

Supporting Information for

Edible *Inonotus dryadeus* Fungi with Quick Separation of Water Pollutant Oils and Methylene Blue Dye

Balaprasad Ankamwar

*Bio-Inspired Materials Research Laboratory, Department of Chemistry, Savitribai Phule
Pune University (Formerly University of Pune), Ganeshkhind, Pune-411007, India
Email: bgankamwar@chem.unipune.ac.in*

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1. Experimental Section

1.1. Chemicals and Materials.

Methylene Blue dye (Merck), Congo Red (HiMedia), Eosin Yellowish (Merck), Bromo Cresol Green (HiMedia), 5% Lambda cyhalothrin pesticide solution of boxer brand (Sun and Ocean Agro India Ltd.) HCl (Merck), NaOH (HiMedia), Ammonia (Merck) used as received.

1.2. Isolation of *Inonotus dryadeus* Fungi from Natural Source.

The orange brownish and spongy fungi grow on stipule of the tree during rainy season, which becoming dark on drying; exuding amber-colored droplets when young, through its pores. Fungi sample was collected from stipule of the *Delonix regia* tree in and around University of Pune campus. It was then squeezed to get an extract and the fungi were observed to change color from yellowish orange to dark brown as soon as extract was taken out. When it was kept in a beaker for 20 minutes, this liquid forms two layers; a black brown substance settled down, while a supernatant and completely transparent lemon colored liquid stays above. The supernatant did not show adsorption/separation of MB. The brown sediment at the bottom of the beaker was harvested and dried in hot air oven for 6 hours at 70°C.

1.3. Oils and Pesticide Separation Tests.

LCP, EO and UEO were used in this study. The adsorption capacity values, W (wt/wt) times were obtained by measuring the mass of the dry *Inonotus dryadeus* (DID) before and after adsorption of oils/pesticide. The samples were left submerged in the layer of pesticide or oils formed over de-ionized and marine water overnight to ensure full saturation and it was obtained before weighing; followed by rapid weighing to avoid evaporation of adsorbed oils or pesticides. Here the test was carried out with marine water, to explore possibility of viable solution for oil spillage in sea and oceans during transport.

1.4. Dye Separation Test.

Series of experiments were carried out with different concentrations of methylene blue dye and various amounts of DID. It was found out that the optimum quantity to completely decolorize the solution of MB was 5.5 mg for 10 ml of 5 ppm solution. Another solution of 25 ppm and 50 ml volume was added to 5 mg DID to calculate Q_e value after 24 hours. The DID still decolorized the MB. It should be noted here that fungi extract can be directly used for the same purpose without drying or any other modification. Drying of settled substance in this case was carried out for the purpose of quantification. Decolorization of MB was monitored by UV-visible spectrophotometer (Shimatzu).

2. Physical and Chemical Desorption of MB dye

2.1. Physical Desorption of MB Dye

It was carried out by adding drops of aqueous MB dye solution in DID powder and pressed through filter paper. Desorption of dye did not occur. Photographic images in Figure S1.



Figure S1. Photographic images of physical desorption of MB dye from DID by dropping aqueous MB dye solution on DID powder and followed by pressing through filter paper. Desorption of dye did not occur.

2.2. Chemical Desorption Study of Methylene Blue Dye

Chemical desorption of MB using DID was carried out with different solvents and solutions such as acetone (1), benzene (2), chloroform (3), ethyl alcohol (4), ethyl acetate (5), methanol (6), petroleum ether (7), ammonia (8), HCl (9), H₂SO₄ (10), NaOH (11) and checked at interval of 12 hr (a), 42 hr (b) and 66 hr (c). However desorption did not occur. Photographic images in Figure S2.



Figure S2. Chemical desorption study of methylene blue dye adsorbed on DID was carried out with different solvents and solutions such as acetone (1), benzene (2), chloroform (3), ethyl alcohol (4), ethyl acetate (5), methanol (6), petroleum ether (7), ammonia (8), HCl (9), H₂SO₄

(10), NaOH (11) and checked at interval of 12 hr (a), 42 hr (b) and 66 hr (c). However, desorption did not occur.

3. DID as a Fuel

Combustion test of engine oil, used engine oil and DID compared in **(Figure S3)**

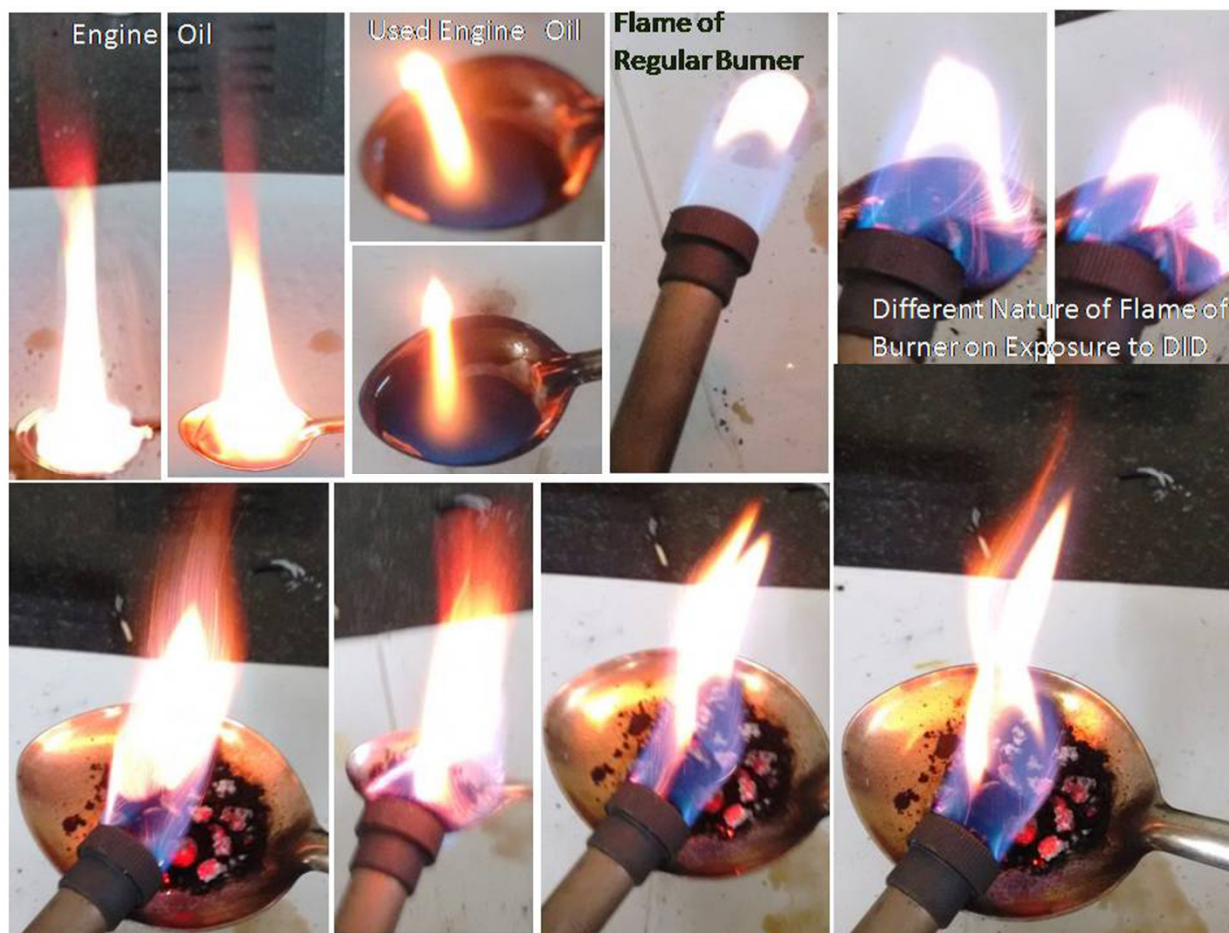


Figure S3. Photographic images of burning test of engine oil, used engine oil and DID.

Different photographic images reveal coal like nature of DID as source of fuel (**Figure S4**).



Figure S4. Different photographic images reveal coal like nature of DID as the fuel.

4. Reusability Test for Oil Extraction

In this study engine oil was adsorbed with DID followed by extraction by pressing and repeating the cycle (**Figure S5**).

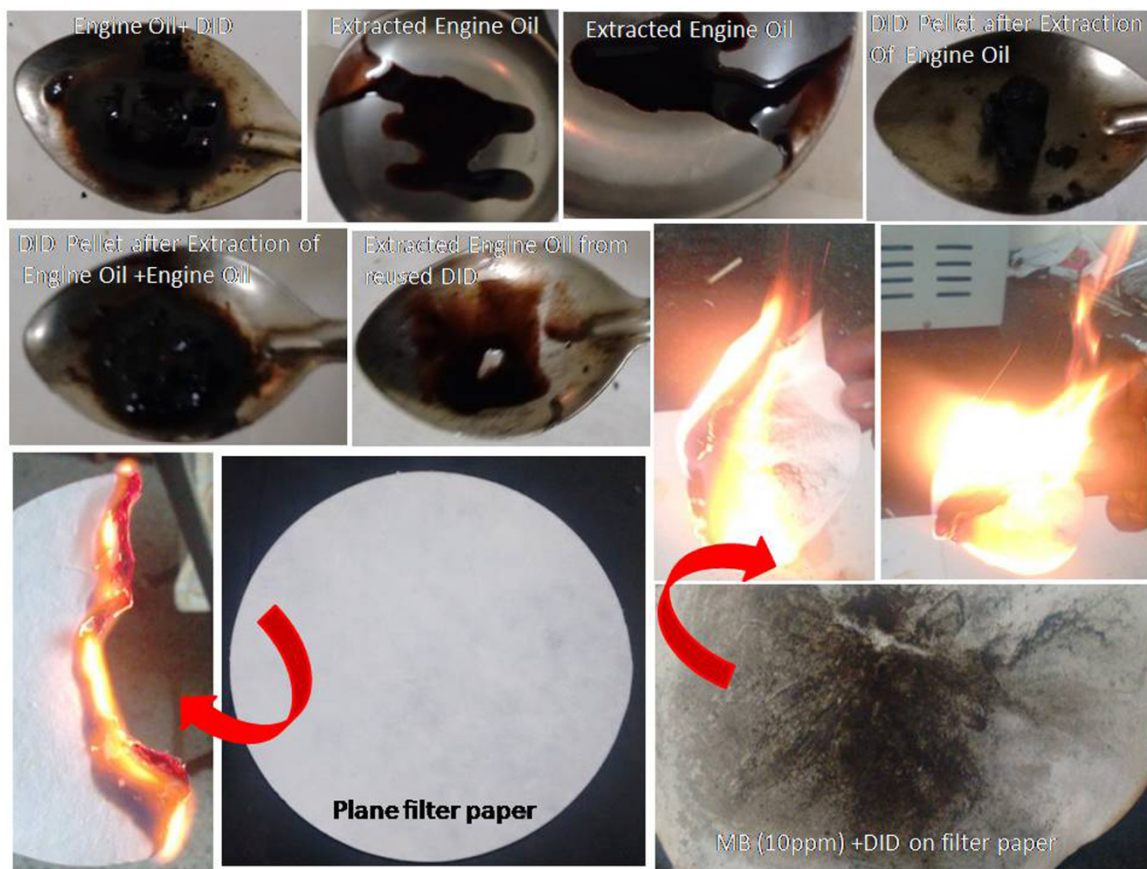


Figure S5. In this study engine oil was adsorbed with DID followed by extraction by pressing and repeating the cycle. Combustion test of plane filter paper and MB dye adsorbed precipitate on filter paper was carried out to check its reusability as the source of fuel.

5. Quantitative Adsorption of MB Dye

The study on the quantitative adsorption of MB dye in the range of 5-20 ppm using DID was fixed after series of trial experiments using simple UV-visible spectrophotometric technique. Supporting Information (**Figure S6**) displays UV-visible spectra of MB samples (1) using various concentrations of MB dye such as 5 ppm (a), 10 ppm (b), 15 ppm (c), 20 ppm (d); and (2) immediately after addition of 5.5 mg of DID. UV-Visible spectra of 5 to 20 ppm MB clearly indicates that MB from 5 ppm sample quick and completely separated by DID. This can be visibly revealed by inset images of S7, which represents 5 ppm MB solution (curve 1) and decolorized solution immediately after addition of 5.5 mg of DID (curve 2). Brown colored DID turns into bluish black colour after it has decolorized MB solution.

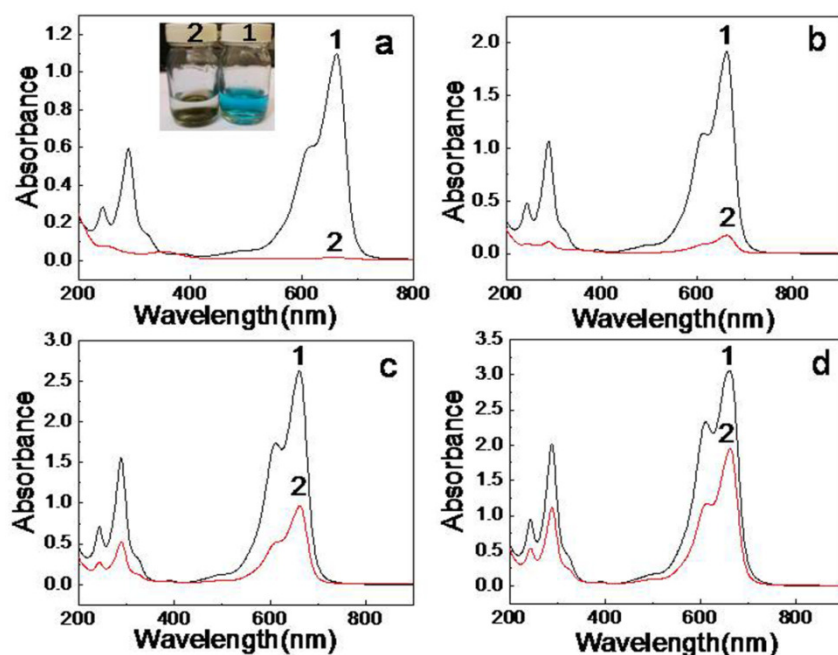


Figure S6. UV-Vis spectrum of (1) MB solution of 5 ppm (a), 10 ppm (b), 15 ppm (c), 20 ppm (d) and (2) immediately after addition of 5.5 mg of DID powder; Inset images of Fig. 1a represent 5 ppm MB solution (1) and decolorized solution immediately after addition of 5.5 mg of DID powder (2).

Table S1. Comparative adsorption investigation and pH effect on removal of dyes

This study was carried out considering four dyes to understand better efficiency, as summarized in the table appended below. Photographic images and UV-visible data of all the dyes at two different concentrations (5ppm and 10ppm) and at various pH values (2, 4, 6, 7, 8, 10, 12) are added in supporting information (**Figure S7 – S11**).

Sr. No.	Name of Dye	Concentration of Dye	pH Adjusted By	pH/pH Range of Complete Adsorption of Dye
1	MB	5ppm and 10ppm	HCl and NaOH	6-12
2	MB	5ppm and 10ppm	HCl and Ammonia	6-12
3	CR	5ppm and 10ppm	HCl and Ammonia	2
4	EY	5ppm and 10ppm	HCl and Ammonia	2
5	BCG	5ppm and 10ppm	HCl and Ammonia	2

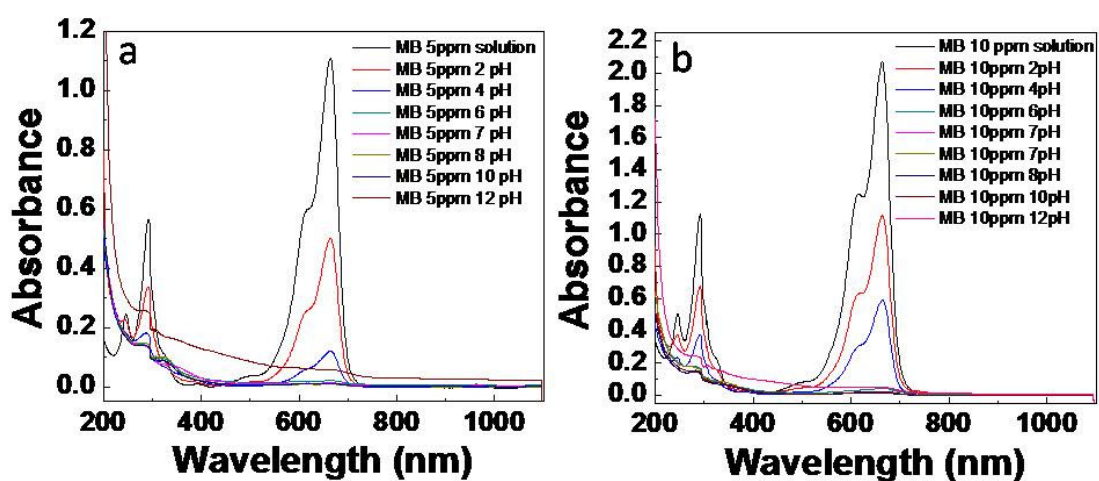
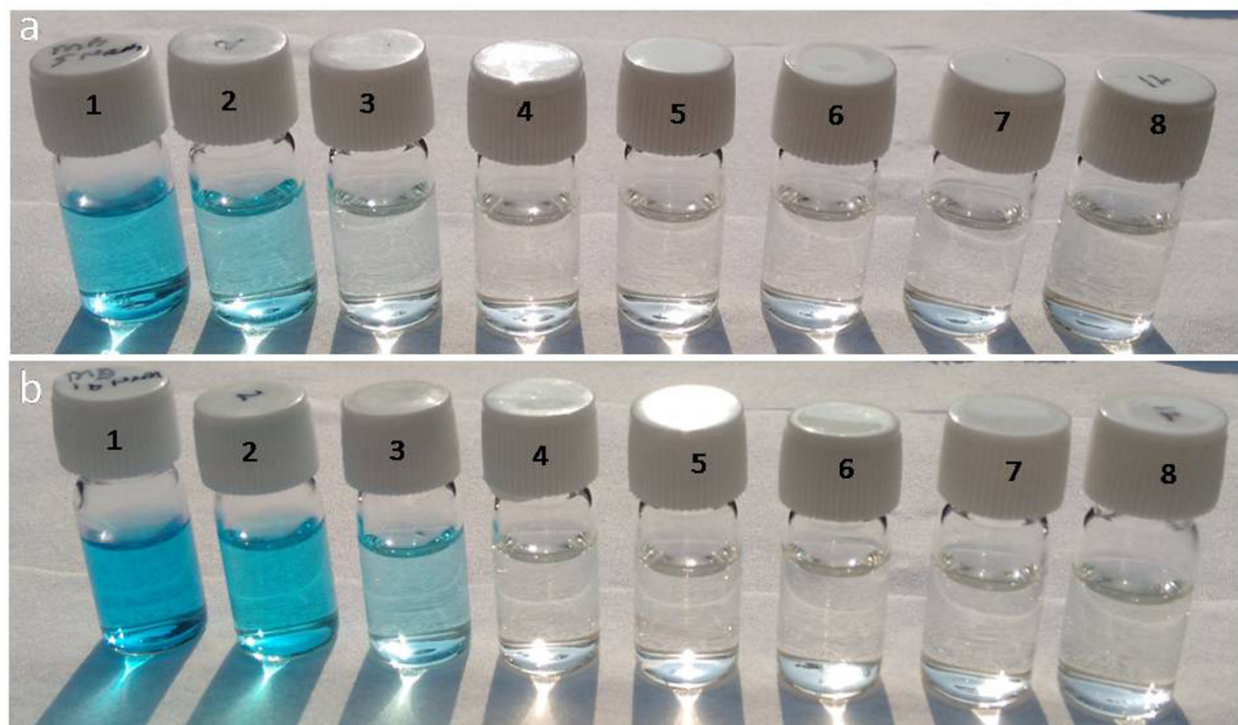


Figure S7. Photographic images of methylene blue (MB) solution at two concentrations 5ppm (a) and 10ppm (1) and after adjusting pH by HCl and NaOH followed by reaction with DID at various pH values pH 2 (2), pH 4 (3), pH 6 (4), pH 7 (5), pH 8 (6), pH 10 (7) and pH 12 (8). Corresponding UV-visible spectra a and b for 5 and 10 ppm respectively.

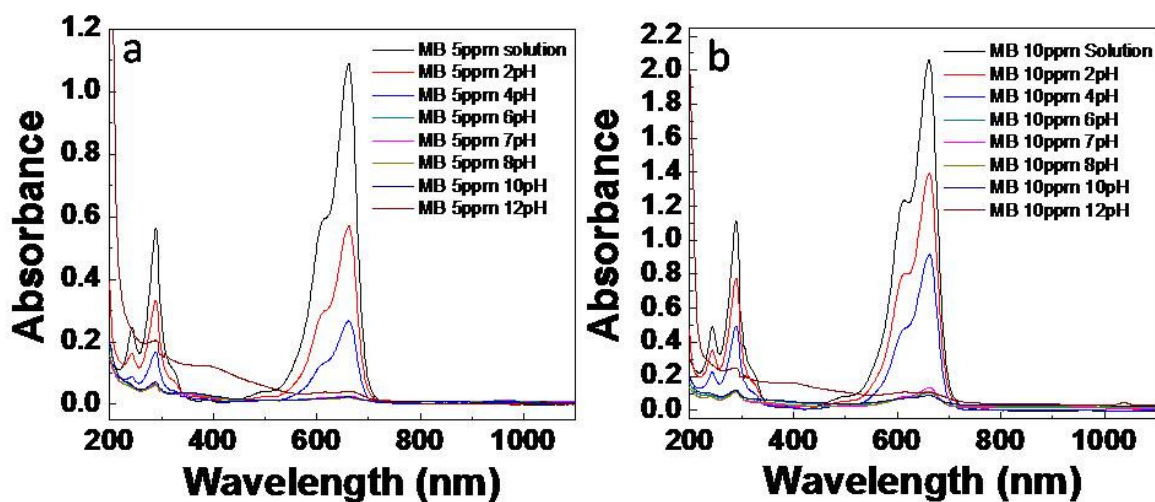
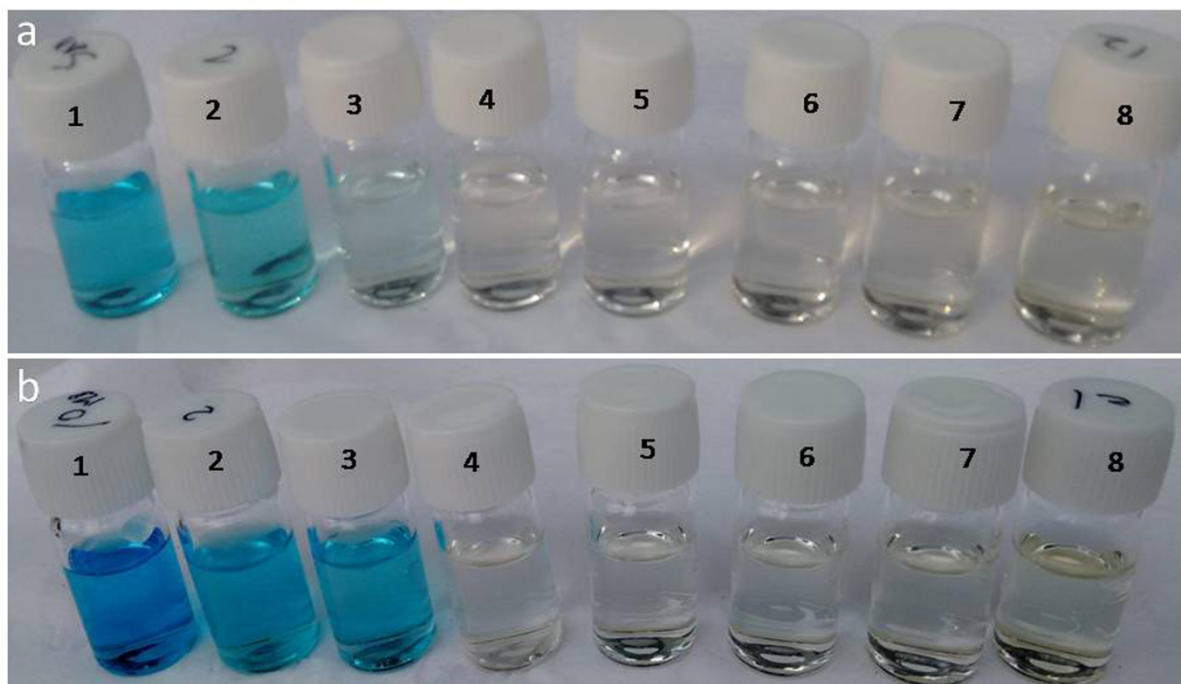


Figure S8. Photographic images of MB solution at two concentrations 5ppm (a) and 10ppm (1) and after adjusting pH by HCl and ammonia followed by reaction with DID at various pH values; pH 2 (2), pH 4 (3), pH 6 (4), pH 7 (5), pH 8 (6), pH 10 (7) and pH 12 (8). Corresponding UV-visible spectra a and b for 5 and 10 ppm respectively.

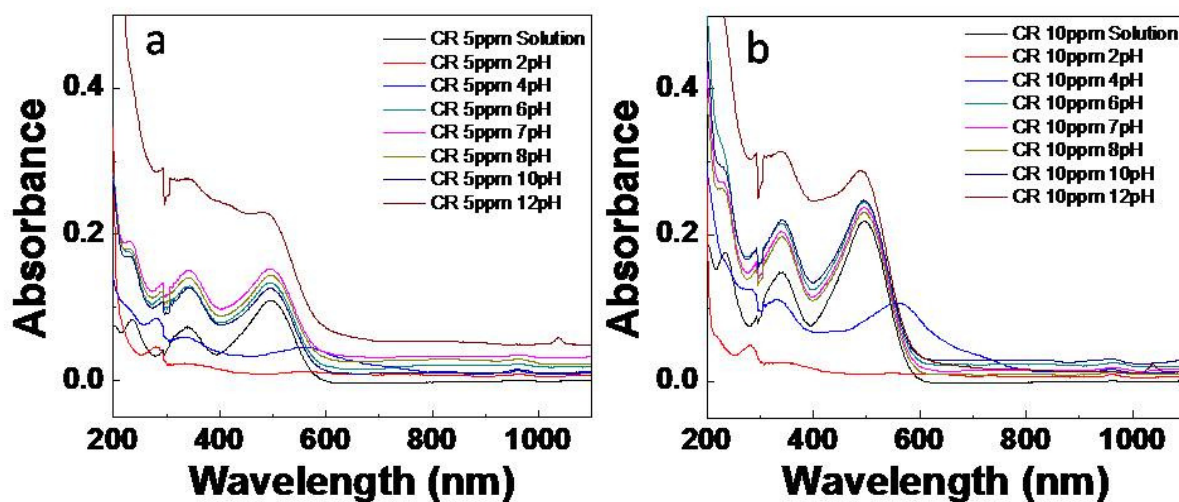
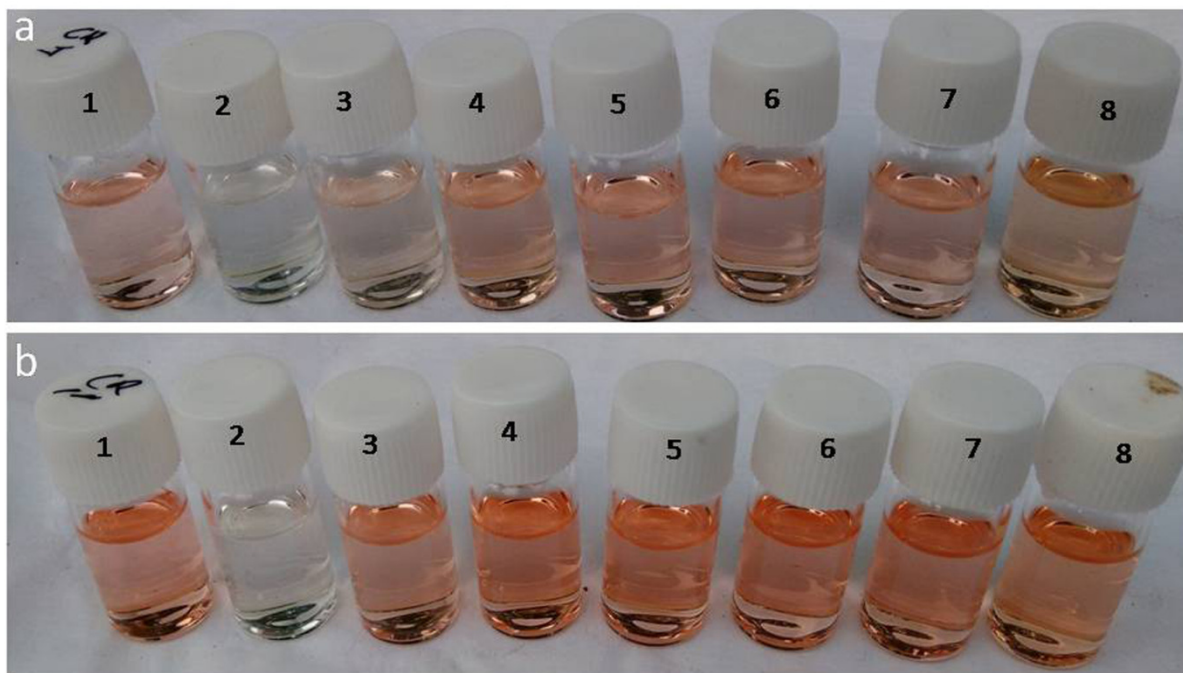


Figure S9. Photographic images of Congo Red (CR) solution at two concentrations 5ppm (a) and 10ppm (1) and after adjusting pH by HCl and ammonia followed by reaction with DID at various pH values; pH 2 (2), pH 4 (3), pH 6 (4), pH 7 (5), pH 8 (6), pH 10 (7) and pH 12 (8). Corresponding UV-visible spectra a and b for 5 and 10 ppm respectively.

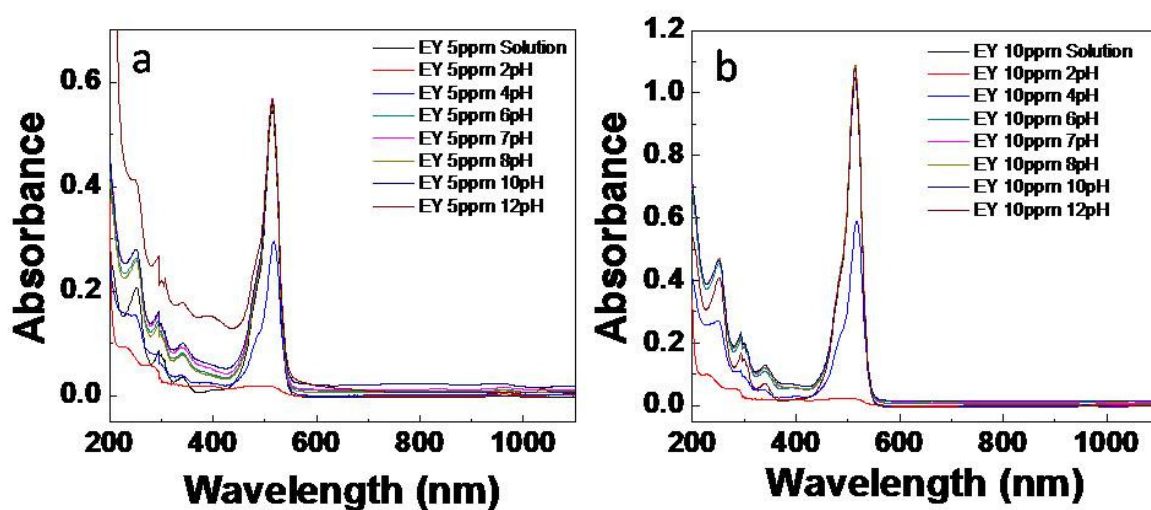
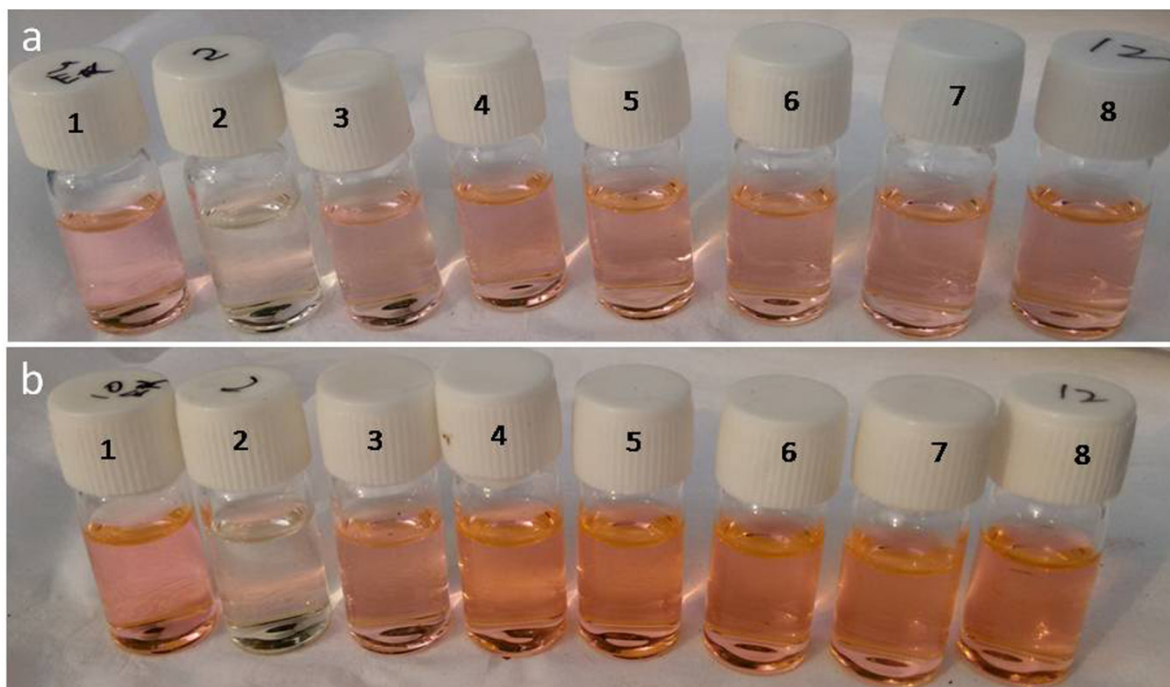


Figure S10. Photographic images of Eosin Yellowish (EY) solution at two concentrations 5ppm (a) and 10ppm (1) and after adjusting pH by HCl and ammonia followed by reaction with DID at various pH values; pH 2 (2), pH 4 (3), pH 6 (4), pH 7 (5), pH 8 (6), pH 10 (7) and pH 12 (8). Corresponding UV-visible spectra a and b for 5 and 10 ppm respectively.

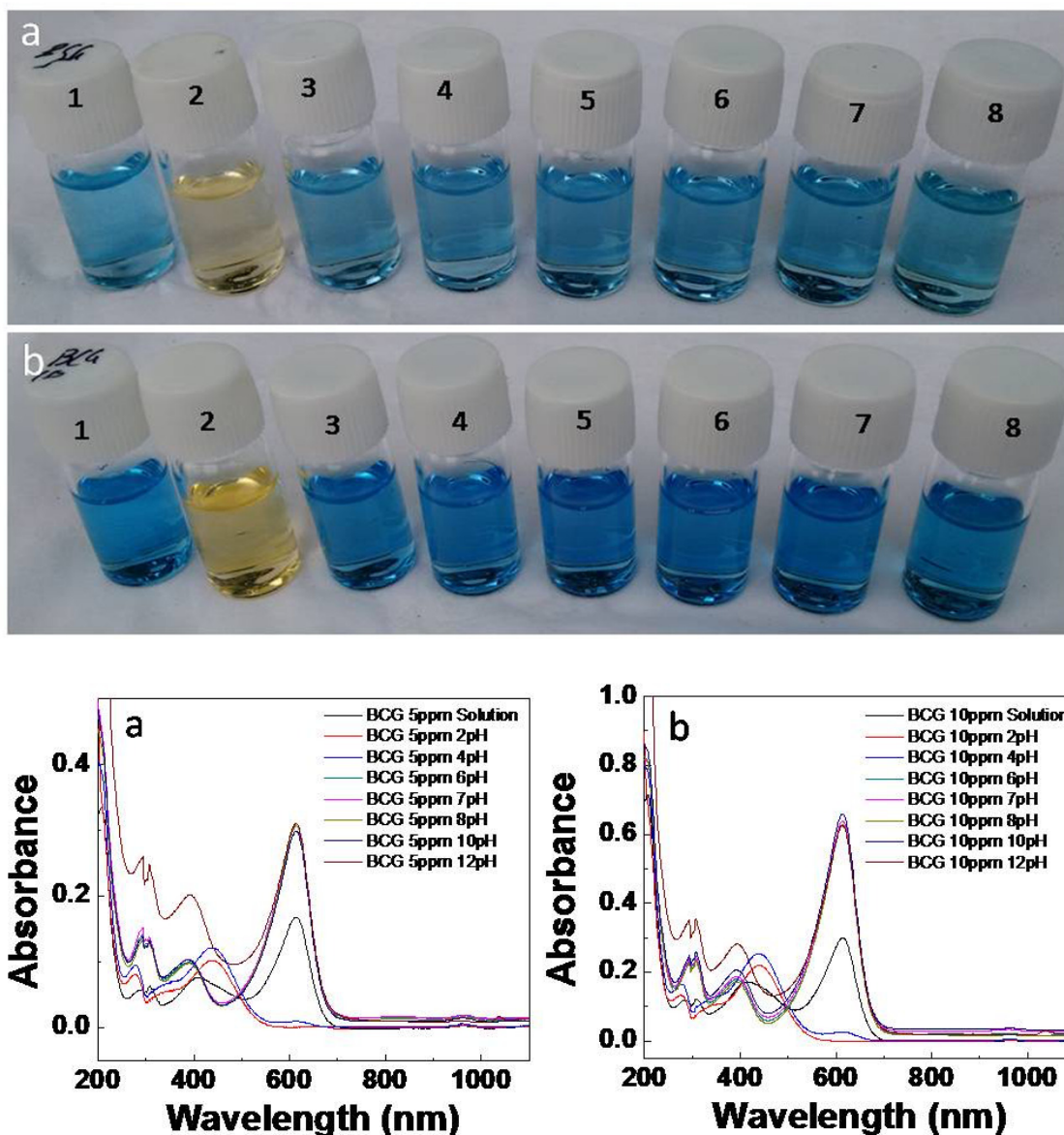


Figure S11. Photographic images of Bromo Cresol Green (BCG) solution at two concentrations 5ppm (a) and 10ppm (1) and after adjusting pH by HCl and ammonia followed by reaction with DID at various pH values; pH 2 (2), pH 4 (3), pH 6 (4), pH 7 (5), pH 8 (6), pH 10 (7) and pH 12 (8). Corresponding UV-visible spectra a and b for 5 and 10 ppm respectively.

Figures S12. GCMS analysis data of *Inonotus dryadeus* (Solvent-Methanol)

Instrument used for analysis: Shimatzu, GC 2010 Plus

Column Oven Temperature 80°C

Injection Temperature 260°C

Injection Mode: Split

Carrier Gas: Helium Prim. Press. 500-900

Flow Control Mode: Linear Velocity

Pressure: 80.4 kPa

Total Flow: 33.9 ml/min

Column Flow: 1.19 ml/min

Linear Velocity: 40.2 cm/sec

Purge Flow: 30 ml/min

Column Oven Temperature

	Rate	Final Temperature	Hold Time
0	-	80.0	0.00
1	15.0	240.0	4.00
2	10.0	290.0	8.00
3	0.00	0.00	0.00

Total Programme Time: 27.67 min.

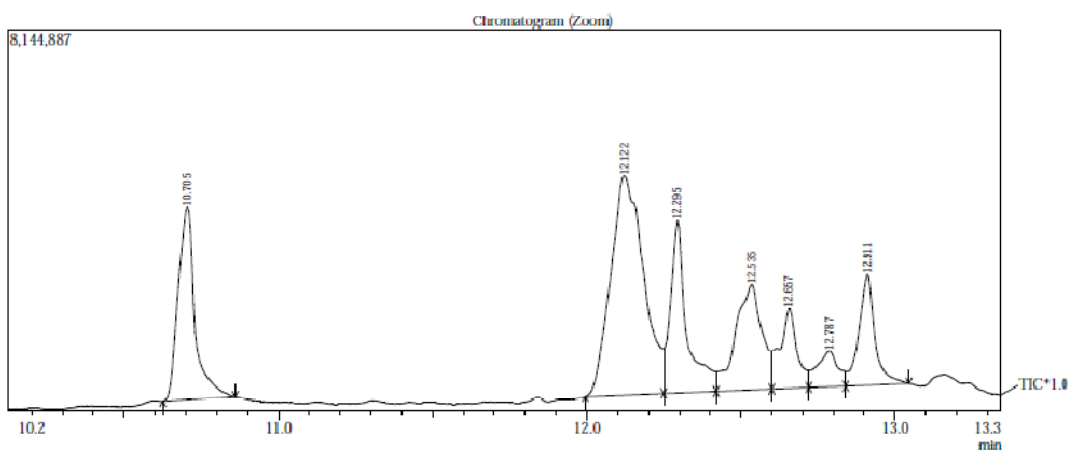
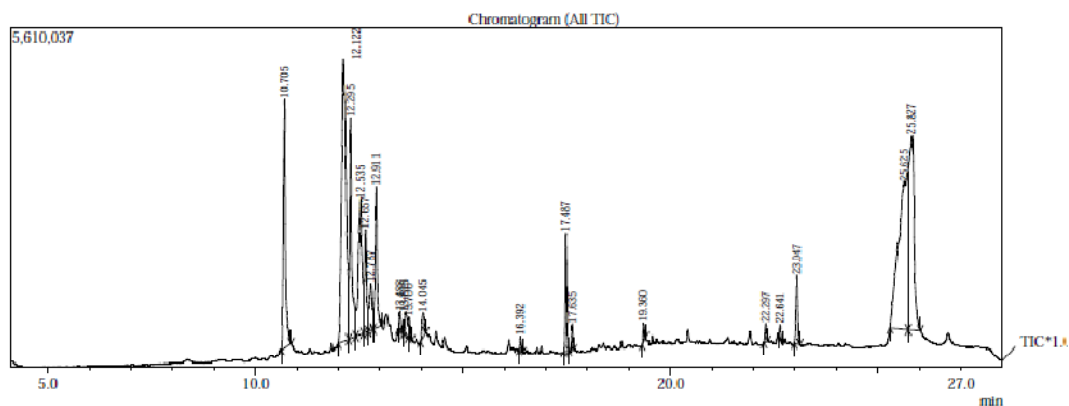
Column

Name: Rtx 5MS

Thickness: 0.25µm

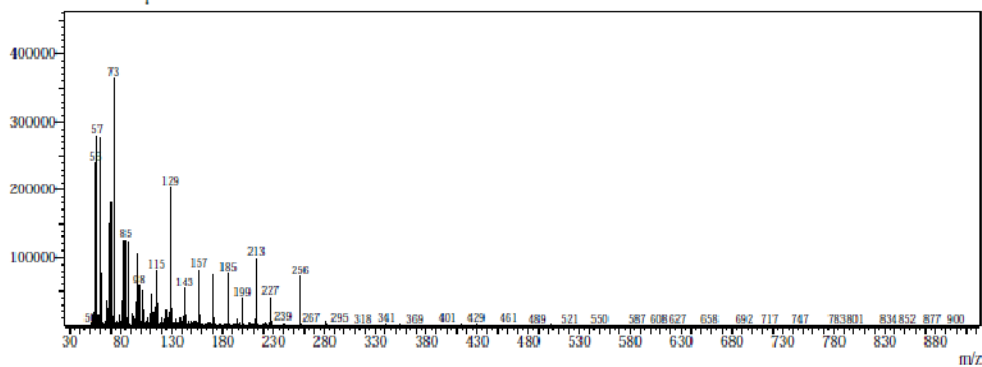
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Diameter: 0.25µm



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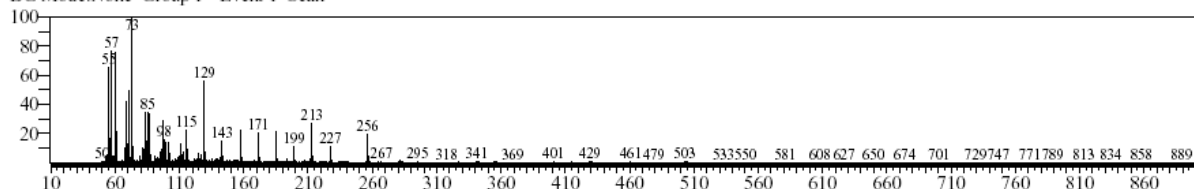
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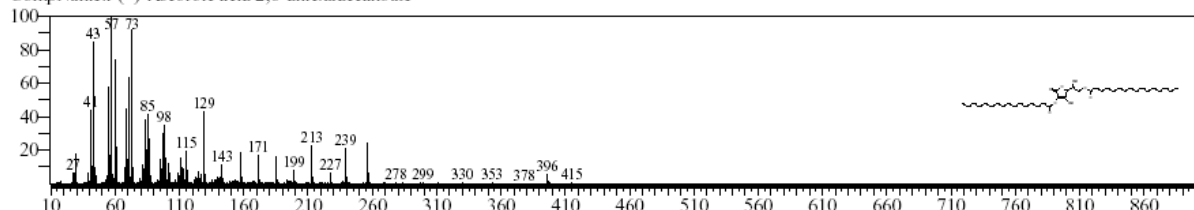
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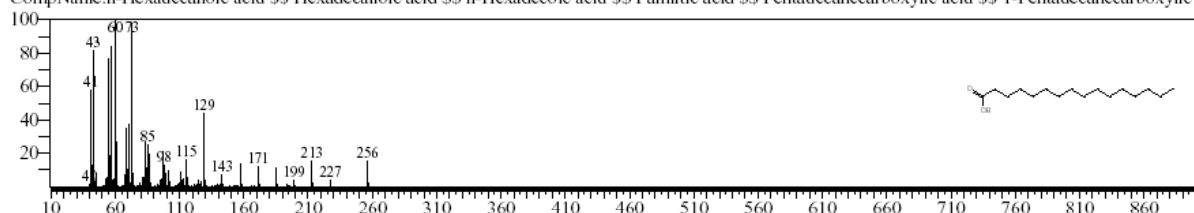
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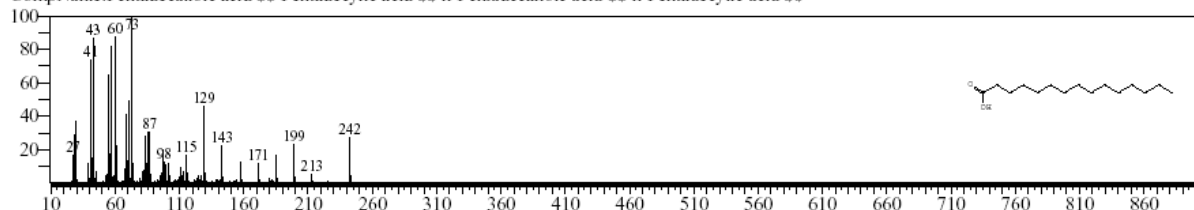
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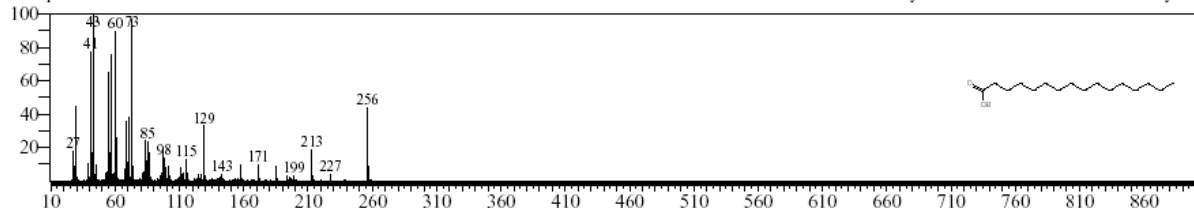
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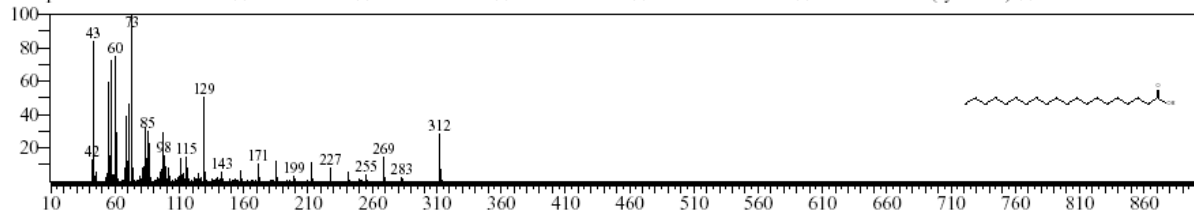
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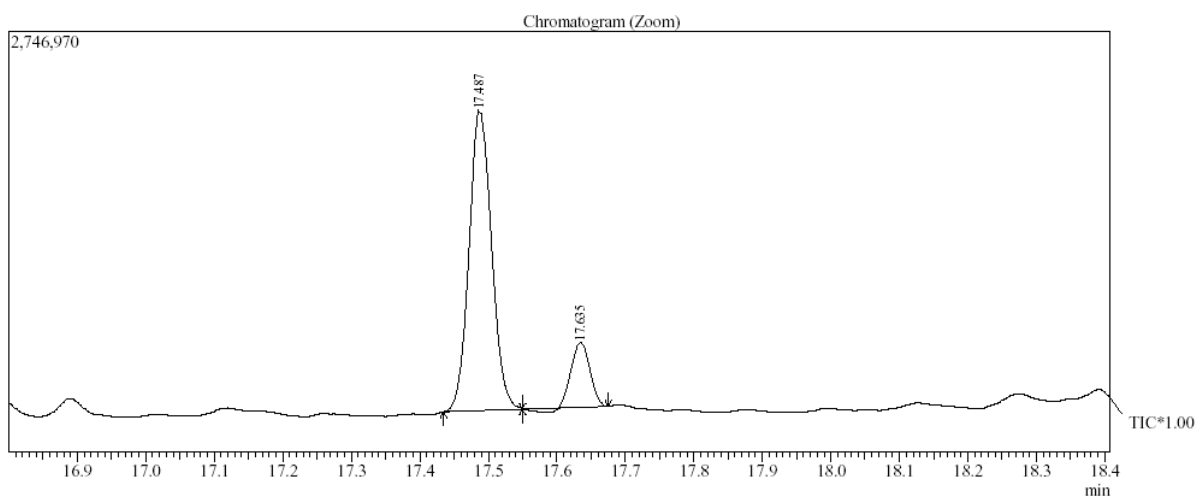
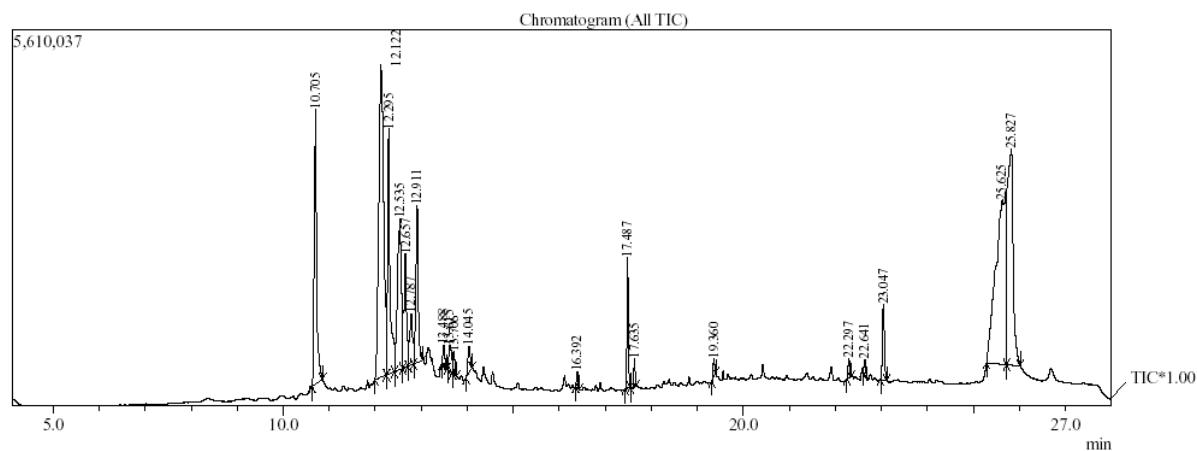


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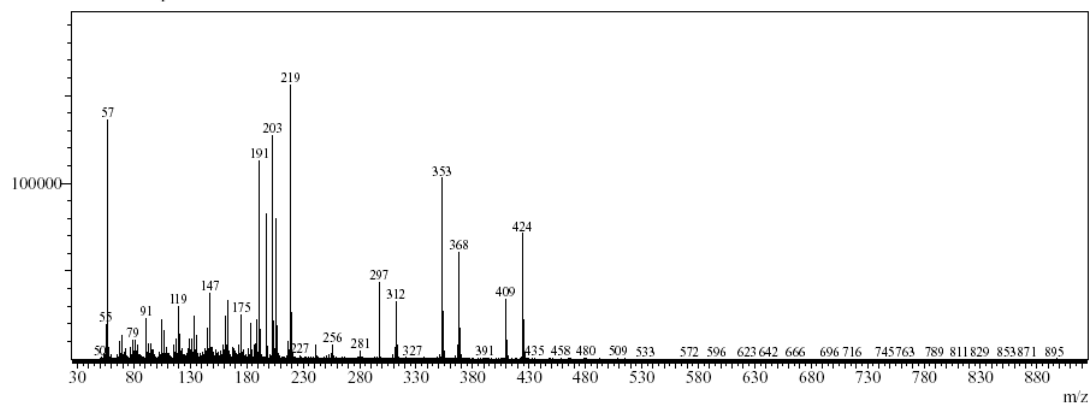
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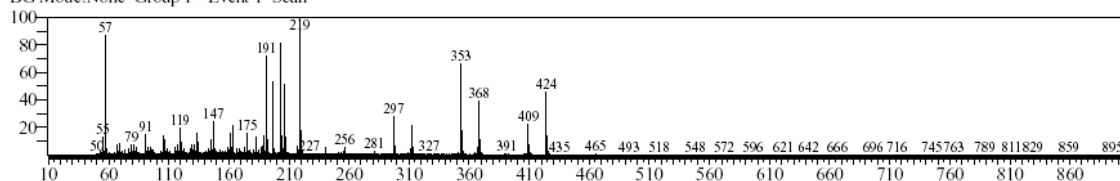
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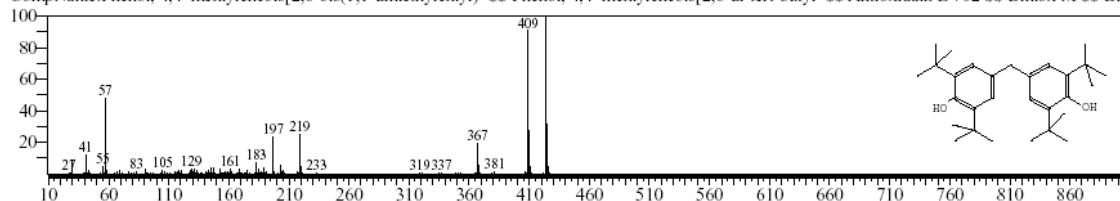
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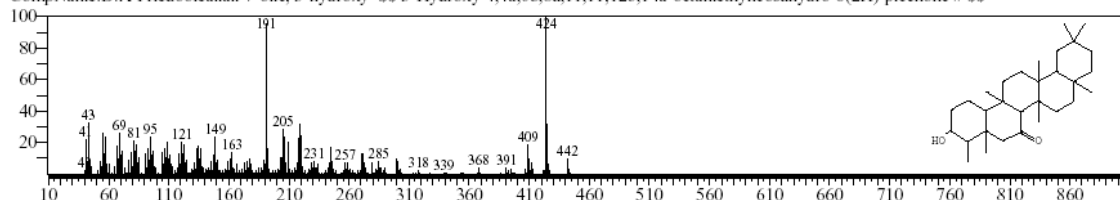
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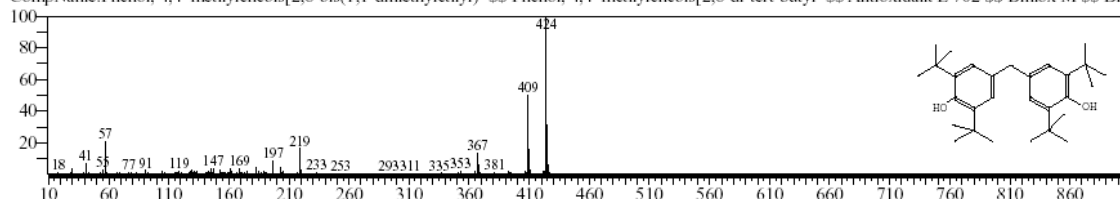
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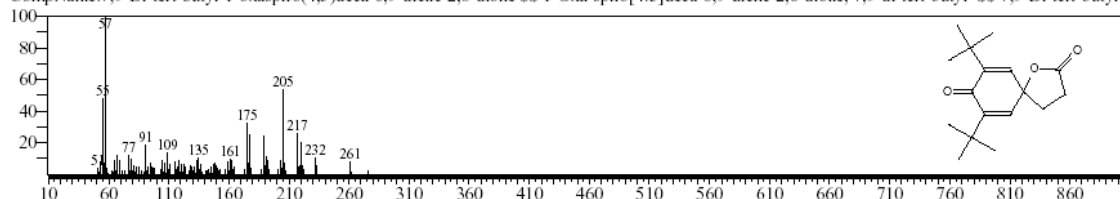
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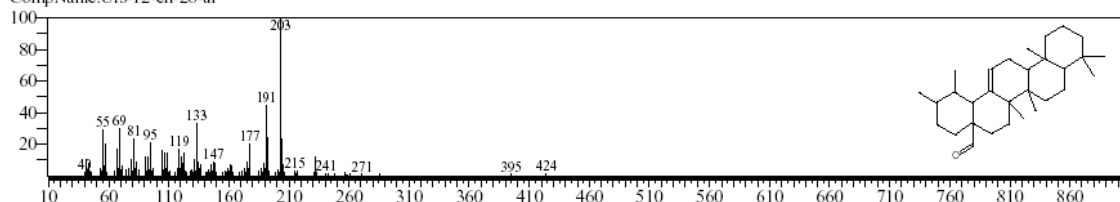
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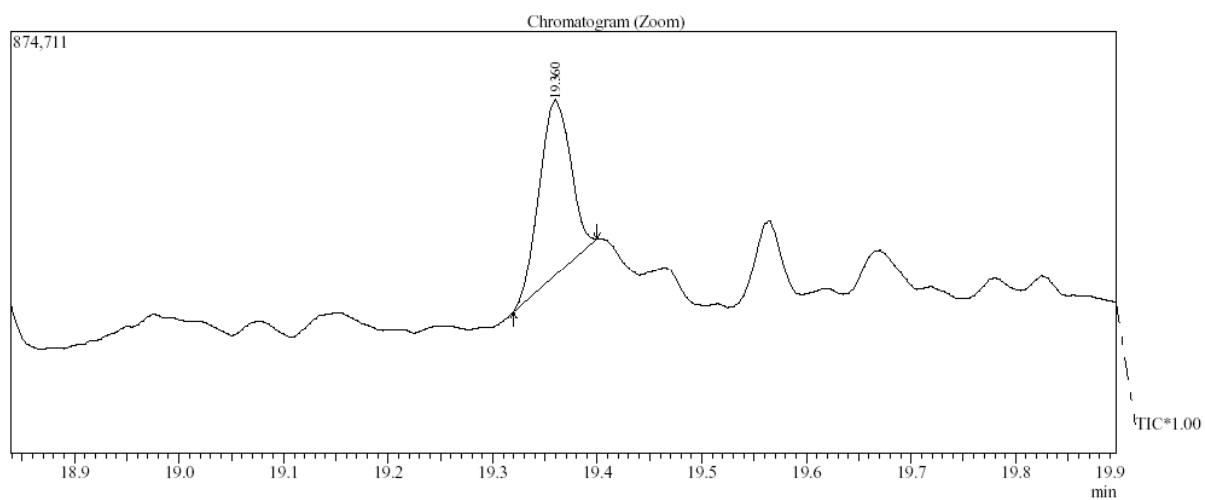
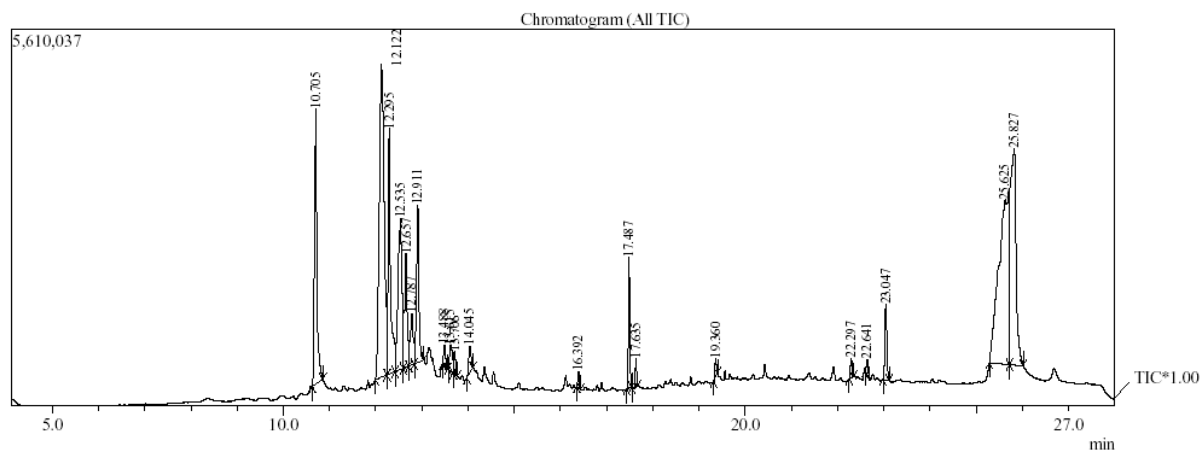


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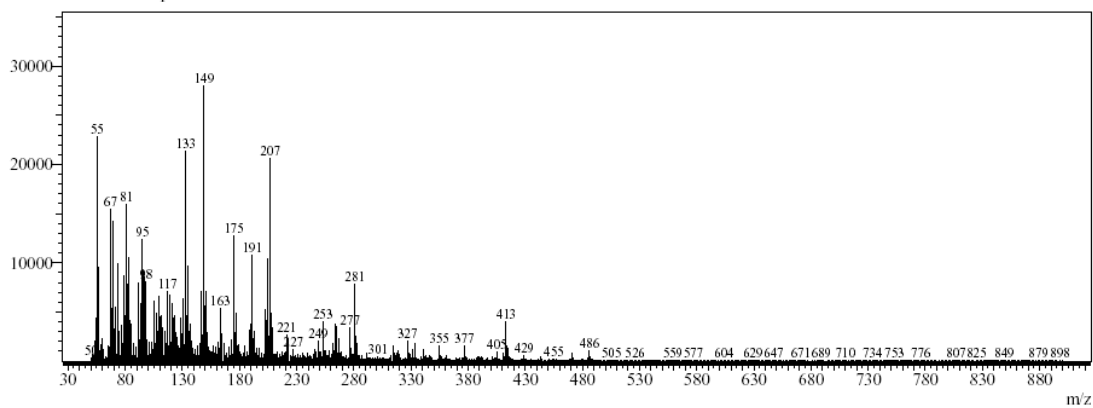
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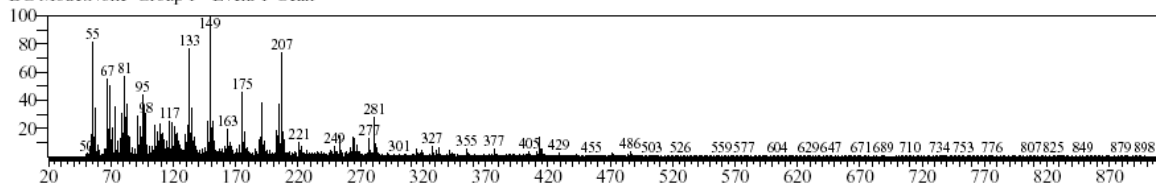
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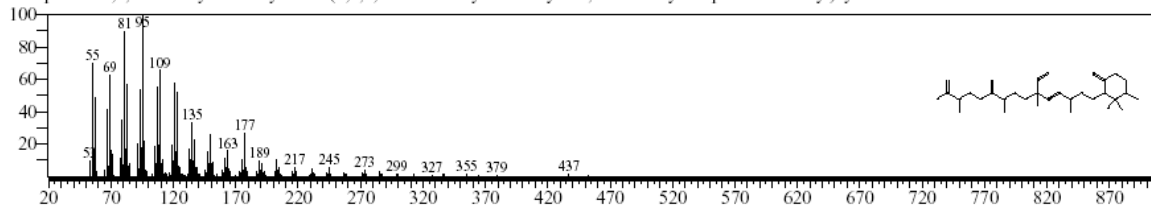
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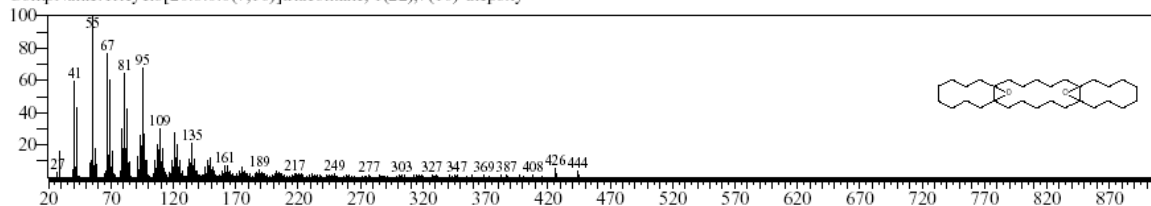
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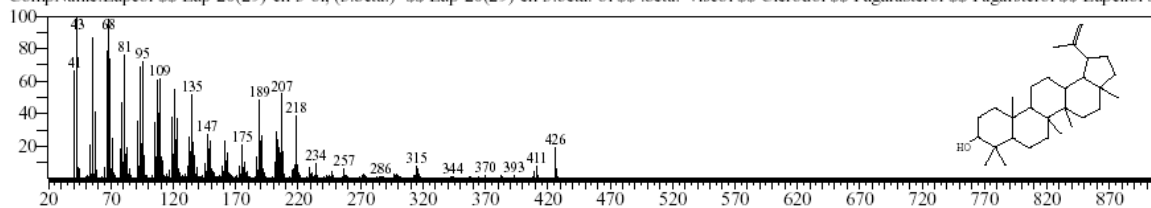
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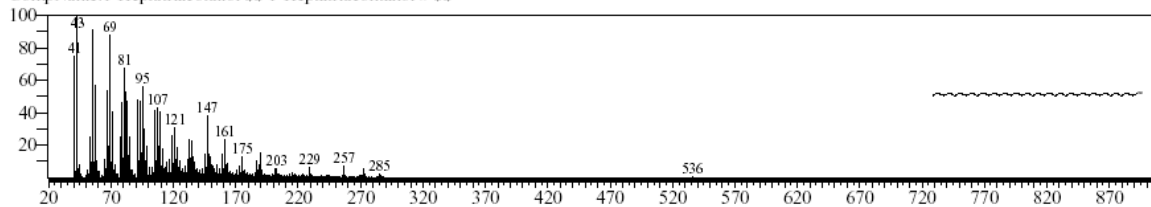
CompName:Lupcol \$\$ Lup-20(29)-en-3-ol, (3.beta.)- \$\$ Lup-20(29)-en-3.beta.-ol \$\$.beta.-Viscol \$\$ Clerodol \$\$ Fagarasterol \$\$ Fagarsterol \$\$ Lupenol \$



Hit#:4 Entry:207593 Library:NIST11.lib

SI:68 Formula:C37H76O CAS:105794-58-9 MolWeight:536 RetIndex:3942

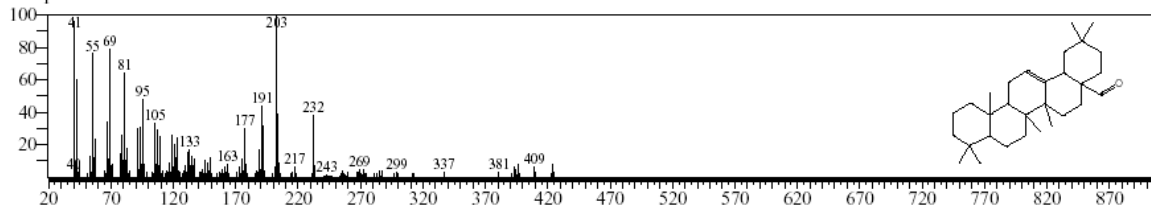
CompName:1-Heptatriacontanol \$\$ 1-Heptatriacontanol # \$\$

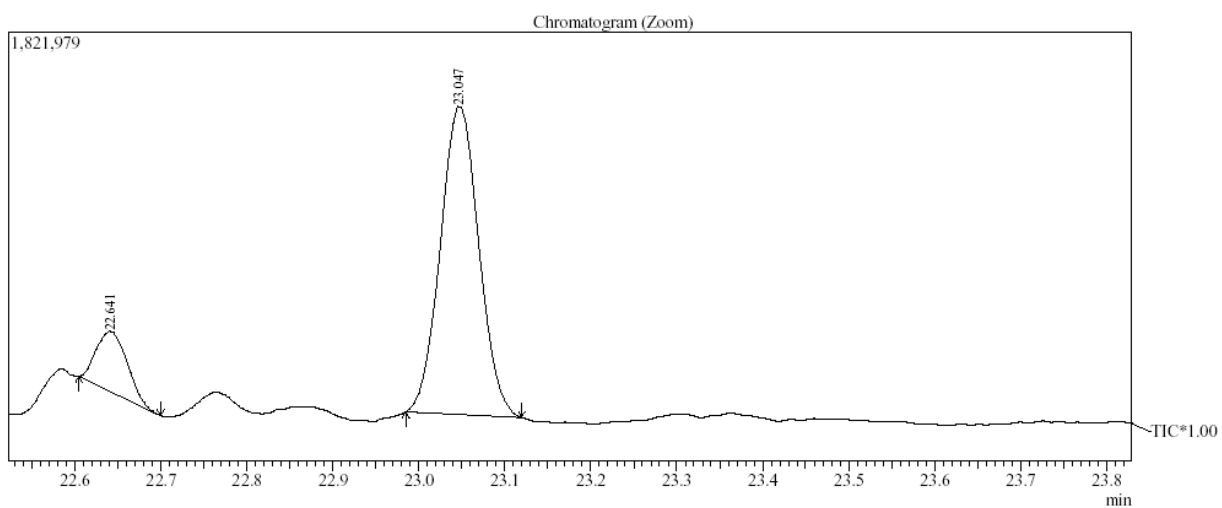
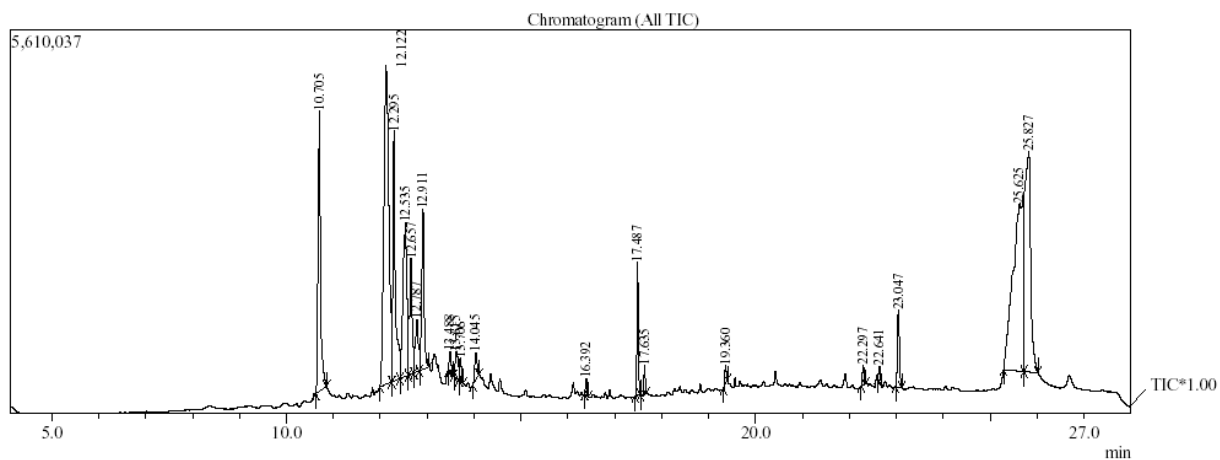


Hit#:5 Entry:190447 Library:NIST11.lib

SI:68 Formula:C30H48O CAS:10070-76-5 MolWeight:424 RetIndex:2886

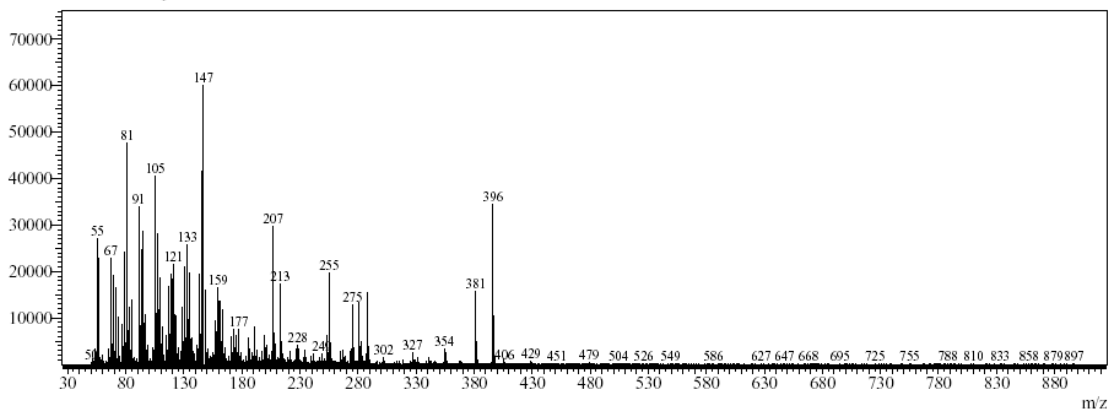
CompName:Olean-12-en-28-al





Spectrum

Line#:1 R.Time:23.050(Scan#:3791)
 MassPeaks:822
 RawMode:Single 23.050(3791) BasePeak:147.05(60015)
 BG Mode:None Group 1 - Event 1 Scan



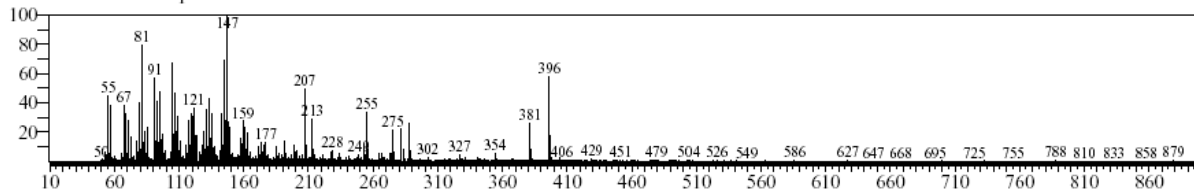
Library Search

<< Target >>

Line#:1 R.Time:23.050(Scan#:3791) MassPeaks:822

RawMode:Single 23.050(3791) BasePeak:147.05(10000)

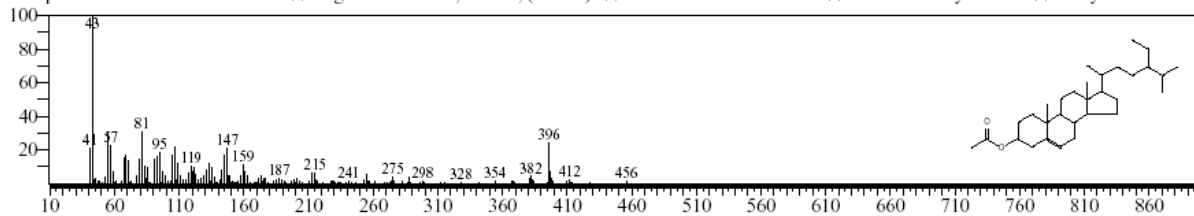
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:30335 Library:NIST11s.lib

SI:83 Formula:C31H52O2 CAS:915-05-9 MolWeight:456 RetIndex:2871

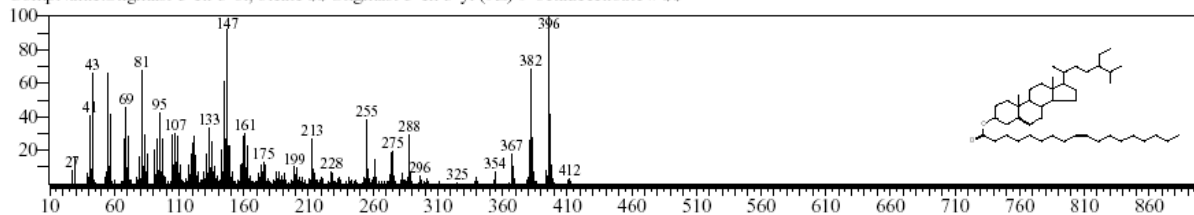
CompName:.beta.-Sitosterol acetate \$\$ Stigmast-5-en-3-ol, acetate, (3.beta.)- \$\$.beta.-Sitosterol 3-acetate \$\$.beta.-Sitoseryl acetate \$\$ Acetyl-.beta.-sitoste



Hit#:2 Entry:211748 Library:NIST11s.lib

SI:82 Formula:C47H82O2 CAS:0-00-0 MolWeight:678 RetIndex:4469

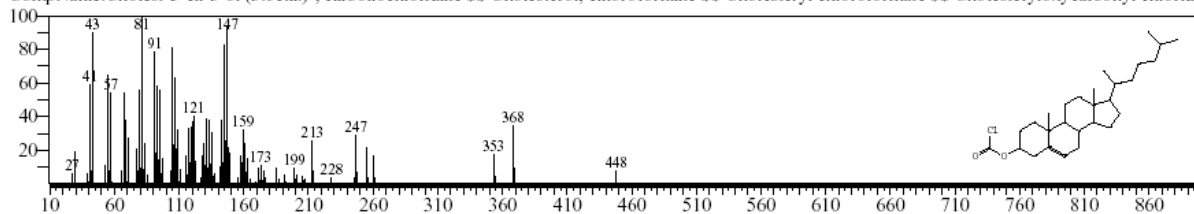
CompName:Stigmast-5-en-3-ol, oleate \$\$ Stigmast-5-en-3-yl (9Z)-9-octadecenoate # \$\$



Hit#:3 Entry:30283 Library:NIST11s.lib

SI:82 Formula:C28H45ClO2 CAS:7144-08-3 MolWeight:448 RetIndex:2813

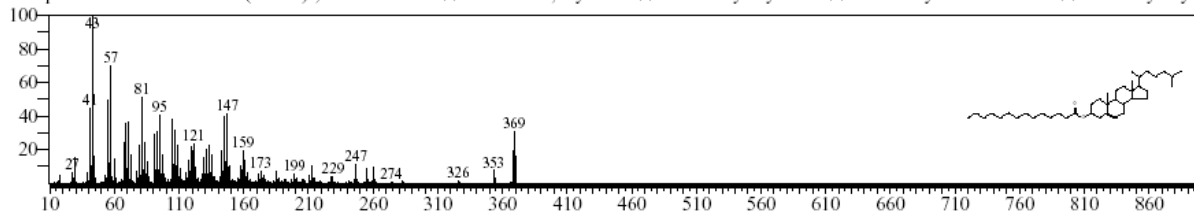
CompName:Cholest-5-en-3-ol (3.beta.)-, carbonochloride \$\$ Cholesterol, chloroformate \$\$ Cholesteryl chloroformate \$\$ Cholesteryloxycarbonyl chloride



Hit#:4 Entry:210195 Library:NIST11s.lib

SI:80 Formula:C41H72O2 CAS:1989-52-2 MolWeight:596 RetIndex:3929

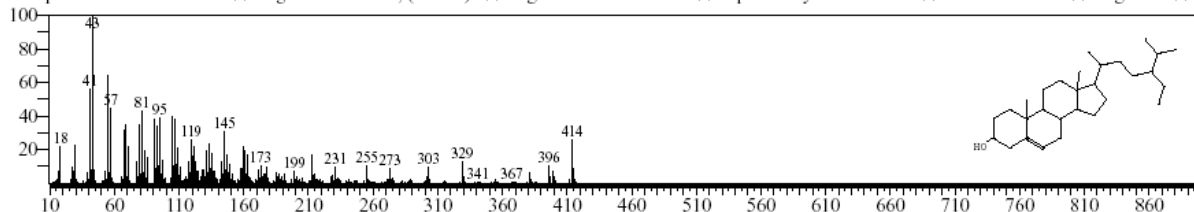
CompName:Cholest-5-en-3-ol (3.beta.)-, tetradecanoate \$\$ Cholesterol, myristate \$\$ Cholesteryl myristate \$\$ Cholesteryl tetradecanoate \$\$ Cholesteryl myri

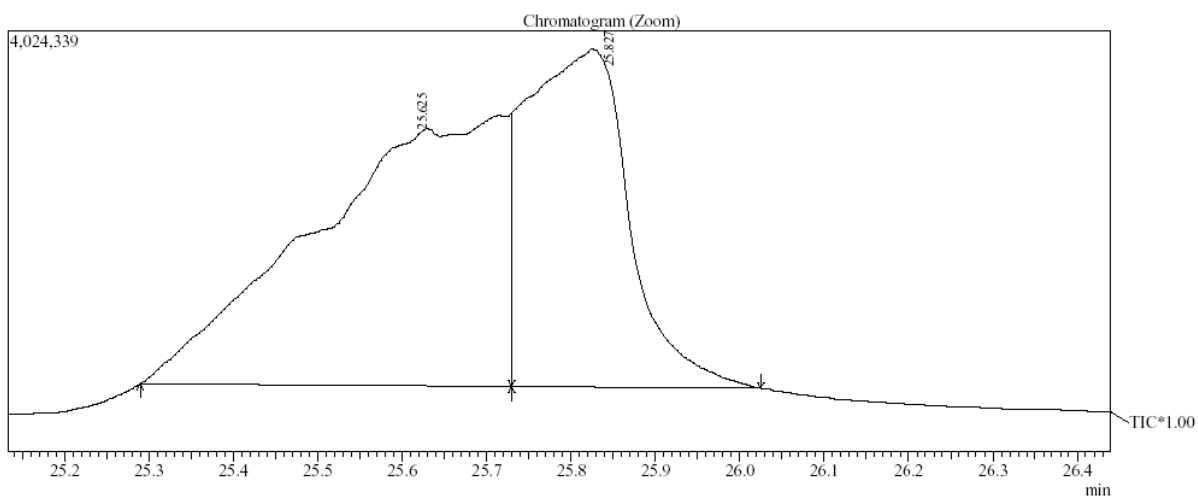
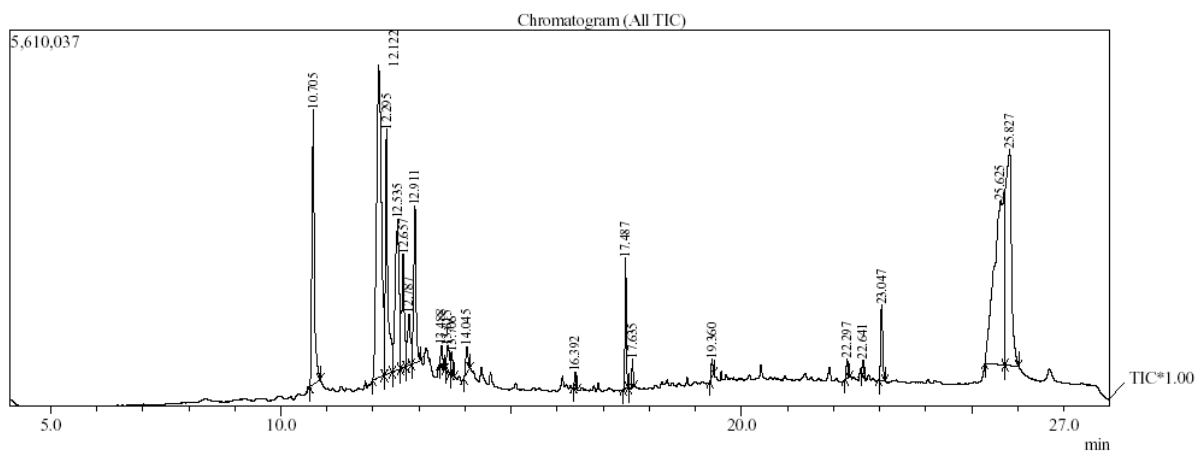


Hit#:5 Entry:29932 Library:NIST11s.lib

SI:79 Formula:C29H50O CAS:83-46-5 MolWeight:414 RetIndex:2731

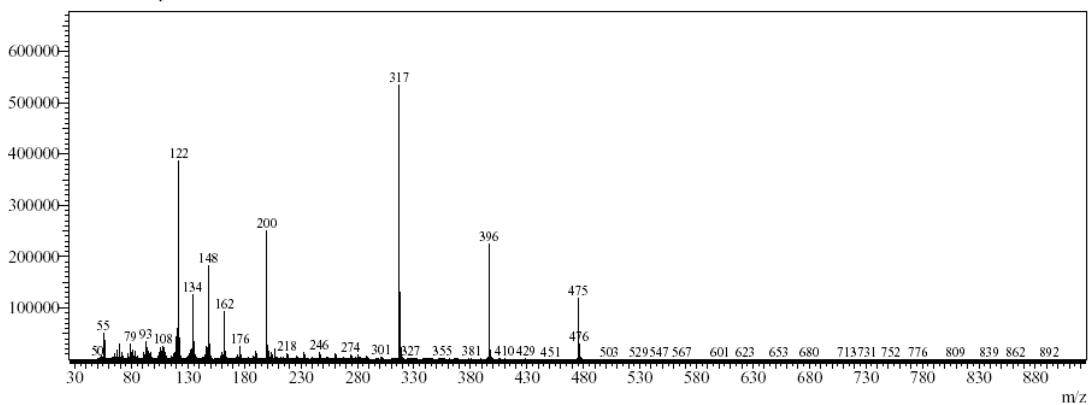
CompName:.beta.-Sitosterol \$\$ Stigmast-5-en-3-ol, (3.beta.)- \$\$ Stigmast-5-en-3.beta.-ol \$\$.alpha.-Dihydrofucosterol \$\$.beta.-Sitosterin \$\$ Angelicin \$\$ /





Spectrum

Line#:1 R.Time:25.825(Scan#:4346)
 MassPeaks:814
 RawMode:Single 25.825(4346) BasePeak:317.15(534028)
 BG Mode:None Group 1 - Event 1 Scan



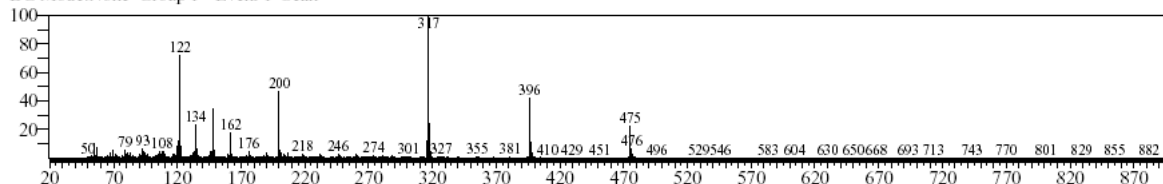
Library Search

<< Target >>

Line#:1 R.Time:25.825(Scan#:4346) MassPeaks:814

RawMode:Single 25.825(4346) BasePeak:317.15(10000)

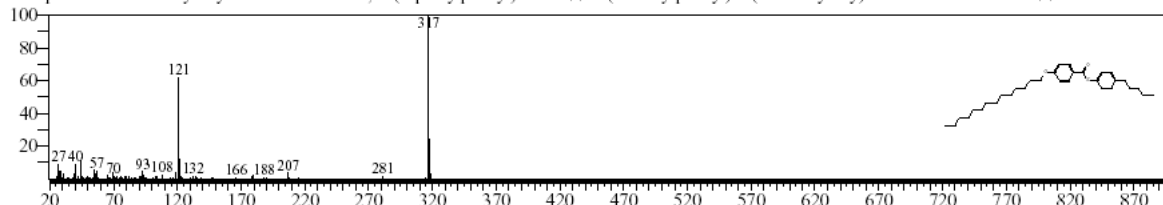
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:204322 Library:NIST11.lib

SI:54 Formula:C32H48O2S CAS:77638-16-5 MolWeight:496 RetIndex:3846

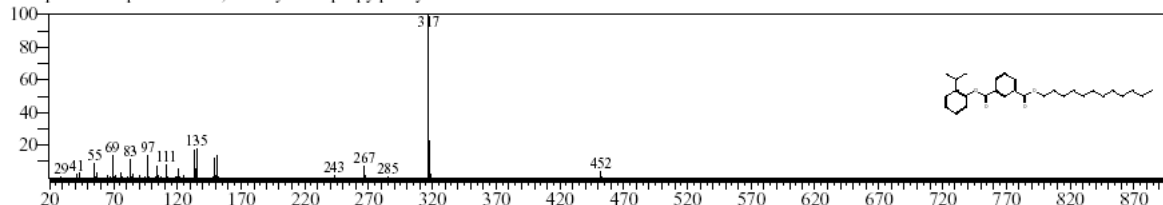
CompName:4-Tetradecyloxybenzenethiolic acid, S-(4-pentylphenyl)- ester SS S-(4-Pentylphenyl) 4-(tetradecyloxy)benzenecarbothioate # SS



Hit#:2 Entry:197326 Library:NIST11.lib

SI:53 Formula:C29H40O4 CAS:0-00-0 MolWeight:452 RetIndex:3355

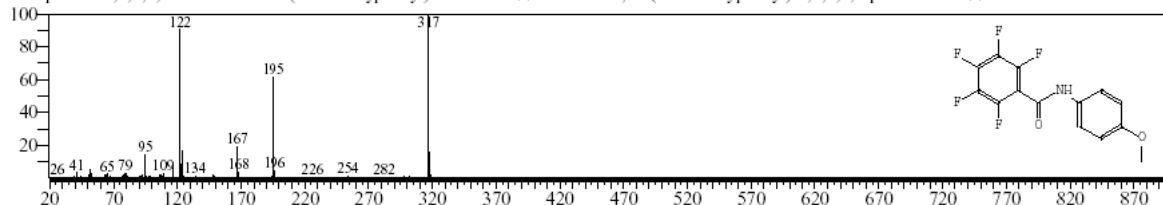
CompName:Isophthalic acid, dodecyl 2-isopropylphenyl ester



Hit#:3 Entry:131492 Library:NIST11.lib

SI:53 Formula:C14H8F5NO2 CAS:297149-72-5 MolWeight:317 RetIndex:1930

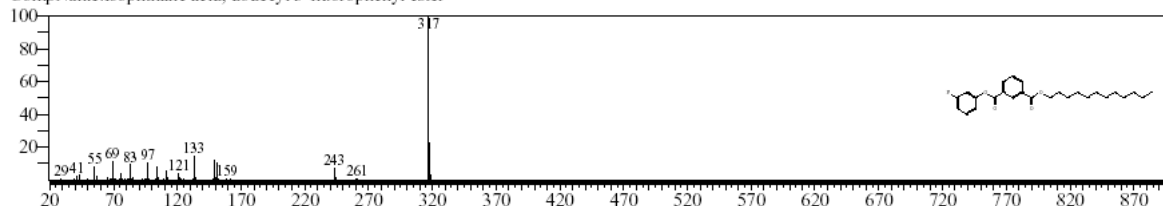
CompName:2,3,4,5,6-Pentafluoro-N-(4-methoxyphenyl)benzamide SS Benzamide, N-(4-methoxyphenyl)-2,3,4,5,6-pentafluoro- SS



Hit#:4 Entry:191586 Library:NIST11.lib

SI:53 Formula:C26H33FO4 CAS:0-00-0 MolWeight:428 RetIndex:3082

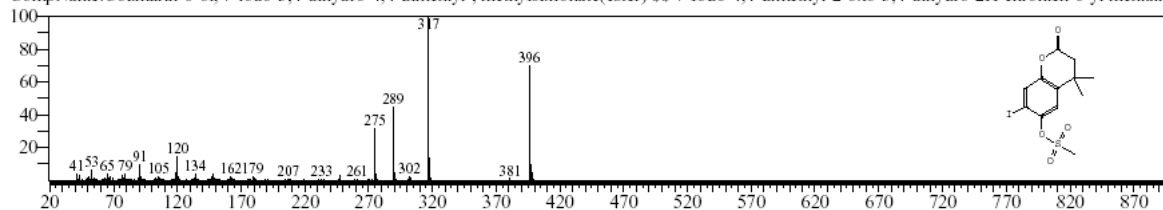
CompName:Isophthalic acid, dodecyl 3-fluorophenyl ester

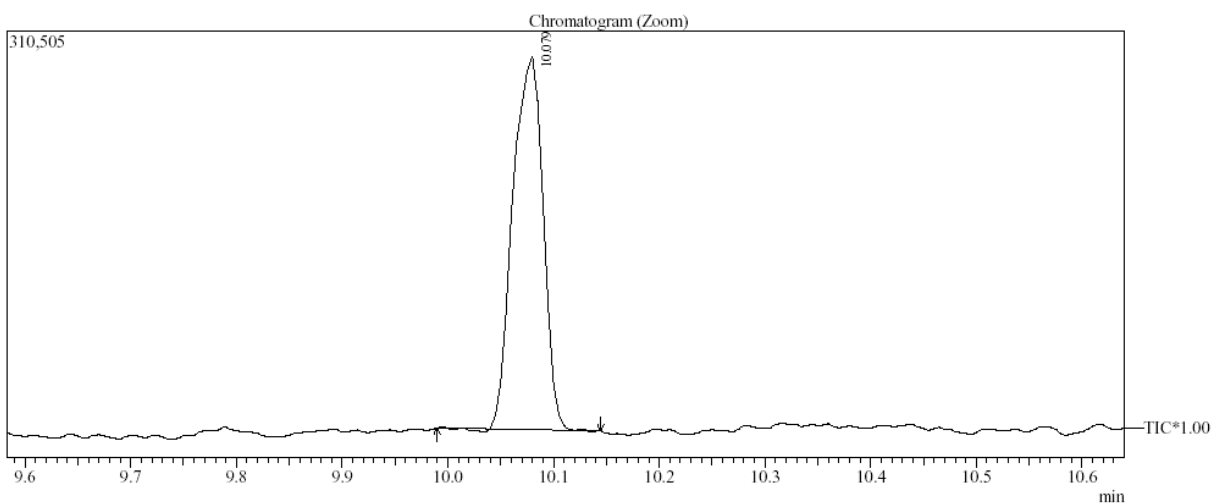
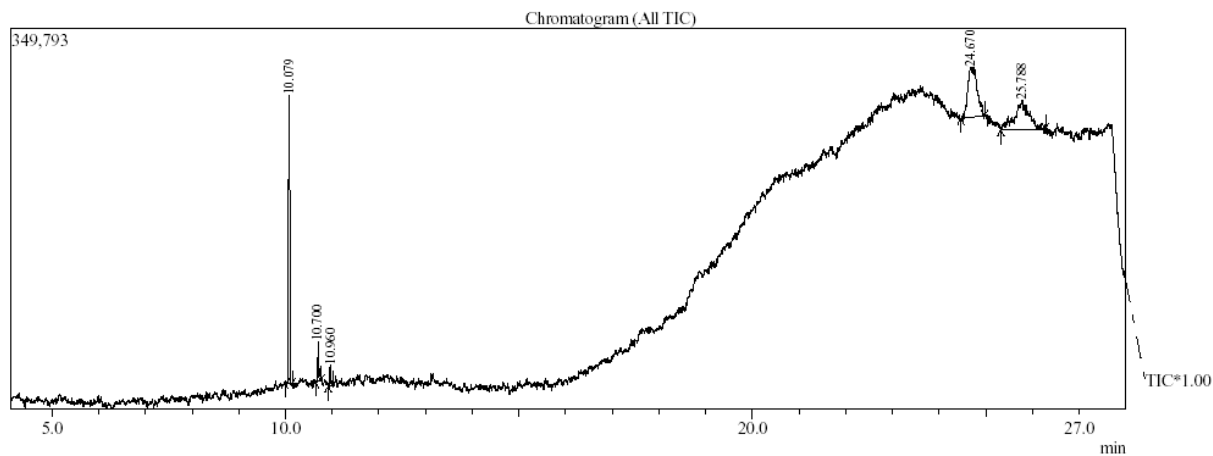


Hit#:5 Entry:180274 Library:NIST11.lib

SI:52 Formula:C12H13IO5S CAS:0-00-0 MolWeight:396 RetIndex:2626

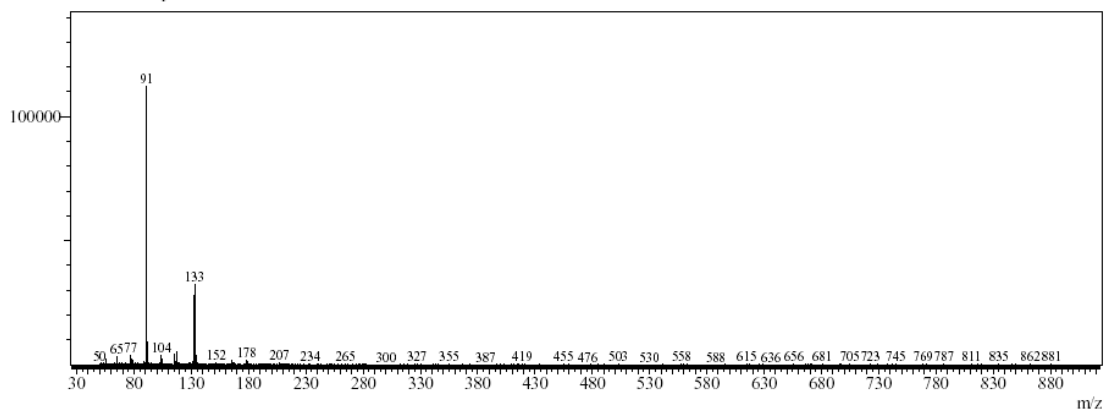
CompName:Coumarin-6-ol, 7-iodo-3,4-dihydro-4,4-dimethyl-, methylsulfonate(ester) SS 7-Iodo-4,4-dimethyl-2-oxo-3,4-dihydro-2H-chromen-6-yl methane-





Spectrum

Line#:1 R.Time:10.075(Scan#:1196)
 MassPeaks:766
 RawMode:Single 10.075(1196) BasePeak:91.00(112060)
 BG Mode:None Group 1 - Event 1 Scan



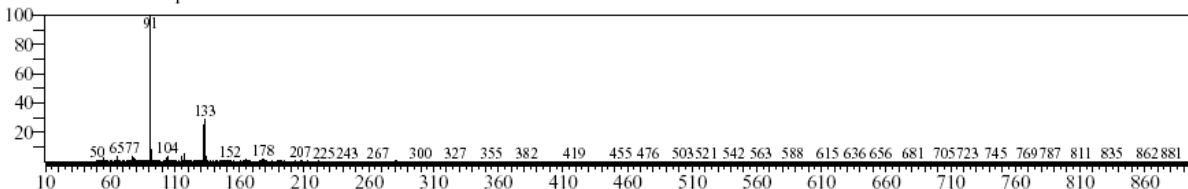
Library Search

<< Target >>

Line#:1 R.Time:10.075(Scan#:1196) MassPeaks:766

RawMode:Single 10.075(1196) BasePeak:91.00(10000)

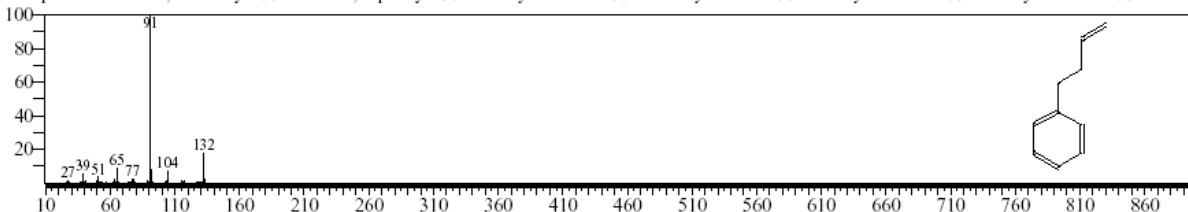
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:8586 Library:NIST11.lib

SI:86 Formula:C10H12 CAS:768-56-9 MolWeight:132 RetIndex:1082

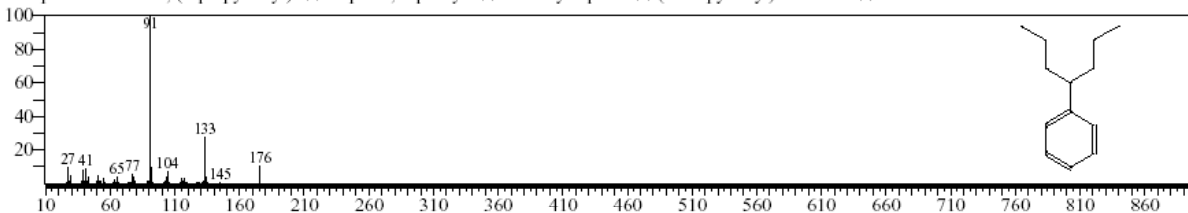
CompName:Benzene, 3-butenyl- \$\$ 1-Butene, 4-phenyl- \$\$ 1-Phenyl-3-butene \$\$ 3-Butenylbenzene \$\$ 4-Phenyl-1-butene \$\$ 4-Phenylbut-1-ene \$\$ 4-Phenyl



Hit#:2 Entry:29321 Library:NIST11.lib

SI:86 Formula:C13H20 CAS:2132-86-7 MolWeight:176 RetIndex:1326

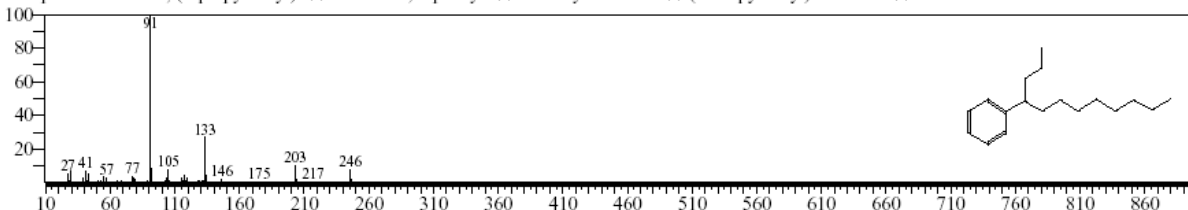
CompName:Benzene, (1-propylbutyl)- \$\$ Heptane, 4-phenyl- \$\$ 4-Phenylheptane \$\$ (1-Propylbutyl)benzene # \$\$



Hit#:3 Entry:76887 Library:NIST11.lib

SI:86 Formula:C18H30 CAS:2719-64-4 MolWeight:246 RetIndex:1823

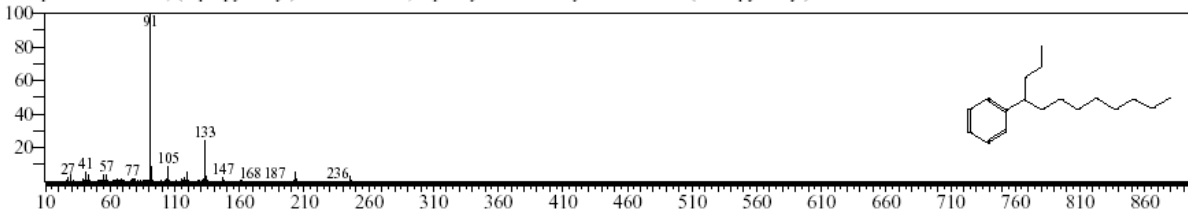
CompName:Benzene, (1-propylnonyl)- \$\$ Dodecane, 4-phenyl- \$\$ 4-Phenyl-dodecane \$\$ (1-Propylnonyl)benzene # \$\$



Hit#:4 Entry:22495 Library:NIST11s.lib

SI:86 Formula:C18H30 CAS:2719-64-4 MolWeight:246 RetIndex:1823

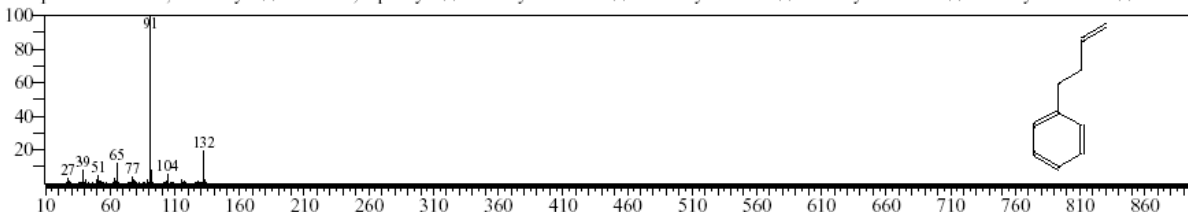
CompName:Benzene, (1-propylnonyl)- \$\$ Dodecane, 4-phenyl- \$\$ 4-Phenyl-dodecane \$\$ (1-Propylnonyl)benzene # \$\$

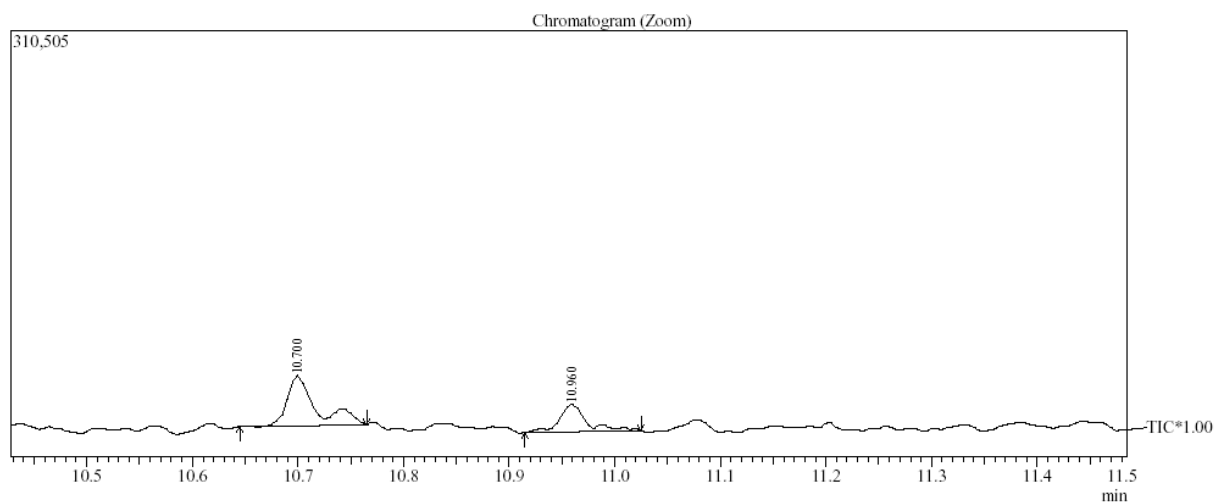
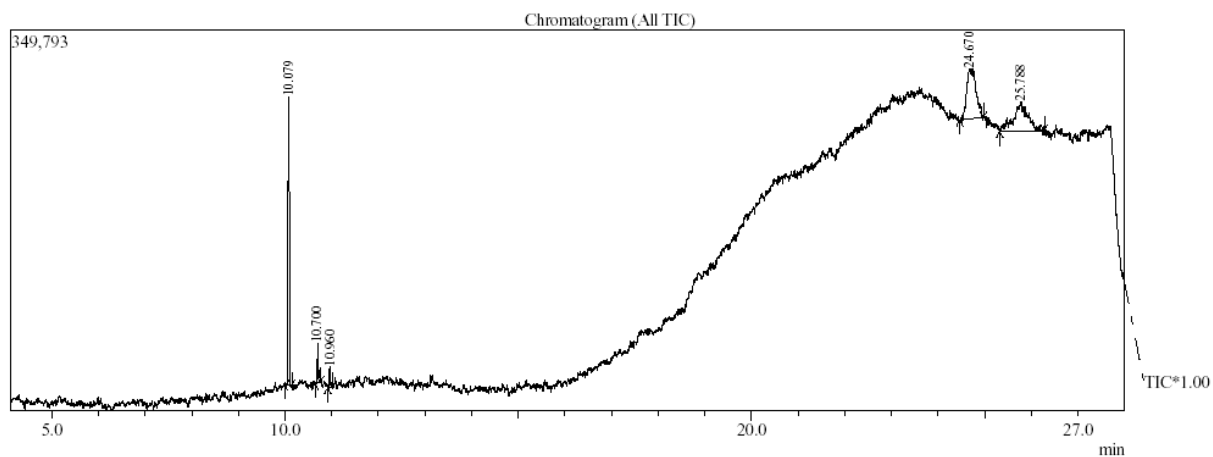


Hit#:5 Entry:5918 Library:NIST11s.lib

SI:86 Formula:C10H12 CAS:768-56-9 MolWeight:132 RetIndex:1082

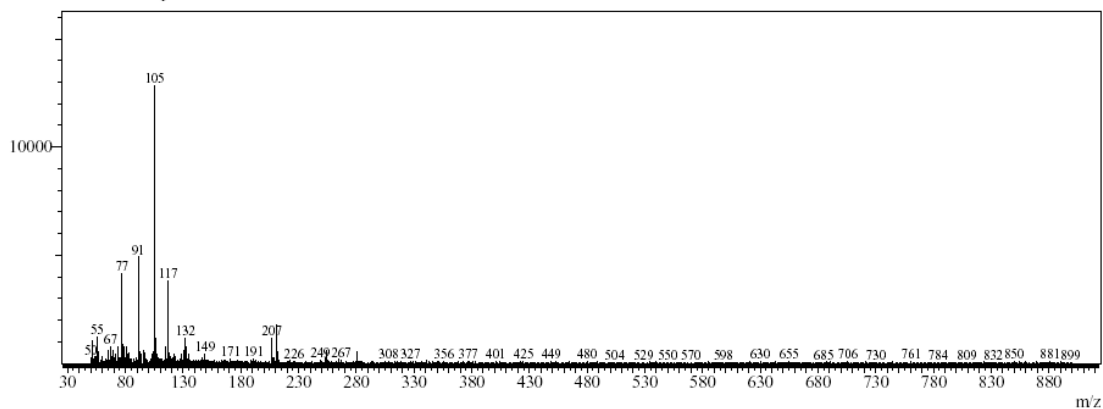
CompName:Benzene, 3-butenyl- \$\$ 1-Butene, 4-phenyl- \$\$ 1-Phenyl-3-butene \$\$ 3-Butenylbenzene \$\$ 4-Phenyl-1-butene \$\$ 4-Phenylbut-1-ene \$\$ 4-Phenyl





Spectrum

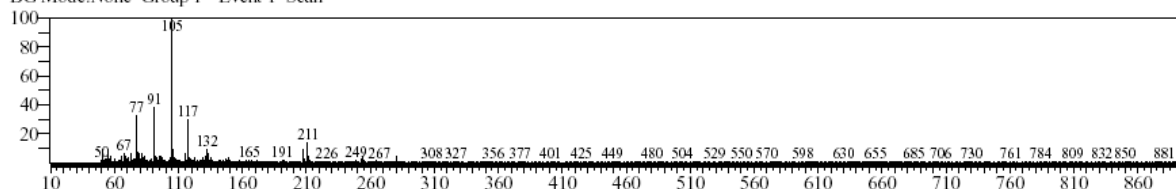
Line#:1 R.Time:10.700(Scan#:1321)
 MassPeaks:745
 RawMode:Single 10.700(1321) BasePeak:105.00(12815)
 BG Mode:None Group 1 - Event 1 Scan



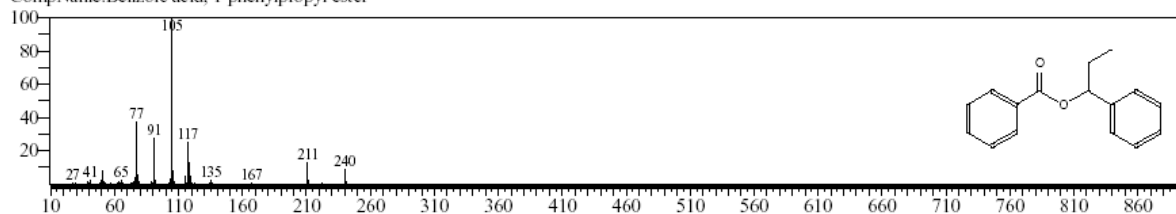
Library Search

<< Target >>

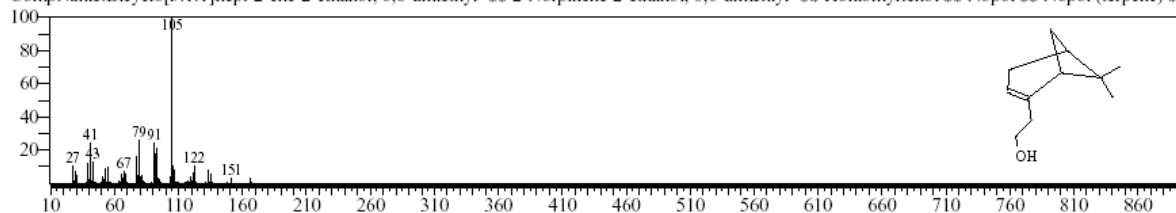
Line#:1 R.Time:10.700(Scan#:1321) MassPeaks:745
RawMode:Single 10.700(1321) BasePeak:105.00(10000)
BG Mode:None Group 1 - Event 1 Scan



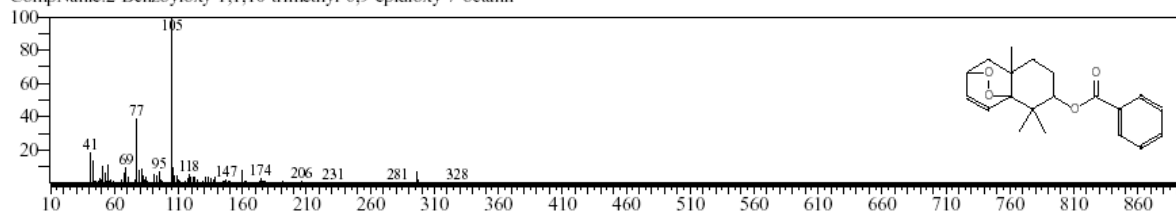
Hit#:1 Entry:72377 Library:NIST11.lib
SI:76 Formula:C16H16O2 CAS:0-00-0 MolWeight:240 RetIndex:1868
CompName:Benzoic acid, 1-phenylpropyl ester



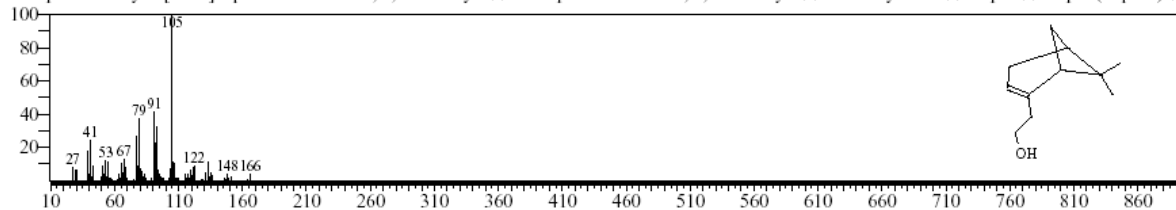
Hit#:2 Entry:23625 Library:NIST11.lib
SI:75 Formula:C11H18O CAS:128-50-7 MolWeight:166 RetIndex:1290
CompName:Bicyclo[3.1.1]hept-2-ene-2-ethanol, 6,6-dimethyl- \$\$ 2-Norpinene-2-ethanol, 6,6-dimethyl- \$\$ Homomyrtenol \$\$ Nopol \$\$ Nopol (terpene) \$\$



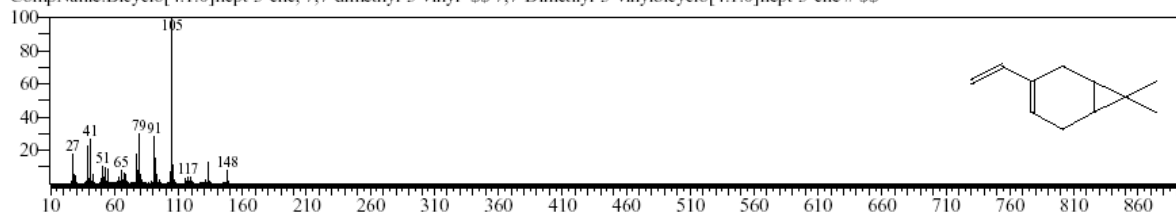
Hit#:3 Entry:140172 Library:NIST11.lib
SI:75 Formula:C20H24O4 CAS:108511-78-0 MolWeight:328 RetIndex:2325
CompName:2-Benzoyloxy-1,1,10-trimethyl-6,9-epidioxy-7-octalin

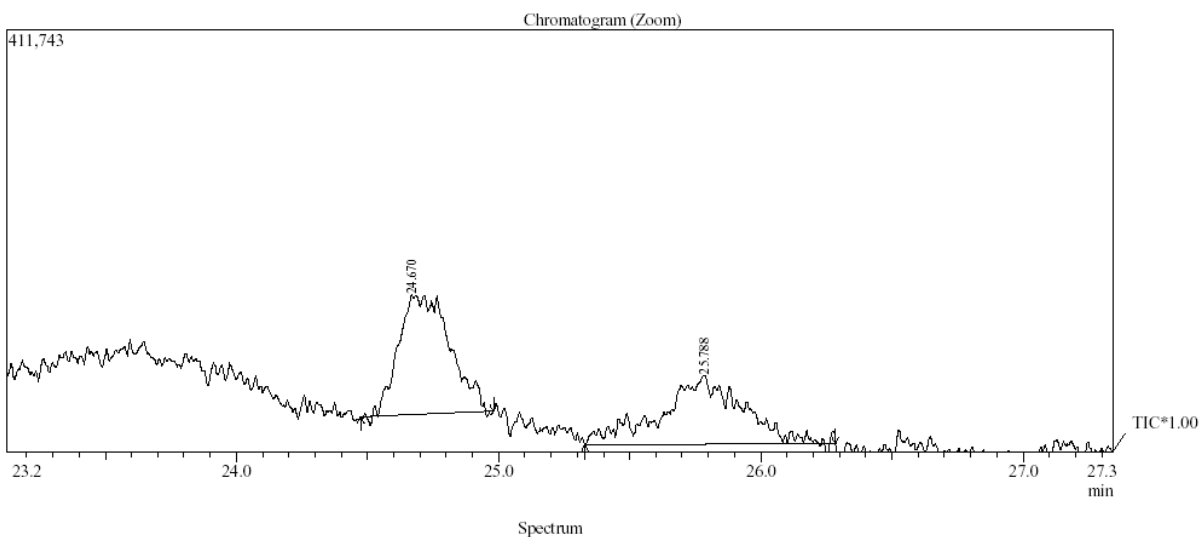
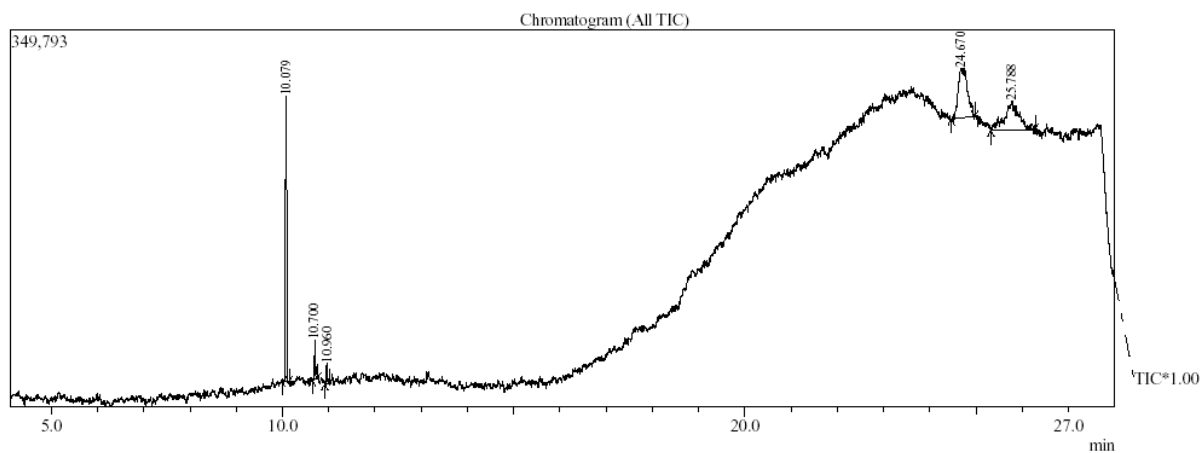


Hit#:4 Entry:12090 Library:NIST11s.lib
SI:75 Formula:C11H18O CAS:128-50-7 MolWeight:166 RetIndex:1290
CompName:Bicyclo[3.1.1]hept-2-ene-2-ethanol, 6,6-dimethyl- \$\$ 2-Norpinene-2-ethanol, 6,6-dimethyl- \$\$ Homomyrtenol \$\$ Nopol \$\$ Nopol (terpene) \$\$

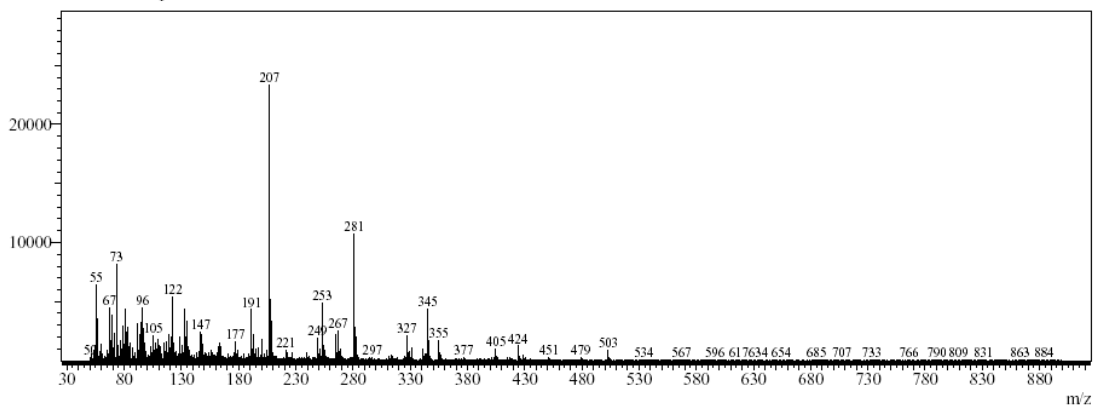


Hit#:5 Entry:14666 Library:NIST11.lib
SI:74 Formula:C11H16 CAS:113003-13-7 MolWeight:148 RetIndex:1037
CompName:Bicyclo[4.1.0]hept-3-ene, 7,7-dimethyl-3-vinyl- \$\$ 7,7-Dimethyl-3-vinylbicyclo[4.1.0]hept-3-ene # \$\$





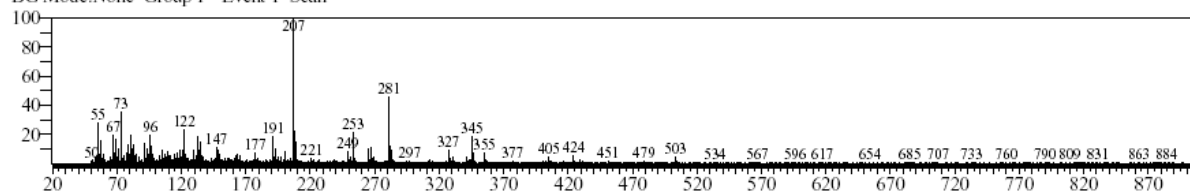
Line#:1 R.Time:24.685(Scan#:4118)
 MassPeaks:816
 RawMode:Single 24.685(4118) BasePeak:206.90(23313)
 BG Mode:None Group 1 - Event 1 Scan



Library Search

<< Target >>

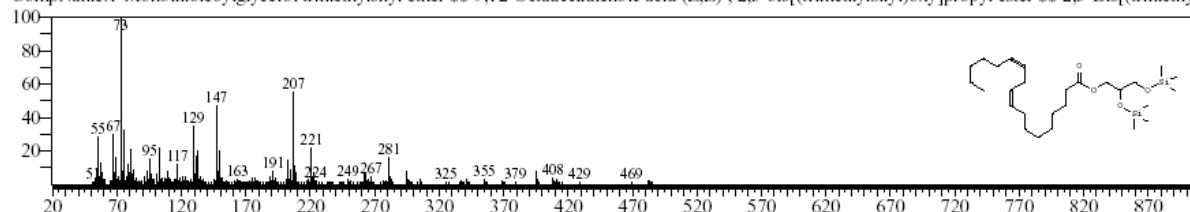
Line#:1 R.Time:24.685(Scan#:4118) MassPeaks:816
RawMode:Single 24.685(4118) BasePeak:206.90(10000)
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:204469 Library:NIST11.lib

SI:60 Formula:C27H54O4Si2 CAS:54284-45-6 MolWeight:498 RetIndex:2796

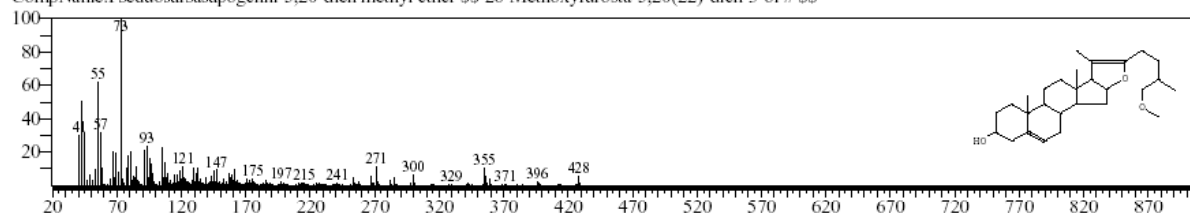
CompName:1-Monolinoleoylglycerol trimethylsilyl ether \$\$ 9,12-Octadecadienoic acid (Z,Z)-, 2,3-bis[(trimethylsilyl)oxy]propyl ester \$\$ 2,3-Bis[(trimethylsilyl)oxy]propyl ester



Hit#:2 Entry:191658 Library:NIST11.lib

SI:58 Formula:C28H44O3 CAS:7604-99-1 MolWeight:428 RetIndex:2889

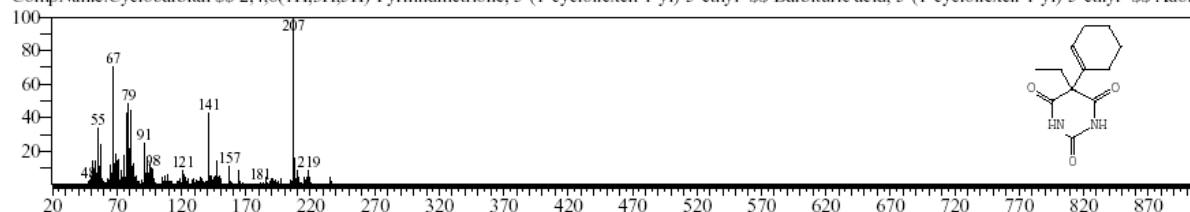
CompName:Pseudoarsasapogenin-5,20-dien methyl ether \$\$ 26-Methoxyfurosta-5,20(22)-dien-3-ol # \$\$



Hit#:3 Entry:21597 Library:NIST11s.lib

SI:57 Formula:C12H16N2O3 CAS:52-31-3 MolWeight:236 RetIndex:2022

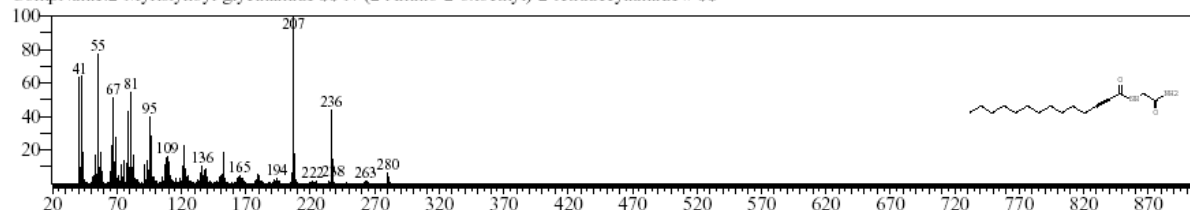
CompName:Cyclobarbitol \$\$ 2,4,6-(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-5-ethyl- \$\$ Barbituric acid, 5-(1-cyclohexen-1-yl)-5-ethyl- \$\$ Adorn



Hit#:4 Entry:102613 Library:NIST11.lib

SI:56 Formula:C16H28N2O2 CAS:0-00-0 MolWeight:280 RetIndex:2439

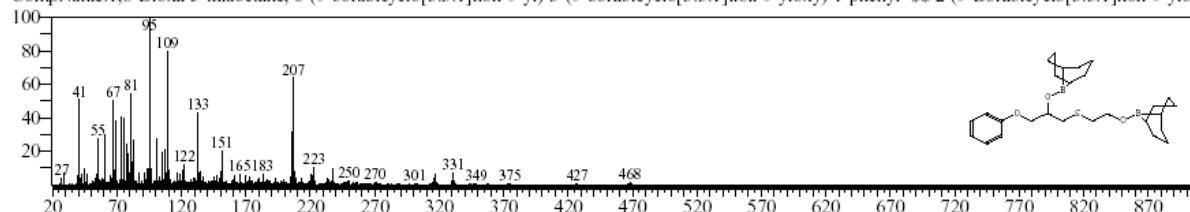
CompName:2-Myristinoyl-glycinamide \$\$ N-(2-Amino-2-oxoethyl)-2-tetradecynamide # \$\$

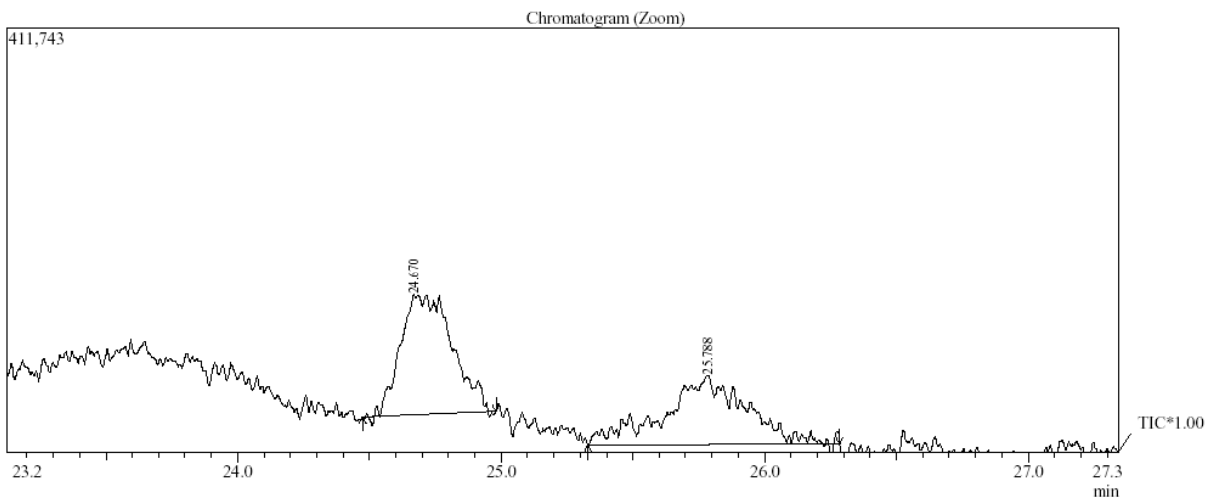
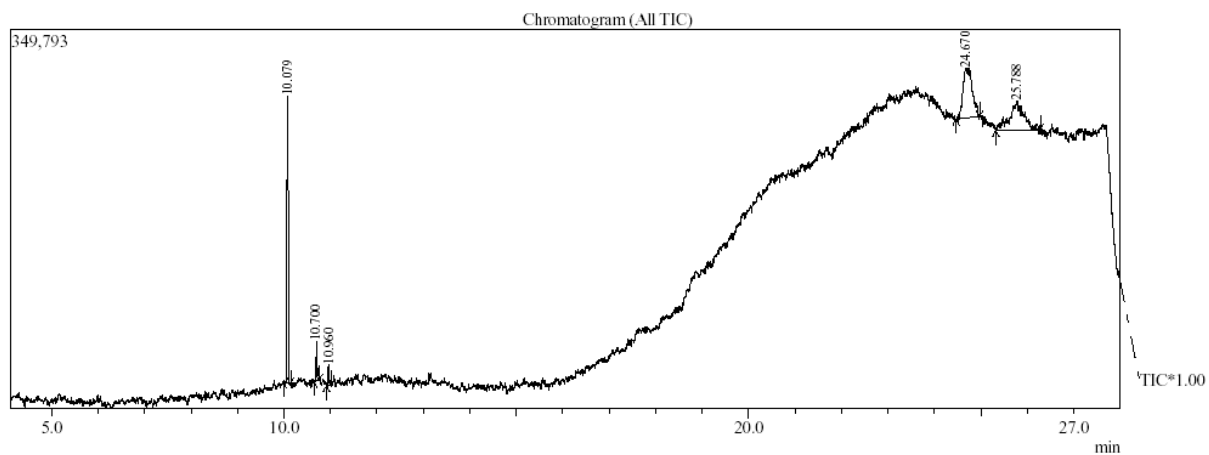


Hit#:5 Entry:200211 Library:NIST11.lib

SI:56 Formula:C27H42B2O3S CAS:0-00-0 MolWeight:468 RetIndex:0

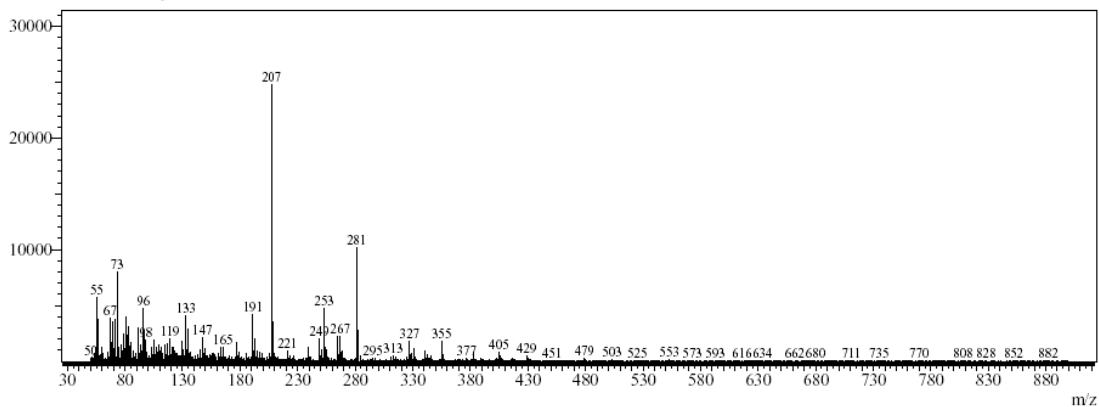
CompName:1,8-Dioxo-5-thiaoctane, 8-(9-borabicyclo[3.3.1]non-9-yl)-3-(9-borabicyclo[3.3.1]non-9-yloxy)-1-phenyl- \$\$ 2-(9-Borabicyclo[3.3.1]non-9-yloxy)-1-phenyl-5-thiaoctane-1,8-dione





Spectrum

Line#:1 R.Time:25.775(Scan#:4336)
 MassPeaks:814
 RawMode:Single 25.775(4336) BasePeak:206.90(24750)
 BG Mode:None Group 1 - Event 1 Scan



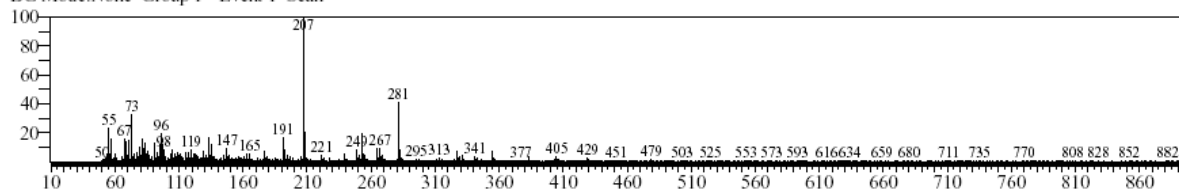
Library Search

<< Target >>

Line#:1 R.Time:25.775(Scan#:4336) MassPeaks:814

RawMode:Single 25.775(4336) BasePeak:206.90(10000)

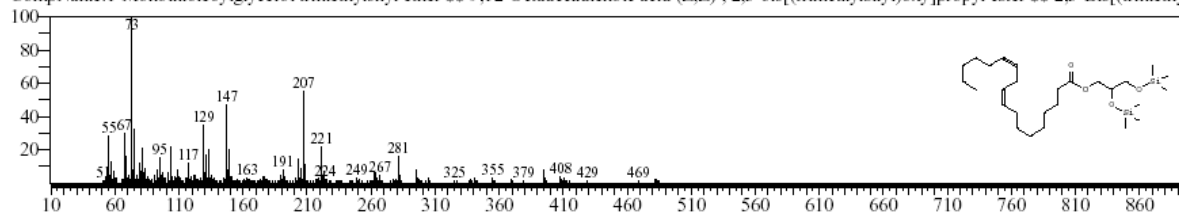
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:204469 Library:NIST11.lib

SI:61 Formula:C₂₇H₅₄O₄Si₂ CAS:54284-45-6 MolWeight:498 RetIndex:2796

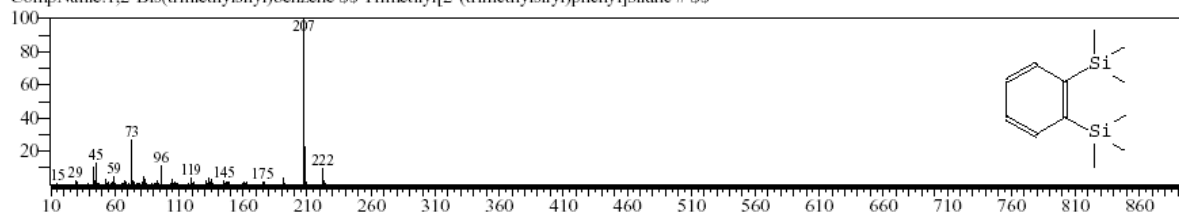
CompName:1-Monolinoleoylglycerol trimethylsilyl ether \$\$ 9,12-Octadecadienoic acid (Z,Z)-, 2,3-bis[(trimethylsilyl)oxy]propyl ester \$\$ 2,3-Bis[(trimethyl-



Hit#:2 Entry:58988 Library:NIST11.lib

SI:58 Formula:C₁₂H₂₂Si₂ CAS:17151-09-6 MolWeight:222 RetIndex:1124

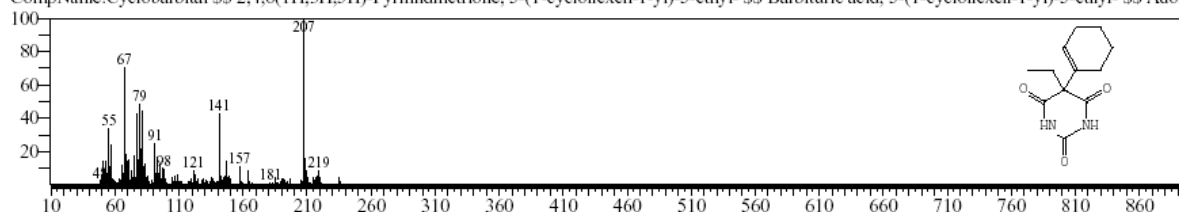
CompName:1,2-Bis(trimethylsilyl)benzene \$\$ Trimethyl[2-(trimethylsilyl)phenyl]silane # \$\$



Hit#:3 Entry:21597 Library:NIST11s.lib

SI:58 Formula:C₁₂H₁₆N₂O₃ CAS:52-31-3 MolWeight:236 RetIndex:2022

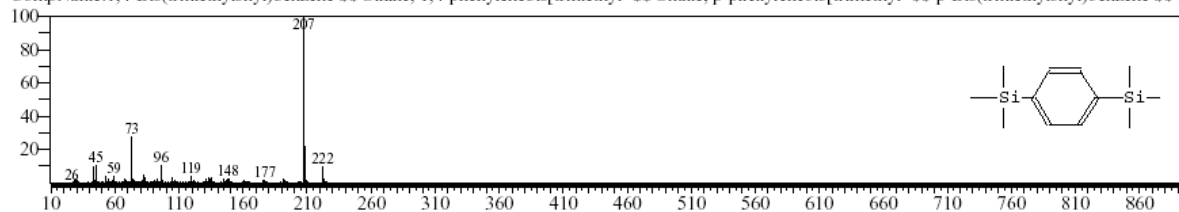
CompName:Cyclobarbitol \$\$ 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-5-ethyl- \$\$ Barbituric acid, 5-(1-cyclohexen-1-yl)-5-ethyl- \$\$ Adorr



Hit#:4 Entry:58989 Library:NIST11.lib

SI:58 Formula:C₁₂H₂₂Si₂ CAS:13183-70-5 MolWeight:222 RetIndex:1124

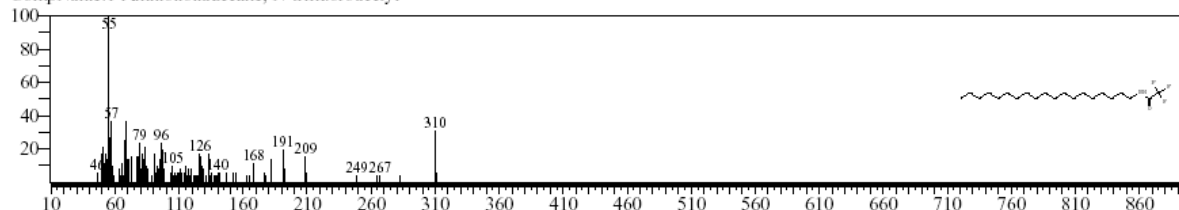
CompName:1,4-Bis(trimethylsilyl)benzene \$\$ Silane, 1,4-phenylenebis[trimethyl- \$\$ Silane, p-phenylenebis[trimethyl- \$\$ p-Bis(trimethylsilyl)benzene \$\$ B-

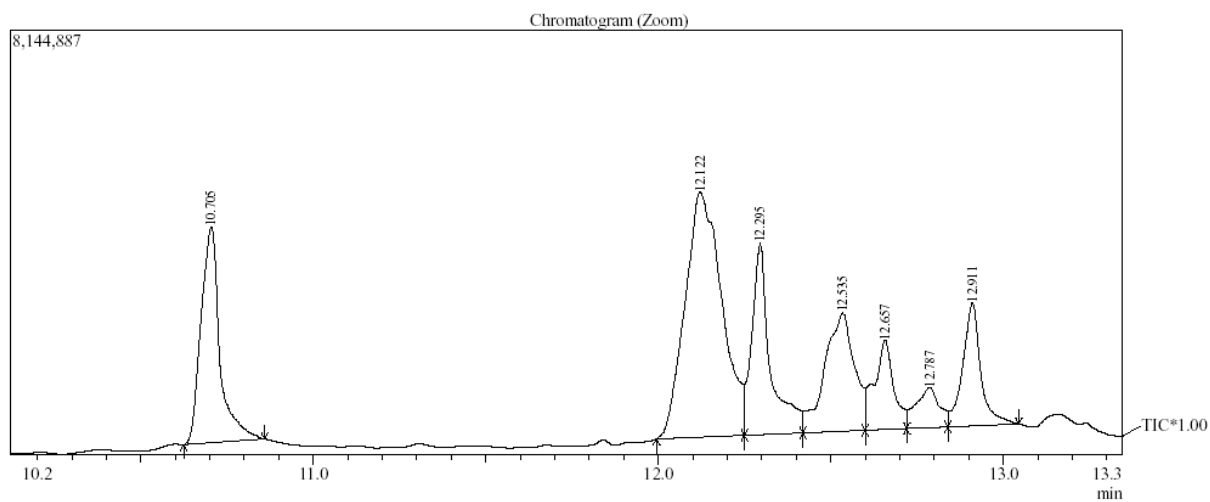
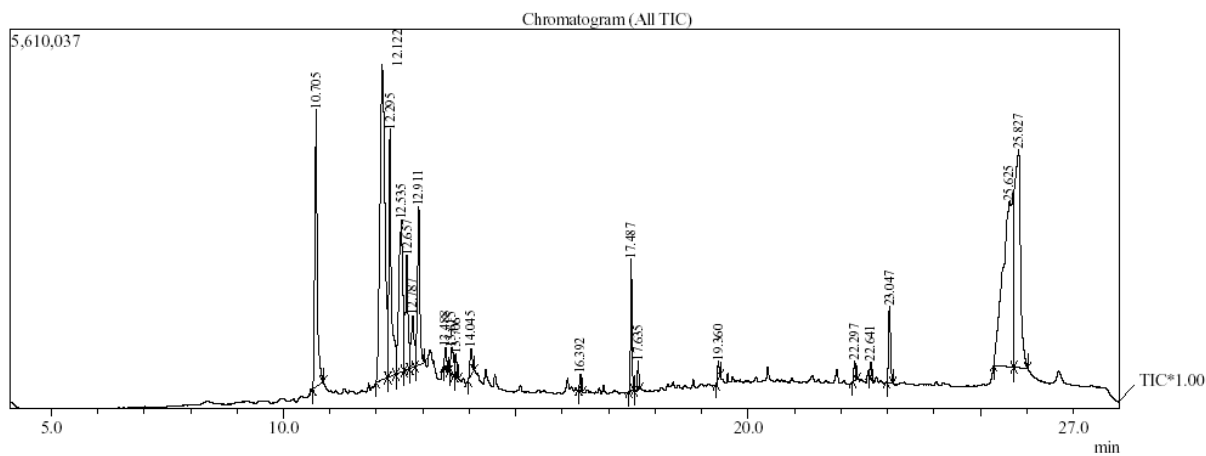


Hit#:5 Entry:172707 Library:NIST11.lib

SI:57 Formula:C₂₁H₄₀F₃NO CAS:0-00-0 MolWeight:379 RetIndex:2343

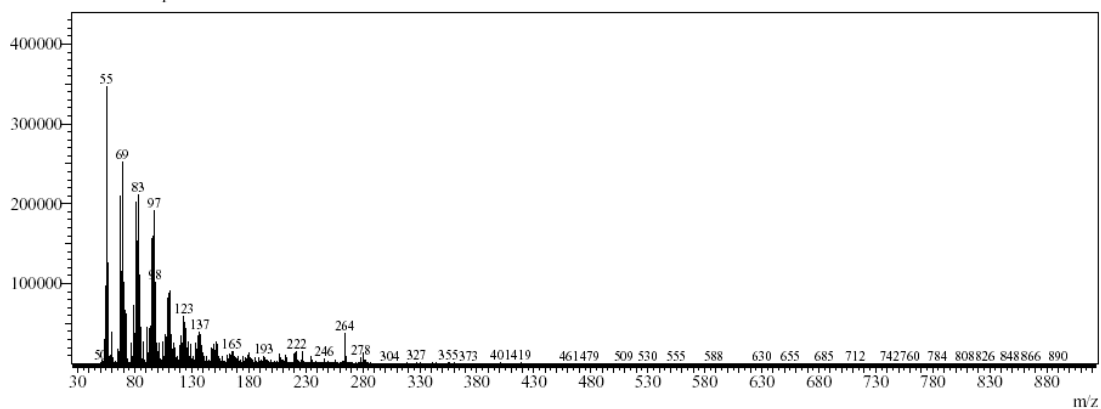
CompName:1-Aminononadecane, N-trifluoroacetyl-





Spectrum

Line#:1 R.Time:12.120(Scan#:1605)
 MassPeaks:767
 RawMode:Single 12.120(1605) BasePeak:55.05(346328)
 BG Mode:None Group 1 - Event 1 Scan



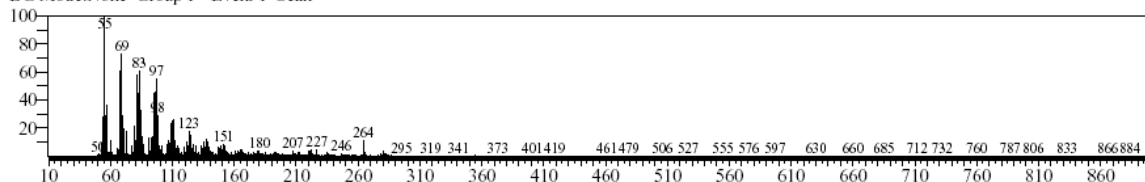
Library Search

<< Target >>

Line#1 R.Time:12.120(Scan#:1605) MassPeaks:767

RawMode:Single 12.120(1605) BasePeak:55.05(10000)

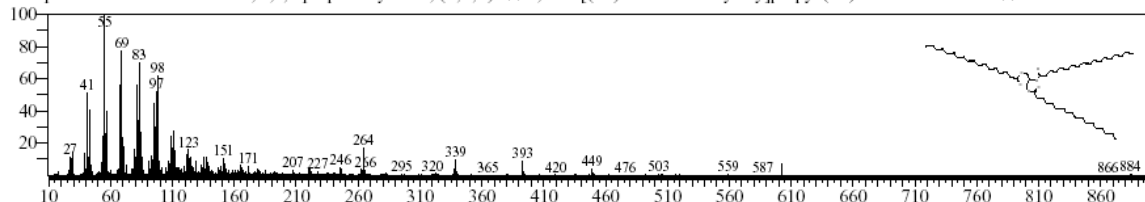
BG Mode:None Group 1 - Event 1 Scan



Hit#1 Entry:212763 Library:NIST11.lib

SI:90 Formula:C57H104O6 CAS:537-39-3 MolWeight:884 RetIndex:6149

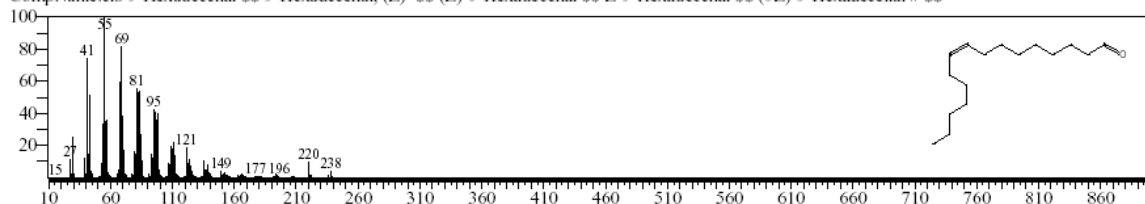
CompName:9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)- \$\$ 2,3-Bis[(9E)-9-octadecenoyloxy]propyl (9E)-9-octadecenoate # \$\$



Hit#2 Entry:70898 Library:NIST11.lib

SI:90 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808

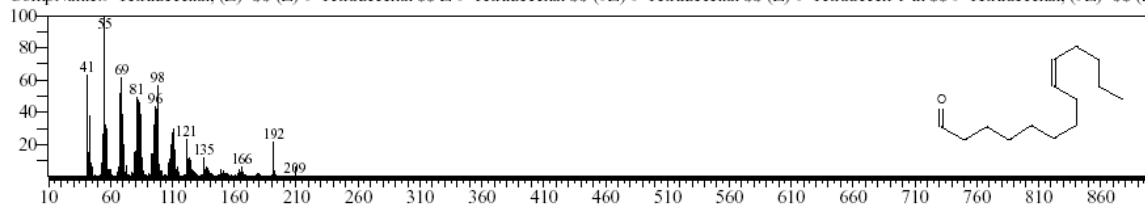
CompName:cis-9-Hexadecenal \$\$ 9-Hexadecenal, (Z)- \$\$ (Z)-9-Hexadecenal \$\$ Z-9-Hexadecenal \$\$ (9Z)-9-Hexadecenal # \$\$



Hit#3 Entry:18866 Library:NIST11s.lib

SI:90 Formula:C14H26O CAS:53939-27-8 MolWeight:210 RetIndex:1609

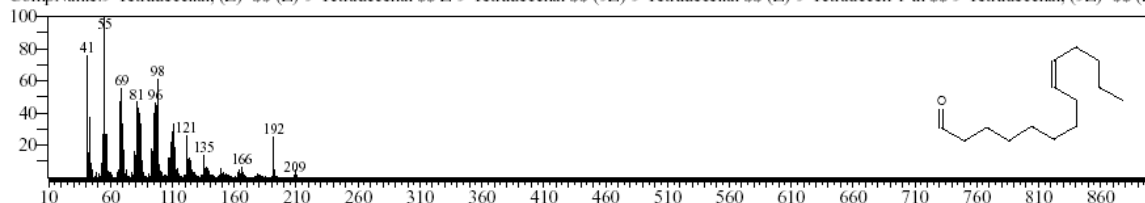
CompName:9-Tetradecenal, (Z)- \$\$ (Z)-9-Tetradecenal \$\$ Z-9-Tetradecenal \$\$ (9Z)-9-Tetradecenal \$\$ (Z)-9-Tetradecen-1-al \$\$ 9-Tetradecenal, (9Z)- \$\$ (Z)-9-Tetradecenal, (Z)- \$\$ (Z)-9-Tetradecenal # \$\$(Z)-9-Tetradecenal



Hit#4 Entry:18867 Library:NIST11s.lib

SI:89 Formula:C14H26O CAS:53939-27-8 MolWeight:210 RetIndex:1609

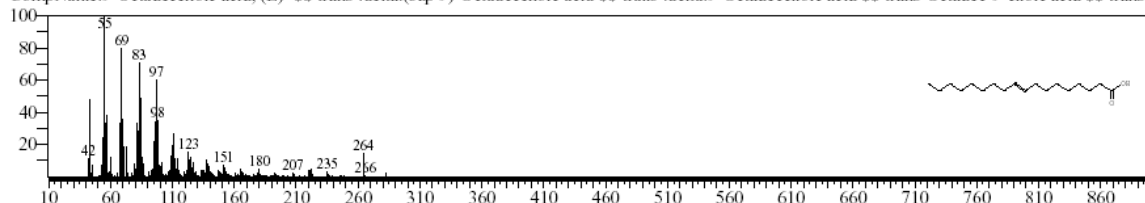
CompName:9-Tetradecenal, (Z)- \$\$ (Z)-9-Tetradecenal \$\$ Z-9-Tetradecenal \$\$ (9Z)-9-Tetradecenal \$\$ (Z)-9-Tetradecen-1-al \$\$ 9-Tetradecenal, (9Z)- \$\$ (Z)-9-Tetradecenal, (Z)- \$\$ (Z)-9-Tetradecenal # \$\$(Z)-9-Tetradecenal

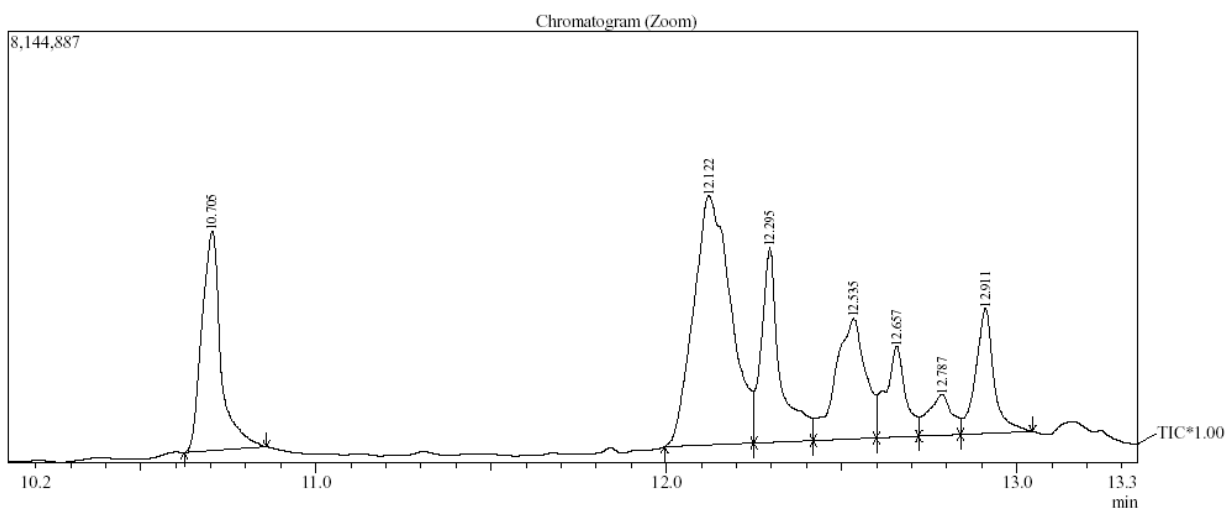
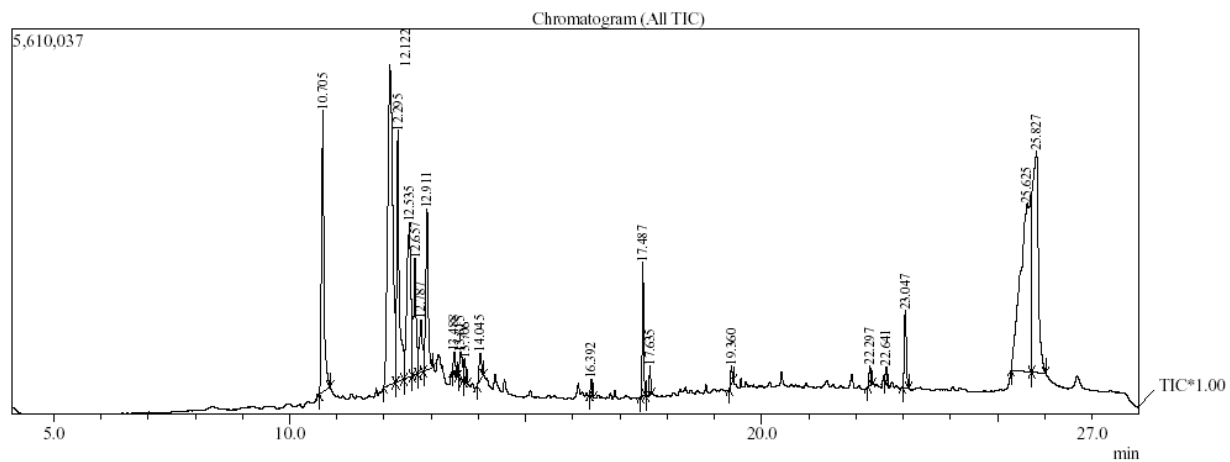


Hit#5 Entry:25042 Library:NIST11s.lib

SI:89 Formula:C18H34O2 CAS:112-79-8 MolWeight:282 RetIndex:2175

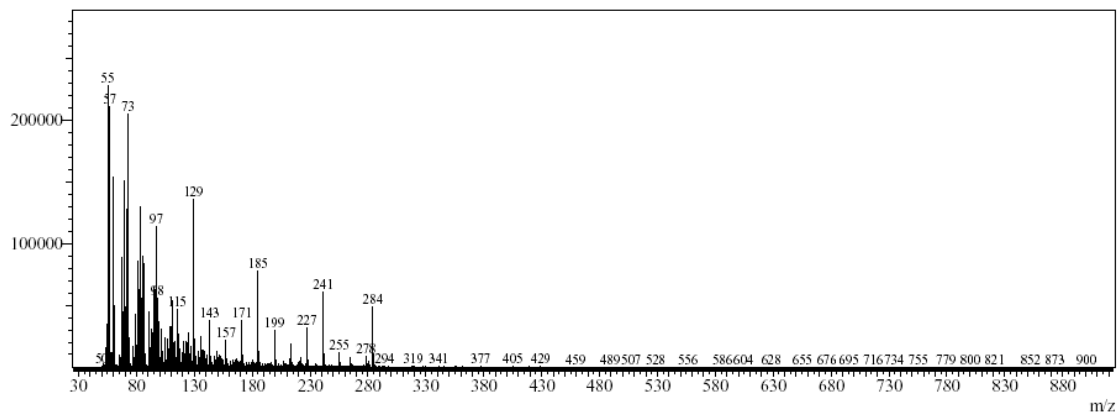
CompName:9-Octadecenoic acid, (E)- \$\$ trans-.delta.(sup 9)-Octadecenoic acid \$\$ trans-.delta.9-Octadecenoic acid \$\$ trans-Octadec-9-enoic acid \$\$ trans-





Spectrum

Line#:1 R.Time:12.295(Scan#:1640)
 MassPeaks:786
 RawMode:Single 12.295(1640) BasePeak:55.05(227756)
 BG Mode:None Group 1 - Event 1 Scan



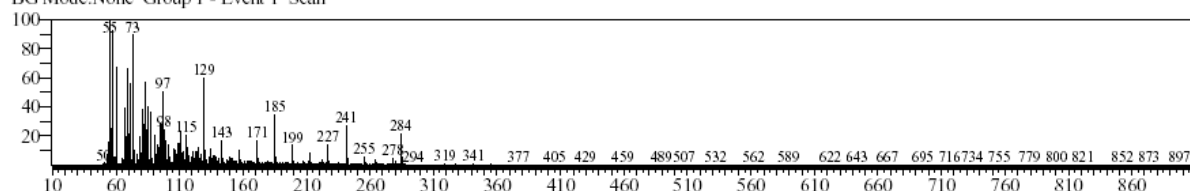
Library Search

<< Target >>

Line#:1 R.Time:12.295(Scan#:1640) MassPeaks:786

RawMode:Single 12.295(1640) BasePeak:55.05(10000)

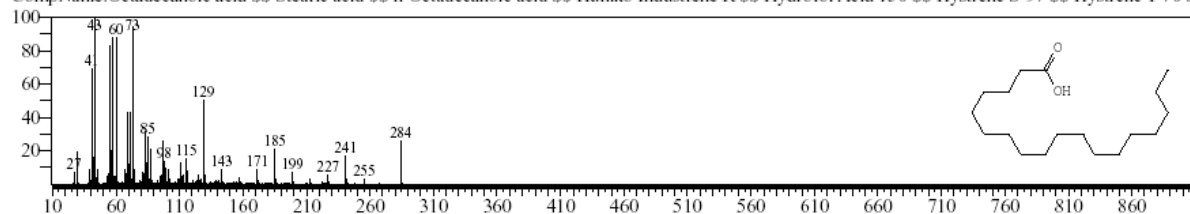
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:106158 Library:NIST11.lib

SI:84 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167

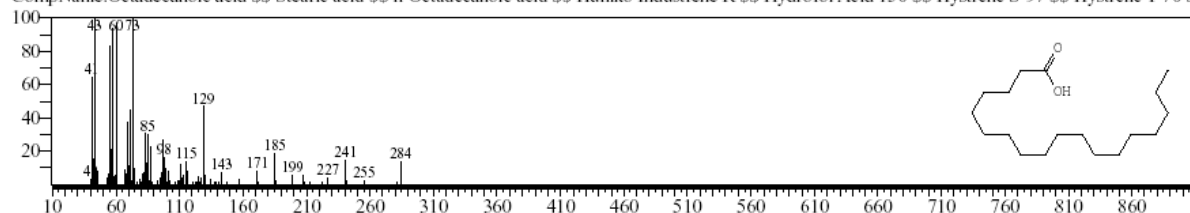
CompName:Octadecanoic acid \$\$ Stearic acid \$\$ n-Octadecanoic acid \$\$ Humko Industrene R \$\$ Hydrofol Acid 150 \$\$ Hystrene S-97 \$\$ Hystrene T-70 S



Hit#:2 Entry:25165 Library:NIST11s.lib

SI:83 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167

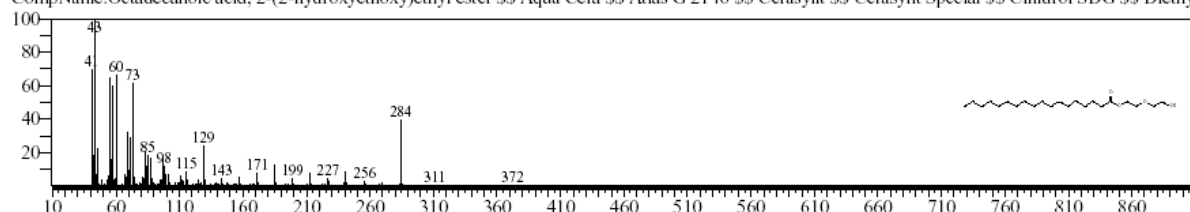
CompName:Octadecanoic acid \$\$ Stearic acid \$\$ n-Octadecanoic acid \$\$ Humko Industrene R \$\$ Hydrofol Acid 150 \$\$ Hystrene S-97 \$\$ Hystrene T-70 S



Hit#:3 Entry:169171 Library:NIST11.lib

SI:83 Formula:C22H44O4 CAS:106-11-6 MolWeight:372 RetIndex:2694

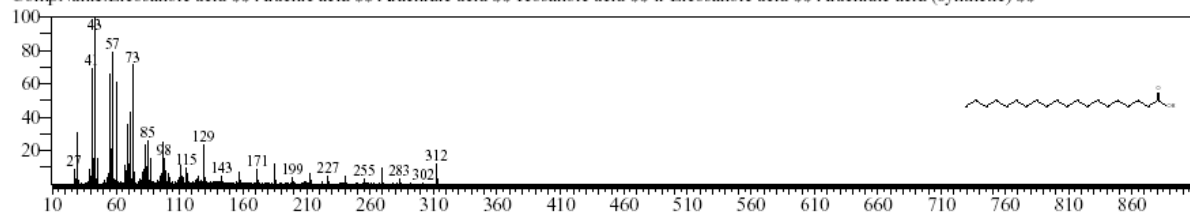
CompName:Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl ester \$\$ Aqua Cera \$\$ Atlas G 2146 \$\$ Cerasynt \$\$ Cerasynt Special \$\$ Clindrol SDG \$\$ Diethyl



Hit#:4 Entry:128151 Library:NIST11.lib

SI:82 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366

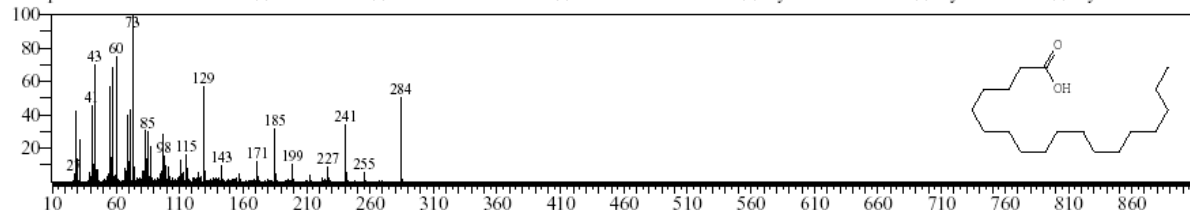
CompName:Eicosanoic acid \$\$ Arachidic acid \$\$ Arachidic acid \$\$ Icosanoic acid \$\$ n-Eicosanoic acid \$\$ Arachidic acid (synthetic) \$\$

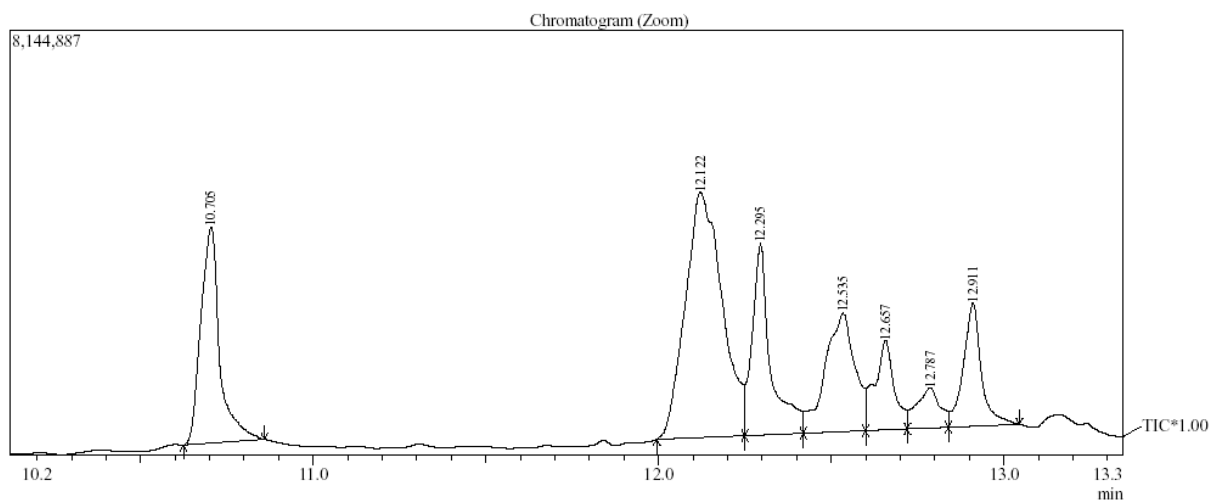
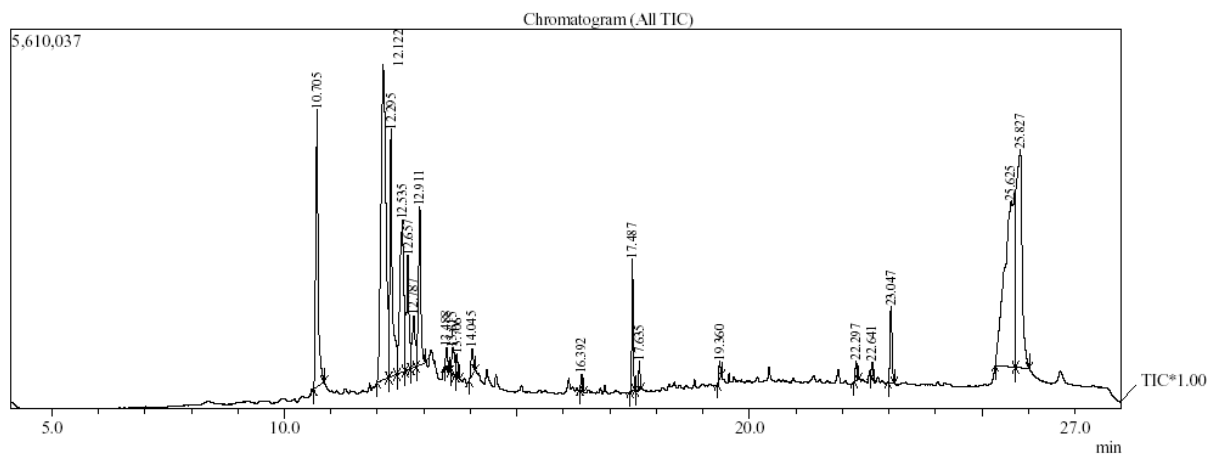


Hit#:5 Entry:25169 Library:NIST11s.lib

SI:82 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167

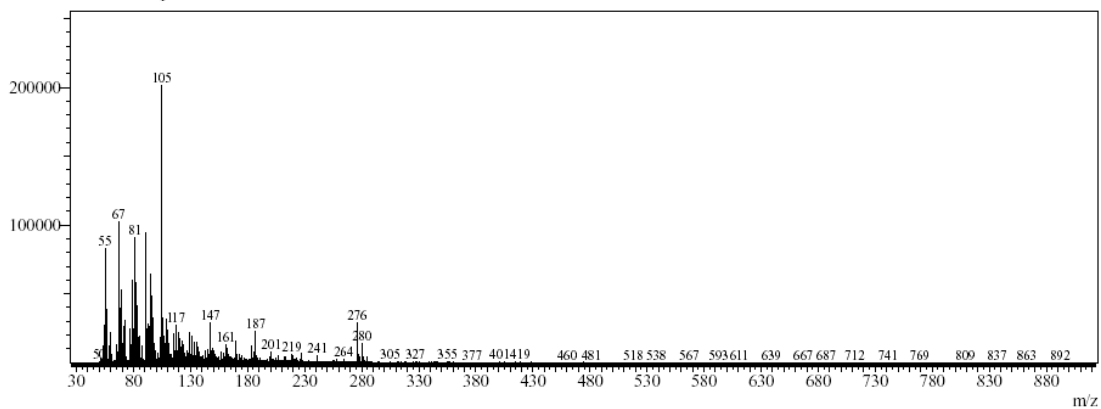
CompName:Octadecanoic acid \$\$ Stearic acid \$\$ n-Octadecanoic acid \$\$ Humko Industrene R \$\$ Hydrofol Acid 150 \$\$ Hystrene S-97 \$\$ Hystrene T-70 S





Spectrum

Line#:1 R.Time:12.550(Scan#:1691)
 MassPeaks:828
 RawMode:Single 12.550(1691) BasePeak:105.05(201169)
 BG Mode:None Group 1 - Event 1 Scan



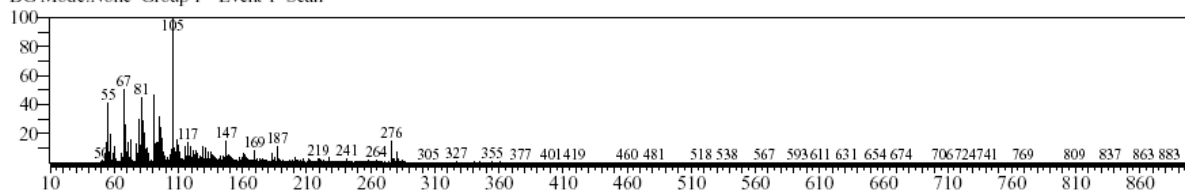
Library Search

<< Target >>

Line#1 RTime:12.550(Scan#:1691) MassPeaks:828

RawMode:Single 12.550(1691) BasePeak:105.05(10000)

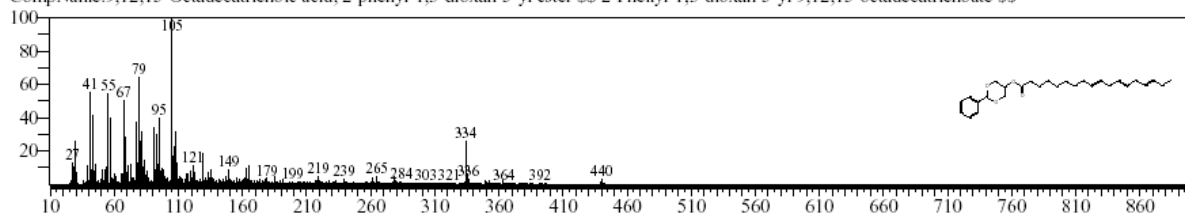
BG Mode:None Group 1 - Event 1 Scan



Hit#1 Entry:194711 Library:NIST11.lib

SI:78 Formula:C28H40O4 CAS:56700-76-6 MolWeight:440 RetIndex:3274

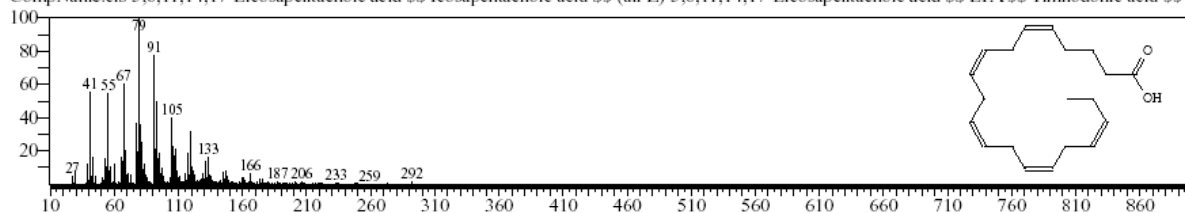
CompName:9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester \$\$ 2-Phenyl-1,3-dioxan-5-yl 9,12,15-octadecatrienoate \$\$



Hit#2 Entry:120338 Library:NIST11.lib

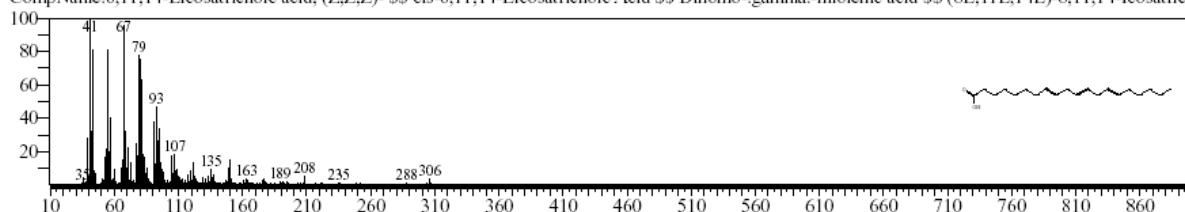
SI:77 Formula:C20H30O2 CAS:10417-94-4 MolWeight:302 RetIndex:2406

CompName:cis-5,8,11,14,17-Eicosapentaenoic acid \$\$ Eicosapentaenoic acid \$\$ (all-Z)-5,8,11,14,17-Eicosapentaenoic acid \$\$ EPA \$\$ Timnodonic acid \$\$



Hit#3 Entry:26468 Library:NIST11s.lib

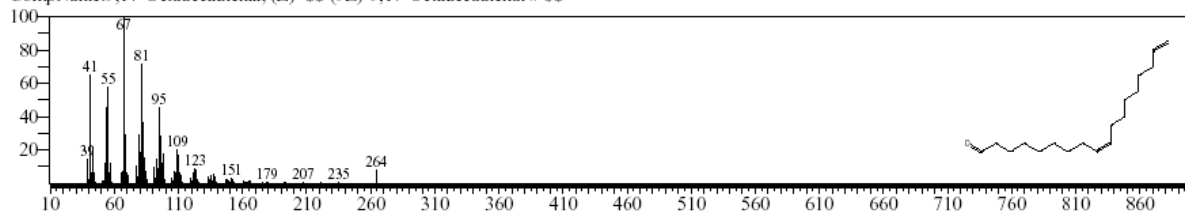
SI:76 Formula:C20H34O2 CAS:1783-84-2 MolWeight:306 RetIndex:2390

CompName:8,11,14-Eicosatrienoic acid, (Z,Z,Z)- \$\$ cis-8,11,14-Eicosatrienoic Acid \$\$ Dihomo- γ -linolenic acid \$\$ (8E,11E,14E)-8,11,14-Icosatrien

Hit#4 Entry:90502 Library:NIST11.lib

SI:76 Formula:C18H32O CAS:56554-35-9 MolWeight:264 RetIndex:1997

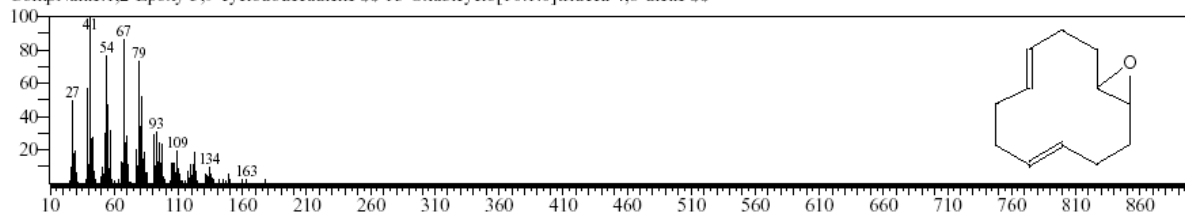
CompName:9,17-Octadecadienal, (Z)- \$\$ (9Z)-9,17-Octadecadienal # \$\$

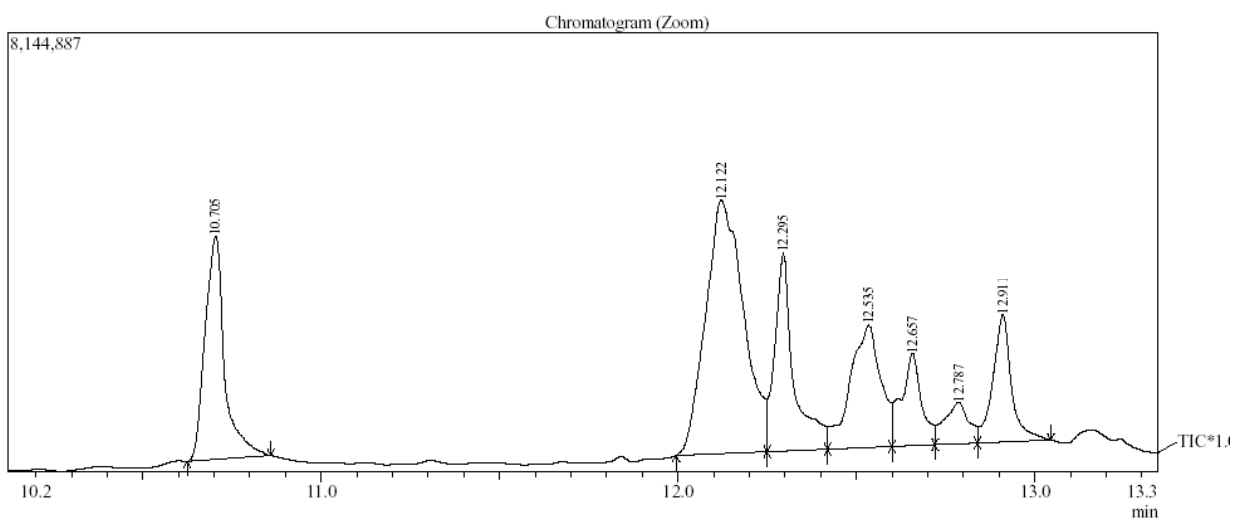
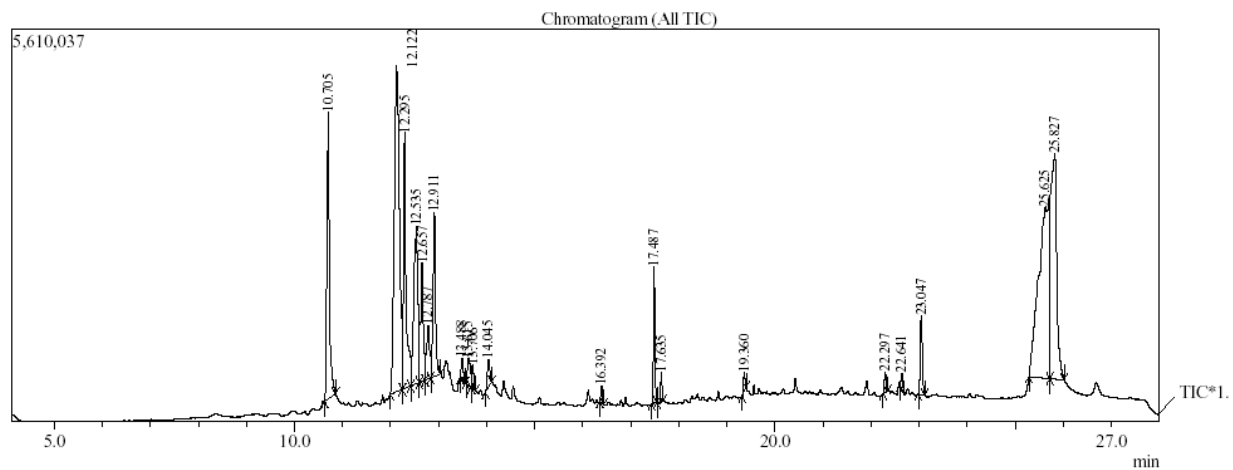


Hit#5 Entry:14066 Library:NIST11s.lib

SI:75 Formula:C12H18O CAS:943-93-1 MolWeight:178 RetIndex:1414

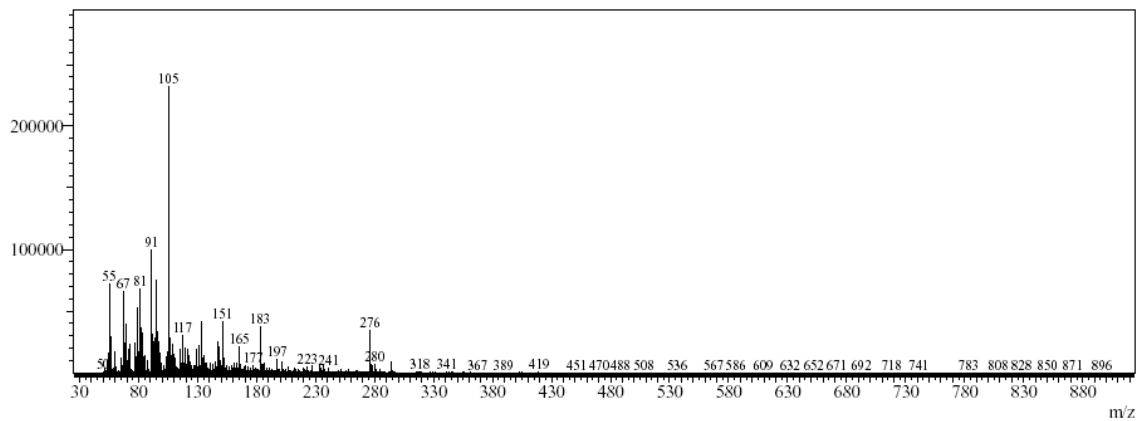
CompName:1,2-Epoxy-5,9-cyclododecadiene \$\$ 13-Oxabicyclo[10.1.0]trideca-4,8-diene \$\$





Spectrum

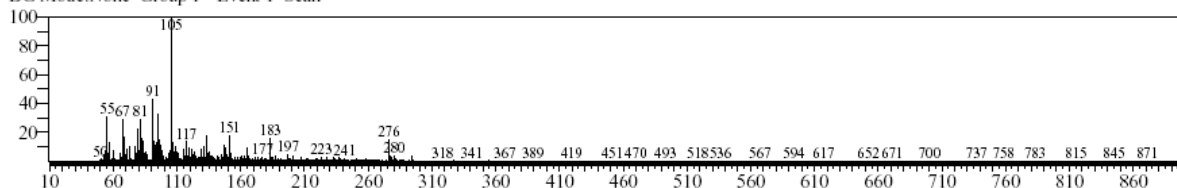
Line#:1 R.Time:12.655(Scan#:1712)
 MassPeaks:816
 RawMode:Single 12.655(1712) BasePeak:105.05(231915)
 BG Mode:None Group 1 - Event 1 Scan



Library Search

<< Target >>

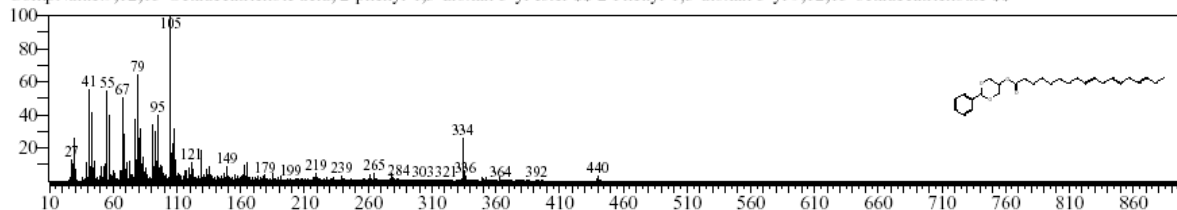
Line#:1 R.Time:12.655(Scan#:1712) MassPeaks:816
RawMode:Single 12.655(1712) BasePeak:105.05(10000)
BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:194711 Library:NIST11.lib

SI:77 Formula:C28H40O4 CAS:56700-76-6 MolWeight:440 RetIndex:3274

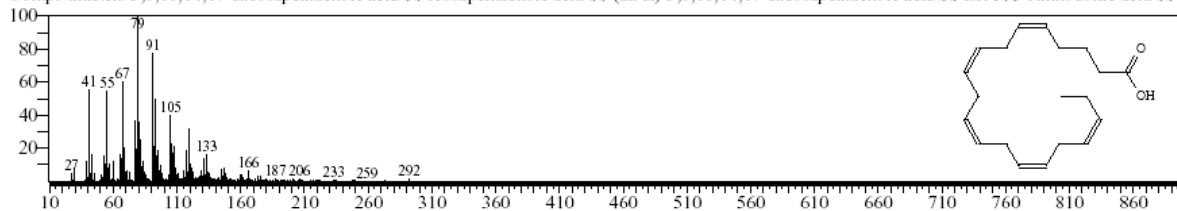
CompName:9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester \$ 2-Phenyl-1,3-dioxan-5-yl 9,12,15-octadecatrienoate \$



Hit#:2 Entry:120338 Library:NIST11.lib

SI:74 Formula:C20H30O2 CAS:10417-94-4 MolWeight:302 RetIndex:2406

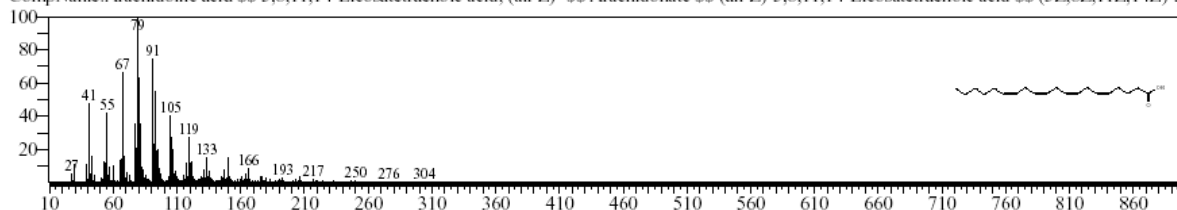
CompName:cis-5,8,11,14,17-Eicosapentaenoic acid \$ Icosapentaenoic acid \$ (all-Z)-5,8,11,14,17-Eicosapentaenoic acid \$ EPA \$ Timnodonic acid \$



Hit#:3 Entry:121879 Library:NIST11.lib

SI:74 Formula:C20H32O2 CAS:506-32-1 MolWeight:304 RetIndex:2398

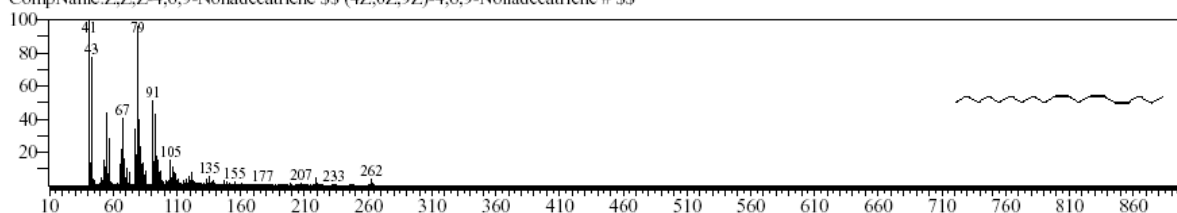
CompName:Arachidonic acid \$ 5,8,11,14-Eicosatetraenoic acid, (all-Z)- \$ Arachidonate \$ (all-Z)-5,8,11,14-Eicosatetraenoic acid \$ (5Z,8Z,11Z,14Z)-5,



Hit#:4 Entry:89045 Library:NIST11.lib

SI:73 Formula:C19H34 CAS:0-00-0 MolWeight:262 RetIndex:1934

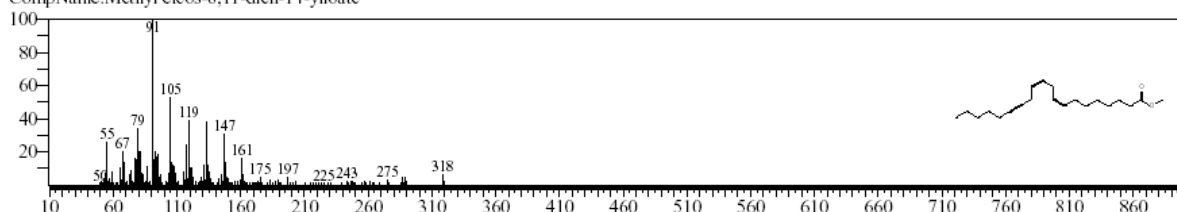
CompName:Z,Z,Z-4,6,9-Nonadecatriene \$ (4Z,6Z,9Z)-4,6,9-Nonadecatriene # \$

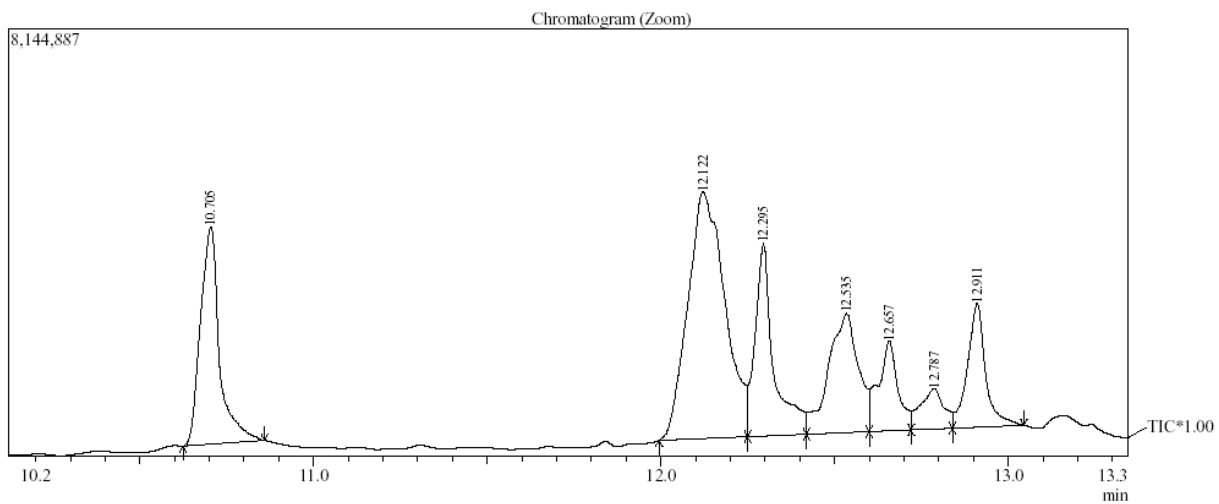
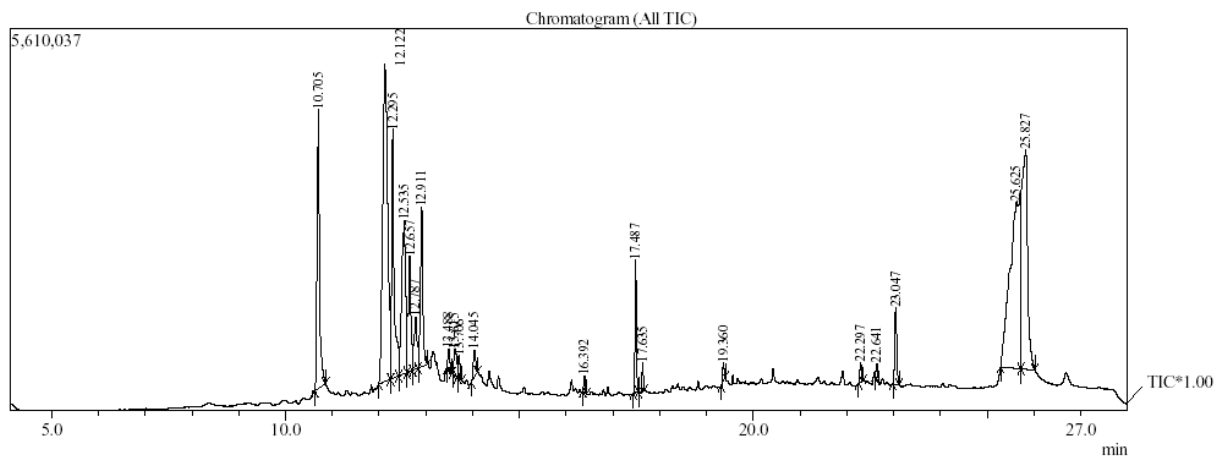


Hit#:5 Entry:132831 Library:NIST11.lib

SI:72 Formula:C21H34O2 CAS:0-00-0 MolWeight:318 RetIndex:2309

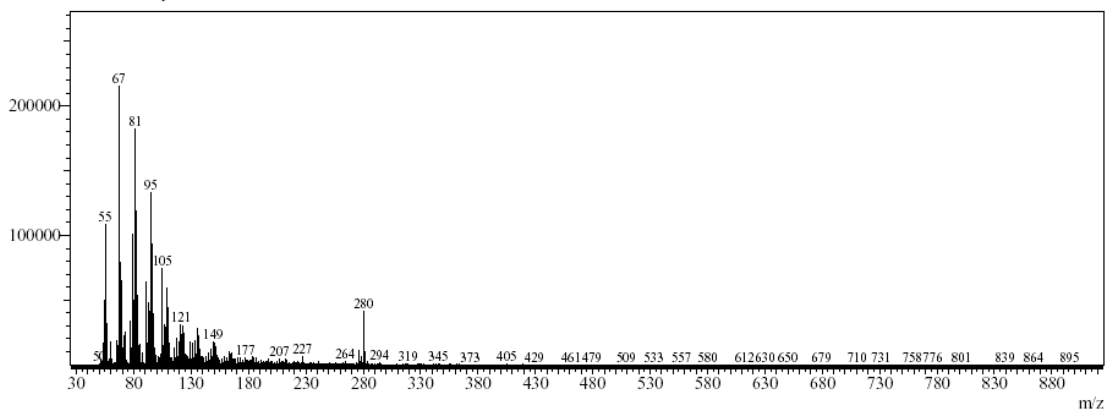
CompName:Methyl eicos-8,11-dien-14-ynoate





Spectrum

Line#:1 R.Time:12.905(Scan#:1762)
 MassPeaks:805
 RawMode:Single 12.905(1762) BasePeak:67.05(215125)
 BG Mode:None Group 1 - Event 1 Scan



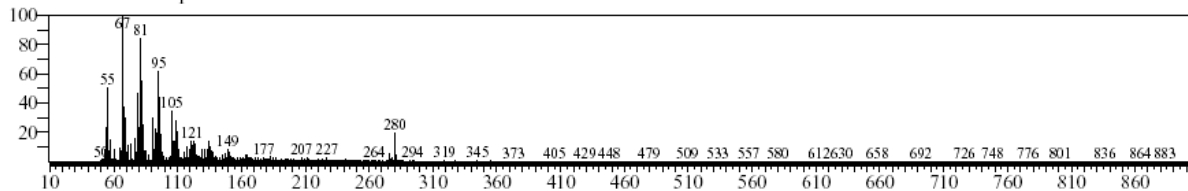
Library Search

<< Target >>

Line#:1 R.Time:12.905(Scan#:1762) MassPeaks:805

RawMode:Single 12.905(1762) BasePeak:67.05(10000)

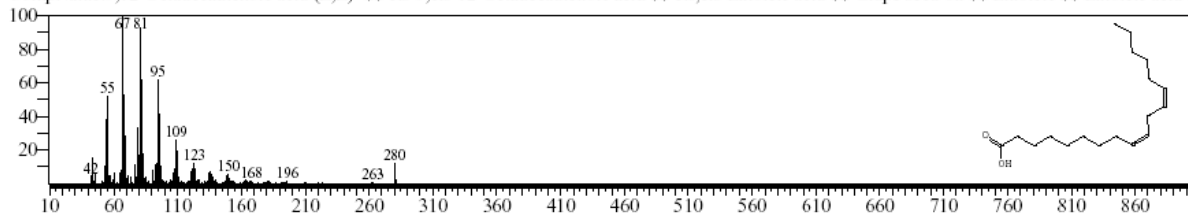
BG Mode:None Group 1 - Event 1 Scan



Hit#1 Entry:24904 Library:NIST11s.lib

SI:90 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183

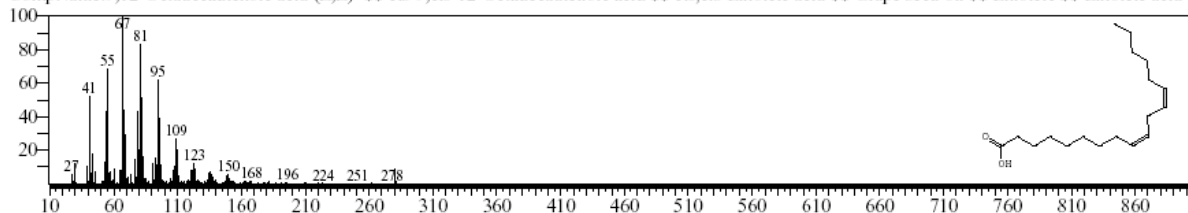
CompName:9,12-Octadecadienoic acid (Z,Z)- \$\$ cis-9,cis-12-Octadecadienoic acid \$\$ cis,cis-Linoleic acid \$\$ Grape seed oil \$\$ Linoleic acid \$



Hit#2 Entry:24903 Library:NIST11s.lib

SI:89 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183

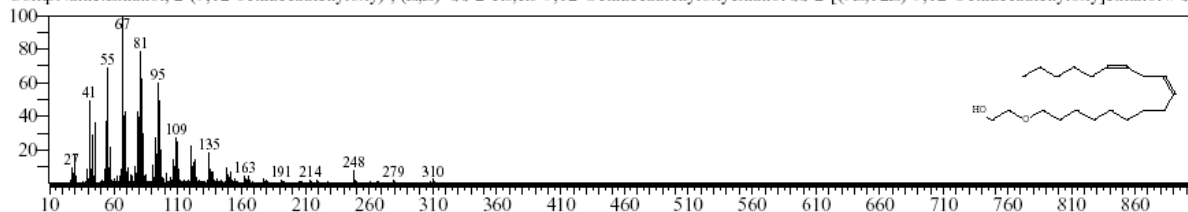
CompName:9,12-Octadecadienoic acid (Z,Z)- \$\$ cis-9,cis-12-Octadecadienoic acid \$\$ cis,cis-Linoleic acid \$\$ Grape seed oil \$\$ Linoleic acid \$



Hit#3 Entry:126507 Library:NIST11.lib

SI:87 Formula:C20H38O2 CAS:17367-08-7 MolWeight:310 RetIndex:2344

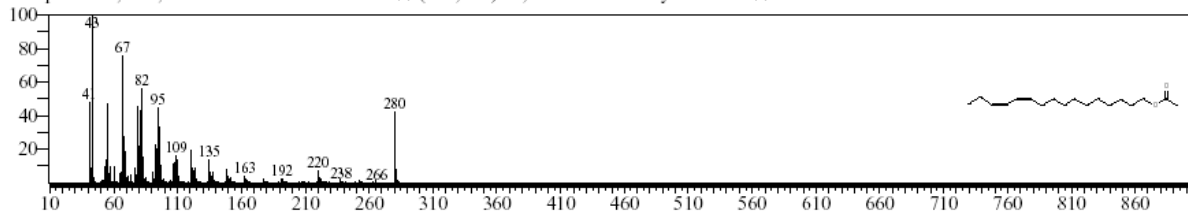
CompName:Ethanol, 2-(9,12-octadecadienyloxy)-, (Z,Z)- \$\$ 2-cis,cis-9,12-Octadecadienyloxyethanol \$\$ 2-[(9Z,12Z)-9,12-Octadecadienyloxy]ethanol # \$\$



Hit#4 Entry:102805 Library:NIST11.lib

SI:86 Formula:C18H32O2 CAS:0-00-0 MolWeight:280 RetIndex:1994

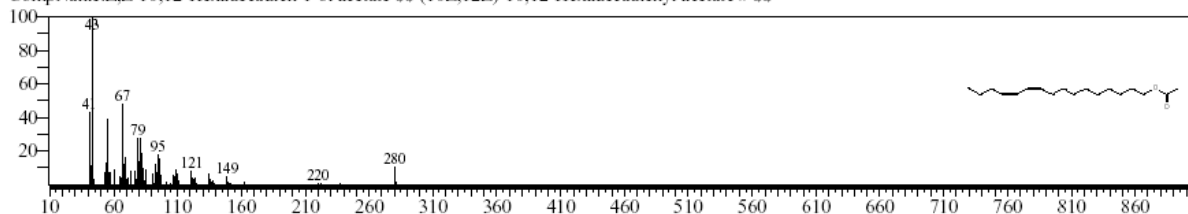
CompName:Z,Z-11,13-Hexadecadien-1-ol acetate \$\$ (11Z,13Z)-11,13-Hexadecadienyl acetate # \$\$



Hit#5 Entry:102804 Library:NIST11.lib

SI:86 Formula:C18H32O2 CAS:0-00-0 MolWeight:280 RetIndex:1994

CompName:Z,Z-10,12-Hexadecadien-1-ol acetate \$\$ (10Z,12Z)-10,12-Hexadecadienyl acetate # \$\$



Figures S13. HRMS Details of instruments used for analysis followed by analyzed data from next page

Liquid Chromatography Mass Spectrometer



FACILITY:

HR-MS

HR-MS/MS

U-HPLC-MS

U-HPLC-MS/MS

(Mode for MSMS: Auto MSMS, MRM)

MODEL AND SPECIFICATIONS:

U-HPLC:

Thermo scientific

Dionex Ultimate 3000

Detector: DAD (Diode Array Detector)

Mass Spectrometer:

Bruker Daltonik GmbH, Germany

Impact II UHR-ToF Mass Spectrometer System

(Impact II Ultra-High-Resolution Time-of-Flight Mass Spectrometer)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info

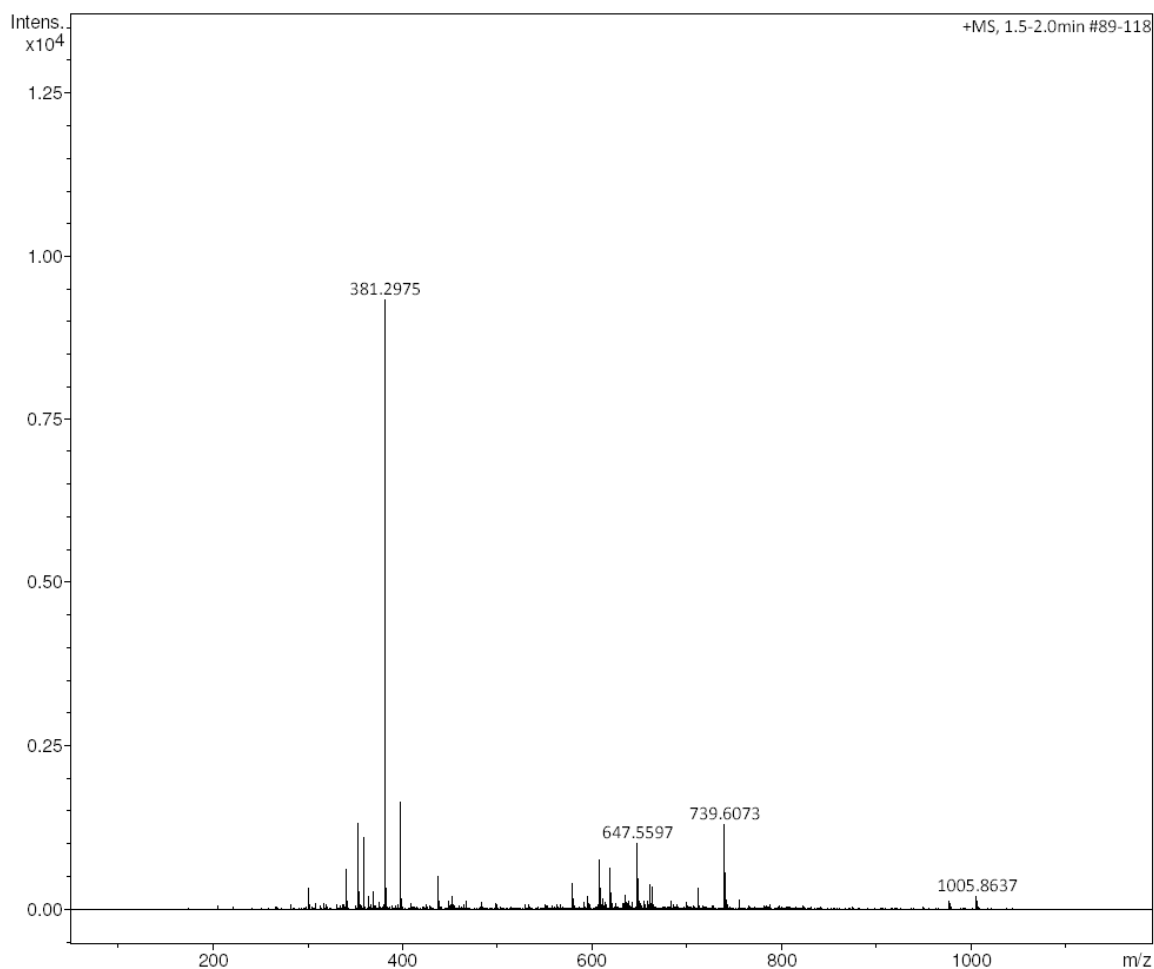
Analysis Name D:\Data\Dr. ANKAMWAR\ID_RE8_01_1717.d
Method dlc_mz1000_10min.m
Sample Name ID
Comment

Acquisition Date 11/26/2015 12:41:48 PM

Operator CIF
Instrument impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



ID_RE8_01_1717.d

Bruker Compass DataAnalysis 4.2

printed: 11/26/2015 1:36:25 PM

by: CIF

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Analysis Info

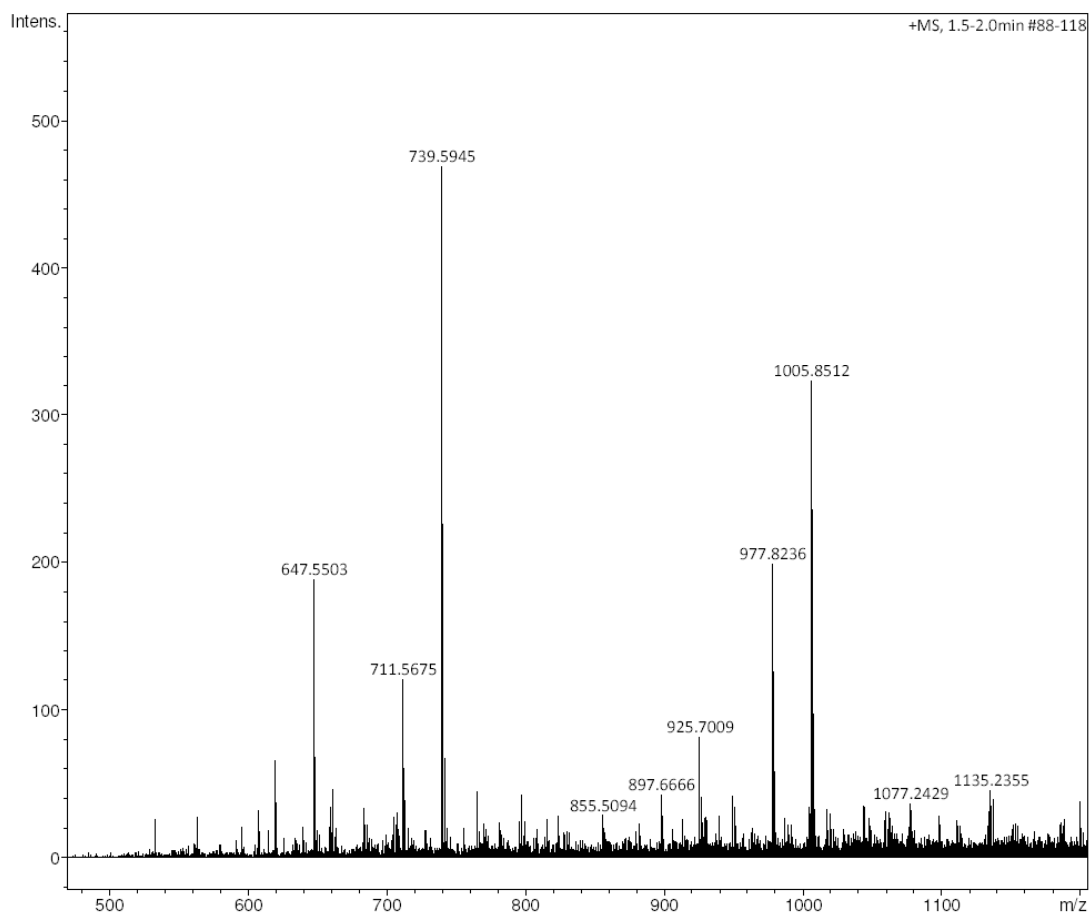
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Sample Name ID
Comment

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Operator CIF
Instrument impact HD 1819696.00184

Acquisition Parameter

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ID_RE8_01_1718.d

Bruker Compass DataAnalysis 4.2

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Analysis Info

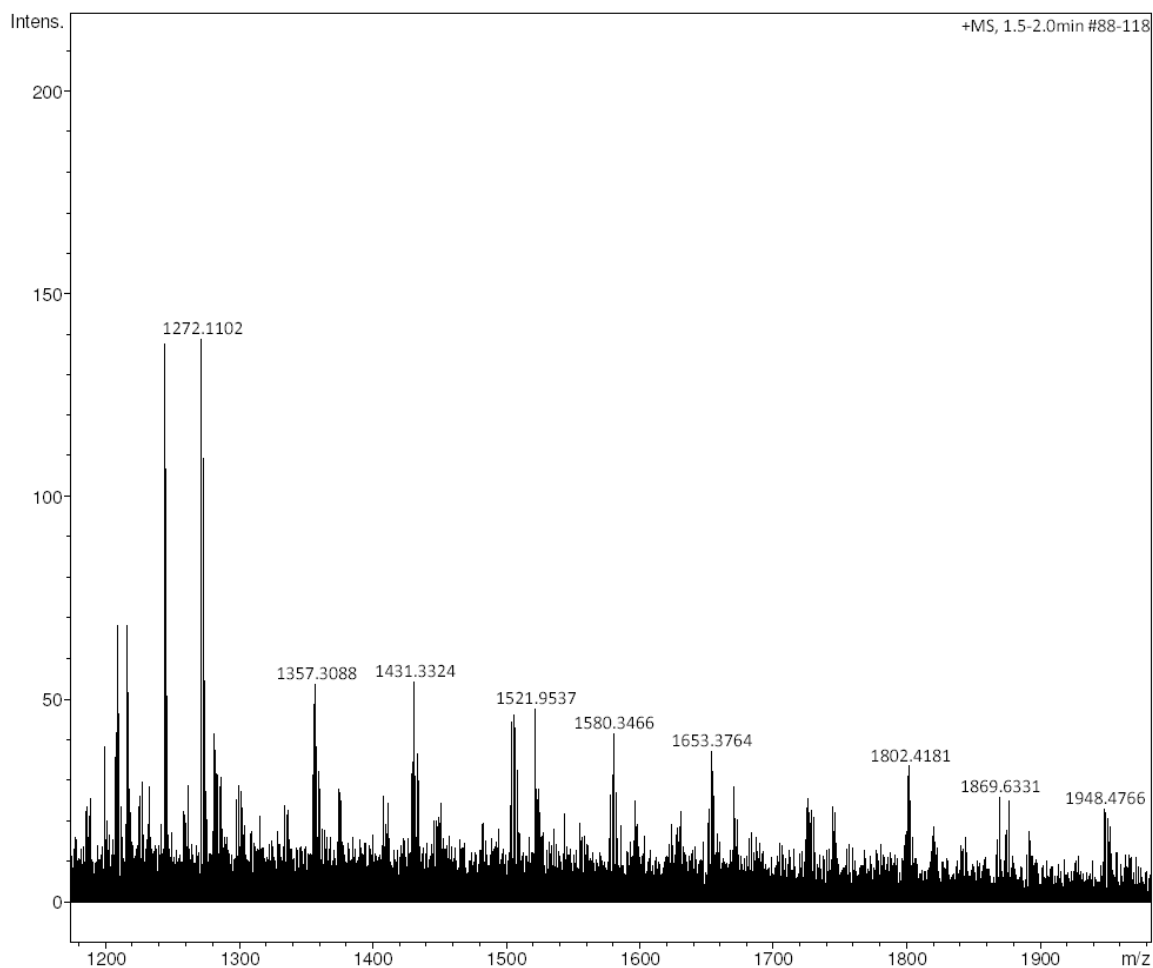
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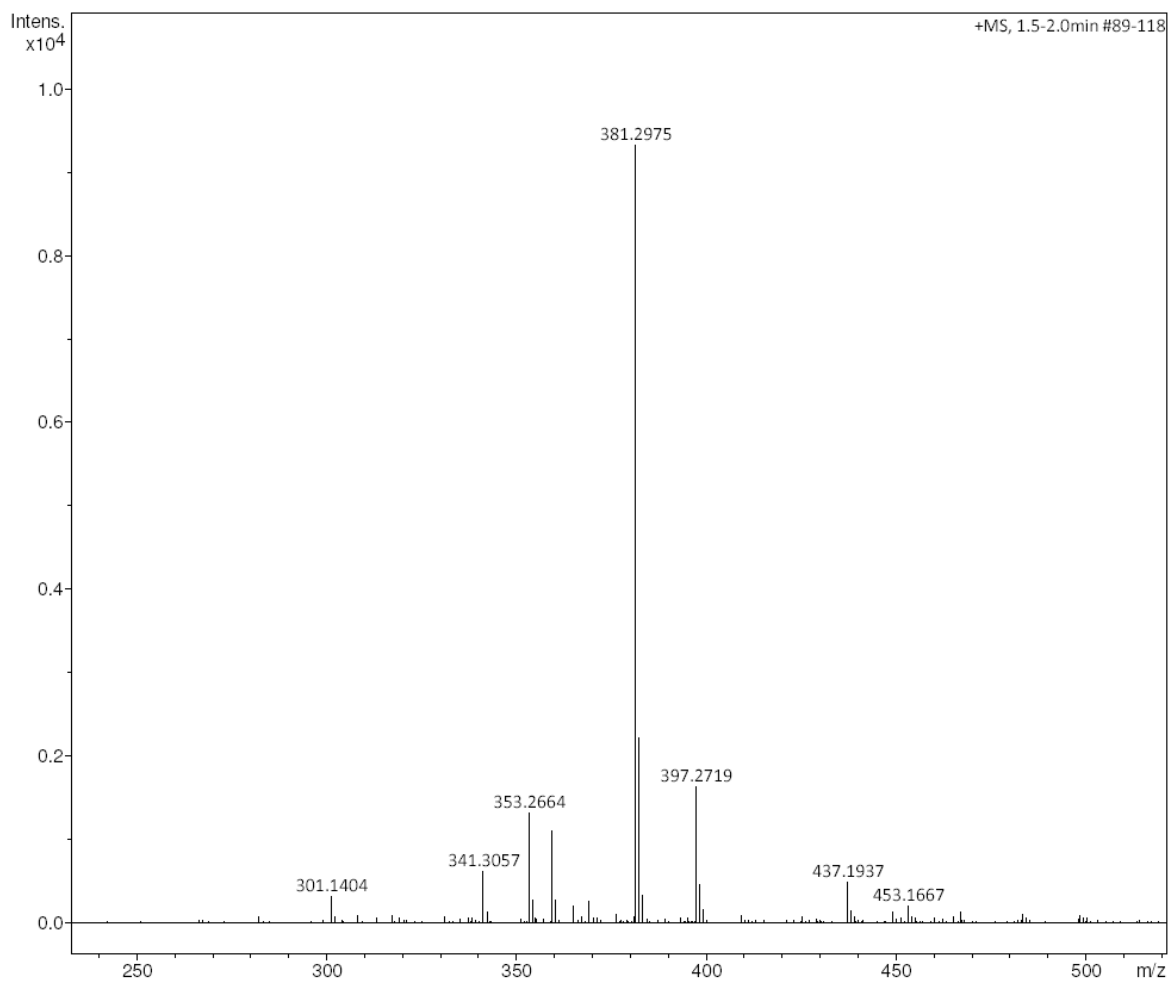
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Operator CIF
Instrument impact HD 1819696.00184

Acquisition Parameter

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Analysis Info

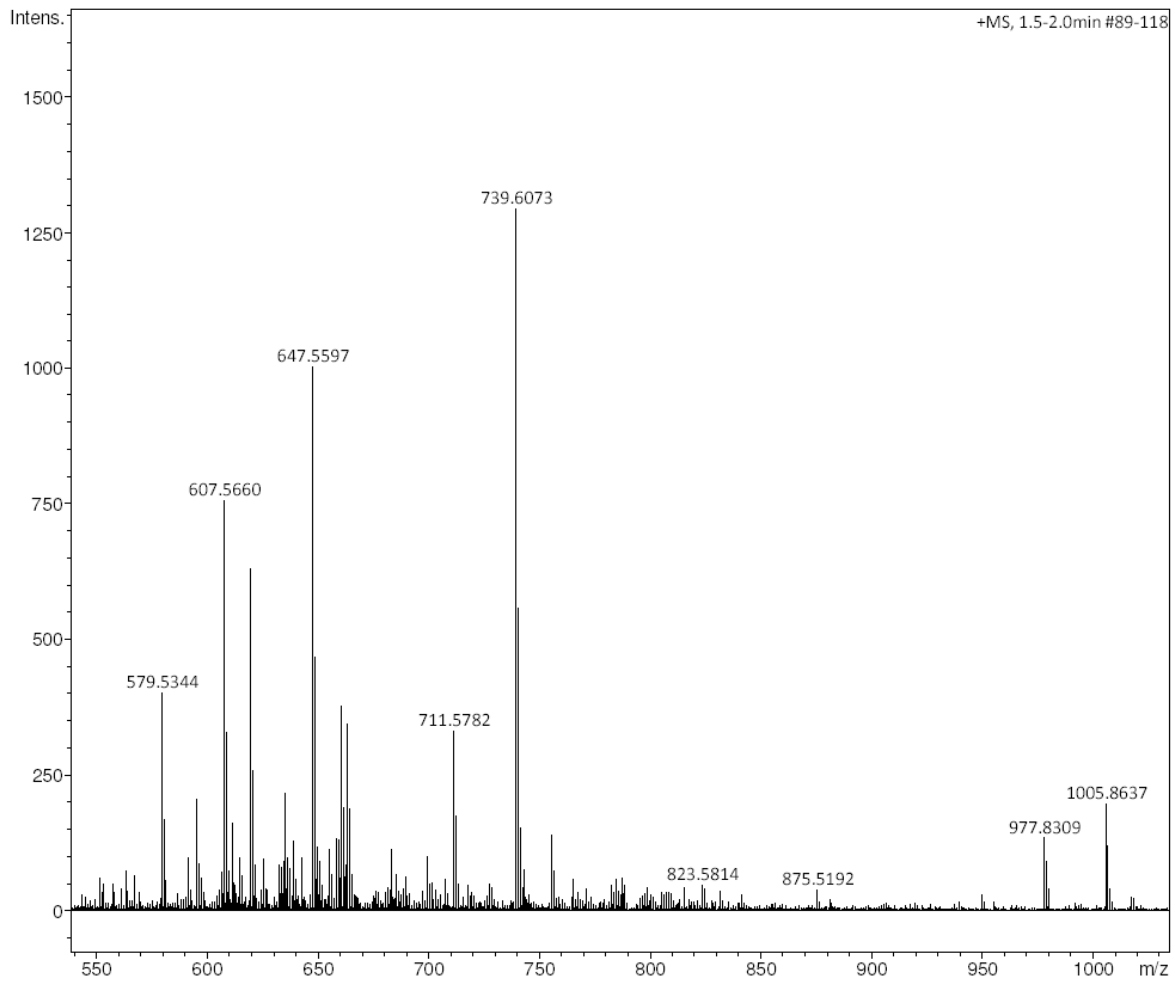
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Instrument impact HD 1819696.00184

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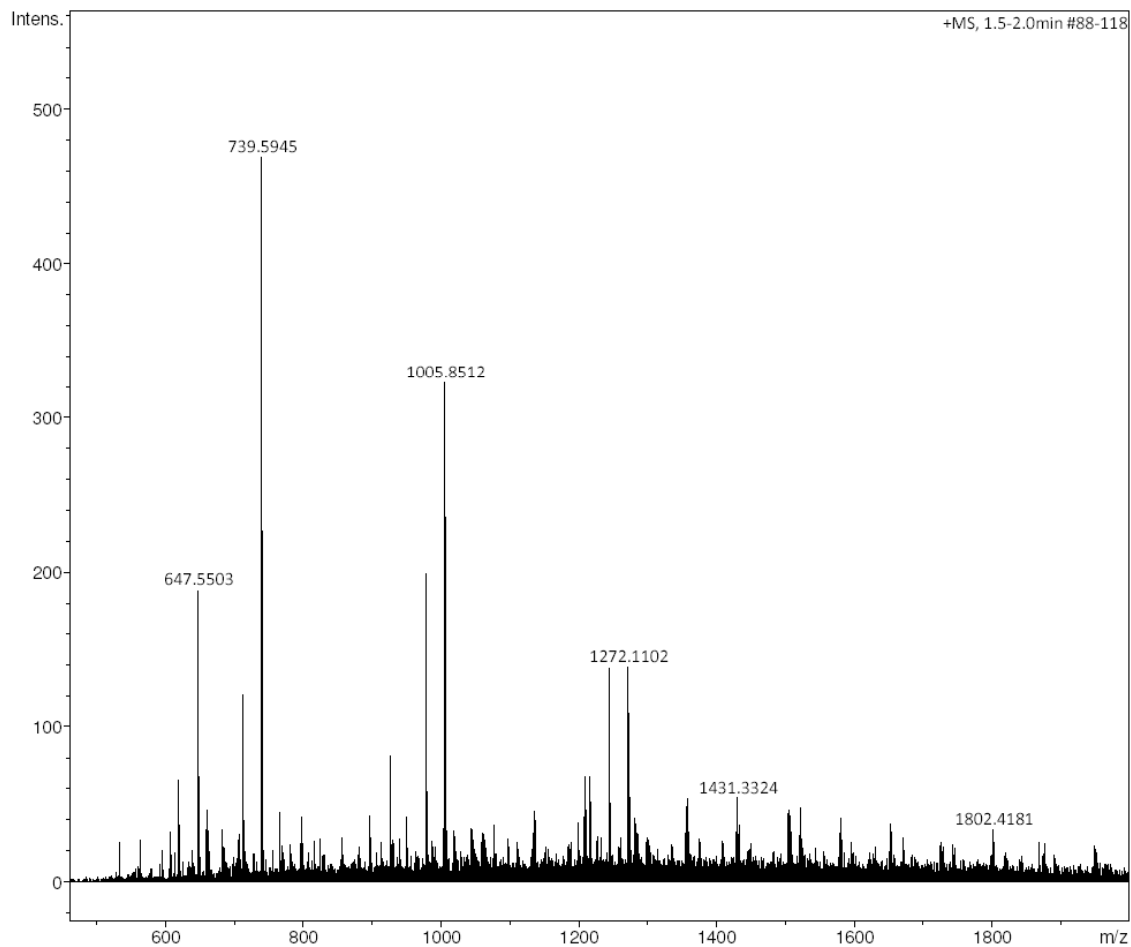
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Instrument impact HD 1819696.00184

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Figure S14. ^1H NMR of *Inonotus dryadeus* (Solvent: DMSO) Instrument: Bruker Ascend 400 MHz

Characteristics chemical shifts were observed in ^1H NMR for alcohols (~1-3ppm) and phenols, amides (~3-7 ppm), however acid peaks didn't, hence ^{13}C NMR was carried out.

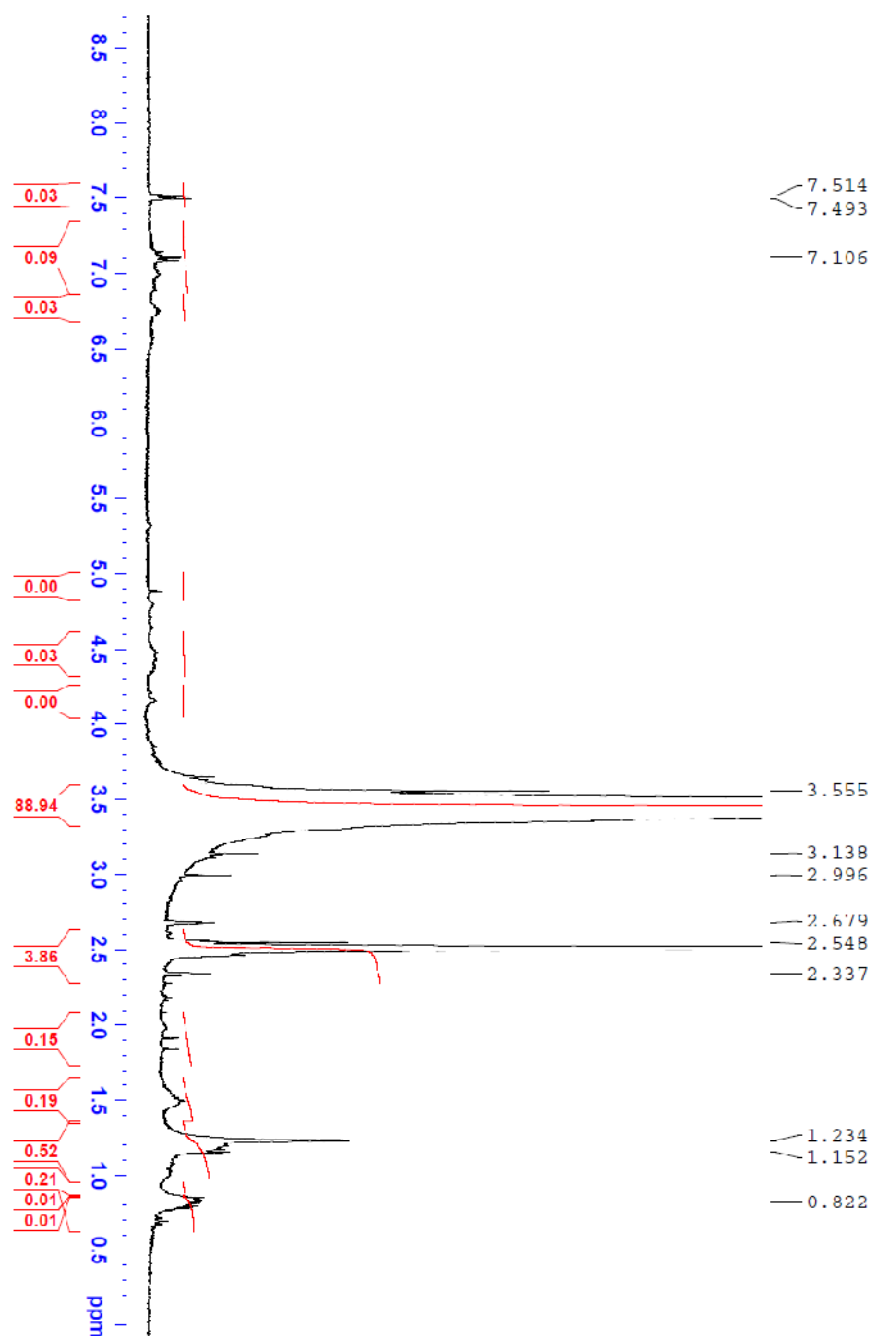


Figure S15. ^{13}C NMR of *Inonotus dryadeus* (Solvent: DMSO) Instrument: Bruker Ascend 400 MHz

Characteristics chemical shifts were observed in ^{13}C NMR for alcohols and amides (~45-75ppm)

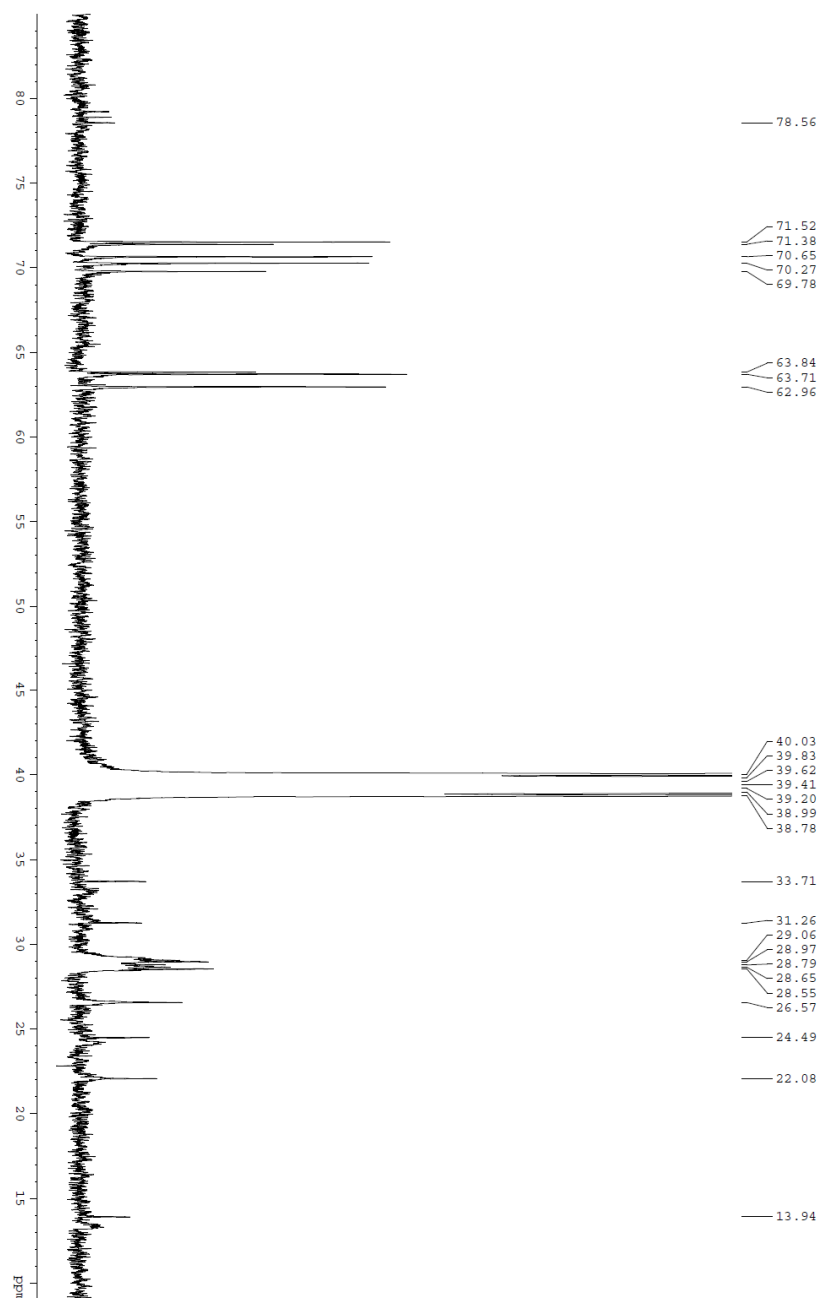
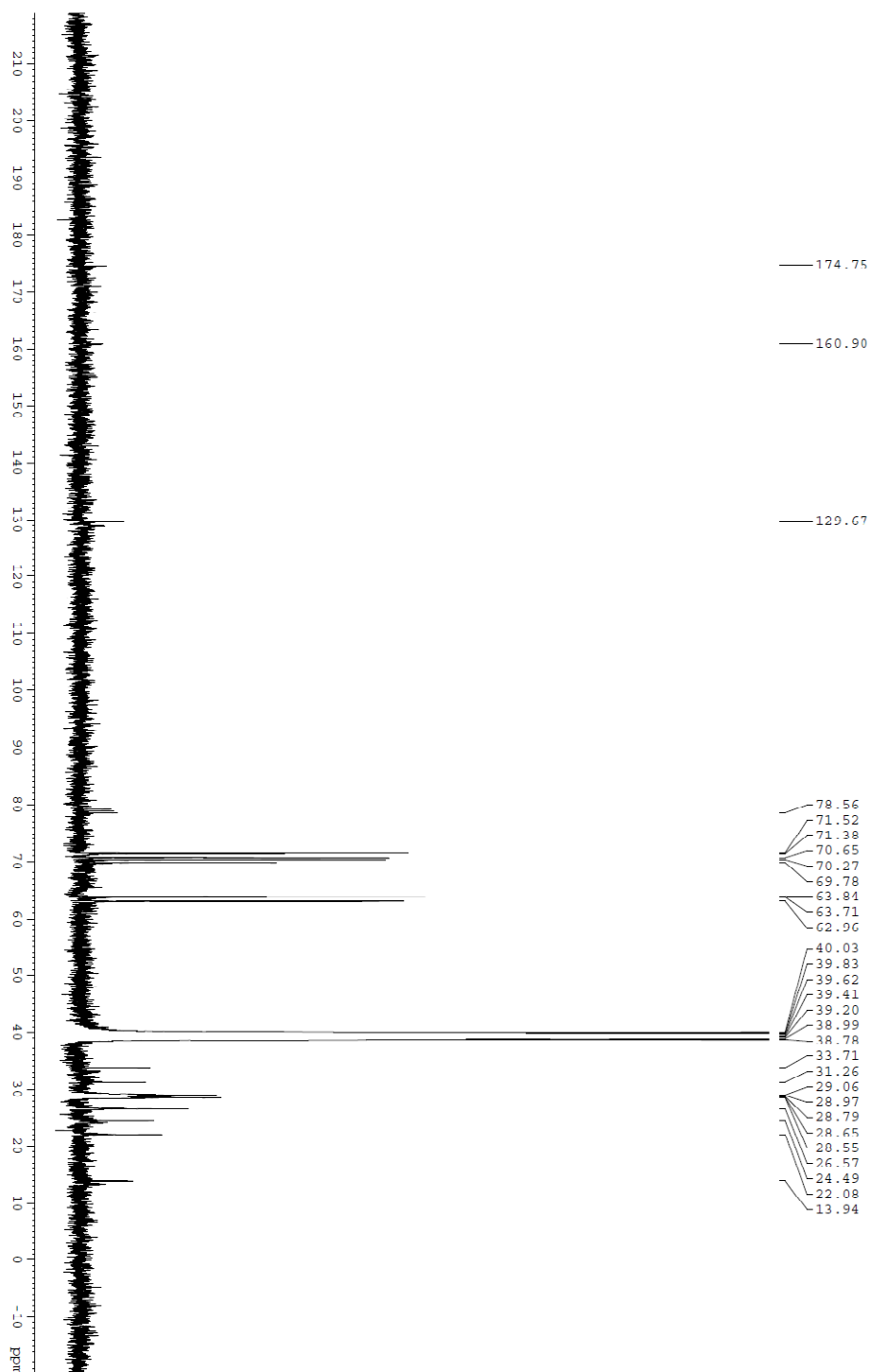


Figure S16. ^{13}C NMR of *Inonotus dryadeus* (Solvent: DMSO) Expanded

Characteristics chemical shifts were observed in ^{13}C NMR for Acids, carboxylic acid derivatives e.g. ester, amide, acid halide, acid anhydride (~160-190 ppm) and phenols (~148-160 ppm).



Figures S17. Most probable molecules of acids, phenol, alcohol, amide and esters from *Inonotus dryadeus* within the bounds of reasonable and acceptable experimental evidences provided here.

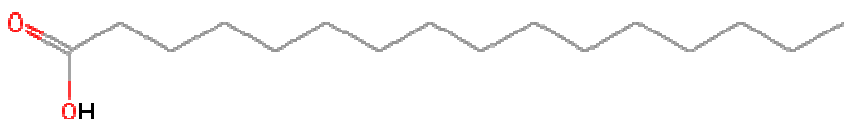
1. Pentadecanoic acid Molecular weight: 242.3975 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) low intensity



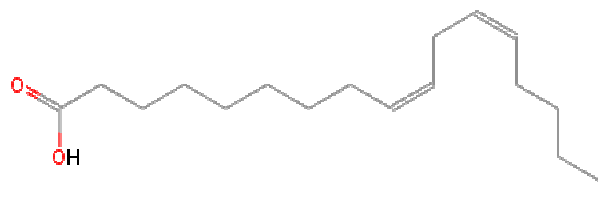
2. Hexadecanoic acid Molecular weight: 256.4241 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) low intensity



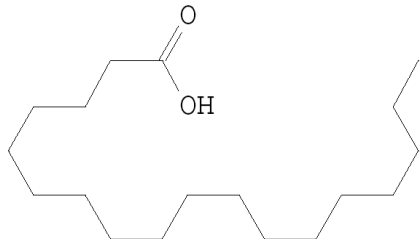
3. 9,12-Octadecadienoic acid (Z,Z)-Molecular weight: 280.4455 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) ~ 281 (low intensity)



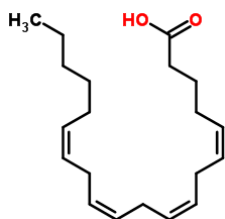
4. Octadecanoic acid Molecular weight: 284 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) ~281 (low intensity)



5. Arachidonic acid Molecular weight: 304.4669 g/mol

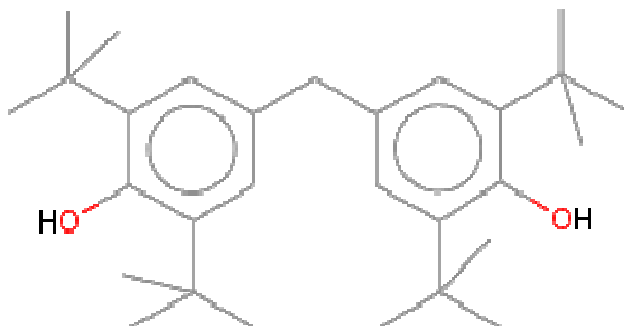
Mass observed by High Resolution Mass Spectroscopy (HRMS) 301.1404



Phenol

1. Phenol, 4,4'-methylenebis[2,6-bis(1,1-dimethylethyl)- Mol. Wt.: 424.6585 g/mol

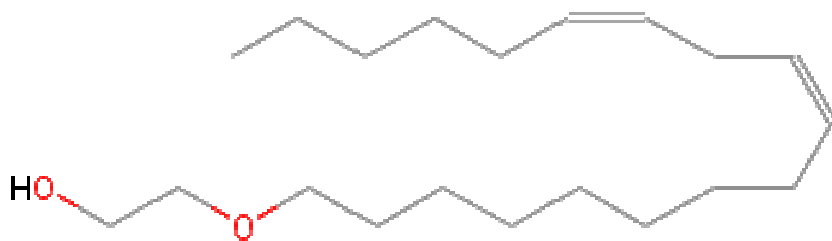
Mass observed by High Resolution Mass Spectroscopy (HRMS) 437.6585



Ethanol

1. Ethanol, 2-(9,12-octadecadienyloxy)-, (Z,Z) Mol. Wt.: 310.5145 g/mol

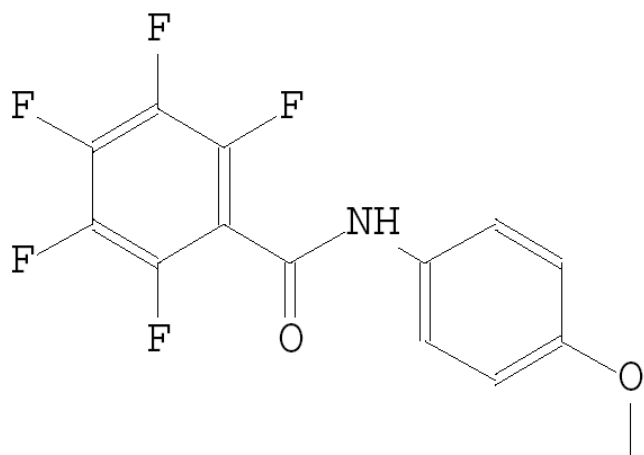
Mass observed by High Resolution Mass Spectroscopy (HRMS) 301.1404



Amide

1. 2,3,4,5,6-Pentafluoro-N-(4-methoxyphenyl) benzamide Mol. Wt.: 285.1938 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) ~281 (low intensity)



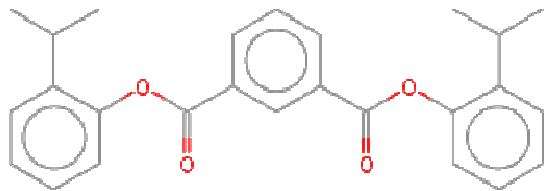
Esters

1. Isophthalic acid, di(2-isopropylphenyl) ester

Mol. Wt.: 402.4822 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS)

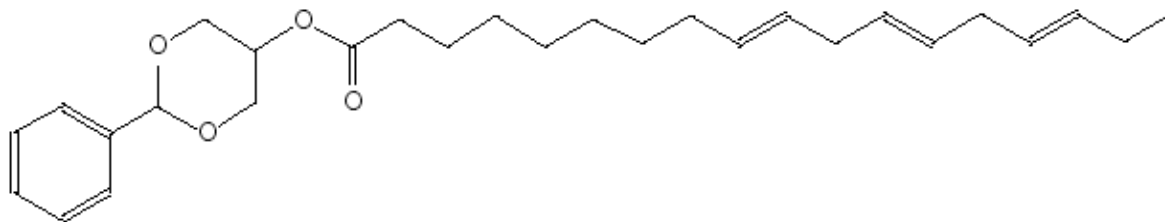
397.2718



2. 9,12,15-Octadecatrienoic acid, 2-phenyl-1,3-dioxan-5-yl ester

Mol. Wt.: 440 g/mol

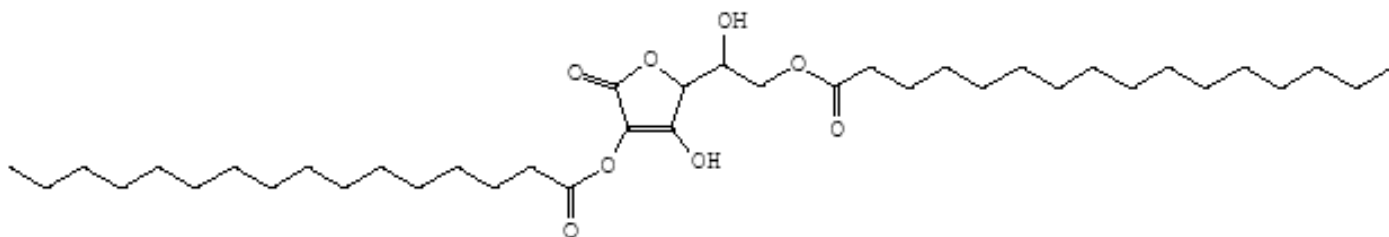
Mass observed by High Resolution Mass Spectroscopy (HRMS) 437.1937



3. L-(+)-Ascorbic acid 2,6-dihexadecanoate

Molecular weight: 652.94172 g/mol

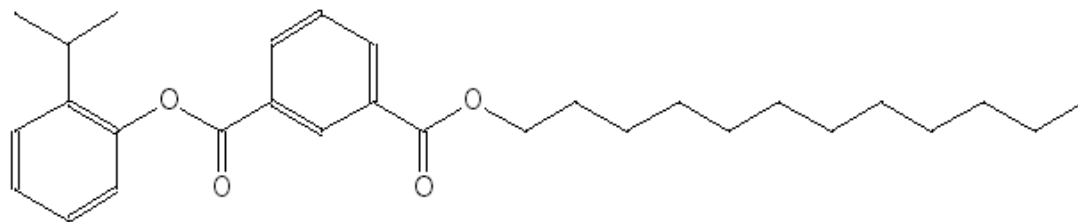
Mass observed by High Resolution Mass Spectroscopy (HRMS) 647.5597



4. Isophthalic acid, dodecyl 2-isopropylphenyl ester

Mol. Wt.: 452 g/mol

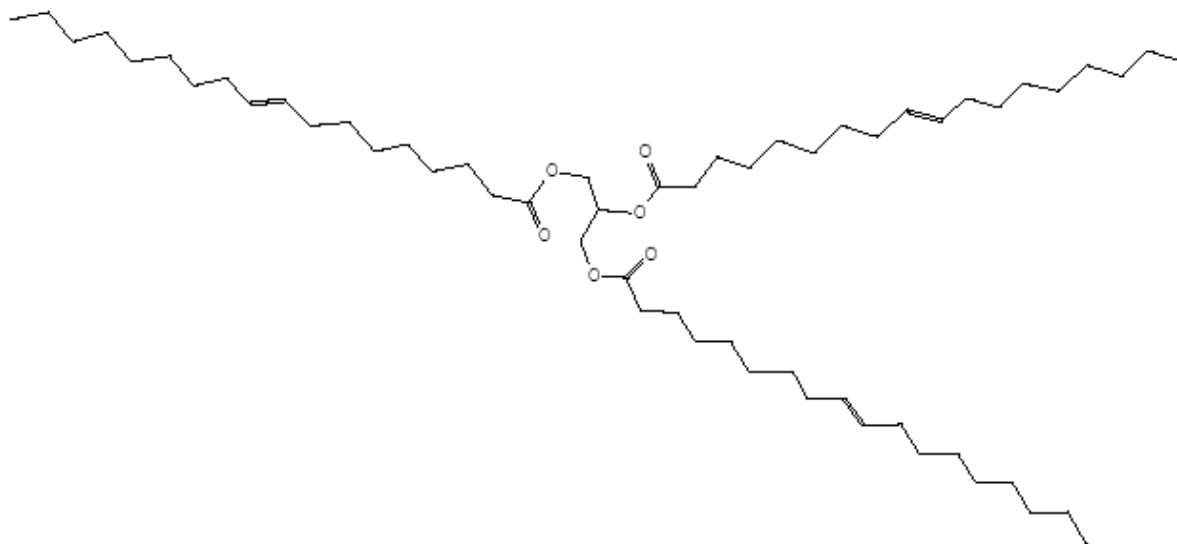
Mass observed by High Resolution Mass Spectroscopy (HRMS) 453.1667



5. 9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-

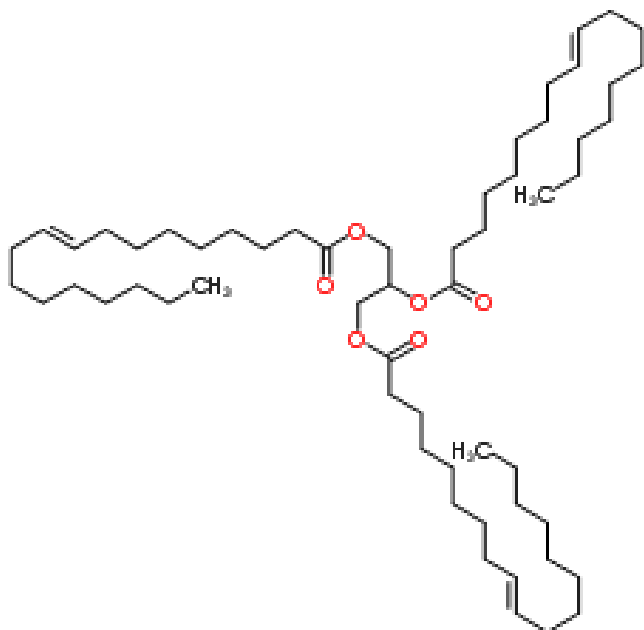
Mol. Wt.: 884 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) 884 matching with low intensity



6. 9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-Mol. Wt.: 884 g/mol

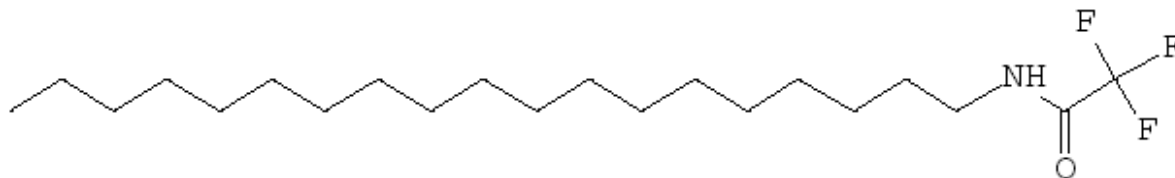
Mass observed by High Resolution Mass Spectroscopy (HRMS) 875.5192



Other molecules

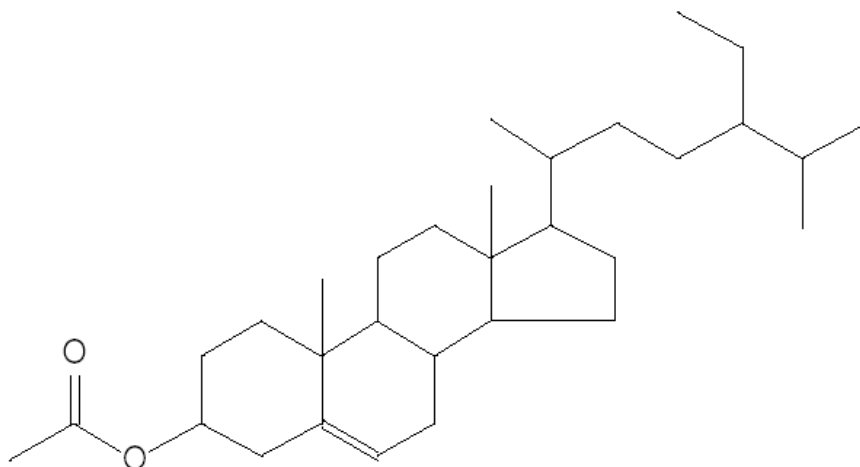
1. 1-Aminononadecane, N-trifluoroacetyl-Mol. Wt.: 379 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) 381.2975 high intensity



2. Sitosterol acetate Molecular weight: 456 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) 453.1667



3. Stigmast-5-en-3-ol, oleate \$\$ Stigmast-5-en-3-yl (9Z)-9-octadecenoate

Mol. Wt.: 678 g/mol

Mass observed by High Resolution Mass Spectroscopy (HRMS) ~678 matching

