	6.89	86.10	--	--
Tetracosane	23.46	9.64	120.52*	--	--
Styrene	8.26	--	--	5.54	69.19
Propylbenzene	9.72	--	--	8.45	105.57

\* Out of the acceptable range for %recovery (60-120%)

### Formal Quantitation

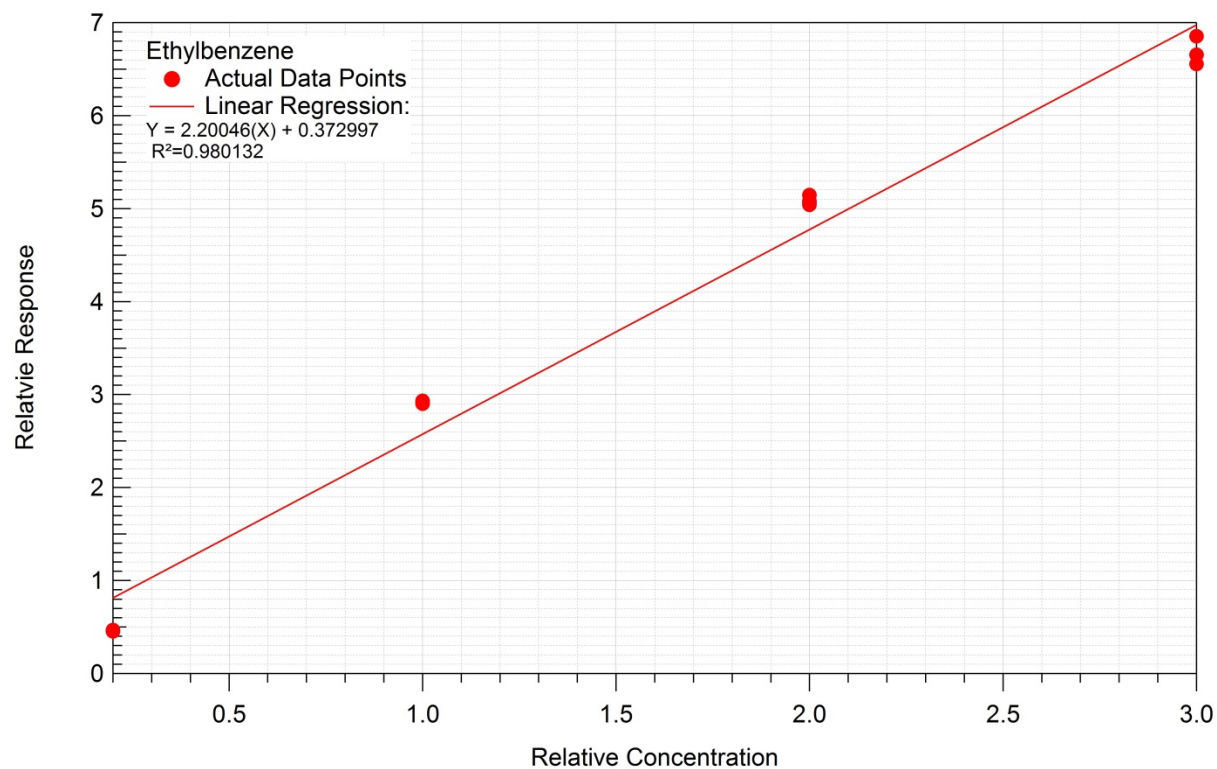
A formal quantitation involves injecting the compound of interest (the twelve compounds in this instance) at various concentrations to create a calibration curve based on the peak areas of the compound. For this study, the twelve compounds were injected at 1, 5, 10, 15 and 25 ppm levels (four injections for each level, to obtain an average) and the peak areas were used to create a calibration curve for each compound. The calibration curve for each target compound are presented in **Figure 1-11**. The calibration equation, the corresponding linearity ( $R^2$ ), and the formal quantitation results for each compound are presented in **Table 3**. The percent recovery was calculated using **Equation 2**.

The accuracy of formal quantitation was significantly better than that produced using relative quantitation. The calculated values ranged from 7-9 ppm (actual value 8 ppm). Recovery values were excellent ranging from 96-111% with just one exception which was stearic acid at 88%. This compound shows very limited volatility and is difficult to quantitate by GCMS. Irganox 1010 showed no signal at the 8 ppm level and was therefore not quantitated.

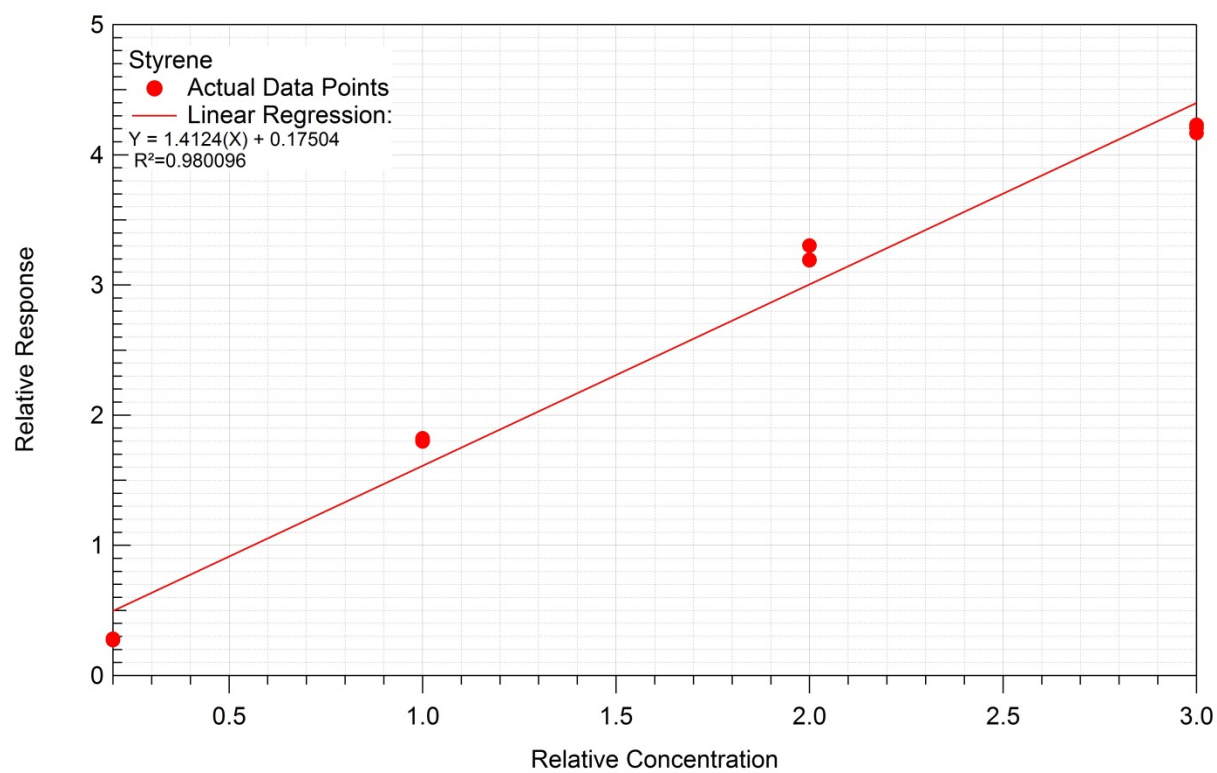


Table 3: Formal Quantitation Results							
Target Compound	RT (min)	Calibration Equation	Calculated Concentration (ppm)				% Recovery
			Injection 1	Injection 2	Injection 3	Average	
Ethylbenzene	7.54	$Y = 2.200 \cdot X + 0.3730$ $R^2 = 0.9801$	8.78	8.71	8.94	8.81	110.1%
Styrene	8.26	$Y = 1.412 \cdot X + 0.1750$ $R^2 = 0.9810$	8.81	8.70	8.85	8.79	109.8%
Cyclohexanone	8.36	$Y = 0.3178 \cdot X + 0.04754$ $R^2 = 0.9806$	8.75	8.61	8.72	8.69	108.7%
Propylbenzene	9.72	$Y = 2.936 \cdot X + 0.1344$ $R^2 = 0.9866$	8.17	8.13	8.16	8.15	101.9%
Diphenyl ether	16.54	$Y = 0.2642 \cdot X + 0.2968$ $R^2 = 0.9805$	8.31	8.37	8.75	8.48	106.0%
Hexadecane	18.18	$Y = 0.1818 \cdot X + 0.01712$ $R^2 = 0.9855$	8.22	8.06	8.11	8.13	101.6%
Eicosane	21.07	$Y = 0.1924 \cdot X + 0.01923$ $R^2 = 0.9805$	8.05	7.94	8.12	8.04	100.5%
Stearic acid	22.08	$Y = 0.003255 \cdot X - 0.002873$ $R^2 = 0.9210$	7.00	6.93	7.25	7.06	88.3%
Tetracosane	23.46	$Y = 0.2103 \cdot X + 0.019677$ $R^2 = 0.9769$	8.07	7.97	8.18	8.07	100.9%
Erucamide	25.47	$Y = 0.06029 \cdot X - 0.05171$ $R^2 = 0.9901$	7.40	7.69	8.03	7.71	96.3%
Didecylphthalate	25.47	$Y = 1.1830 \cdot X - 0.05543$ $R^2 = 0.9863$	8.67	8.95	8.99	8.87	110.9%
Irganox 1010	ND	--	--	--	--	--	--

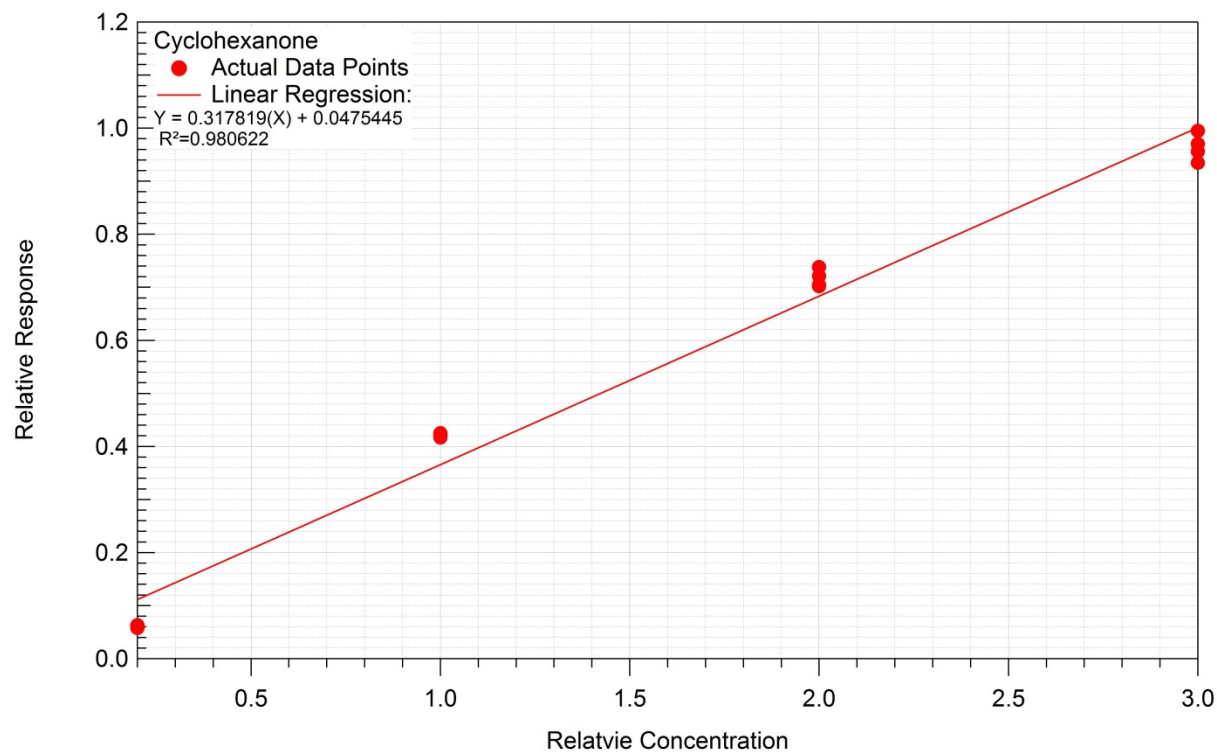
ND – Not Detected



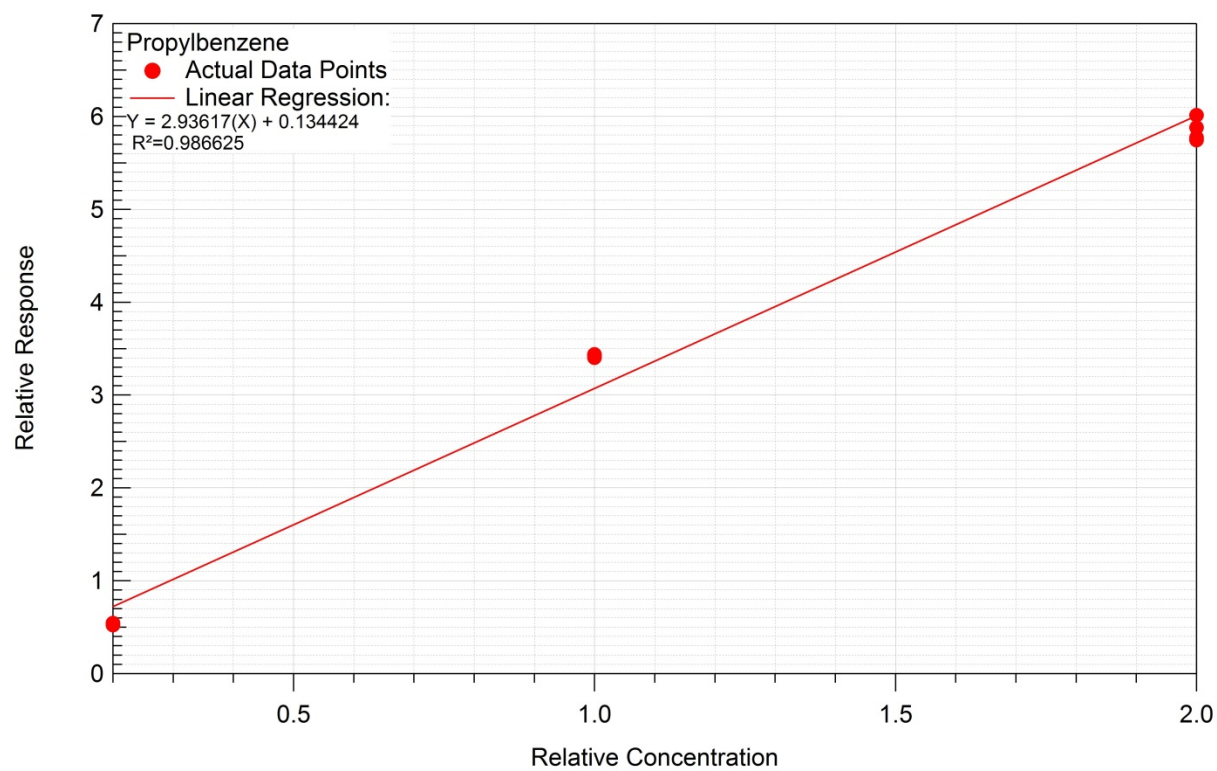
**Figure 1** - Calibration curve prepared for Ethylbenzene.



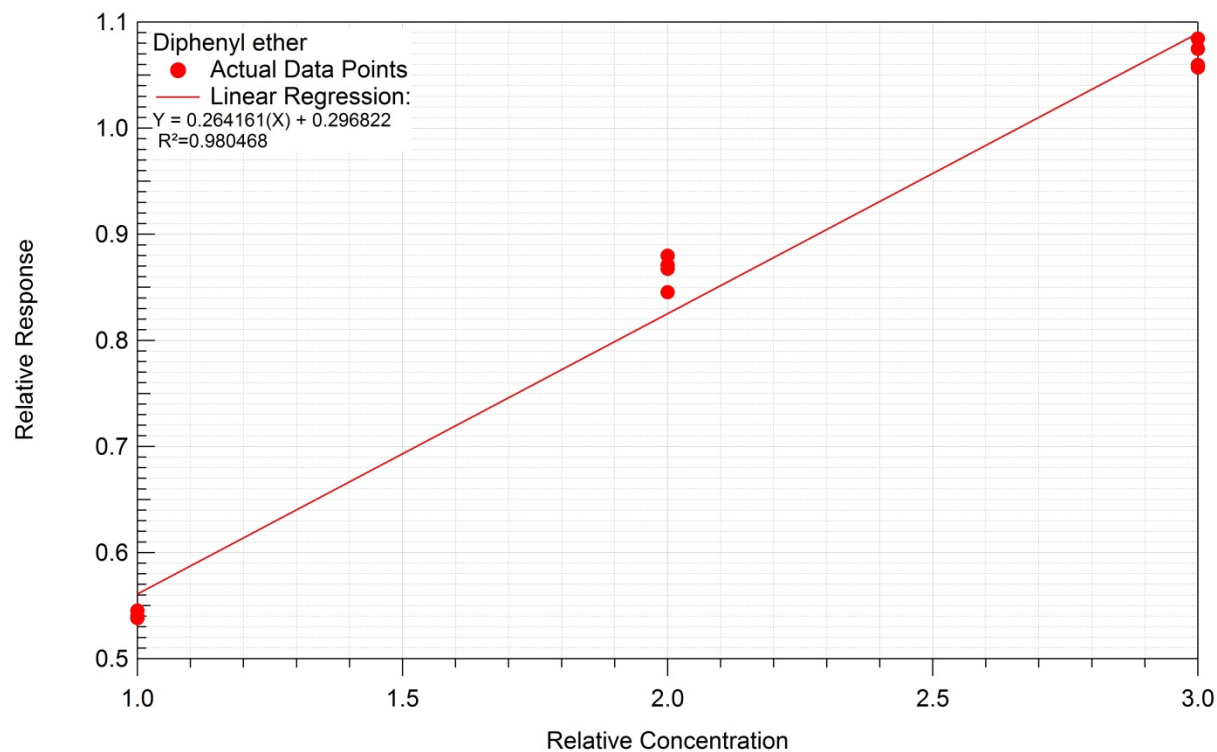
**Figure 2** - Calibration curve prepared for Styrene.



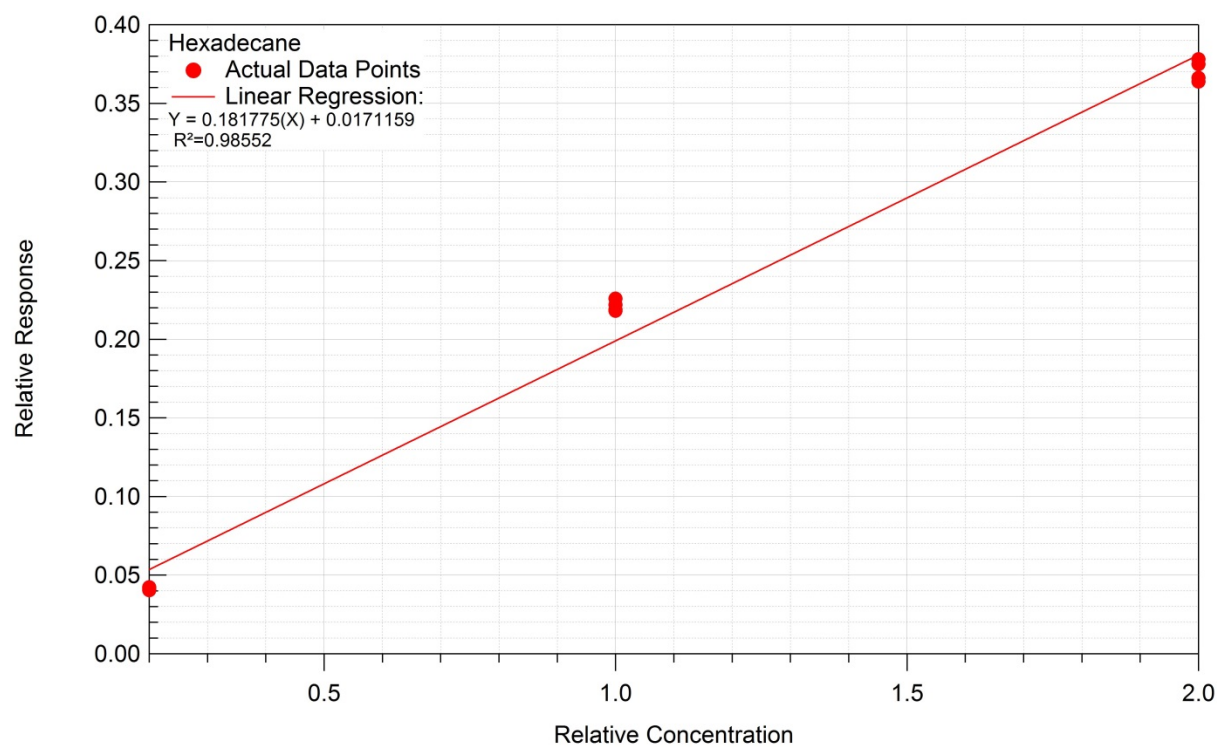
**Figure 3** - Calibration curve prepared for Cyclohexanone.



**Figure 4** - Calibration curve prepared for Propylbenzene.

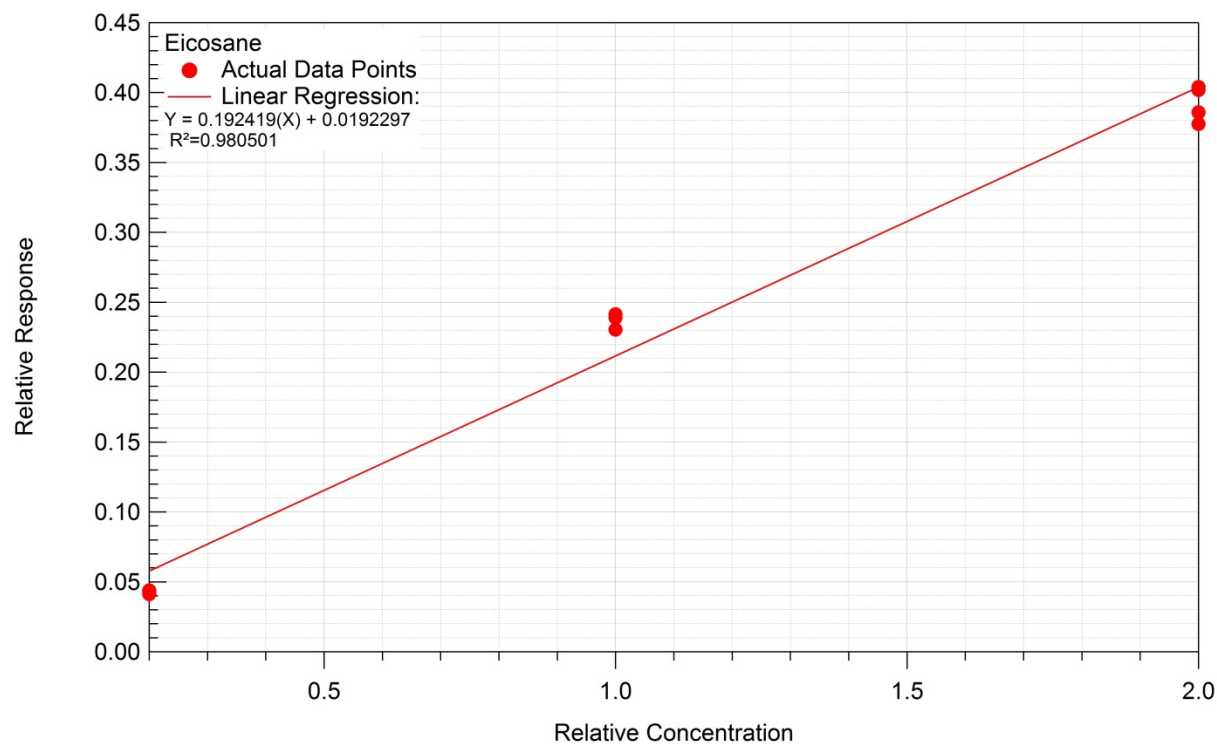


**Figure 5** - Calibration curve prepared for Diphenyl ether.

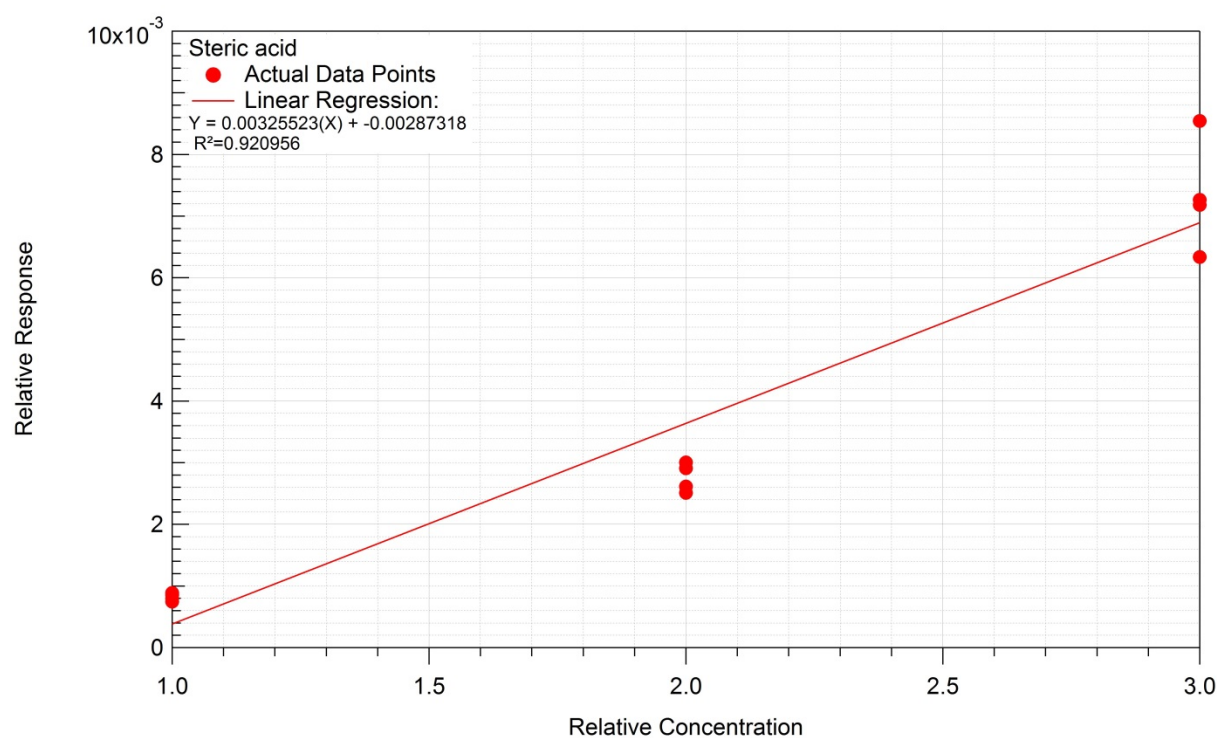


**Figure 6** - Calibration curve prepared for Hexadecane.

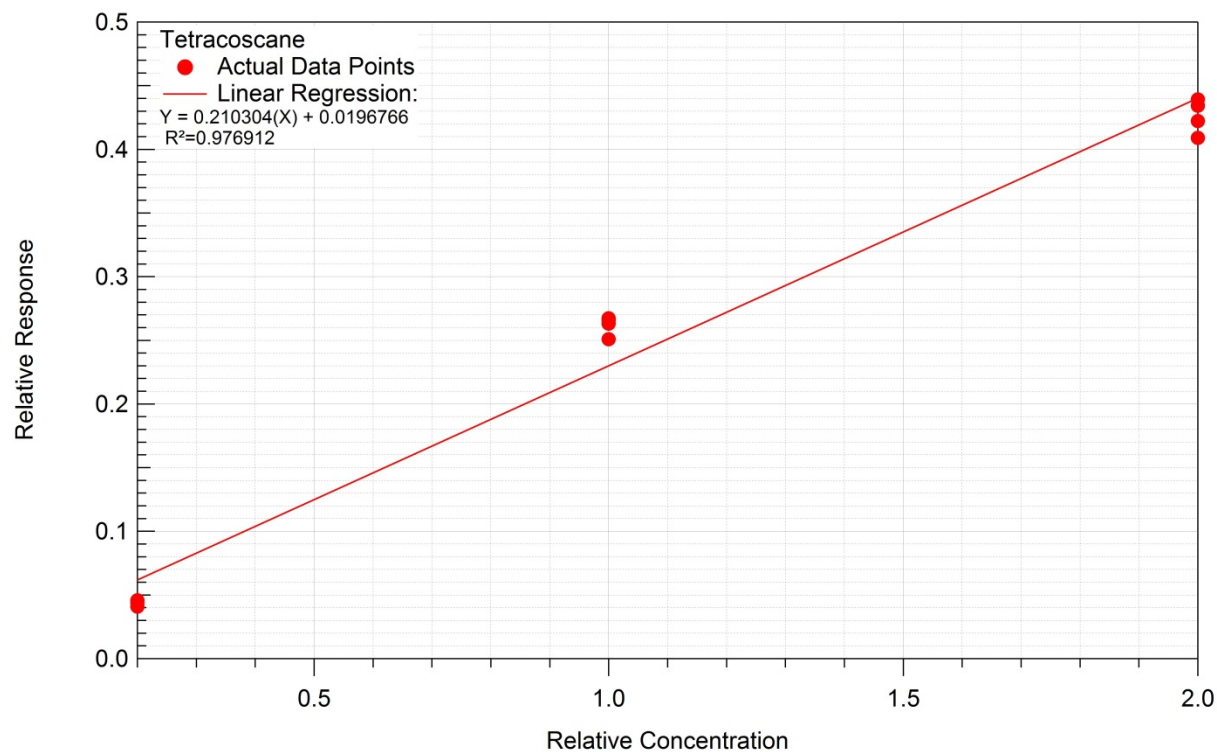




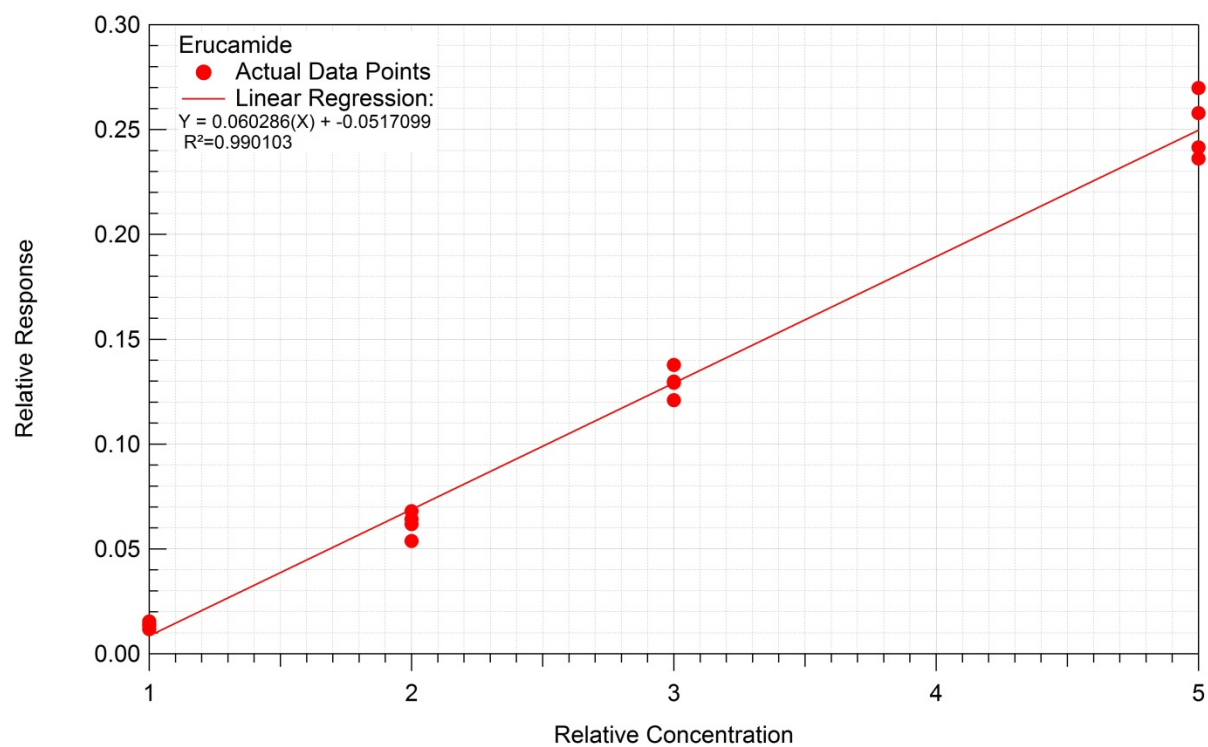
**Figure 7** - Calibration curve prepared for Eicosane.



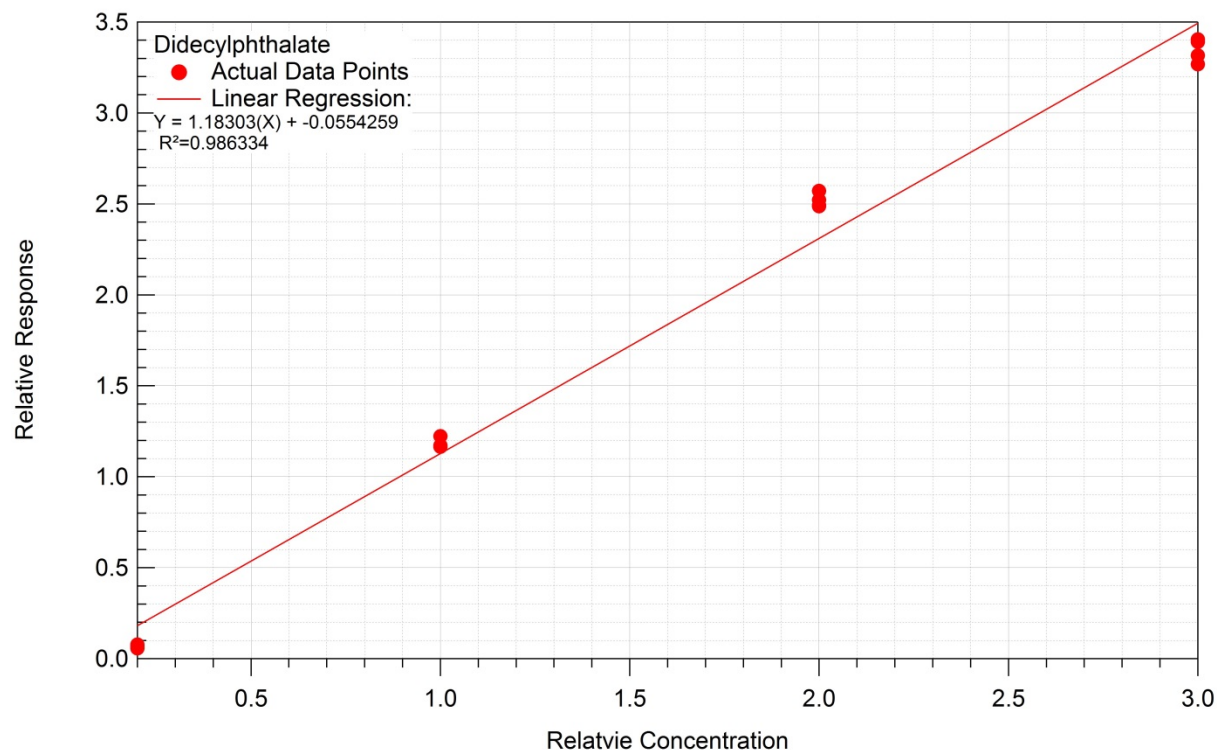
**Figure 8** - Calibration curve prepared for Steric acid.



**Figure 9** - Calibration curve prepared for Tetracosane.



**Figure 10** - Calibration curve prepared for Erucamide.



**Figure 11** - Calibration curve prepared for Didecylphthalate.

## Analysis Conditions

### QTOF GCMS

The samples were analyzed using an Agilent 7890B gas chromatograph in conjunction with a 7200 QTOF mass selective detector using liquid injection. Data acquisition was accomplished using MassHunter software. Sample peaks were compared with over 796,613 reference compounds using the NIST/EPA/NIH mass spectral search program.

The following run conditions were applied for Gas Chromatographic analysis:

Ionization Mode: Electron Impact

Injection Size = 2uL

Initial Delay = 4.0 minutes

Initial Temperature: 50°C

Final Temperature: 320°C

Temperature Ramp Rate 1: 15°C per minute

Injector Port Temperature: 310°C

Hold Time: 10 minutes

Detector Temperature: 320°C

Injector Split = NA

Mass Range: Low Mass = 29, High Mass = 550

Column = DB-5MS 30m x 0.25 x 0.25µm film

## Closing Comments

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 deformulations. 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,

*Zejing Xu*

Zejing Xu, Ph. D  
Senior Chemist  
Jordi Labs LLC

*Anthony Grice*

Anthony Grice, Ph. D.  
Senior Chemist  
Jordi Labs LLC

*Mark Jordi*

Mark Jordi, Ph. D.  
President  
Jordi Labs LLC



# QTOF-GCMS

## Data

# Qualitative Analysis Report

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<b>Sample Type</b>		<b>Position</b>	11
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<b>Acq Method</b>	J8674.M	<b>Acquired Time</b>	6/19/2015 12:54:34 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

**Expected Barcode**

**Sample Amount**

<b>Dual Inj Vol</b>	1	<b>TuneName</b>	atunes.ei.tune.xml
<b>TunePath</b>	D:\MassHunter\GCMS\1\7200 \	<b>TuneDateStamp</b>	42172.83935

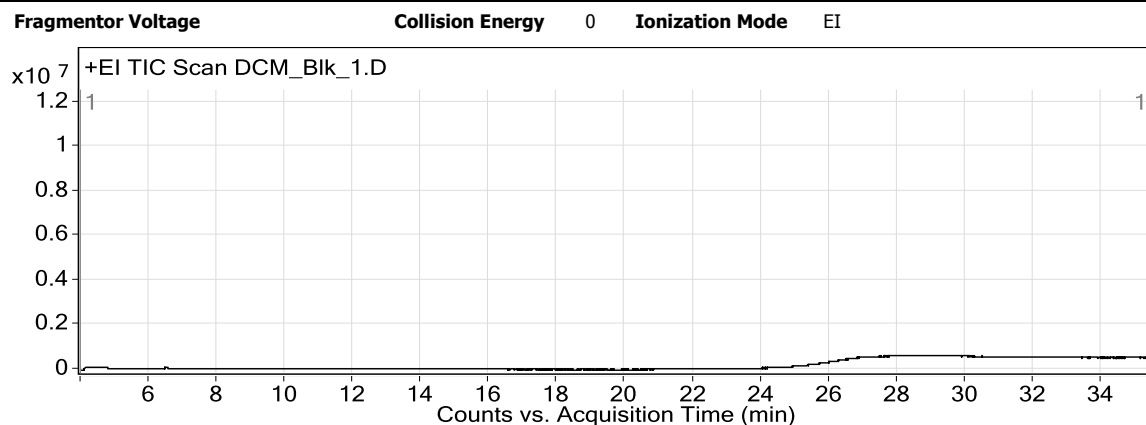
**MSFirmwareVersion** G.7200.01.13

**OperatorName**

**RunCompletedFlag** TRUE

**Acquisition SW Version**  
MassHunter GC/MS  
Acquisition B.07.00  
SP2.1654 29-Aug-2013  
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Agilent Technologies, Inc.

## User Chromatograms



--- End Of Report ---

# Qualitative Analysis Report

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<b>Sample Type</b>		<b>Position</b>	14
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<b>Acq Method</b>	J8674.M	<b>Acquired Time</b>	6/19/2015 9:36:03 PM
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<b>Comment</b>			

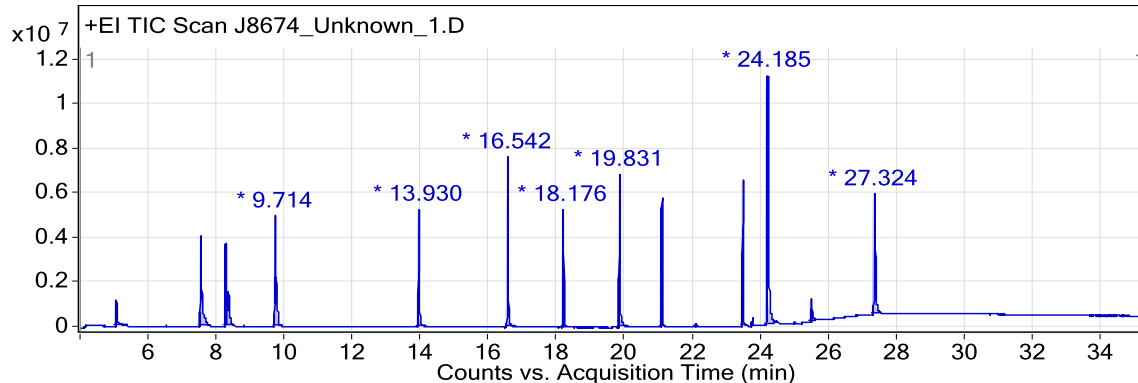
**Expected Barcode**

**Sample Amount**

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<b>MSFirmwareVersion</b>	G.7200.01.13	<b>OperatorName</b>	
<b>RunCompletedFlag</b>	TRUE	<b>Acquisition SW Version</b>	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc.

## User Chromatograms

**Fragmentor Voltage**      **Collision Energy** 0      **Ionization Mode** EI



## Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.981	5.038	5.407	1170004.68	4111315.49	10.77
2	7.478	7.525	7.818	4081370.45	13362322.52	34.99
3	8.21	8.251	8.308	3739134.6	9287264.8	24.32
4	8.308	8.331	8.512	1582934.1	5473107.5	14.33
5	9.667	9.714	9.949	4940484.14	14089441.15	36.9
6	13.89	13.93	14.168	5268614.04	11004698.76	28.82
7	16.503	16.542	16.81	7625960.46	13448060.66	35.22
8	18.141	18.176	18.314	5268854.7	7636166.6	20
9	19.795	19.831	20.117	6844633.49	13259287.73	34.72
10	21.033	21.07	21.214	5771948.72	8793358.04	23.03
11	22.037	22.08	22.158	178755.34	358670.27	0.94
12	23.415	23.45	23.601	6509206.03	10600456.69	27.76
13	24.127	24.185	24.41	11168961.49	38186925.56	100
14	25.424	25.467	25.628	1039444.3	3046272.11	7.98
15	27.267	27.324	27.501	5396177.89	14736118.36	38.59

# Qualitative Analysis Report

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--- End Of Report ---

# Qualitative Analysis Report

<b>Data Filename</b>	J8674_Unknown_2.D	<b>Sample Name</b>	Unknown
<b>Sample Type</b>		<b>Position</b>	14
<b>Instrument Name</b>	GC-QTOF	<b>User Name</b>	
<b>Acq Method</b>	J8674.M	<b>Acquired Time</b>	6/19/2015 10:19:00 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

**Expected Barcode**

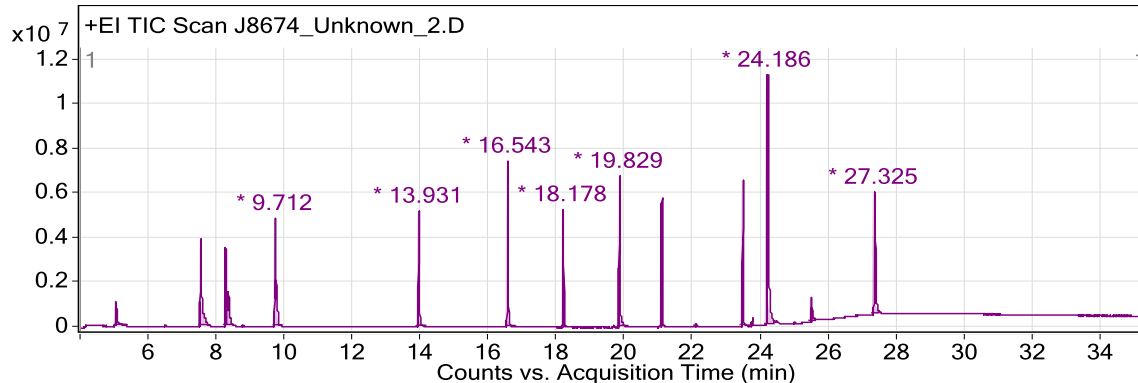
**Sample Amount**

<b>Dual Inj Vol</b>	1	<b>TuneName</b>	atunes.ei.tune.xml
<b>TunePath</b>	D:\MassHunter\GCMS\1\7200	<b>TuneDateStamp</b>	42172.83935
<b>MSFirmwareVersion</b>	G.7200.01.13	<b>OperatorName</b>	

<b>RunCompletedFlag</b>	TRUE	<b>Acquisition SW Version</b>	MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc.
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## User Chromatograms

**Fragmentor Voltage**      **Collision Energy** 0      **Ionization Mode** EI



## Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.986	5.033	5.385	1081412.05	3973756.48	10.31
2	7.48	7.523	7.815	3925608.41	13083492.55	33.93
3	8.207	8.248	8.306	3550924.03	8935557.78	23.17
4	8.306	8.332	8.51	1556395.68	5542931.01	14.38
5	9.665	9.712	9.95	4823944.92	13883756.51	36.01
6	13.888	13.931	14.17	5174719.25	10761390.98	27.91
7	16.502	16.543	16.812	7432697.79	13276349.78	34.43
8	18.143	18.178	18.312	5256252.12	7567760.67	19.63
9	19.793	19.829	20.118	6754156.52	13334535.53	34.58
10	21.034	21.071	21.216	5768770.73	8794002.75	22.81
11	22.038	22.078	22.155	179638.64	355736.84	0.92
12	23.411	23.451	23.602	6543977.36	10633574.92	27.58
13	24.126	24.186	24.411	11218363.08	38558919.94	100
14	25.425	25.472	25.63	1102849.3	3161038.32	8.2
15	27.271	27.325	27.496	5468253.94	15225657.63	39.49

# Qualitative Analysis Report

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--- End Of Report ---

# Qualitative Analysis Report

**Data Filename** J8674\_Unknown\_3.D **Sample Name** Unknown  
**Sample Type** **Position** 14  
**Instrument Name** GC-QTOF **User Name**  
**Acq Method** J8674.M **Acquired Time** 6/19/2015 11:01:50 PM  
**IRM Calibration Status** Success **DA Method** Default.m  
**Comment**

**Expected Barcode** **Sample Amount**

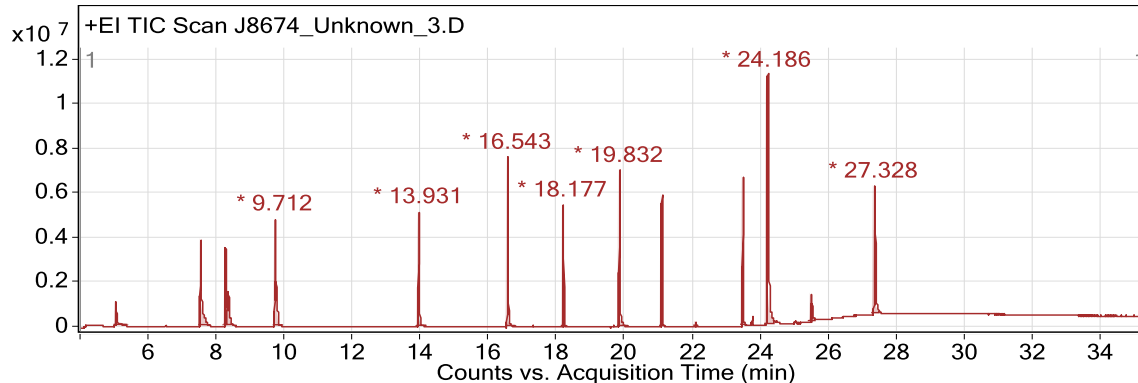
**Dual Inj Vol** 1 **TuneName** atunes.ei.tune.xml  
**TunePath** D:\MassHunter\GCMS\1\7200 **TuneDateStamp** 42172.83935  
 \

**MSFirmwareVersion** G.7200.01.13 **OperatorName**

**RunCompletedFlag** TRUE **Acquisition SW** MassHunter GC/MS  
**Version** Acquisition B.07.00  
 SP2.1654 29-Aug-2013  
 Copyright © 1989-2013  
 Agilent Technologies, Inc.

## User Chromatograms

**Fragmentor Voltage** **Collision Energy** 0 **Ionization Mode** EI



## Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.984	5.026	5.395	1066809.14	3897227.57	9.7
2	7.478	7.523	7.818	3883796.71	13009694.96	32.39
3	8.204	8.248	8.308	3544177.07	9076815.37	22.6
4	8.308	8.332	8.517	1542616.94	5345908.71	13.31
5	9.668	9.712	9.95	4806682.62	13679834.13	34.06
6	13.891	13.931	14.169	5154619.84	10878606.7	27.08
7	16.504	16.543	16.808	7605619.6	13476542.78	33.55
8	18.141	18.177	18.315	5467595.38	7888417.75	19.64
9	19.793	19.832	20.118	7016457.69	13905721.02	34.62
10	21.034	21.071	21.215	5931752.82	9237027.81	23
11	22.038	22.081	22.158	205944.98	405182.16	1.01
12	23.418	23.451	23.602	6682768.32	11092219.15	27.61
13	24.126	24.186	24.411	11245297.86	40169052.11	100
14	25.431	25.472	25.619	1271220.5	3607106.65	8.98
15	27.274	27.328	27.499	5739314.88	15779295.91	39.28

# Qualitative Analysis Report

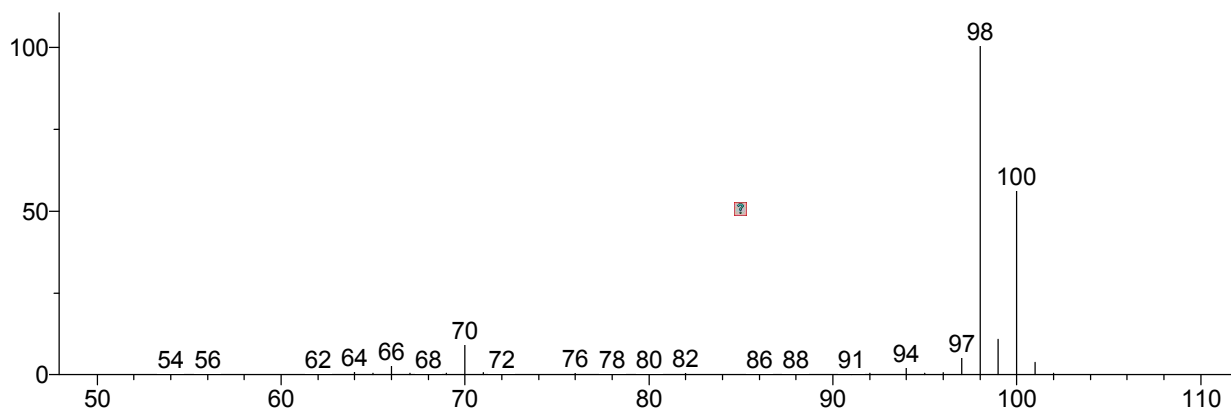
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--- End Of Report ---

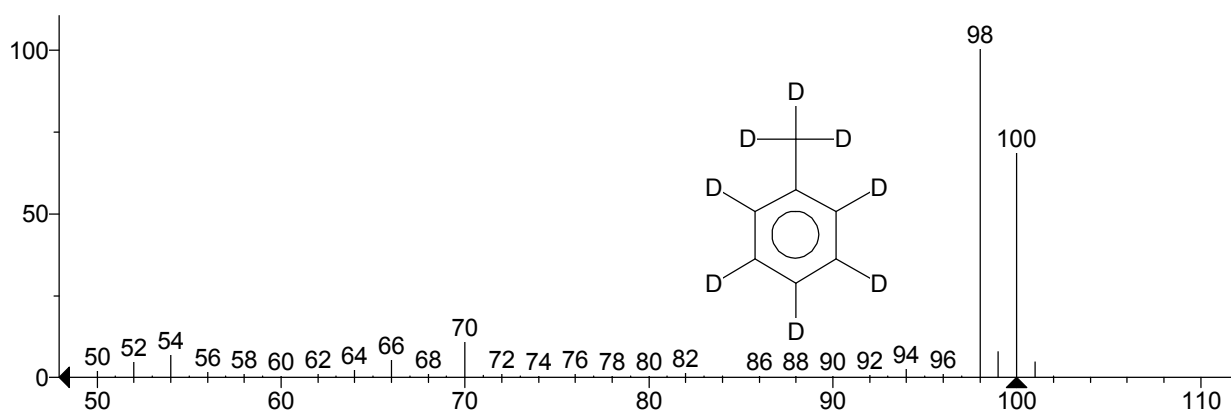


\*\* Search Report Page 1 of 1 \*\*

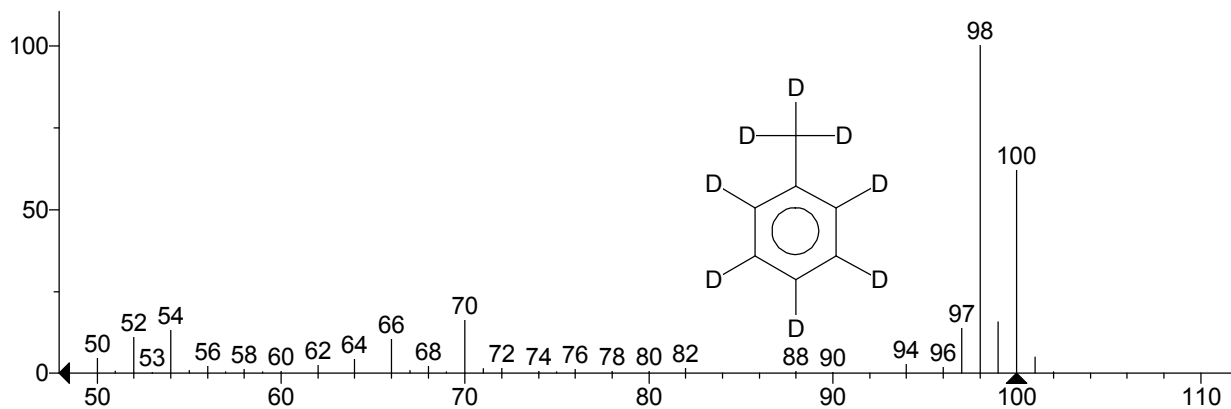
Unknown: +EI Scan (rt: 5.006-5.143 min, 42 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 583



Hit 1 : Toluene-D8  
C7D8; MF: 897; RMF: 913; Prob 91.0%; CAS: 2037-26-5; Lib: mainlib; ID: 64863.

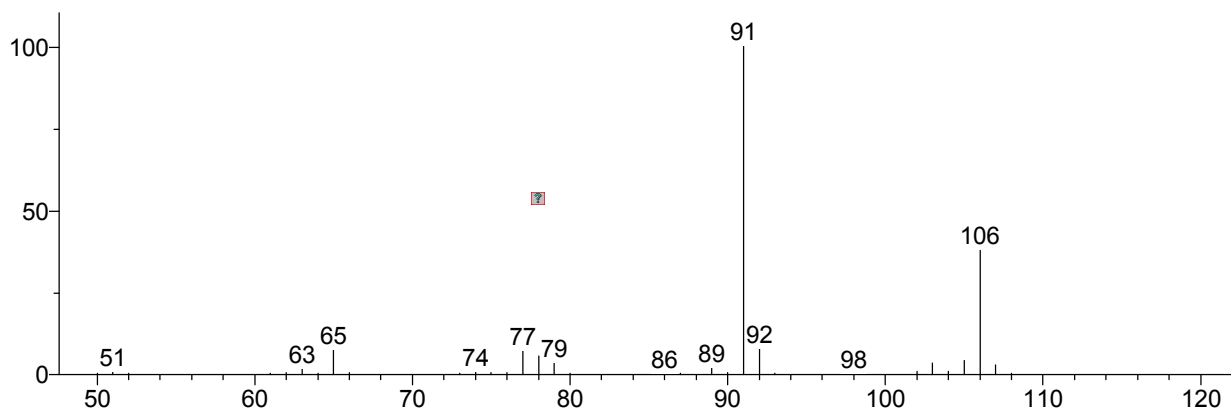


Hit 2 : Toluene-D8  
C7D8; MF: 866; RMF: 867; Prob 91.0%; CAS: 2037-26-5; Lib: replib; ID: 13959.

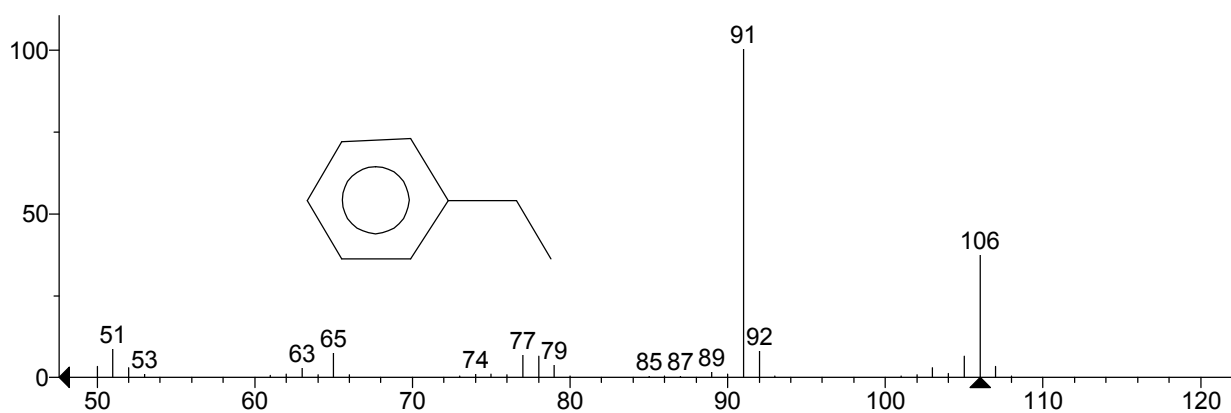


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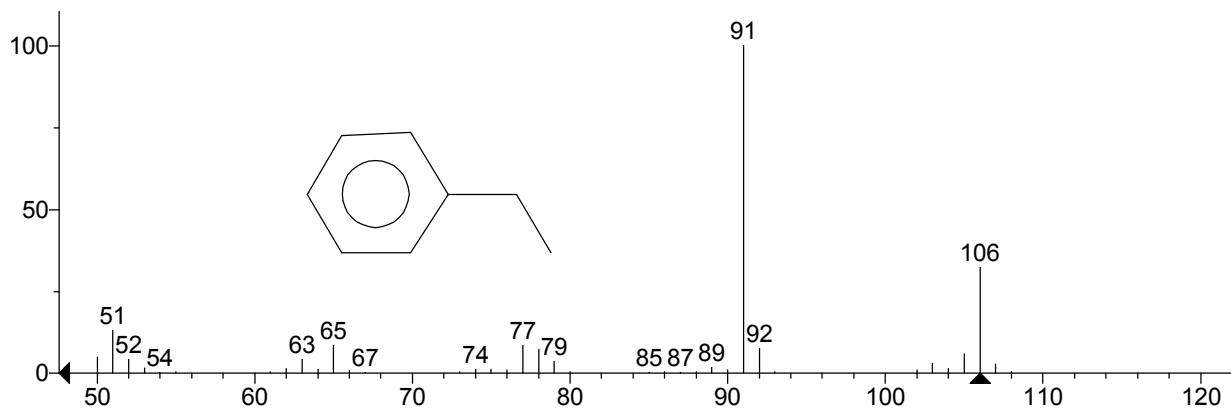
Unknown: +EI Scan (rt: 7.500-7.507, 7.547-7.644 min, 33 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = -117



Hit 1 : Ethylbenzene  
C<sub>8</sub>H<sub>10</sub>; MF: 895; RMF: 895; Prob 54.2%; CAS: 100-41-4; Lib: replib; ID: 12438.

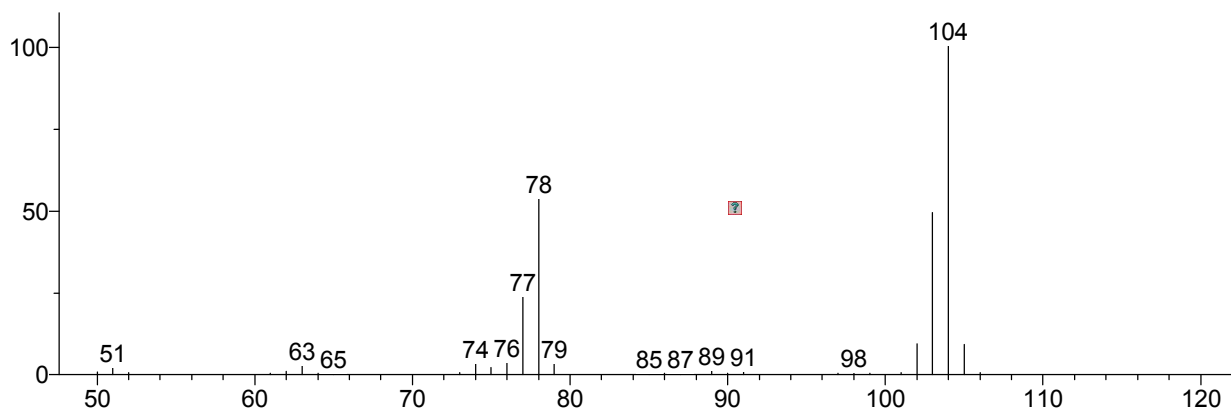


Hit 2 : Ethylbenzene  
C<sub>8</sub>H<sub>10</sub>; MF: 889; RMF: 889; Prob 54.2%; CAS: 100-41-4; Lib: replib; ID: 12436.

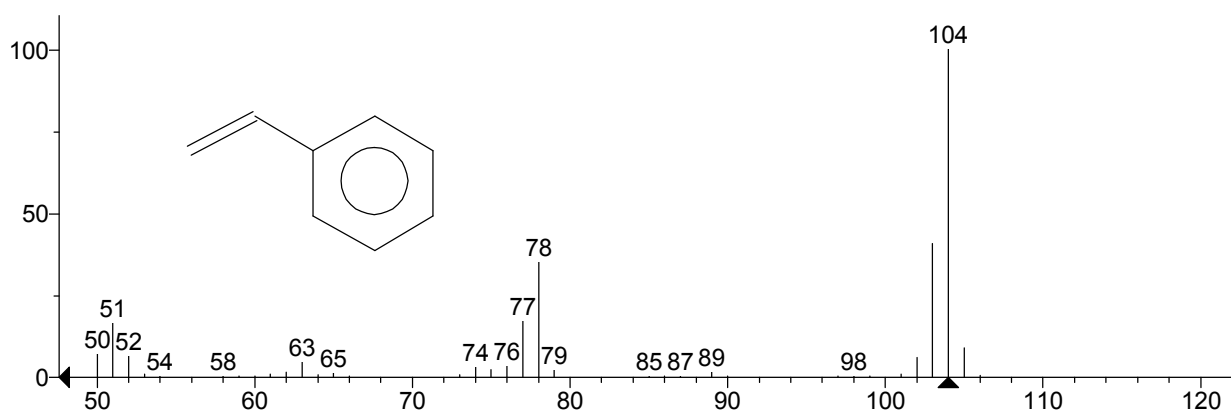


\*\* Search Report Page 1 of 1 \*\*

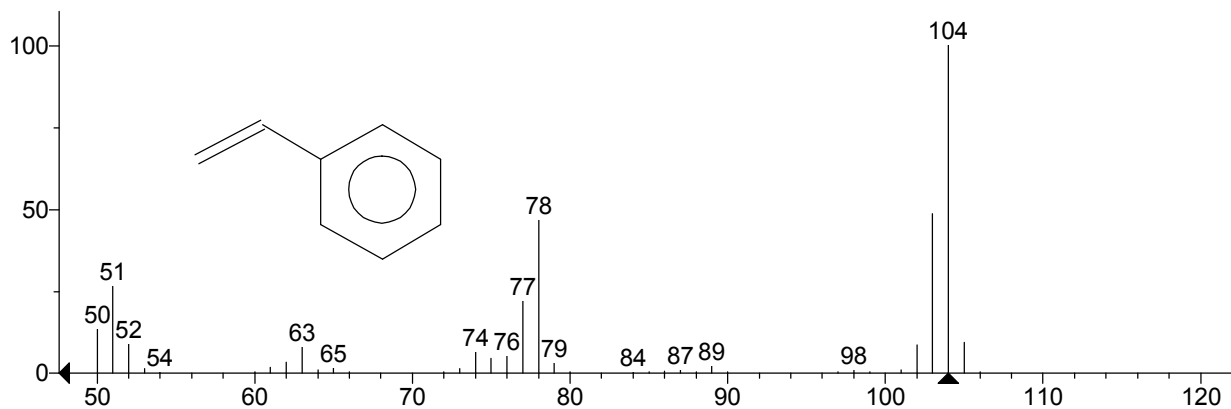
Unknown: +EI Scan (rt: 8.225-8.235, 8.265-8.306 min, 17 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 135



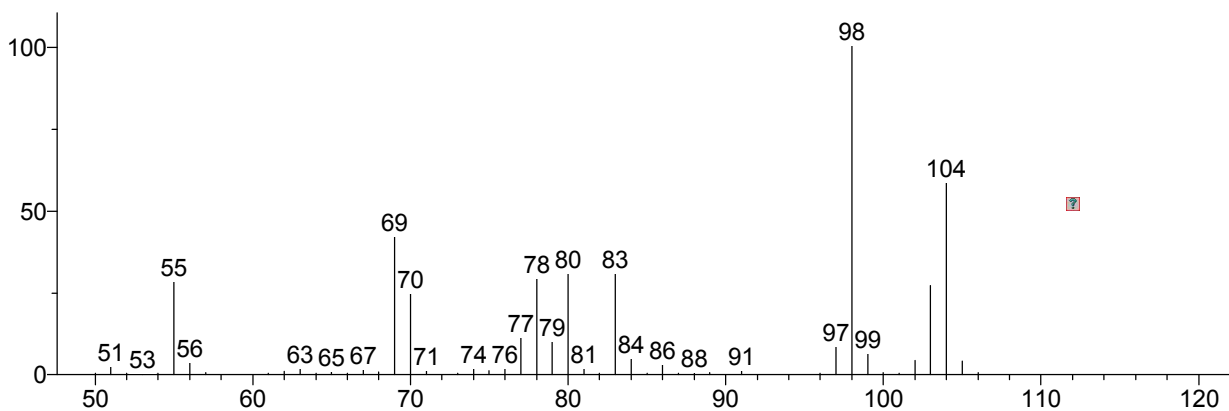
Hit 1 : Styrene  
C<sub>8</sub>H<sub>8</sub>; MF: 903; RMF: 905; Prob 39.8%; CAS: 100-42-5; Lib: replib; ID: 14602.



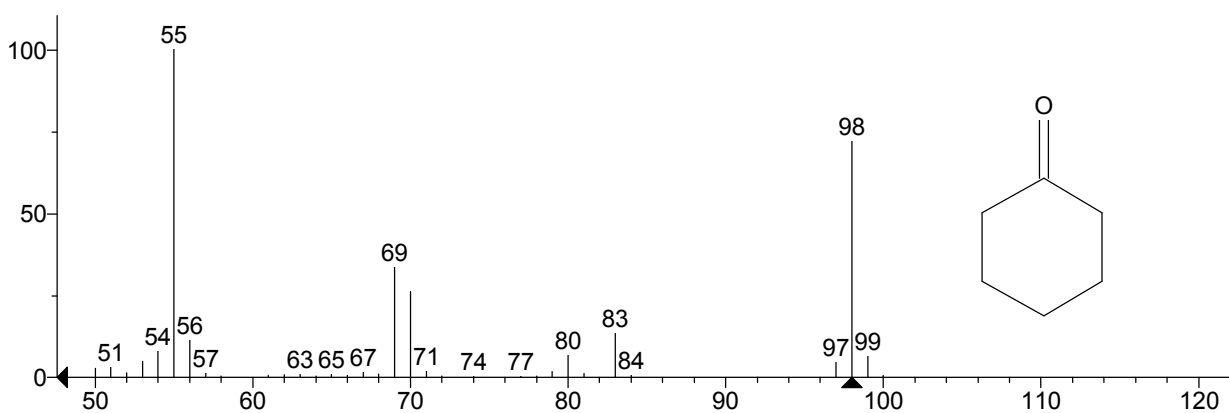
Hit 2 : Styrene  
C<sub>8</sub>H<sub>8</sub>; MF: 898; RMF: 900; Prob 39.8%; CAS: 100-42-5; Lib: mainlib; ID: 69556.



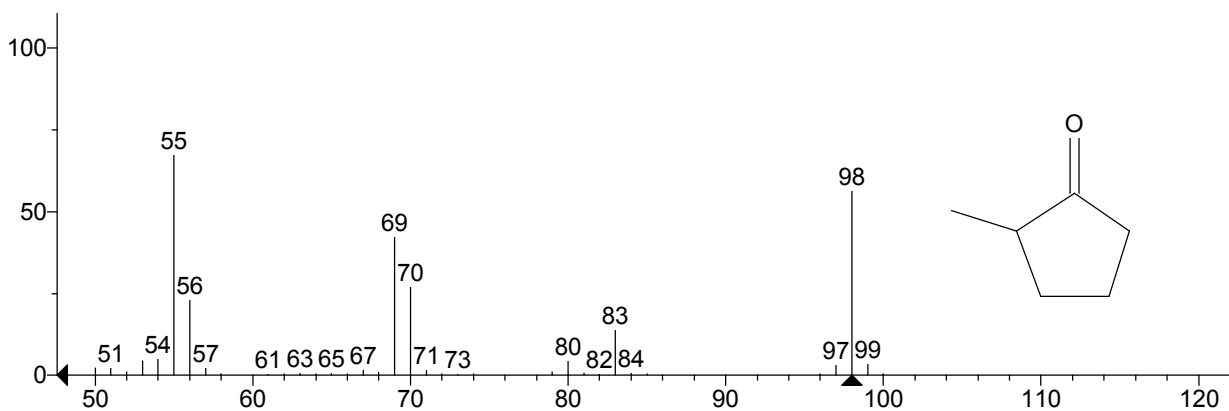
Unknown: +EI Scan (rt: 8.334 min) J8674\_Unknown\_1.D  
Compound in Library Factor = -988



Hit 1 : Cyclohexanone  
C6H10O; MF: 633; RMF: 746; Prob 30.2%; CAS: 108-94-1; Lib: replib; ID: 5014.

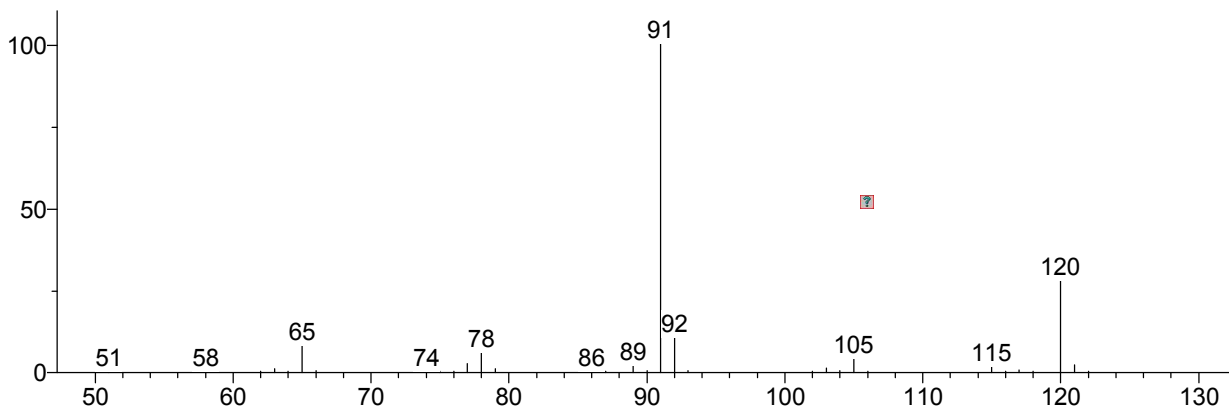


Hit 2 : Cyclopentanone, 2-methyl-  
C6H10O; MF: 629; RMF: 787; Prob 25.5%; CAS: 1120-72-5; Lib: replib; ID: 1445.

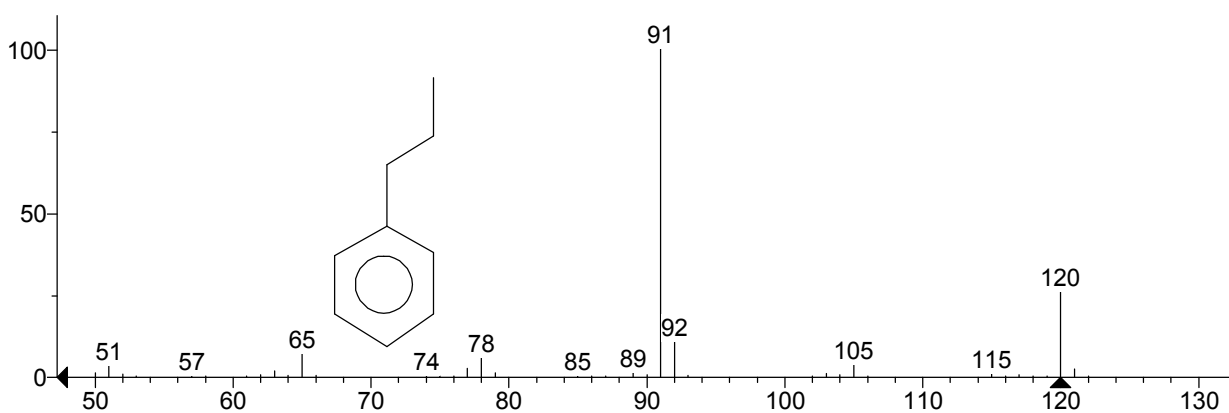


\*\* Search Report Page 1 of 1 \*\*

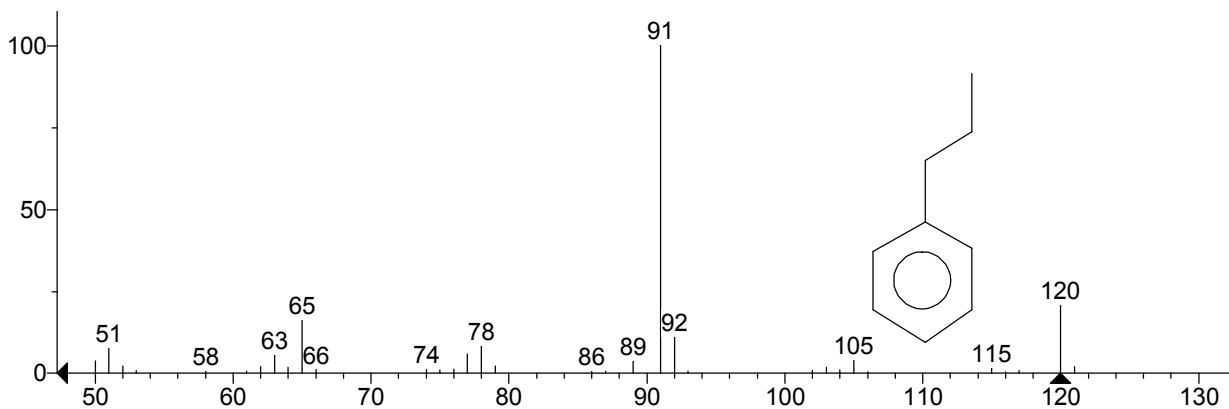
Unknown: +EI Scan (rt: 9.689-9.692, 9.742-9.789 min, 17 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 177



Hit 1 : Benzene, propyl-  
C<sub>9</sub>H<sub>12</sub>; MF: 922; RMF: 922; Prob 75.5%; CAS: 103-65-1; Lib: mainlib; ID: 56127.

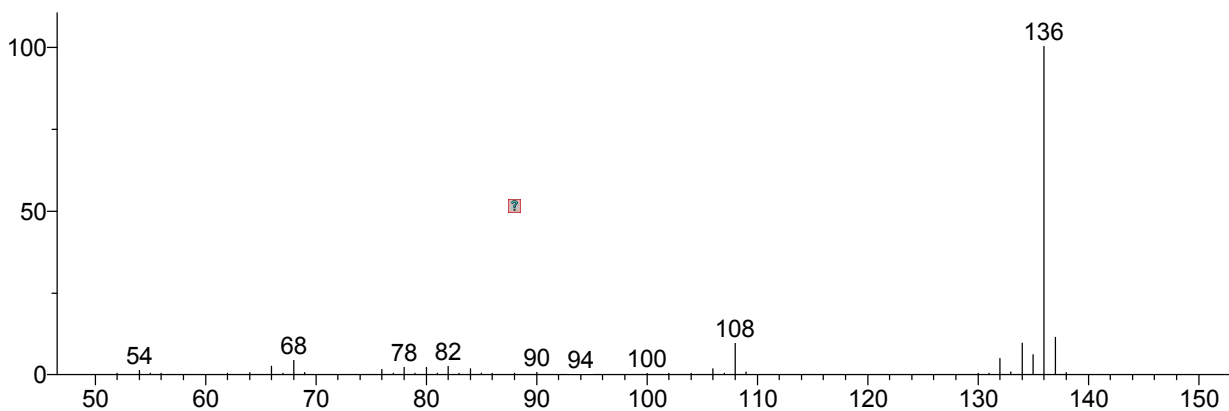


Hit 2 : Benzene, propyl-  
C<sub>9</sub>H<sub>12</sub>; MF: 889; RMF: 890; Prob 75.5%; CAS: 103-65-1; Lib: replib; ID: 12560.



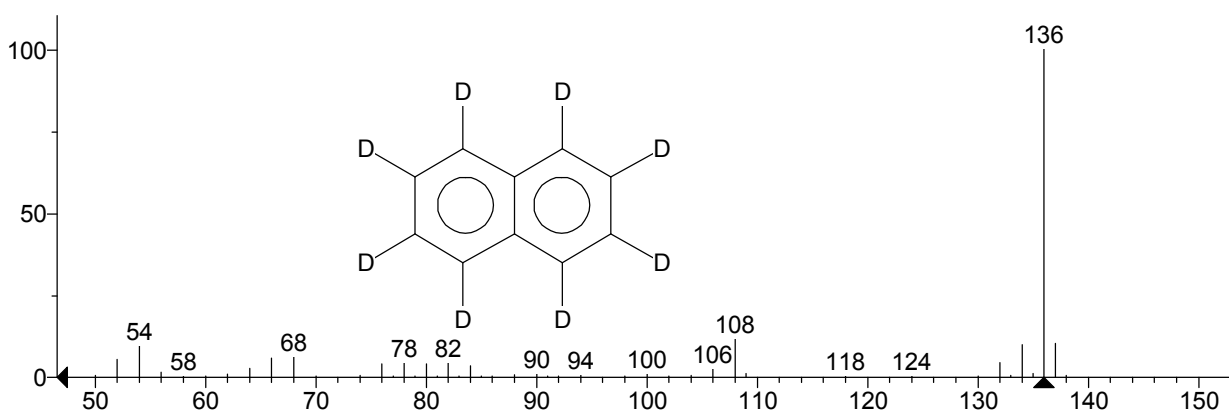
\*\* Search Report Page 1 of 1 \*\*

Unknown: +EI Scan (rt: 13.911, 13.955-13.962 min, 4 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 478



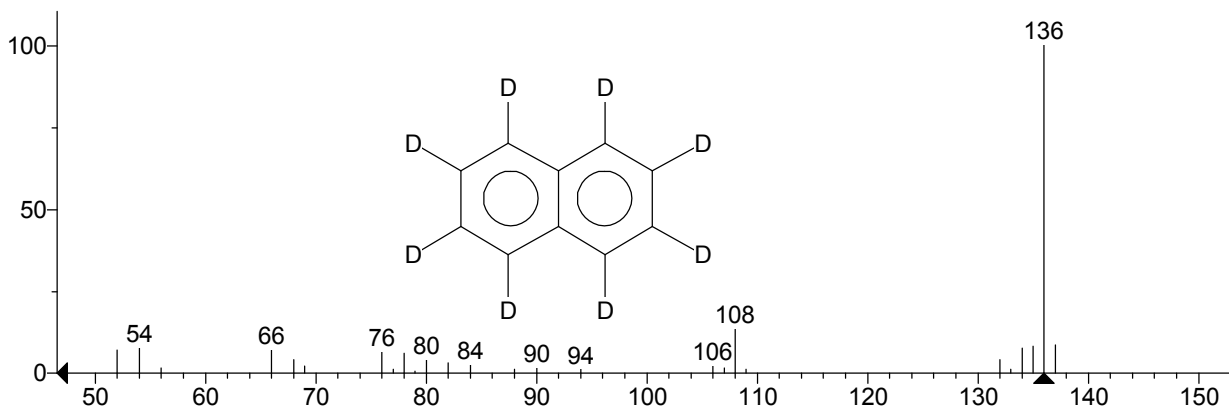
Hit 1 : Naphthalene-D8

C10D8; MF: 892; RMF: 894; Prob 94.0%; CAS: 1146-65-2; Lib: mainlib; ID: 109263.



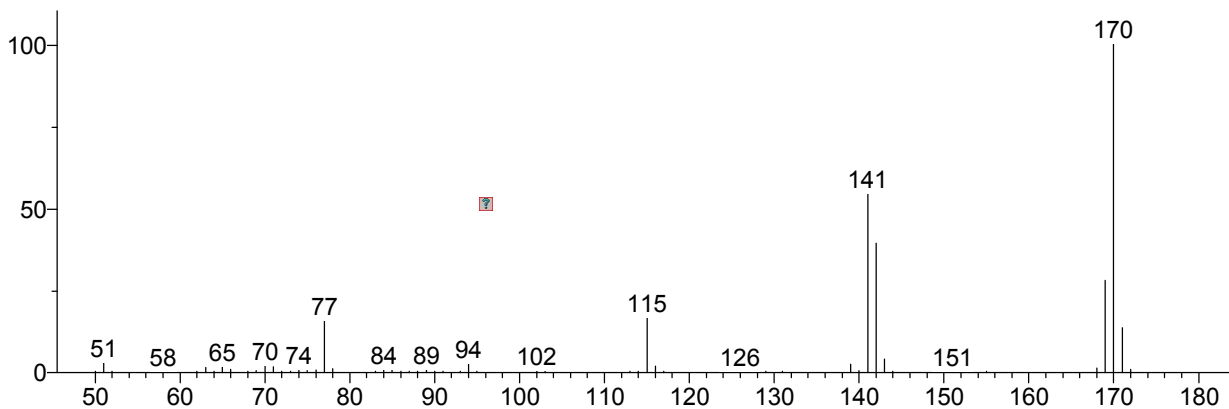
Hit 2 : Naphthalene-D8

C10D8; MF: 845; RMF: 850; Prob 94.0%; CAS: 1146-65-2; Lib: replib; ID: 20132.



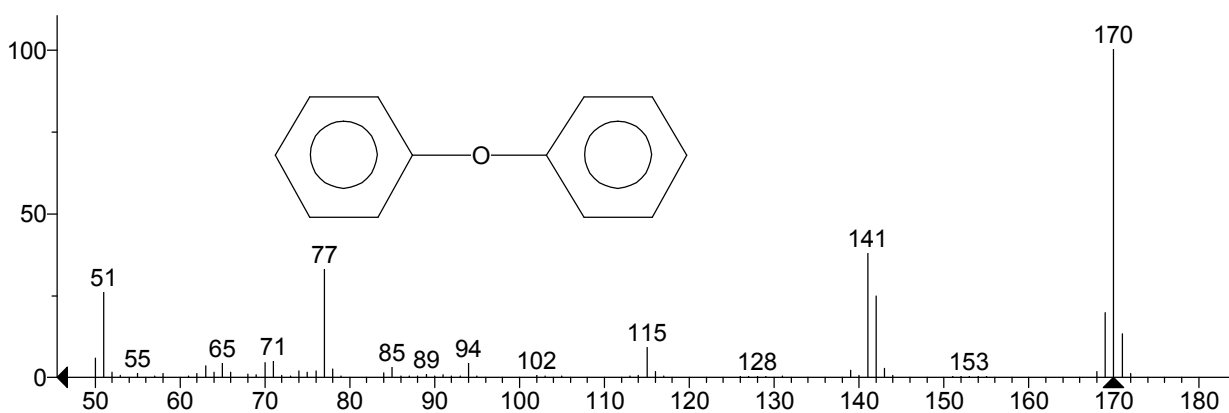
\*\* Search Report Page 1 of 1 \*\*

Unknown: +EI Scan (rt: 16.519-16.523, 16.556-16.563 min, 5 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 162



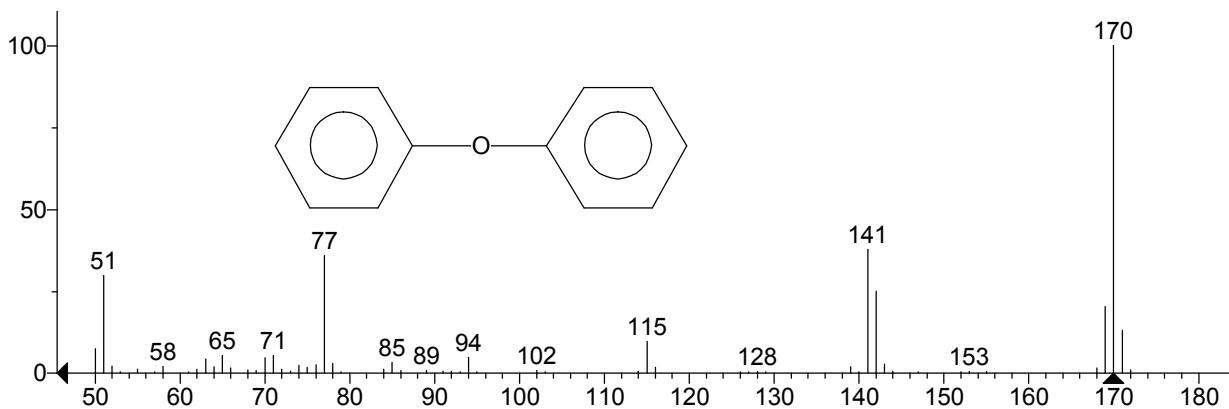
Hit 1 : Diphenyl ether

C<sub>12</sub>H<sub>10</sub>O; MF: 886; RMF: 886; Prob 76.2%; CAS: 101-84-8; Lib: replib; ID: 24092.

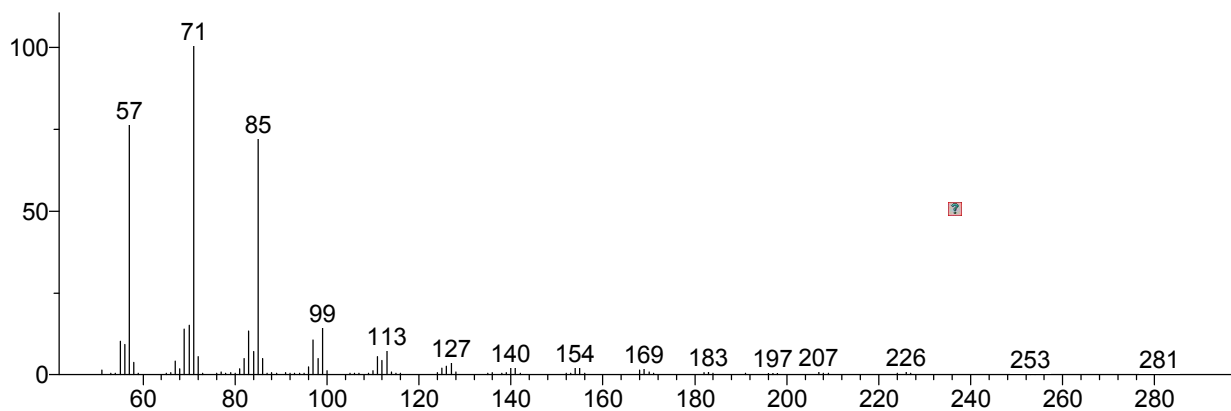


Hit 2 : Diphenyl ether

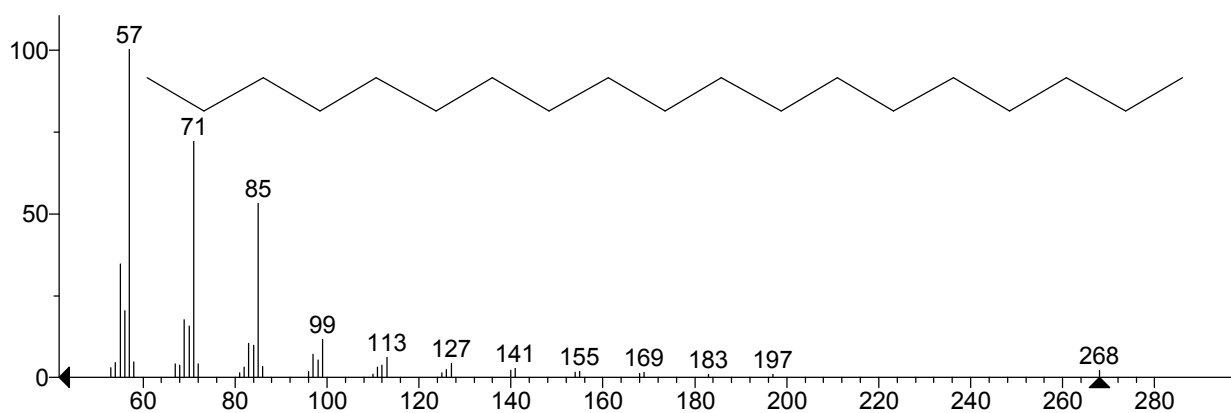
C<sub>12</sub>H<sub>10</sub>O; MF: 875; RMF: 876; Prob 76.2%; CAS: 101-84-8; Lib: replib; ID: 24093.



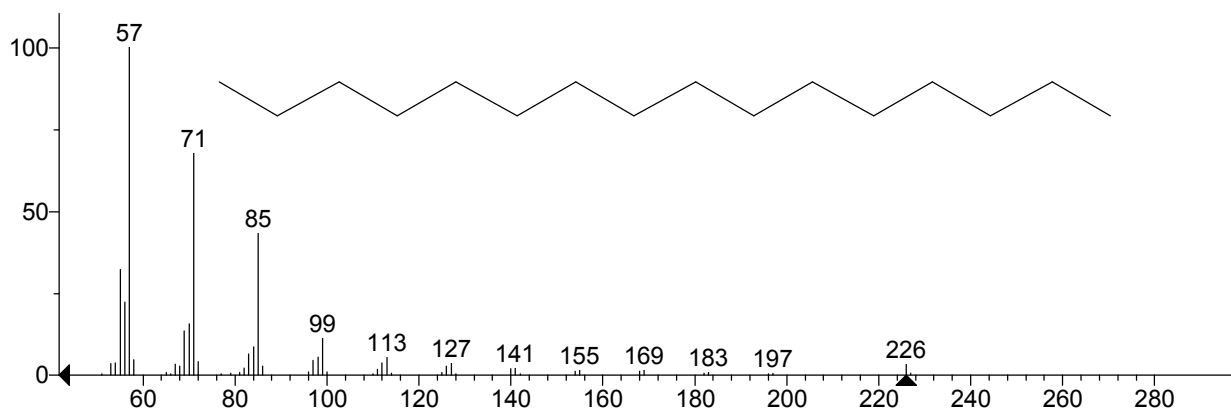
Unknown: +EI Scan (rt: 18.156 min) J8674\_Unknown\_1.D  
Compound in Library Factor = -217



Hit 1 : Nonadecane  
C19H40; MF: 879; RMF: 904; Prob 14.8%; CAS: 629-92-5; Lib: replib; ID: 5836.



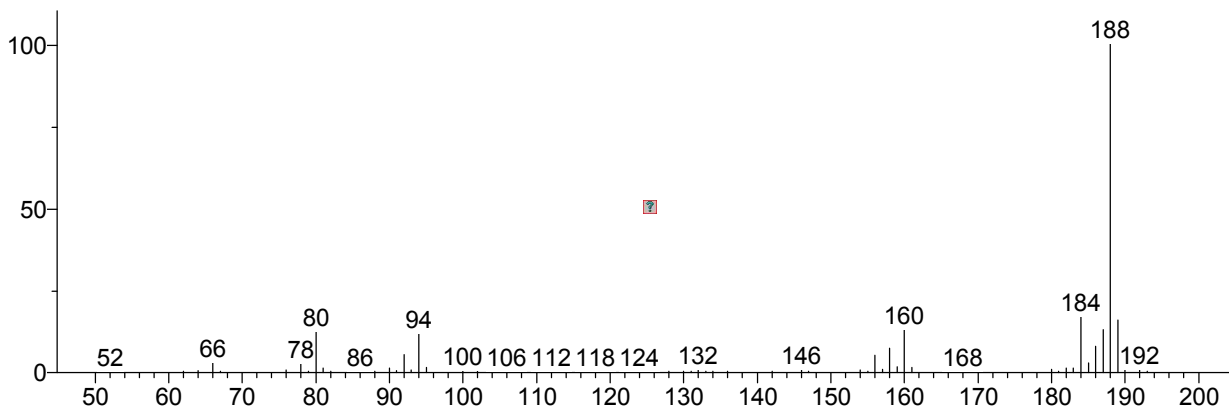
Hit 2 : Hexadecane  
C16H34; MF: 871; RMF: 882; Prob 11.0%; CAS: 544-76-3; Lib: replib; ID: 5861.



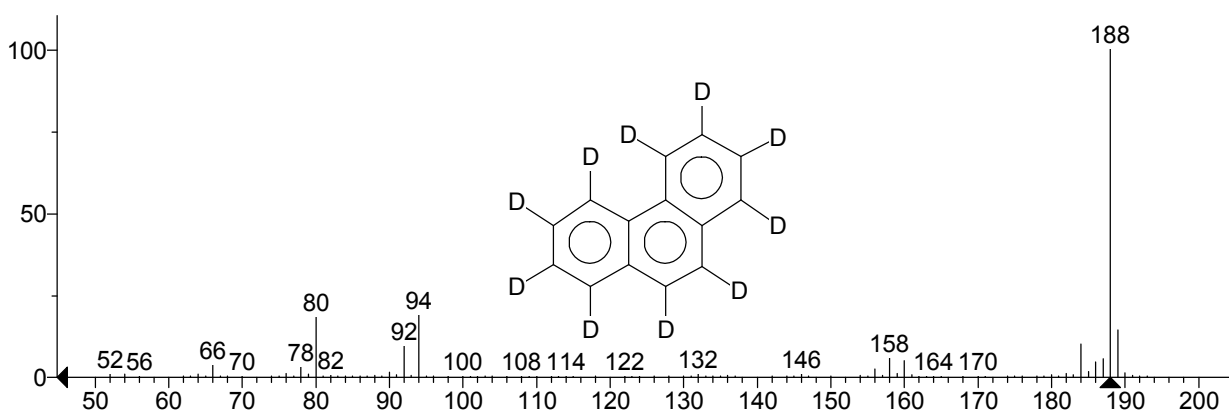


\*\* Search Report Page 1 of 1 \*\*

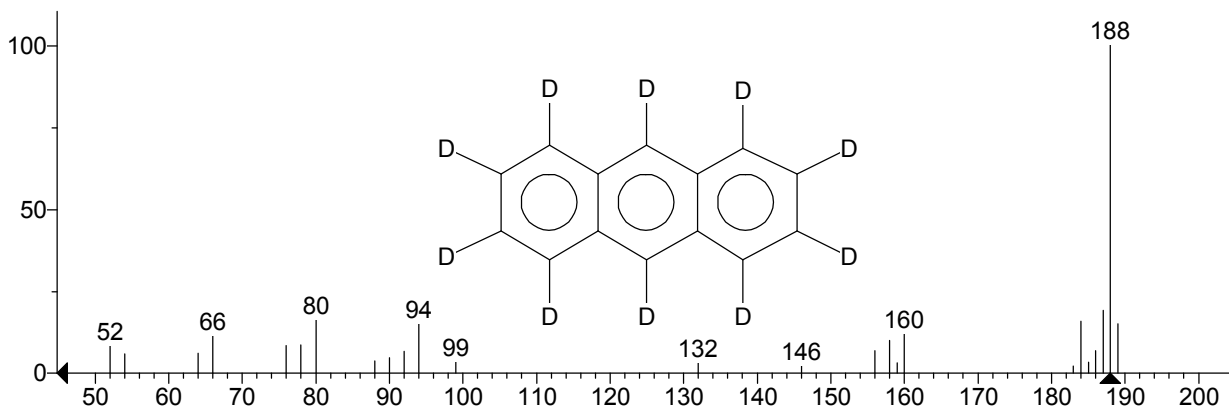
Unknown: +EI Scan (rt: 19.812, 19.849-19.859 min, 5 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 341



Hit 1 : Phenanthrene-D10  
C14D10; MF: 880; RMF: 881; Prob 64.9%; CAS: 1517-22-2; Lib: replib; ID: 25597.

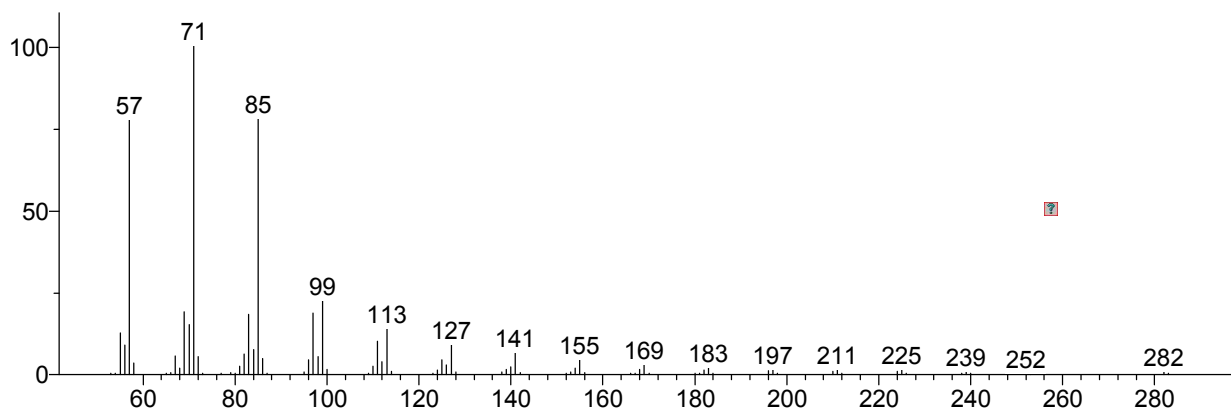


Hit 2 : Anthracene-D10-  
C14D10; MF: 862; RMF: 895; Prob 33.5%; CAS: 1719-06-8; Lib: replib; ID: 25635.

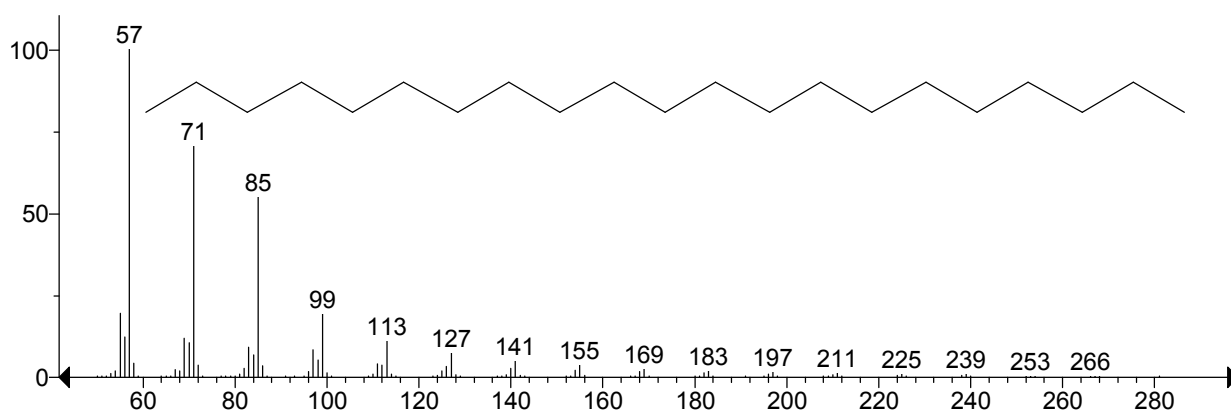


\*\* Search Report Page 1 of 1 \*\*

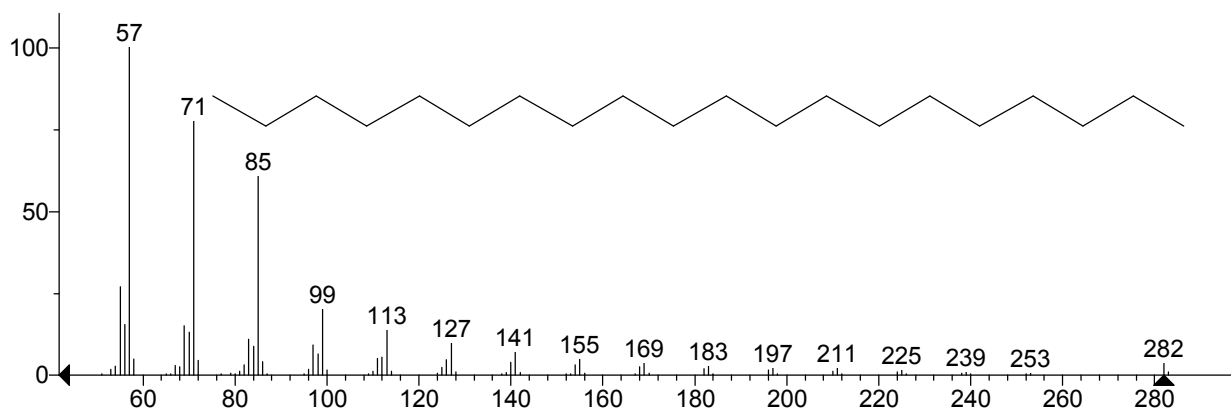
Unknown: +EI Scan (rt: 21.054-21.061, 21.078-21.091 min, 8 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = -138



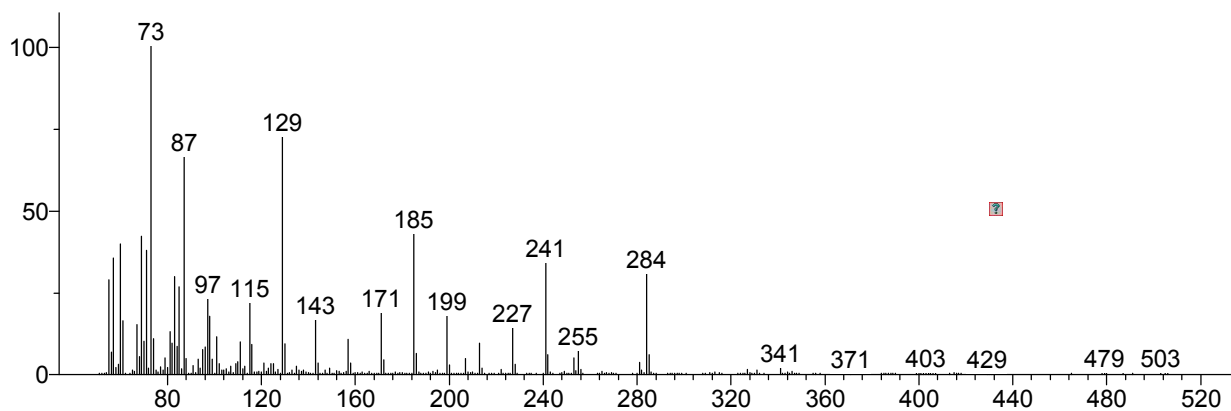
Hit 1 : Heneicosane  
C<sub>21</sub>H<sub>44</sub>; MF: 891; RMF: 893; Prob 15.9%; CAS: 629-94-7; Lib: replib; ID: 6082.



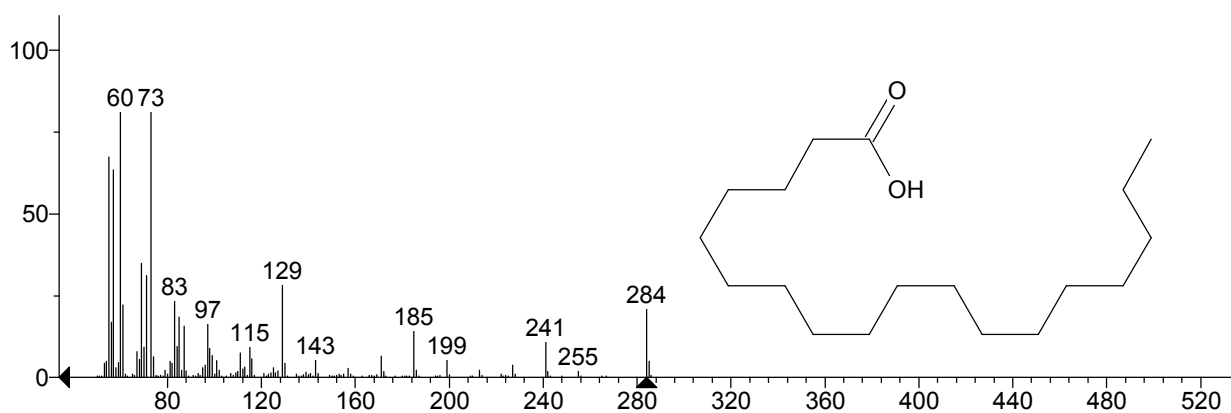
Hit 2 : Eicosane  
C<sub>20</sub>H<sub>42</sub>; MF: 886; RMF: 886; Prob 12.8%; CAS: 112-95-8; Lib: mainlib; ID: 23557.



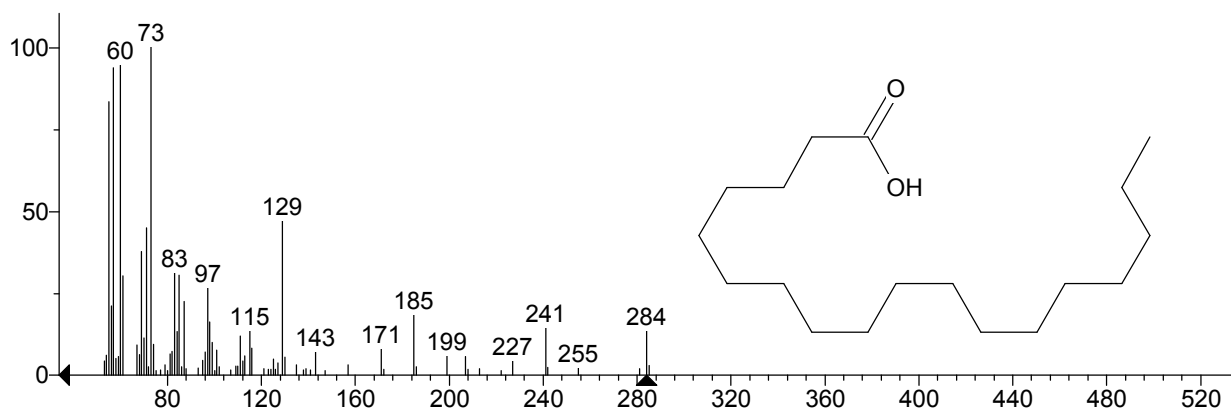
Unknown: +EI Scan (rt: 22.061-22.155 min, 29 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = -279



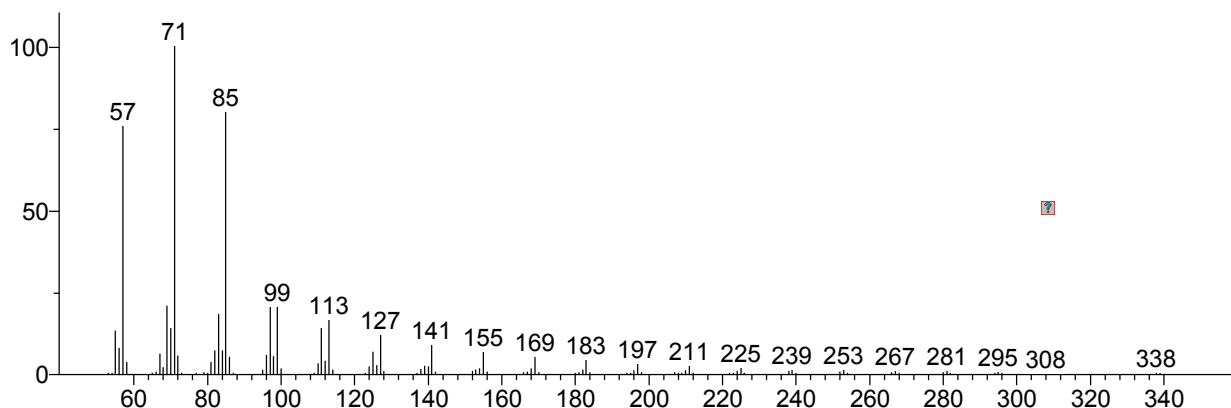
Hit 1 : Octadecanoic acid  
C18H36O2; MF: 796; RMF: 843; Prob 62.7%; CAS: 57-11-4; Lib: replib; ID: 1782.



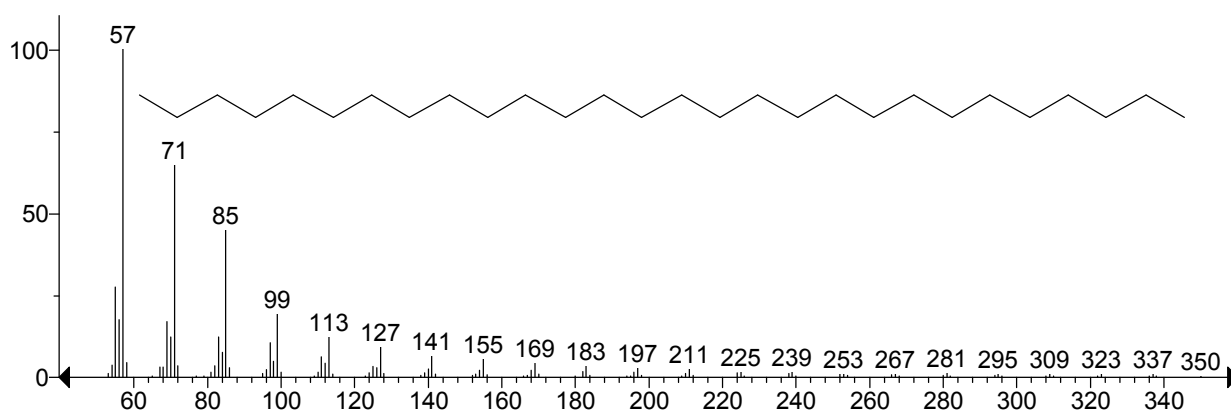
Hit 2 : Octadecanoic acid  
C18H36O2; MF: 795; RMF: 870; Prob 62.7%; CAS: 57-11-4; Lib: replib; ID: 2658.



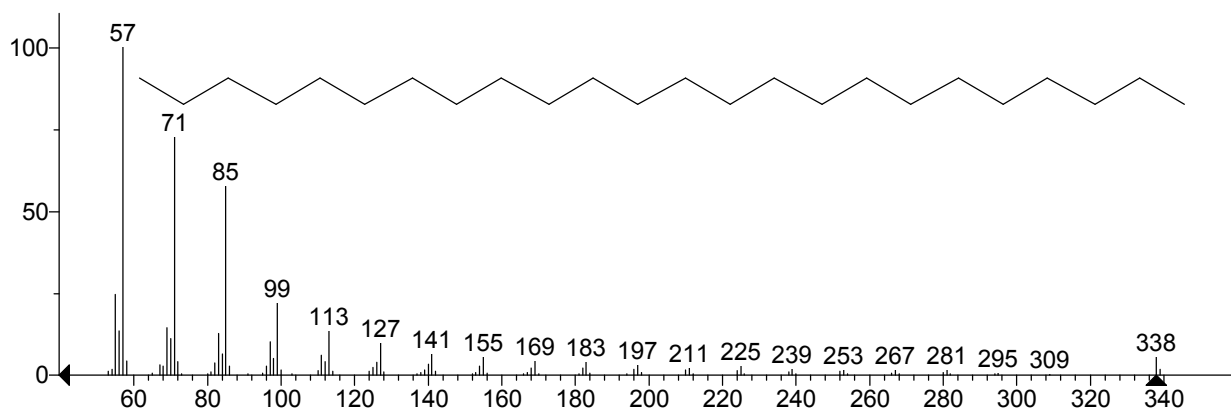
Unknown: +EI Scan (rt: 23.450 min) J8674\_Unknown\_1.D  
Compound in Library Factor = -297



Hit 1 : Octacosane  
C28H58; MF: 876; RMF: 878; Prob 9.77%; CAS: 630-02-4; Lib: replib; ID: 5774.

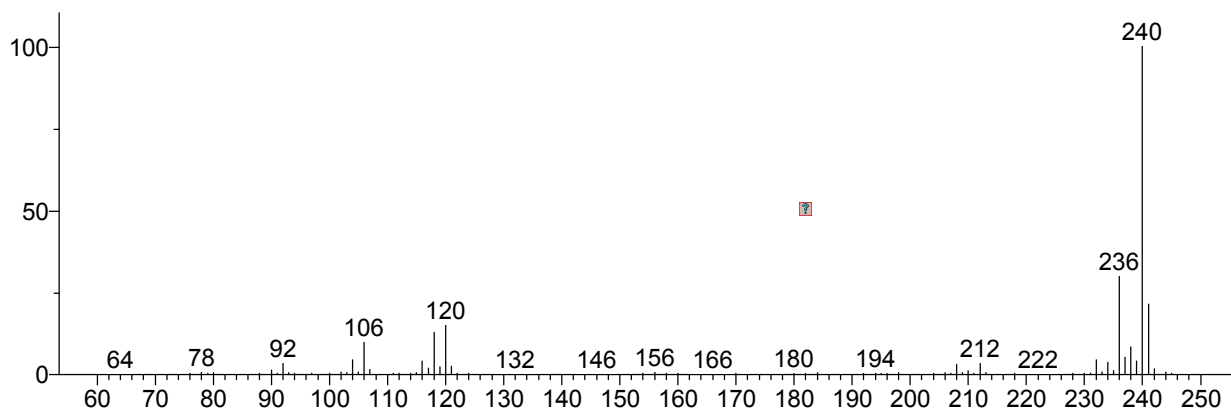


Hit 2 : Tetracosane  
C24H50; MF: 871; RMF: 874; Prob 7.87%; CAS: 646-31-1; Lib: replib; ID: 5841.



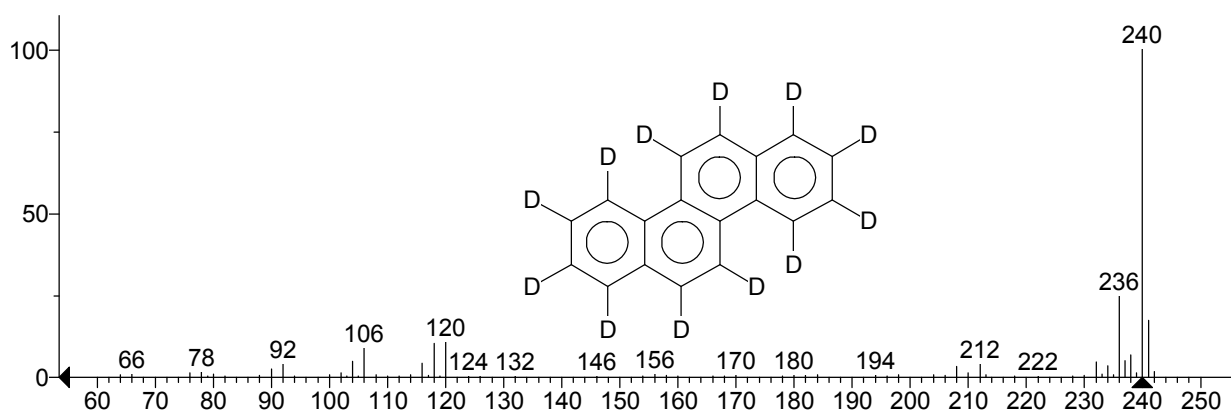
\*\* Search Report Page 1 of 1 \*\*

Unknown: +EI Scan (rt: 24.149, 24.220-24.240 min, 8 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = 333



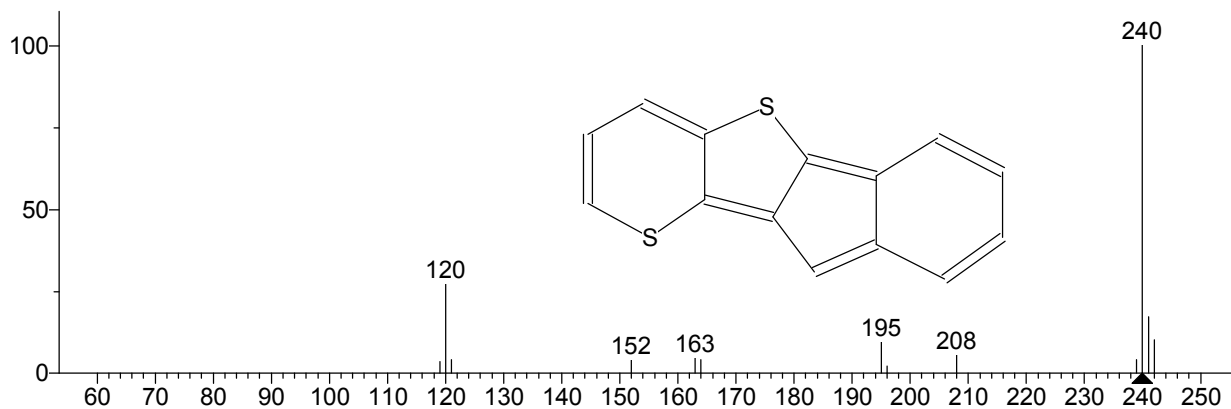
Hit 1 : Chrysene-D12

C18D12; MF: 879; RMF: 888; Prob 97.5%; CAS: 1719-03-5; Lib: mainlib; ID: 180711.

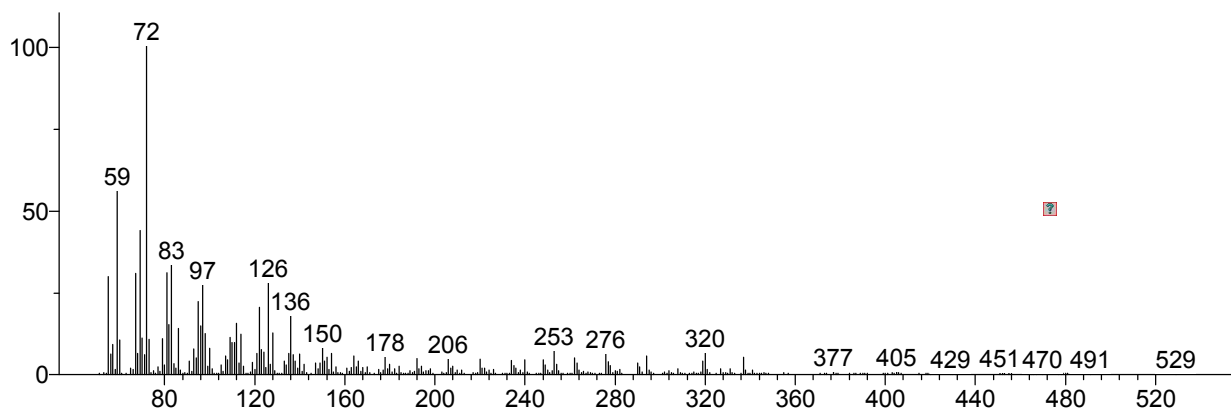


Hit 2 : Indeno[2',1':4,5]thieno[3,2-b]thiopyran

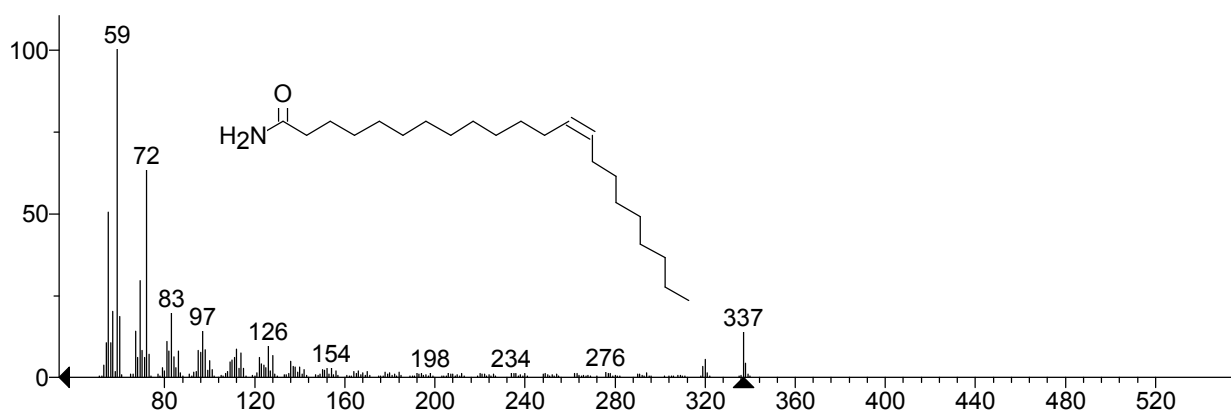
C14H8S2; MF: 656; RMF: 826; Prob 0.97%; CAS: 56830-85-4; Lib: mainlib; ID: 180533.



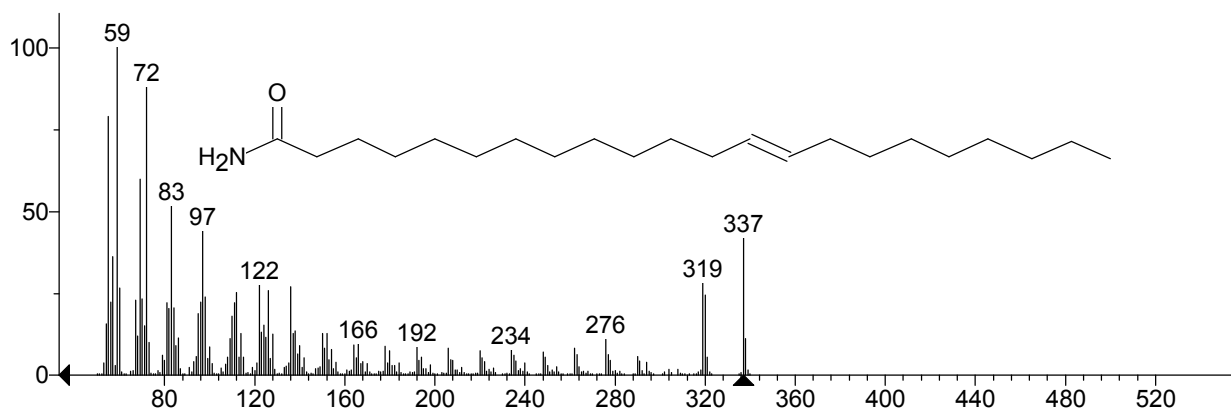
Unknown: +EI Scan (rt: 25.452-25.623 min, 52 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = -223



Hit 1 : 13-Docosenamide, (Z)-  
C<sub>22</sub>H<sub>43</sub>NO; MF: 818; RMF: 840; Prob 53.7%; CAS: 112-84-5; Lib: replib; ID: 6994.

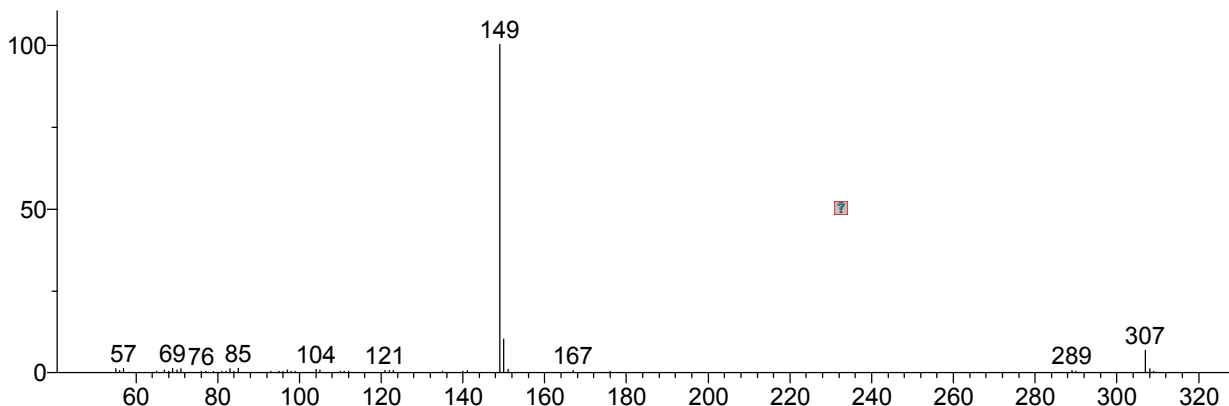


Hit 2 : trans-13-Docosenamide  
C<sub>22</sub>H<sub>43</sub>NO; MF: 806; RMF: 822; Prob 35.8%; CAS: 10436-09-6; Lib: mainlib; ID: 27659.

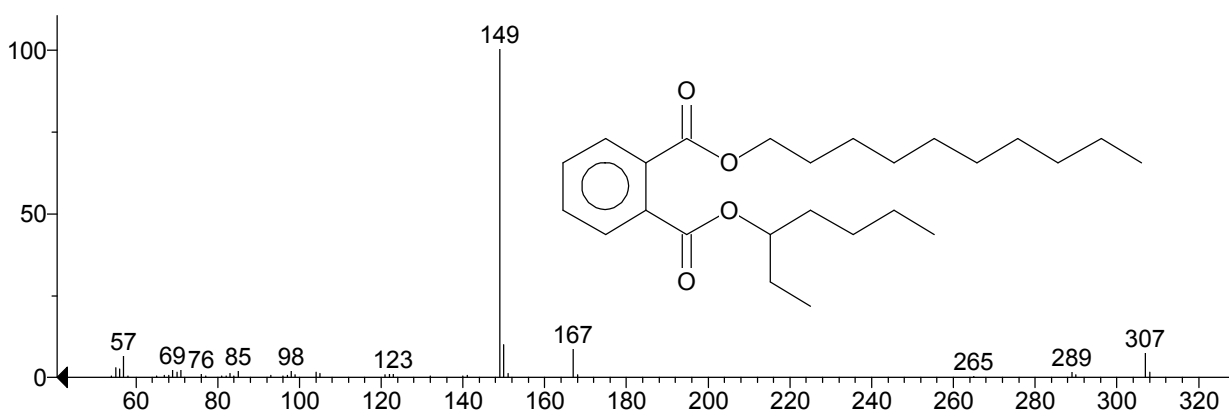


\*\* Search Report Page 1 of 1 \*\*

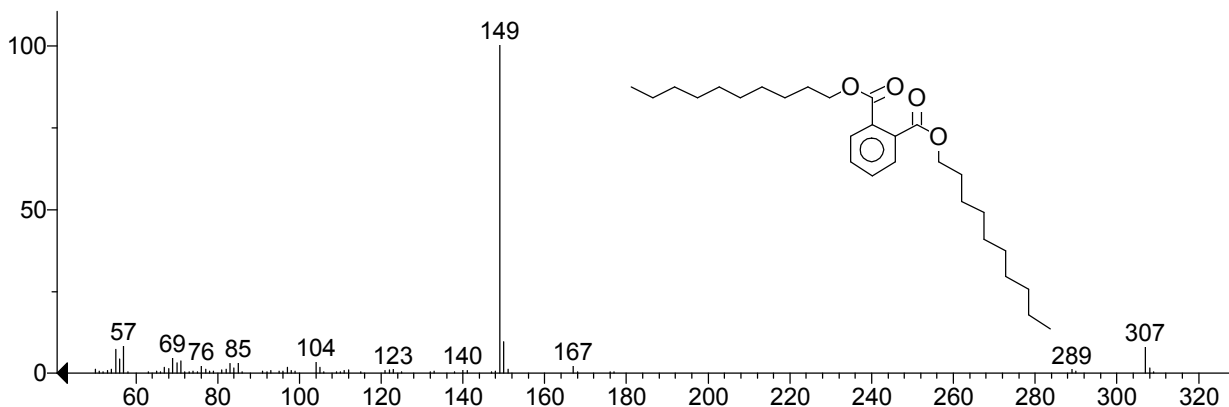
Unknown: +EI Scan (rt: 27.301, 27.362-27.382 min, 8 scans) J8674\_Unknown\_2.D Subtract  
Compound in Library Factor = -253



Hit 1 : Phthalic acid, decyl hept-3-yl ester  
C<sub>25</sub>H<sub>40</sub>O<sub>4</sub>; MF: 883; RMF: 884; Prob 9.81%; Lib: mainlib; ID: 122632.



Hit 2 : Didecyl phthalate  
C<sub>28</sub>H<sub>46</sub>O<sub>4</sub>; MF: 882; RMF: 882; Prob 9.43%; CAS: 84-77-5; Lib: replib; ID: 21755.

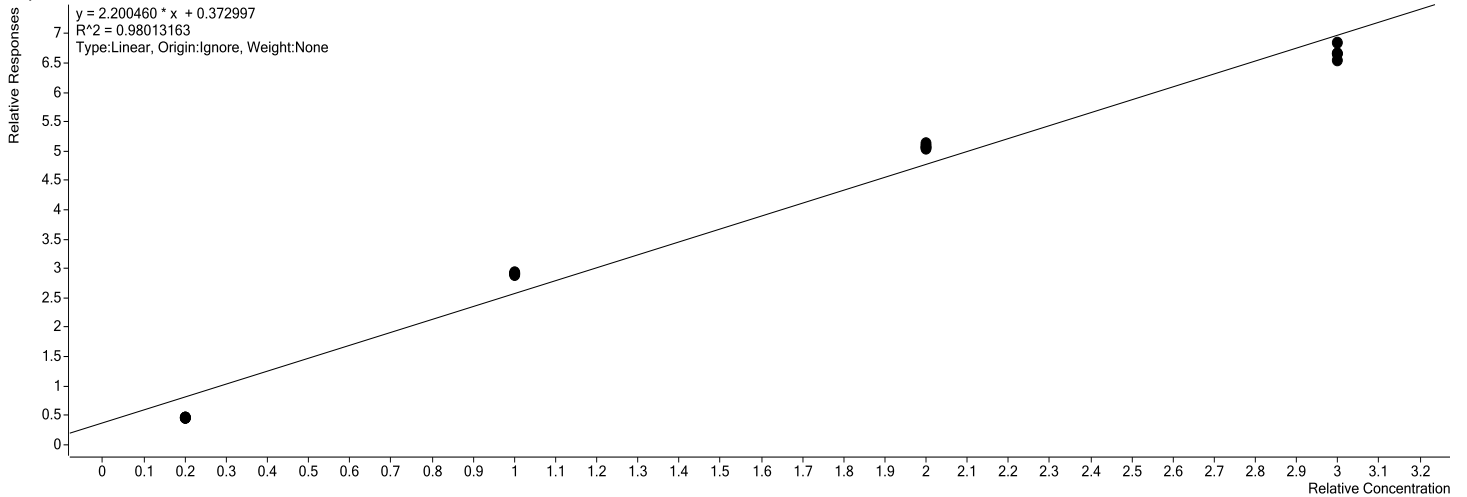


# Quantitative Analysis Compound Report

## Calibration Curve

### Ethylbenzene

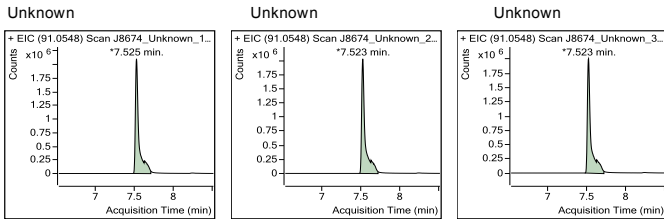
Ethylbenzene - 4 Levels, 4 Levels Used, 16 Points, 16 Points Used, 0 QCs



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Ethylbenzene	Toluene-d8	7.525	8781.6891	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Ethylbenzene	Toluene-d8	7.523	8714.6067	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Ethylbenzene	Toluene-d8	7.523	8942.7585	ng/ml

## Compound Graphics





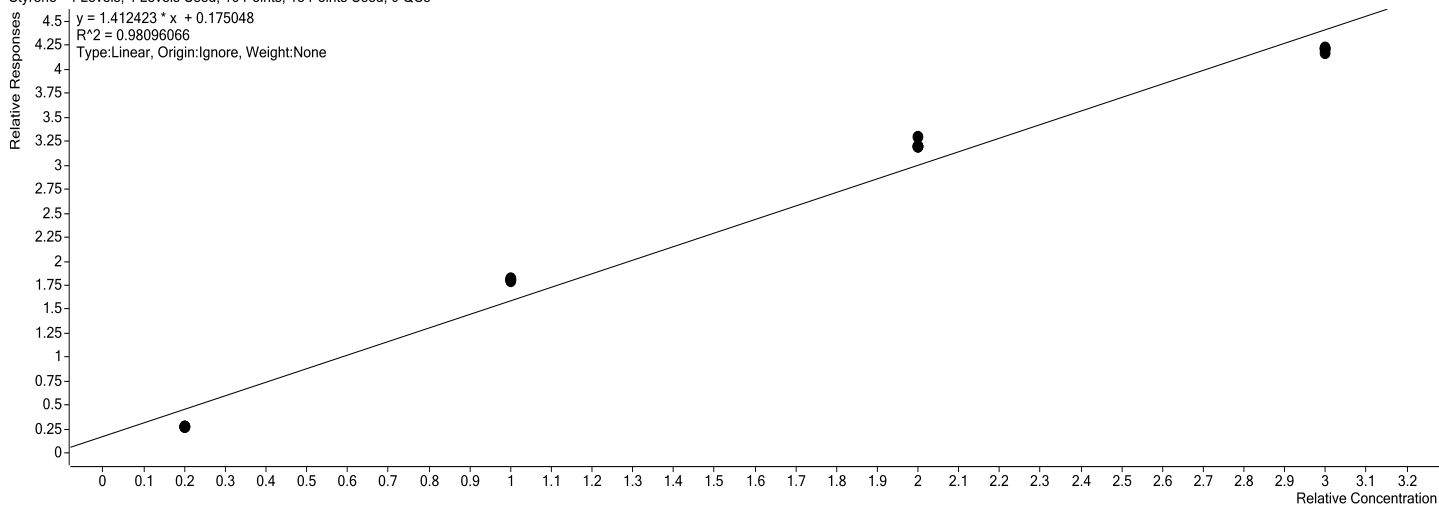
# Quantitative Analysis Compound Report

## Calibration Curve

### Styrene

Styrene - 4 Levels, 4 Levels Used, 16 Points, 13 Points Used, 0 QCs

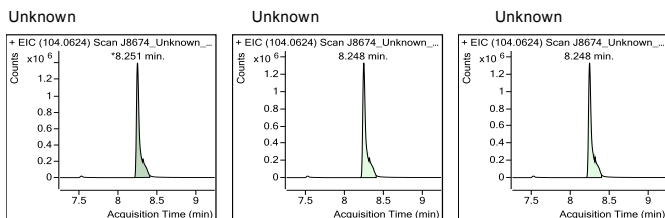
Relative Responses  
 $y = 1.412423 \cdot x + 0.175048$   
 $R^2 = 0.98096066$   
Type: Linear, Origin: Ignore, Weight: None



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Styrene	Toluene-d8	8.251	8810.7953	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Styrene	Toluene-d8	8.248	8695.9538	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Styrene	Toluene-d8	8.248	8848.2162	ng/ml

## Compound Graphics



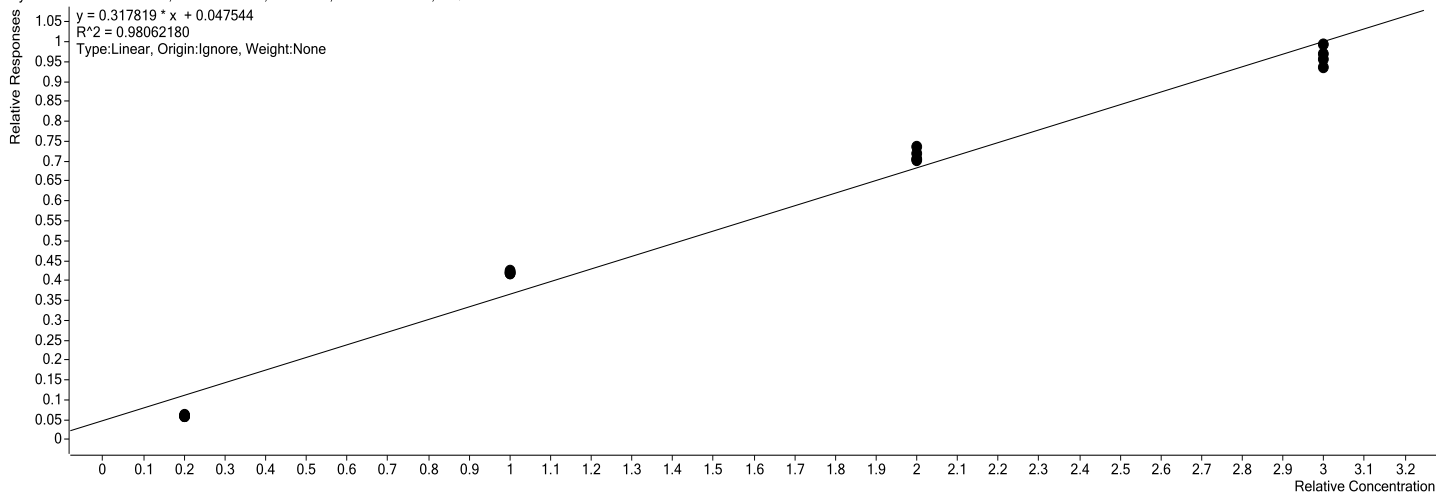
# Quantitative Analysis Compound Report

## Calibration Curve

### Cyclohexanone

Cyclohexanone - 4 Levels, 4 Levels Used, 16 Points, 16 Points Used, 0 QCs

$y = 0.317819 \cdot x + 0.047544$   
 $R^2 = 0.98062180$   
Type: Linear, Origin: Ignore, Weight: None

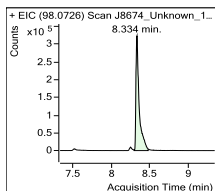


## Quantitation Results

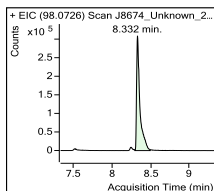
Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Cyclohexanone	Toluene-d8	8.334	8746.2079	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Cyclohexanone	Toluene-d8	8.332	8595.0818	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Cyclohexanone	Toluene-d8	8.332	8724.8747	ng/ml

## Compound Graphics

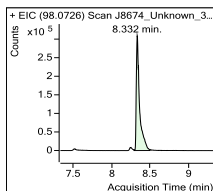
Unknown



Unknown



Unknown

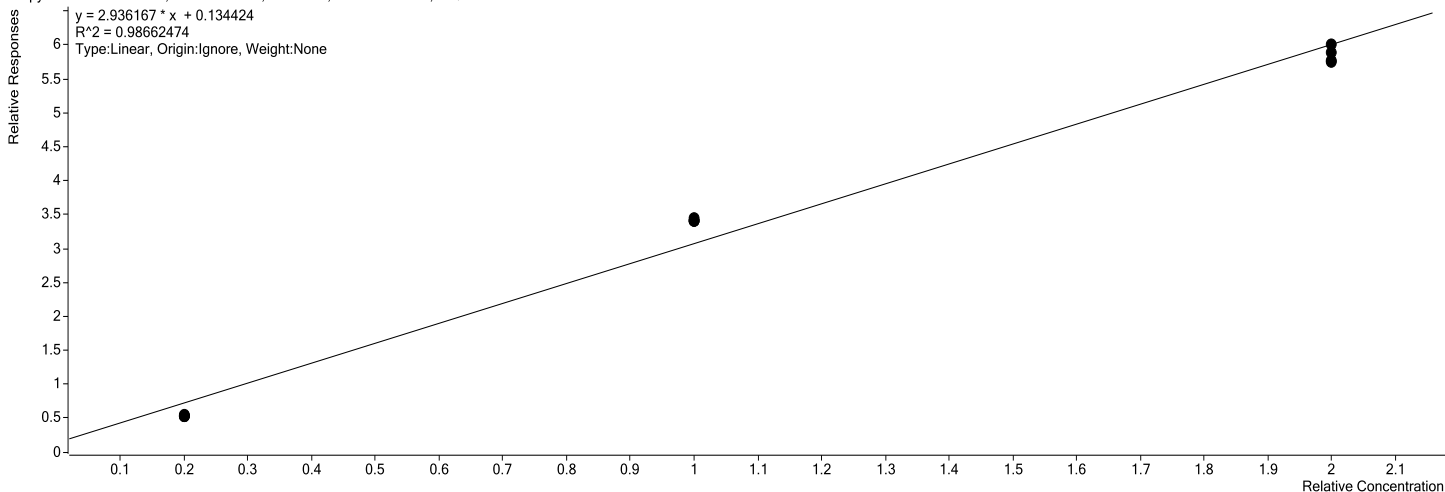


# Quantitative Analysis Compound Report

## Calibration Curve

### Propylbenzene

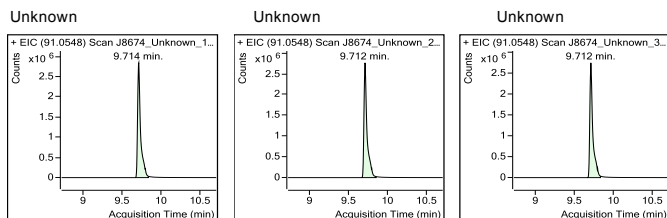
Propylbenzene - 3 Levels, 3 Levels Used, 12 Points, 12 Points Used, 0 QCs



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Propylbenzene	Toluene-d8	9.714	8167.5760	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Propylbenzene	Toluene-d8	9.712	8130.1805	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Propylbenzene	Toluene-d8	9.712	8156.9285	ng/ml

## Compound Graphics

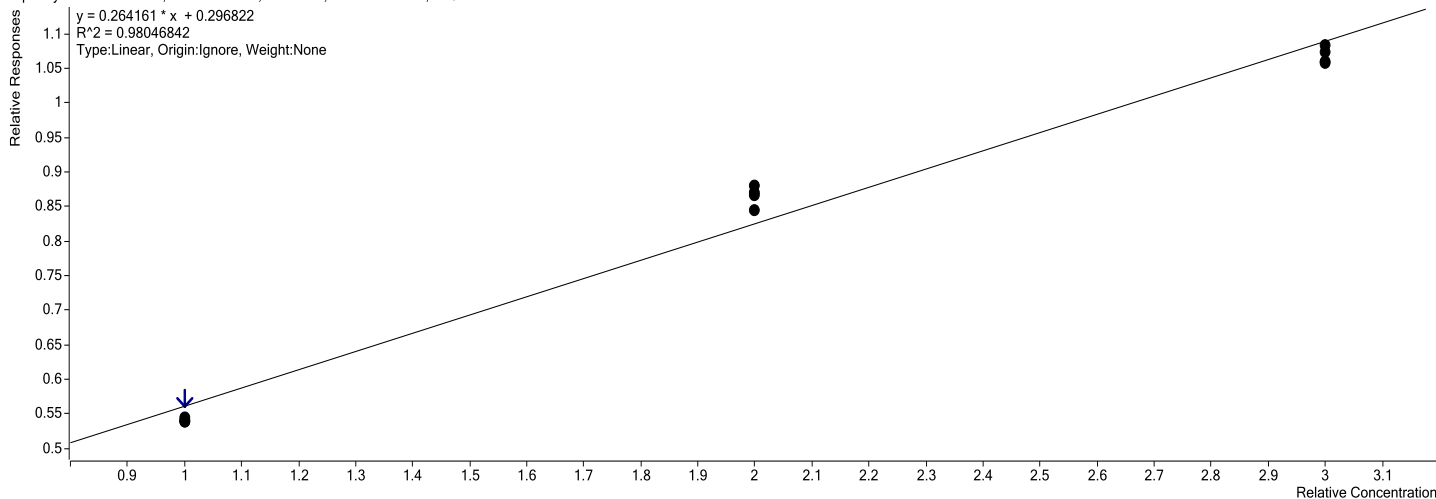


# Quantitative Analysis Compound Report

## Calibration Curve

Diphenyl ether

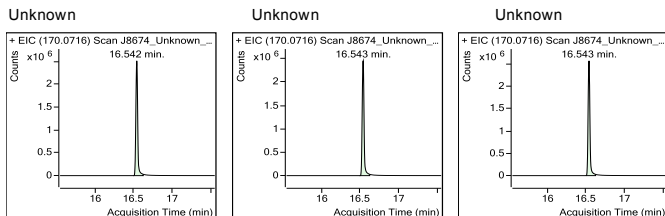
Diphenyl ether - 3 Levels Used, 12 Points, 12 Points Used, 0 QCs



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Diphenyl ether	Naphelene-d8	16.542	8307.1968	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Diphenyl ether	Naphelene-d8	16.543	8368.0811	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Diphenyl ether	Naphelene-d8	16.543	8749.5518	ng/ml

## Compound Graphics



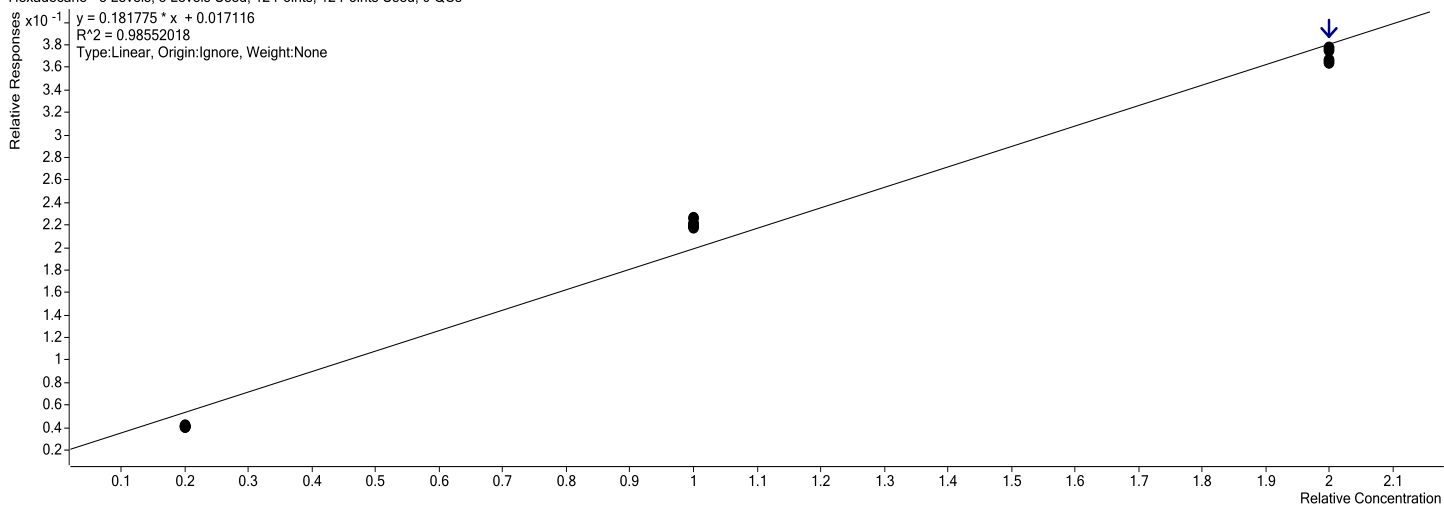
# Quantitative Analysis Compound Report

## Calibration Curve

### Hexadecane

Hexadecane - 3 Levels Used, 12 Points Used, 12 Points Used, 0 QCs

Relative Responses  
x10<sup>-1</sup>  
 $y = 0.181775 * x + 0.017116$   
 $R^2 = 0.98552018$   
Type: Linear, Origin: Ignore, Weight: None

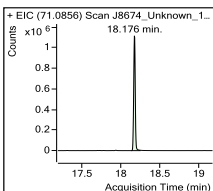


## Quantitation Results

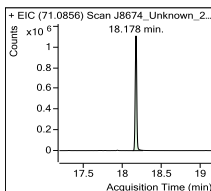
Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Hexadecane	Phenathrene-d10	18.176	8219.6286	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Hexadecane	Phenathrene-d10	18.178	8059.5013	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Hexadecane	Phenathrene-d10	18.177	8112.5690	ng/ml

## Compound Graphics

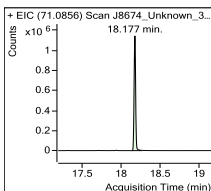
Unknown



Unknown



Unknown



# Quantitative Analysis Compound Report

## Calibration Curve

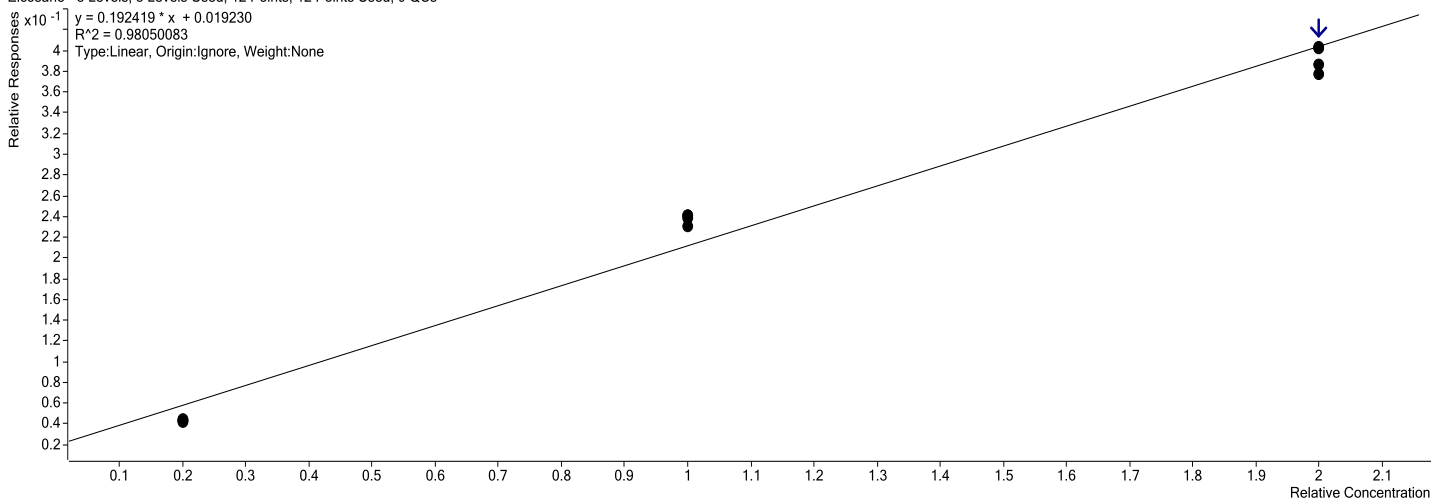
### Eicosane

Eicosane - 3 Levels, 3 Levels Used, 12 Points, 12 Points Used, 0 QCs

$$y = 0.192419 \cdot x + 0.019230$$

$$R^2 = 0.98050083$$

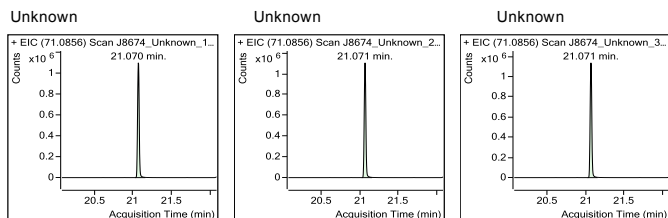
Type: Linear, Origin: Ignore, Weight: None



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Eicosane	Phenathrene-d10	21.070	8046.8813	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Eicosane	Phenathrene-d10	21.071	7941.9010	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Eicosane	Phenathrene-d10	21.071	8123.8427	ng/ml

## Compound Graphics

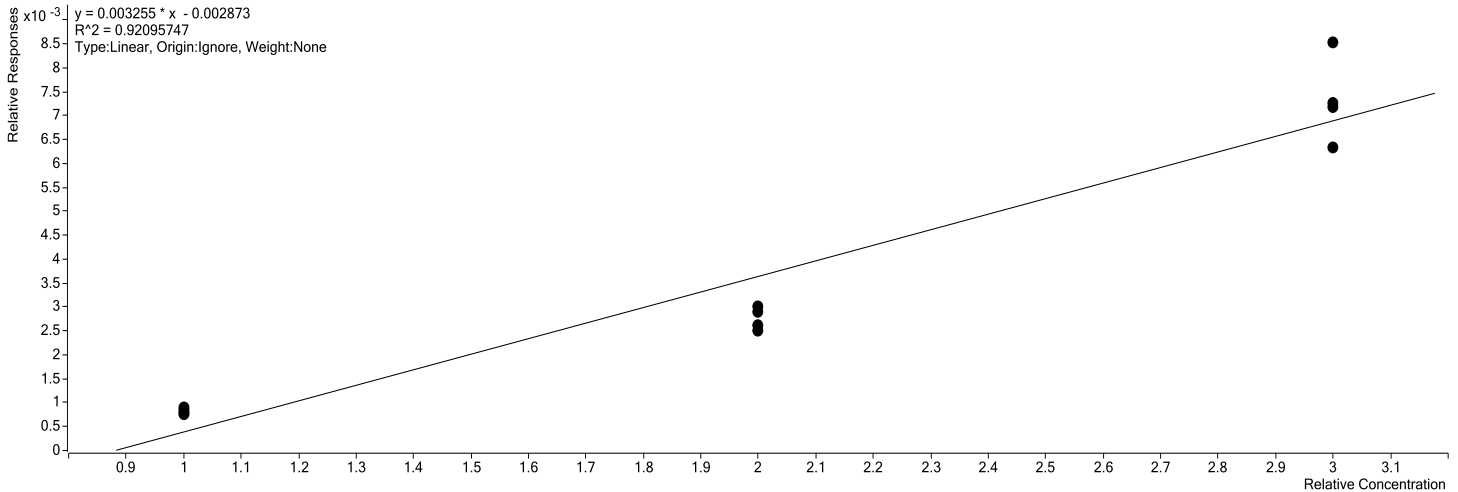


# Quantitative Analysis Compound Report

## Calibration Curve

### Steric acid

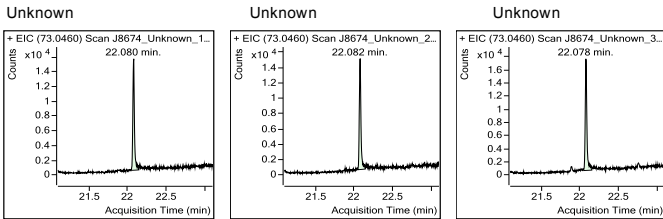
Steric acid - 3 Levels, 3 Levels Used, 12 Points, 12 Points Used, 0 QCs



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Steric acid	Chrysene-d12	22.080	7000.5321	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Steric acid	Chrysene-d12	22.082	6926.7417	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Steric acid	Chrysene-d12	22.078	7249.9159	ng/ml

## Compound Graphics

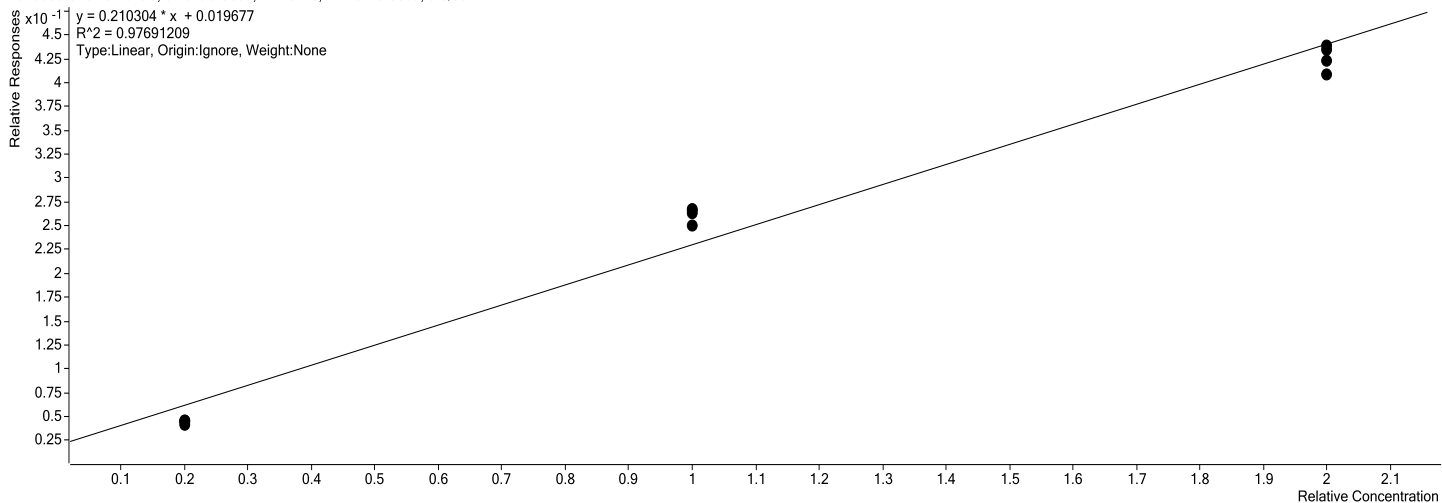


# Quantitative Analysis Compound Report

## Calibration Curve

### Tetracosane

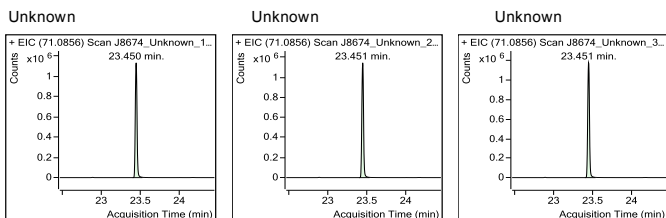
Tetracosane - 3 Levels, 3 Levels Used, 12 Points, 12 Points Used, 0 QCs



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Tetracosane	Phenathrene-d10	23.450	8068.9622	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Tetracosane	Phenathrene-d10	23.451	7973.4124	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Tetracosane	Phenathrene-d10	23.451	8181.3507	ng/ml

## Compound Graphics





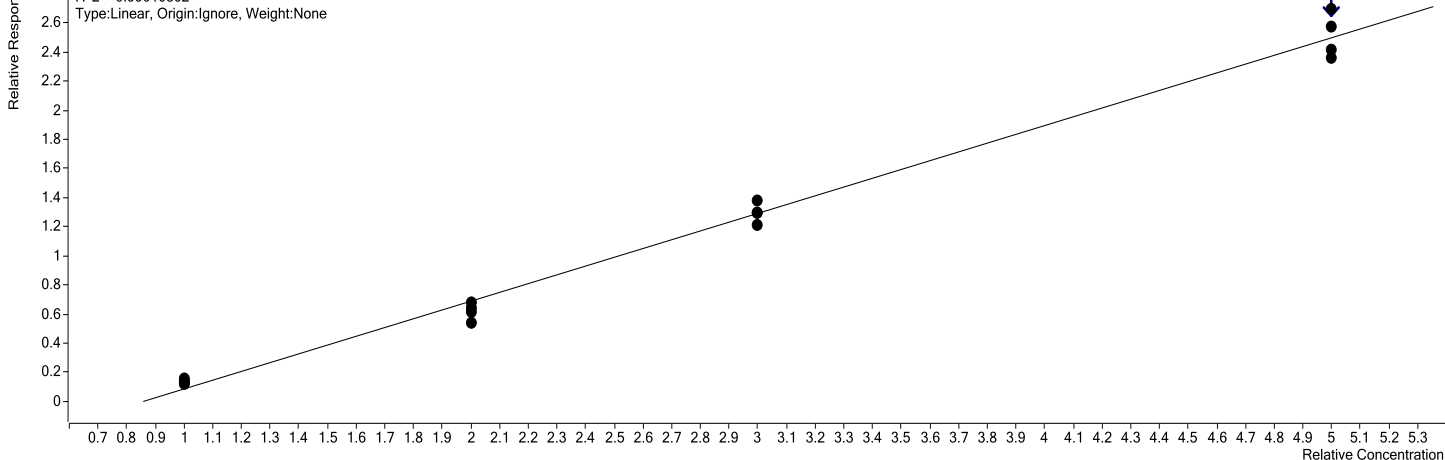
# Quantitative Analysis Compound Report

## Calibration Curve

### Erucamide

Erucamide - 4 Levels, 4 Levels Used, 16 Points, 16 Points Used, 0 QCs

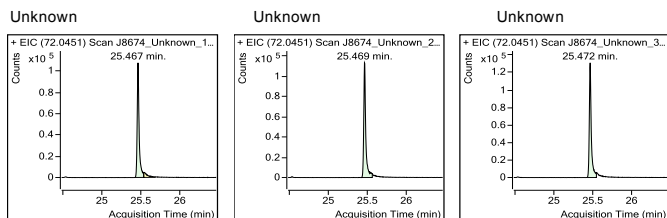
Relative Responses  
x10<sup>-1</sup>  
 $y = 0.060286 * x - 0.051710$   
 $R^2 = 0.99010302$   
Type: Linear, Origin: Ignore, Weight: None



## Quantitation Results

Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Erucamide	Phenathrene-d10	25.467	7402.5067	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Erucamide	Phenathrene-d10	25.469	7690.7770	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Erucamide	Phenathrene-d10	25.472	8025.2478	ng/ml

## Compound Graphics



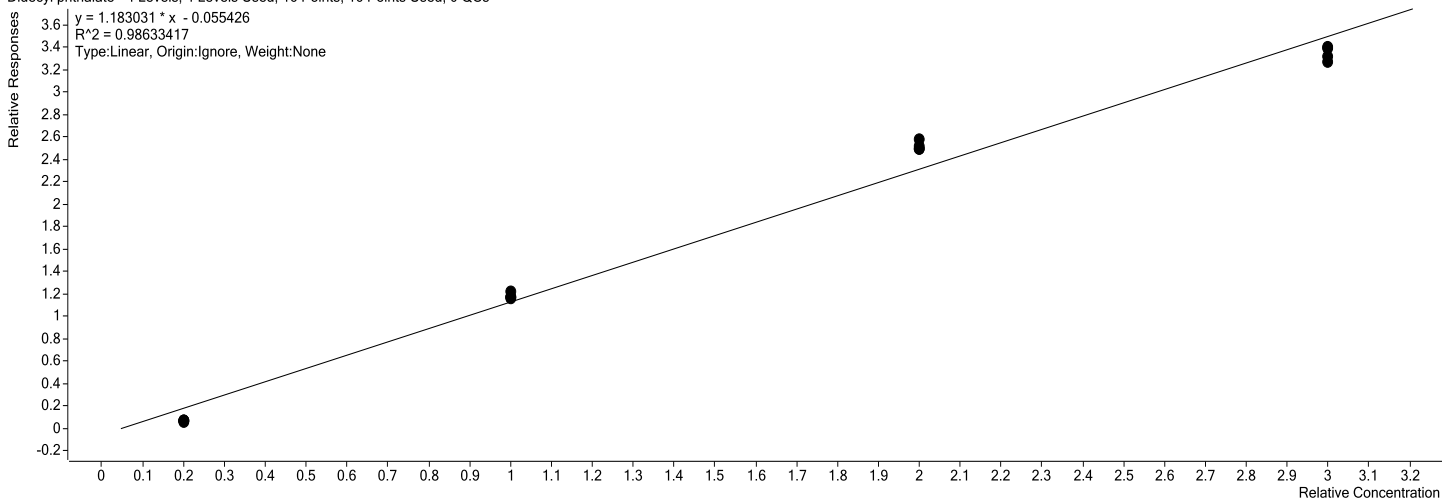
# Quantitative Analysis Compound Report

## Calibration Curve

### Didecyl phthalate

Didecyl phthalate - 4 Levels, 4 Levels Used, 16 Points, 16 Points Used, 0 QCs

$y = 1.183031 \cdot x - 0.055426$   
 $R^2 = 0.98633417$   
Type: Linear, Origin: Ignore, Weight: None

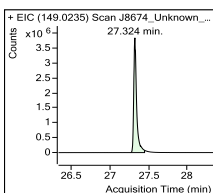


## Quantitation Results

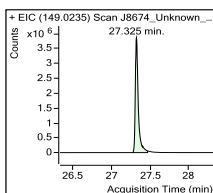
Data File	Type	Sample Name	Compound	ISTD	RT	Final Conc	
J8674_Unknown_1.D	Sample	Unknown	Didecyl phthalate	Phenathrene-d10	27.324	8673.3033	ng/ml
J8674_Unknown_2.D	Sample	Unknown	Didecyl phthalate	Phenathrene-d10	27.325	8952.0678	ng/ml
J8674_Unknown_3.D	Sample	Unknown	Didecyl phthalate	Phenathrene-d10	27.328	8985.6857	ng/ml

## Compound Graphics

Unknown



Unknown



Unknown

