



CASE STUDY FTIR v. PYMS

OBJECTIVE

The objective of this study is to highlight the benefits and limitations of two analytical techniques, FTIR and PYMS.

ANALYTICAL STRATEGY

By analyzing polymers from two common families, nylons and polyesters, we will be able to demonstrate the types of information that Jordi can provide with each technique.

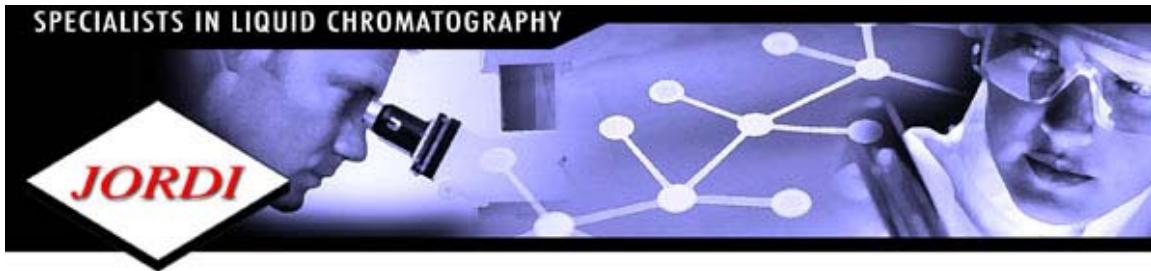
FTIR is sensitive to any component at a concentration of roughly 5% or greater, thus the technique is generally applied for identification of the chemical composition of the polymer matrix but not the additives package or other minor sample components.

PYMS is intended for the analysis of polymer systems and is most useful for the ability to identify polymer and copolymer varieties in addition to many polymer additives (e.g. antioxidants and stabilizers). This powerful technique provides excellent resolution for identifying components in a complex mixture. For most polymer systems, PYMS offers more definitive identification and greater sensitivity than FTIR, down to the single digit ppm range for many compounds.

RESULT

PYMS is a more powerful technique for identifying unknowns within a particular polymer family or identifying any low-concentration additives or impurities. FTIR is a great method for the quick identification of the functionality of an unknown sample, but PYMS analysis can provide a much greater level of information and should be the method of choice when this type of information is preferred.

Read the following report to see the full analysis.



Date

Client Name
Company Name

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

Dear Client,

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

1. *Nylon 6 (N6)*
2. *Nylon 12 (N12)*
3. *Polyethylene terephthalate (PET)*
4. *Polybutylene terephthalate (PBT)*
5. *PET/Di-n-octyl phthalate Mixture (PET/DOP)*

The following tests were performed:

1. Fourier Transform Infrared Spectroscopy (FTIR)
2. Pyrolysis Gas Chromatography Mass Spectroscopy (PYMS)

Objective

The objective of this study is to highlight the benefits and limitations of two analytical techniques, FTIR and PYMS. By analyzing polymers from two common families, nylons and polyesters, we will be able to demonstrate the types of information that Jordi can provide with each technique.

Summary of Results

FTIR was shown to be a useful method for determining the functionality (and by extension, the family) of an unknown polymer sample. The limitations of this method were demonstrated for compounds of similar chemical structures and for additives analysis. PYMS was demonstrated to be generally superior when definitive identification of the monomer structure is required or when performing an analysis of polymer additives.

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.

Background

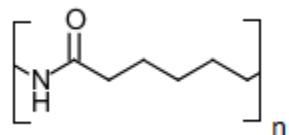
FTIR - A sample is placed into an infrared (IR) source and the absorption characteristics of the material are monitored. Resultant IR absorbance bands are qualitative and characteristic of functional groups that absorb IR light at those frequencies. Careful inspection of the bands present can allow for a general identification of the material in question based on the functional groups associated with those bands. FTIR is useful for identifying the *general class* of a material.

For unknown samples, the collected spectra are compared with reference spectra for thousands of known compounds to aid in major component identification. FTIR is sensitive to any component at a concentration of roughly 5% or greater, thus the technique is generally applied for identifying the chemical composition of the polymer matrix and not the additives package or other minor sample components. To obtain more definitive chemical identification, pyrolysis mass spectroscopy (PYMS) can be employed.

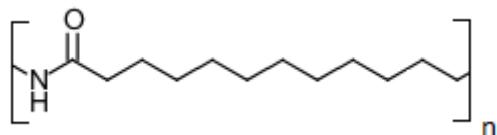
PYMS - In PYMS, the sample is examined using a two-stage heating process while mass spectra are continually monitored. In the first cycle (often called PY1), the sample is heated through a predefined temperature profile while solvents, impurities, additives, and other small molecules are evolved and detected. In the second cycle (often called PY2), the sample is exposed to higher temperatures where thermal dissociation occurs and large molecules cleave at their weakest points. This produces smaller and more volatile fragments that are detected and used to help identify the polymer itself as well as any component left behind during PY1.

PYMS is an excellent tool for the analysis of polymer systems and is most useful for its ability to identify polymers, copolymers and many polymer additives (e.g. antioxidants and stabilizers). This powerful technique provides excellent resolution for identifying components in a complex mixture. For most polymer systems, PYMS offers more definitive identification and greater sensitivity than FTIR, down to the single digit ppm range for many compounds.

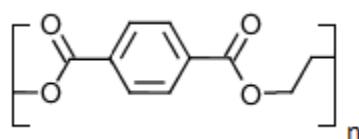
Definitions



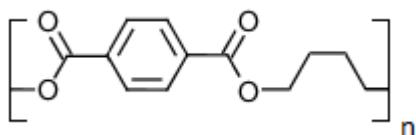
Nylon 6



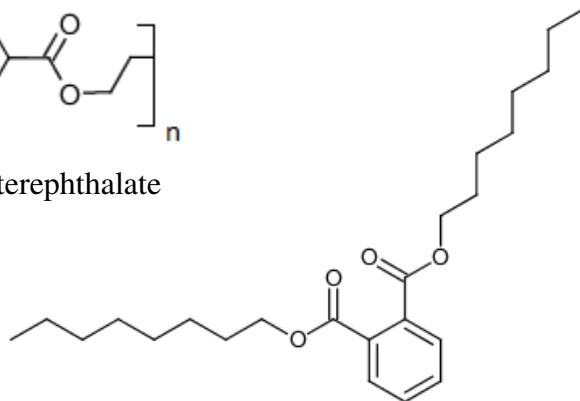
Nylon 12



Polyethylene terephthalate



Polybutylene terephthalate



Di-n-octyl phthalate

Individual Test Results

FTIR

An FTIR spectrum was collected for each polymer sample as well as the PET/phthalate mixture. Figures I and II compare the nylon and polyester FTIR spectra, respectively. We can see that there is very little difference between the two nylon spectra or between the two polyester spectra. We would, however, be able to tell the difference between a nylon and a polyester because of the presence and absence of various functional group absorbance bands.

FTIR is a convenient and powerful technique for determining the functionality (and by extension, the family) of an unknown polymer sample. However, FTIR is not nearly as useful for determining specific chemical structures within a family of polymers.

Another limitation of FTIR can be demonstrated in Figure I. As stated previously, the detection limit of an FTIR is generally 5%. If a component or additive concentration is below this range, it will rarely show up on an FTIR spectrum. We are unable to observe the 400 ppm di-n-octyl phthalate (DOP) additive by FTIR because any would-be peaks are masked by the major component, PET.

Figure I: A comparison of Nylon 6 and Nylon 12 FTIR spectra

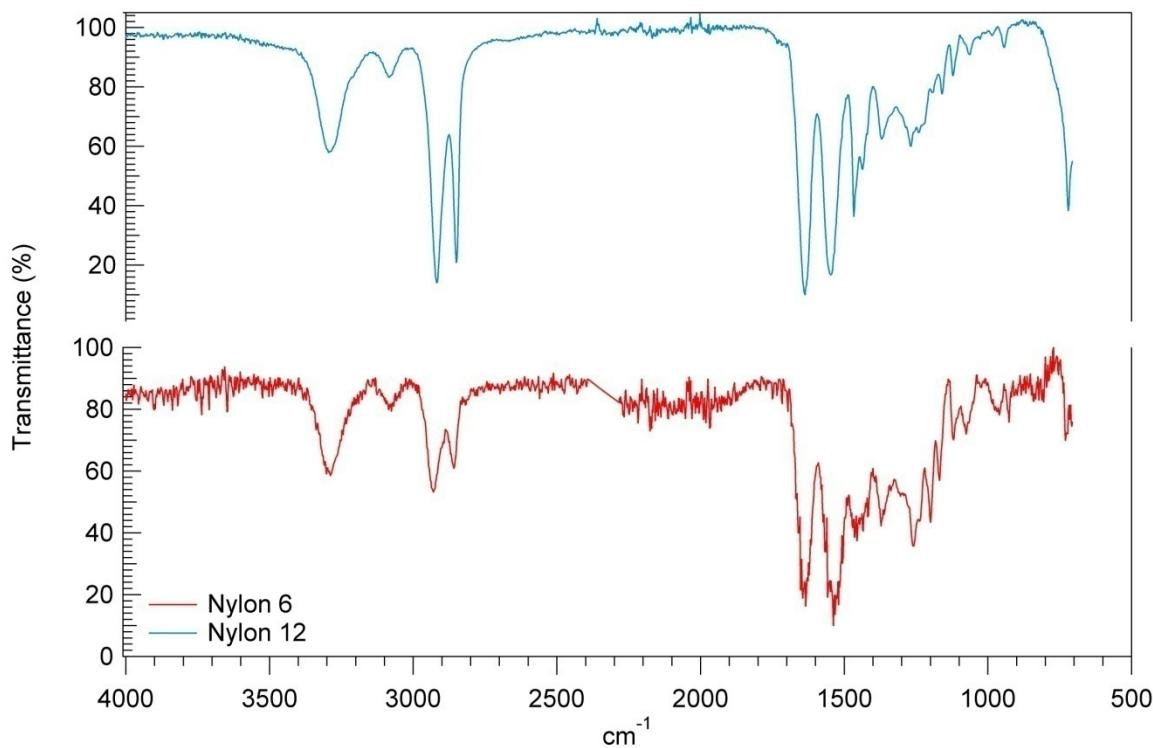
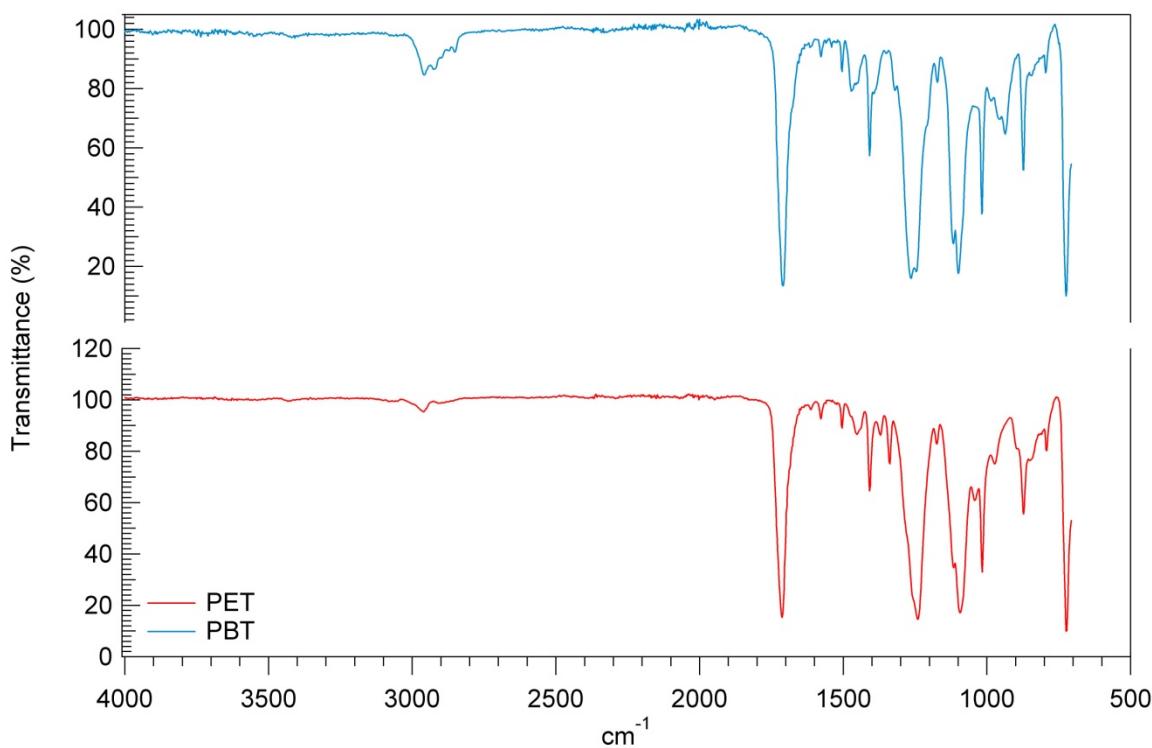
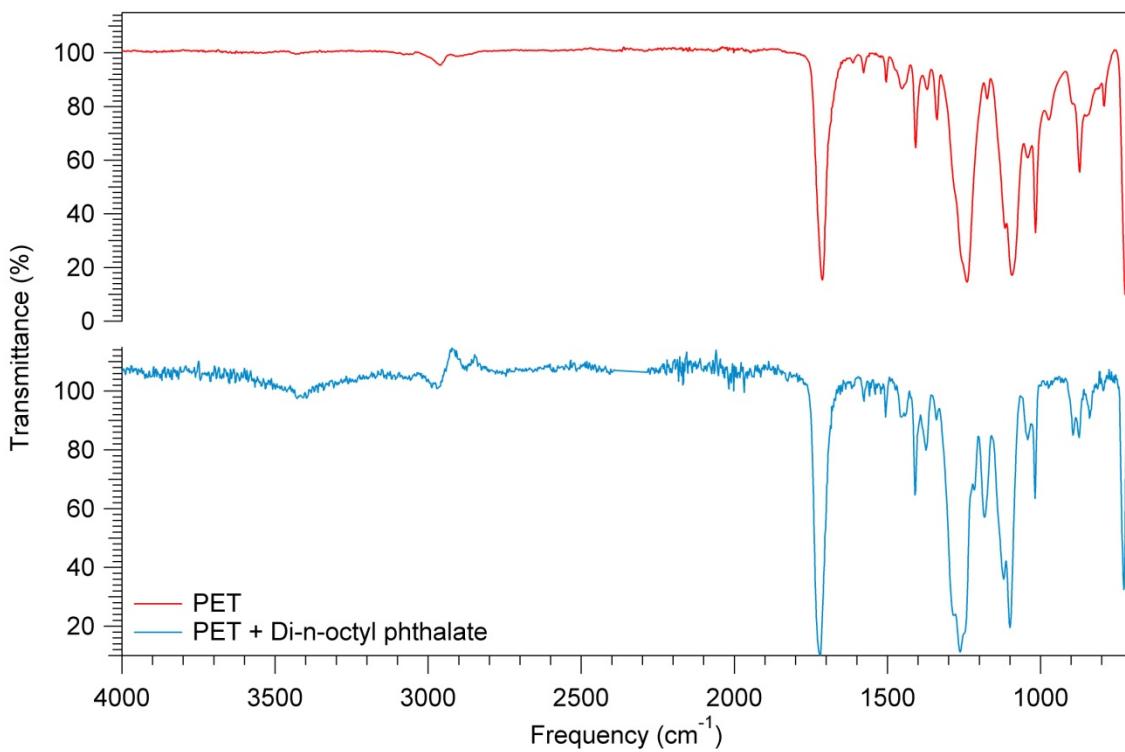


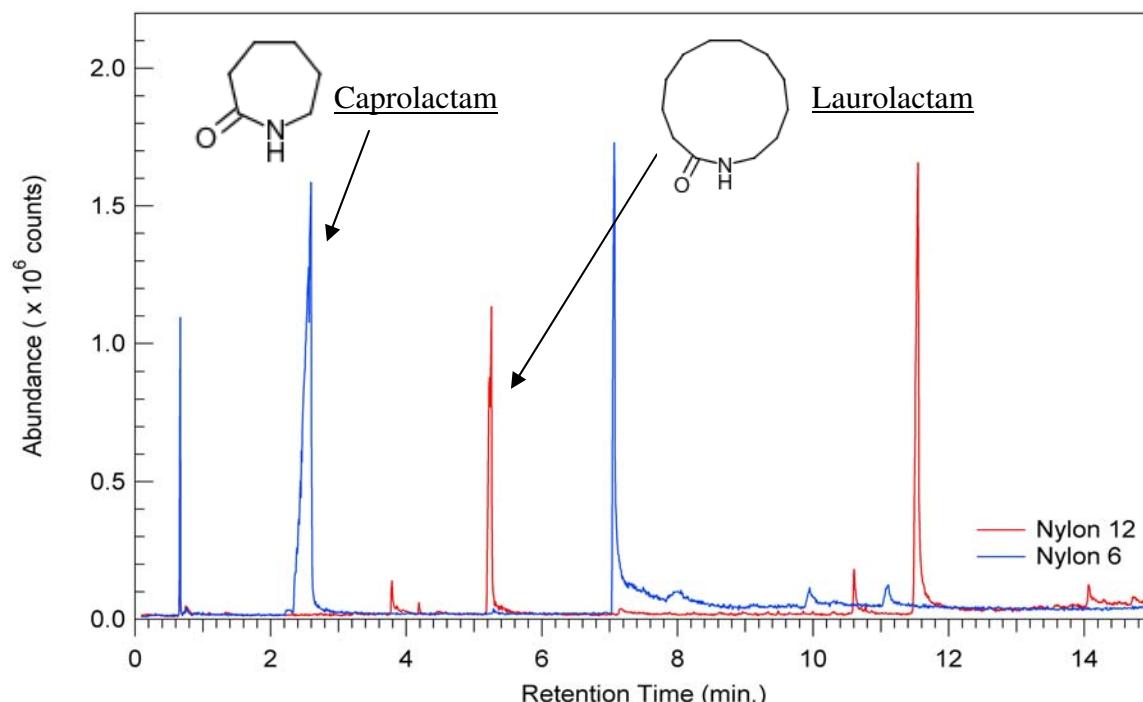
Figure II: A comparison of PET and PBT FTIR spectra**Figure III: A comparison of PET and PET/DOP (400 ppm) mixture FTIR spectra**

PYMS

PYMS, on the other hand, is a powerful technique for determination of specific chemical structures, even for polymers in the same family and components at low concentration. We analyzed the same nylon and polyester samples by PYMS to demonstrate what additional information can be gleaned using this technique.

For the nylon and polyester samples, we are able to isolate specific fragments that allow us to identify the exact chemical structure of our polymer. For the nylons, the polymer breaks down into their original monomers, caprolactam and laurolactam. **Figure IV** shows the PY2 chromatograms and two specific degradation products unique to each material. The presence of these particular fragments in an unknown nylon sample can be compared with the reference library of known spectra to allow a positive identification.

Figure IV: PYMS Chromatograms of Nylon 6 and Nylon 12 (PY2 portion)

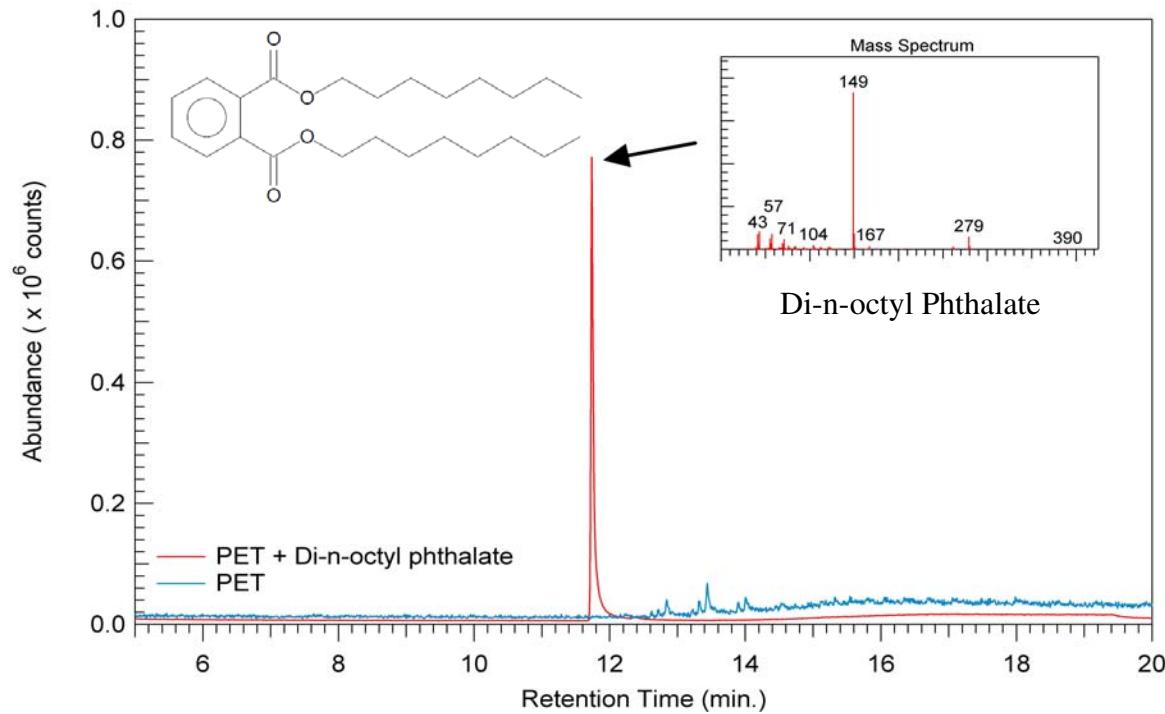


While not the original monomers, PBT and PET have their own unique fragments that are observed during PYMS. Ethyl- and benzyl-containing fragments can be observed throughout the PET chromatogram. PBT, however, contains many similar benzyl fragments as well as two distinct degradation products that demonstrate the presence of a 4-carbon butyl chain: a butadiene at 2.46 minutes and a dicyclobutyl ester-type phthalic acid at 8.67 minutes. In an unknown sample analysis, the presence or absence of any of these fragments would allow the analyst to distinguish between these two very similar polymer structures.

Figure V is an overlay of the PY1 portion of the PYMS for PET and the 400ppm di-n-octyl phthalate/PET mixture. Though it was impossible to identify the DOP by FTIR, we can see it

very clearly identified by PYMS. The DOP was also the highest abundance component in the PY2 portion of the PYMS due to its high volatility, demonstrating that additives could be observed even when present in extremely low ppm values.

Figure V: PYMS Chromatograms of PBT and a PET/DOP (400 ppm) mixture



From this demonstration, it should be clear that PYMS is a more powerful technique for identifying unknowns within a particular polymer family or identifying any low-concentration additives or impurities. FTIR is a great method for the quick identification of the functionality of an unknown sample, but PYMS analysis can provide a much greater wealth of information and should be the method of choice when this type of information is preferred.

Analysis Conditions

FTIR

Solid samples were tested as-is on a Perkin-Elmer PC-16 FT-IR spectrometer fitted with a DuraScope diamond ATR system (an integrated video imaging accessory). The DuraScope is designed for the analysis of all sample types. The PET/DOP mixture was cast onto the FTIR surface from solution using HFIP.

PYMS

The samples were analyzed using an Agilent 6890 gas chromatograph in conjunction with a 5975B mass selective detector using a Frontier Laboratories double shot Pyrolyzer model PY2020ID.

Analysis was conducted using a double shot technique, which consists of heating the sample over a set temperature range while volatiles were cryogenically trapped and then analyzed by GCMS. Following completion of the 1st pass analysis, the remaining portion of the sample was then heated to 500°C rapidly and pyrolyzed components were passed into a gas chromatography column and analyzed by mass spectroscopy.

Prominent peaks found in PY-GCMS typically include polymer fragments as well as monomer, antioxidants and other additives. Sample peaks were compared with over 147,350 reference compounds using the NIST/EPA/NIH mass spectral search program.

Closing Comments

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

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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,



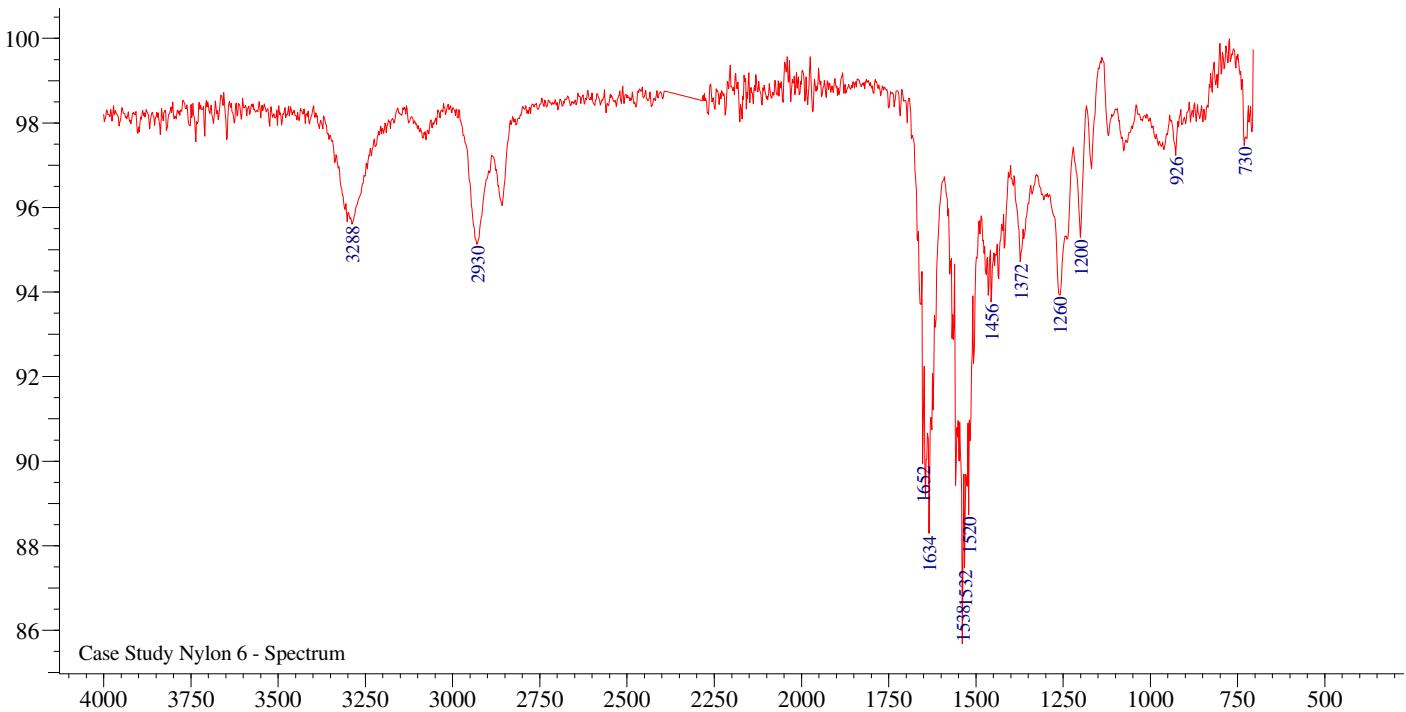
Mark Jordi, Ph. D.
President
Jordi Labs LLC

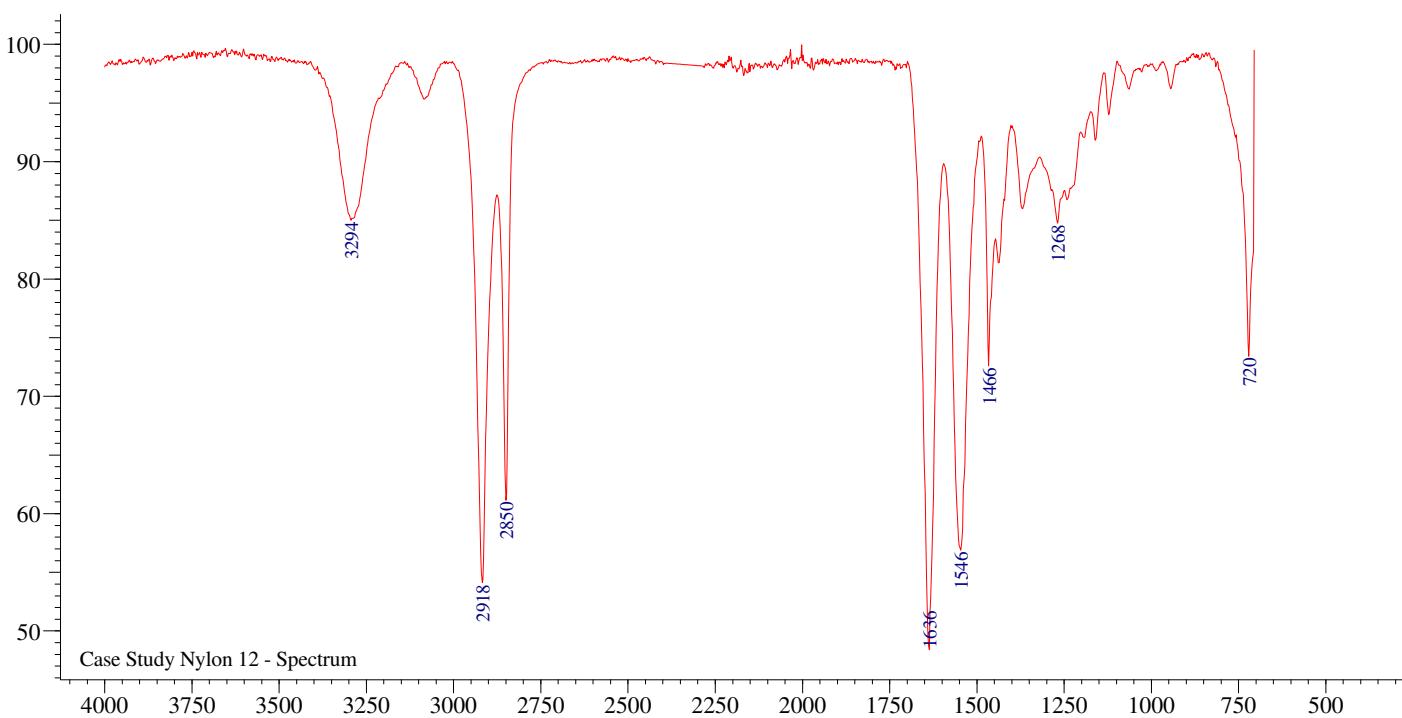
Appendix

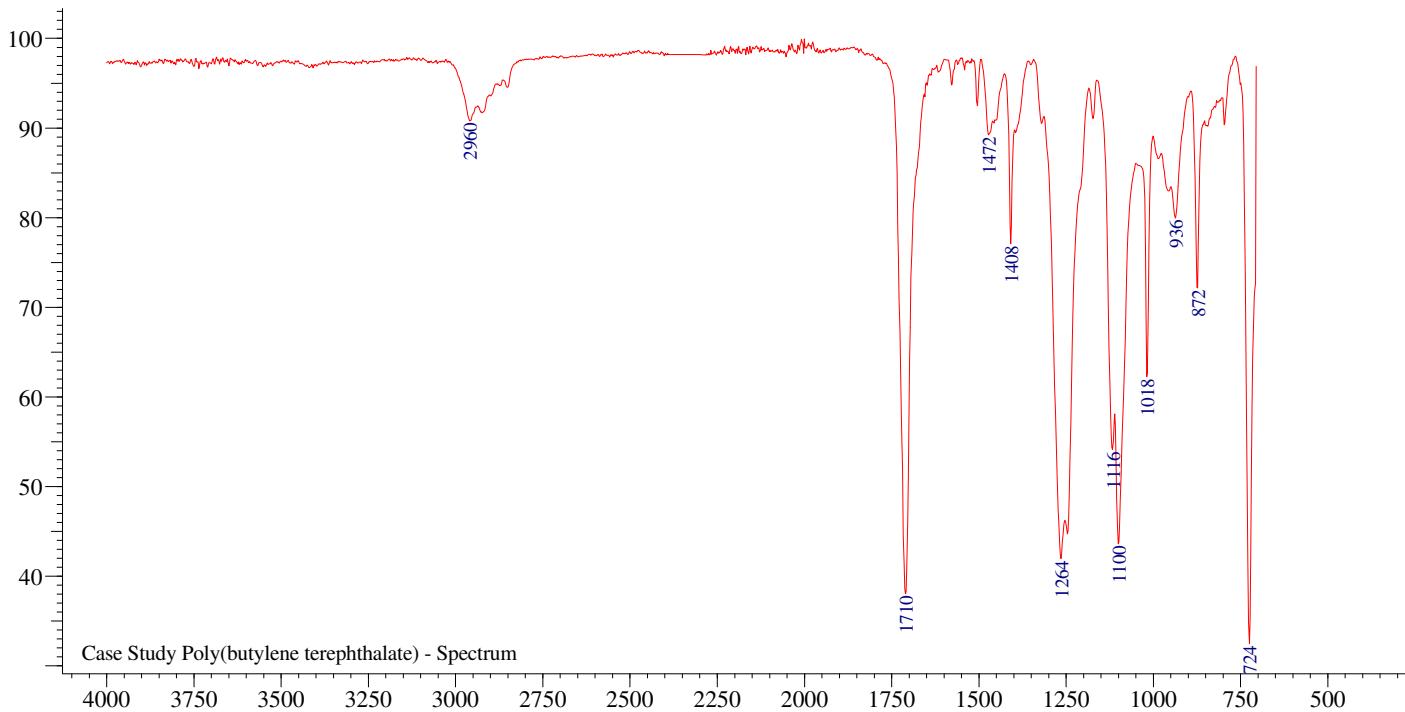
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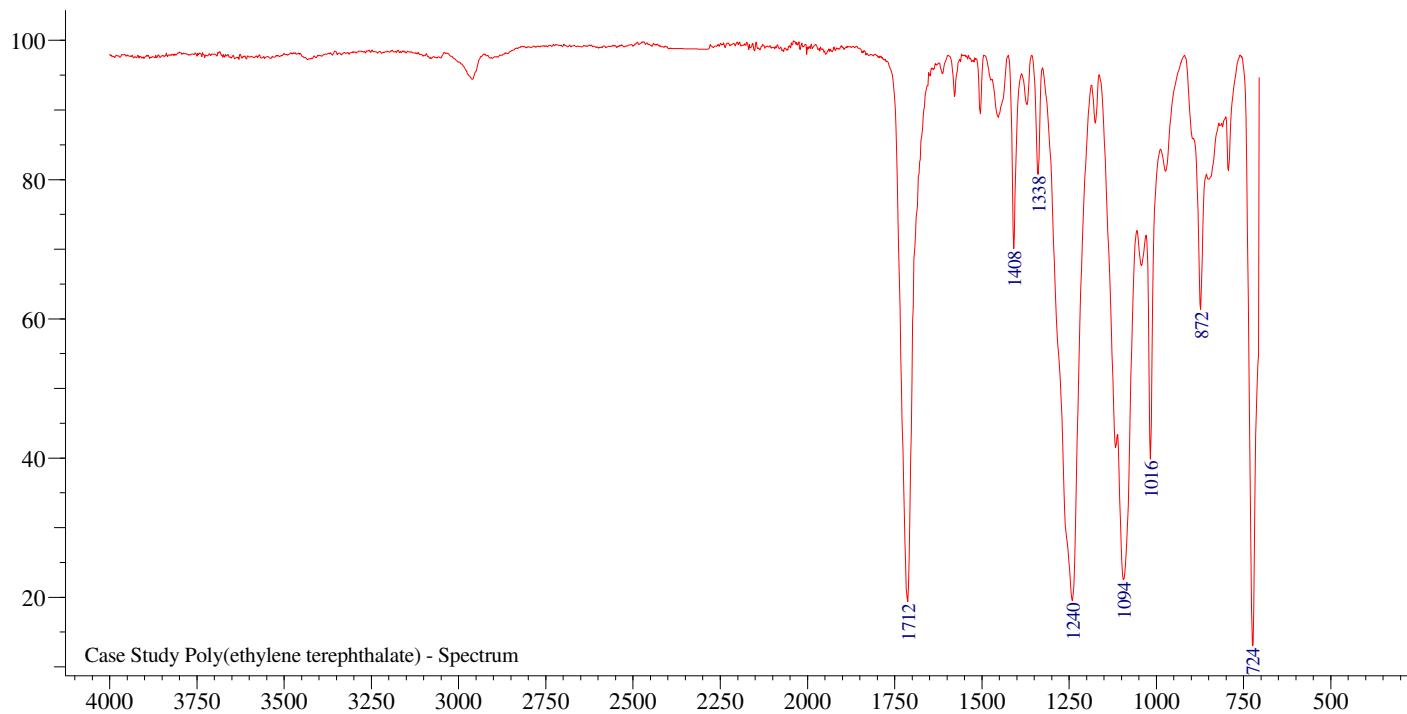
- Pages 11-15 – FTIR Data
- Page 16-54 – PYMS Data

FTIR RESULTS



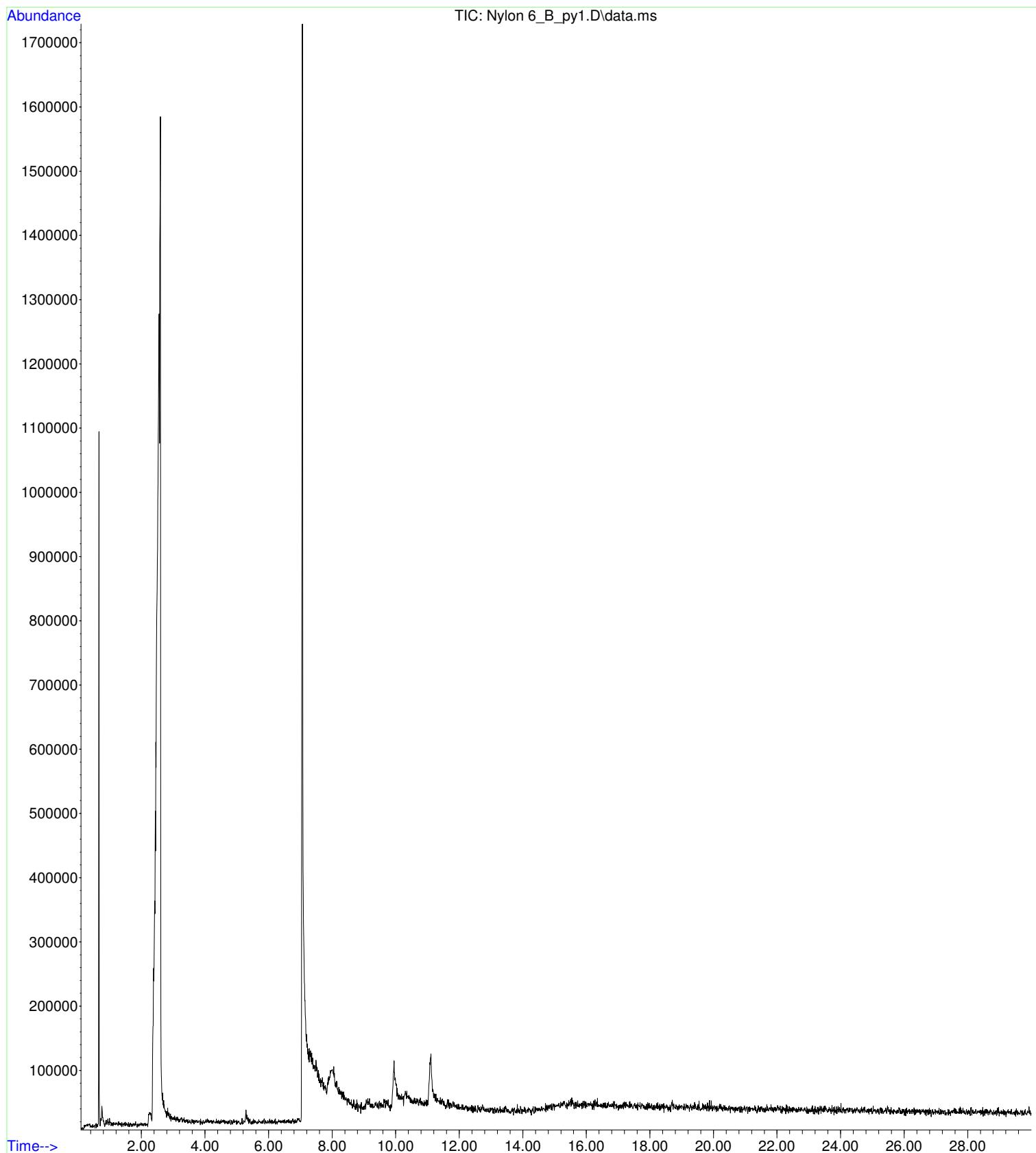






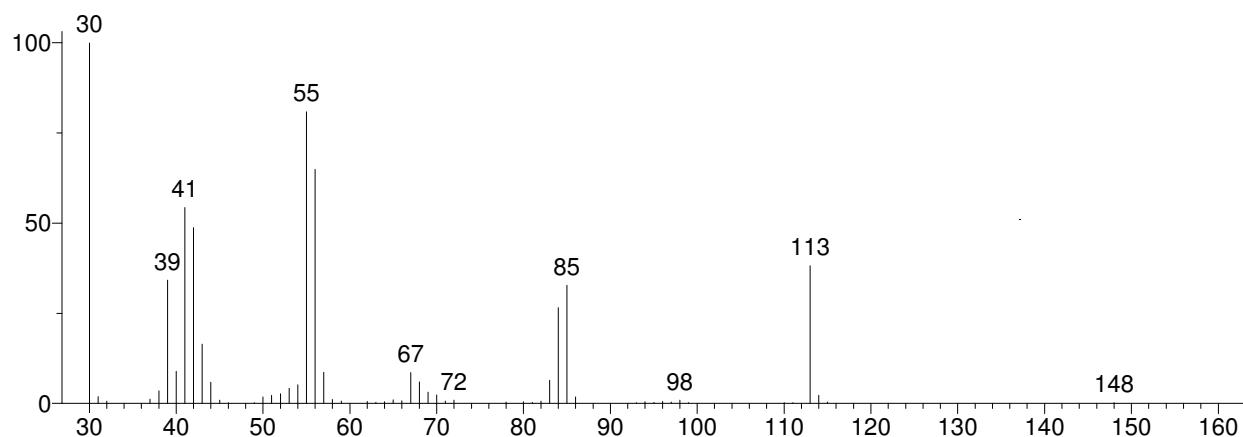
PYMS RESULTS

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Instrument : Instrument #1
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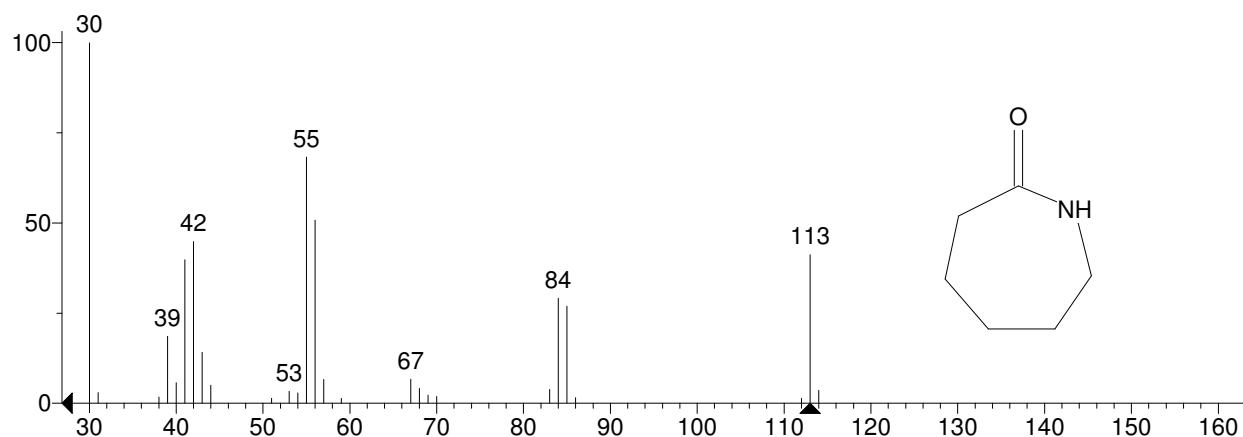


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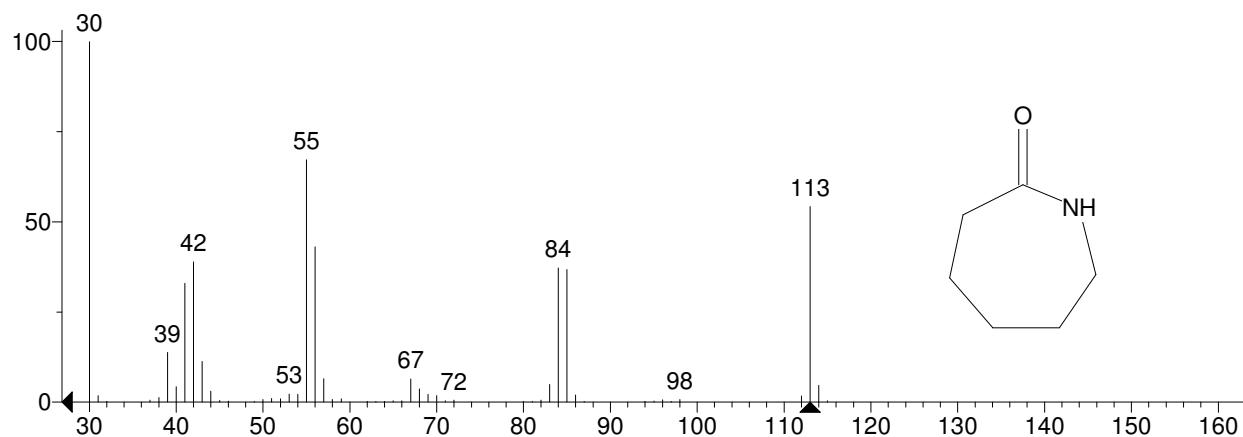
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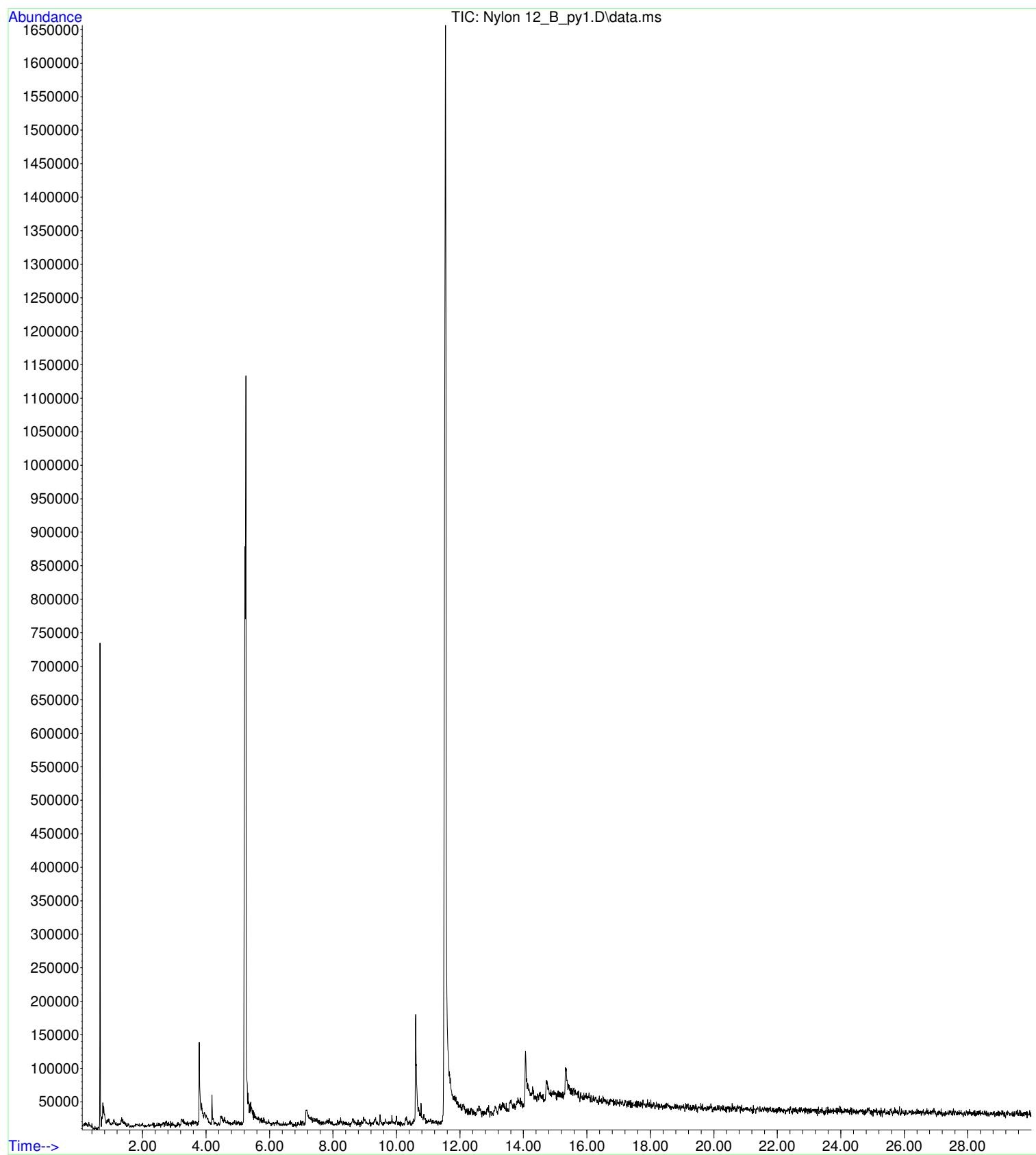
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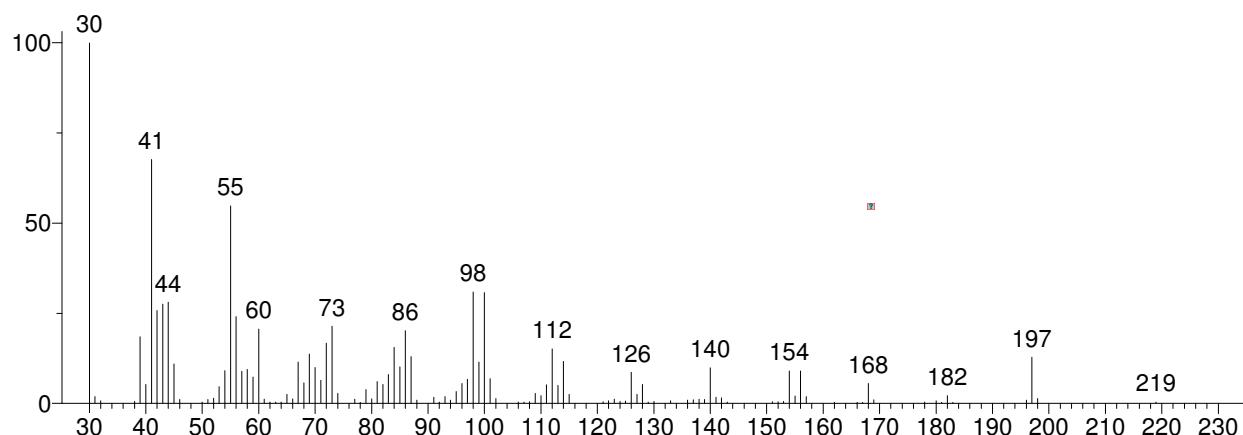


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Misc Info : sp2 P#044

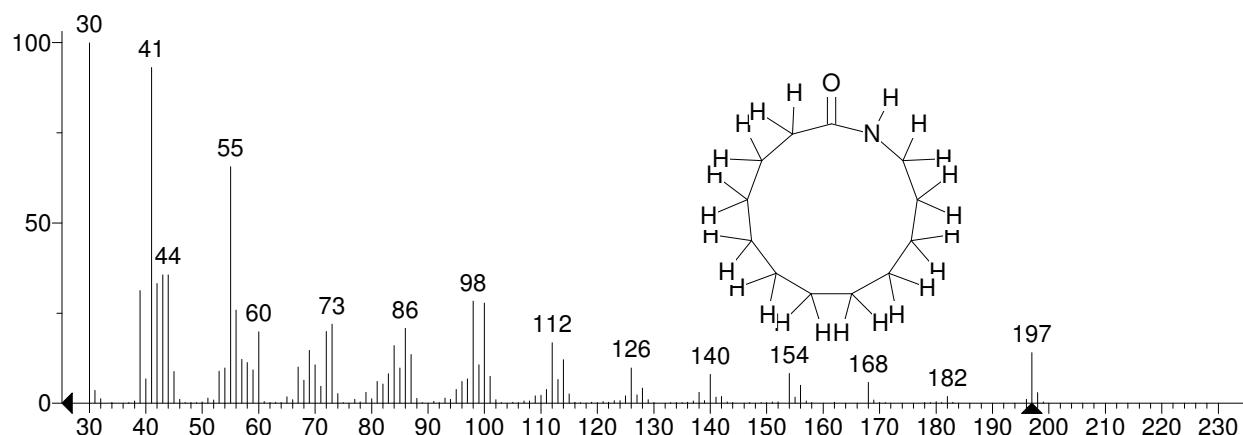


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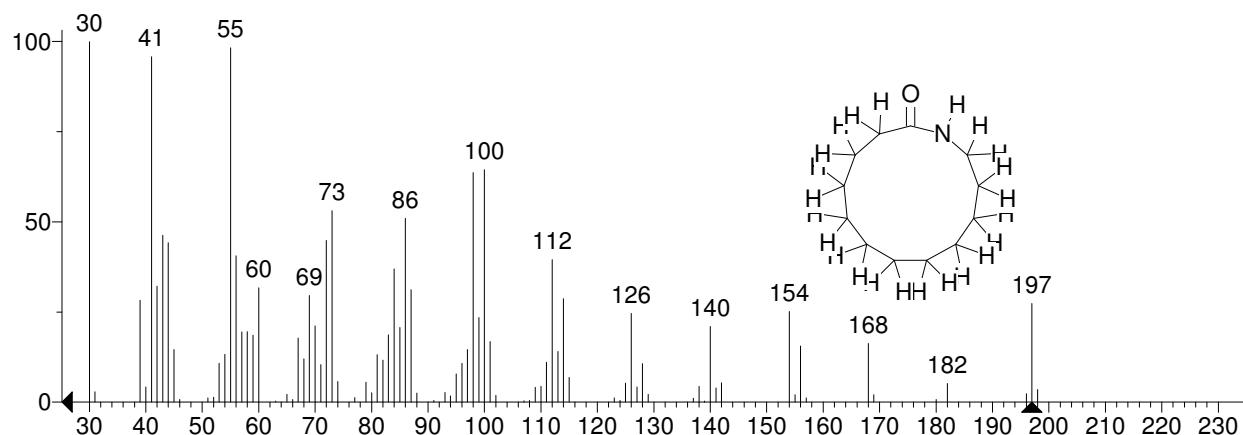
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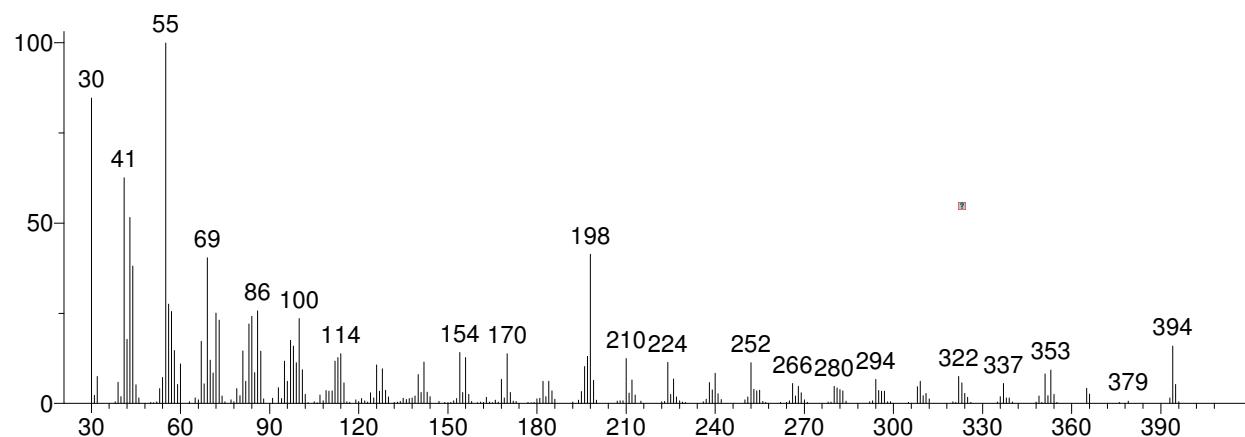


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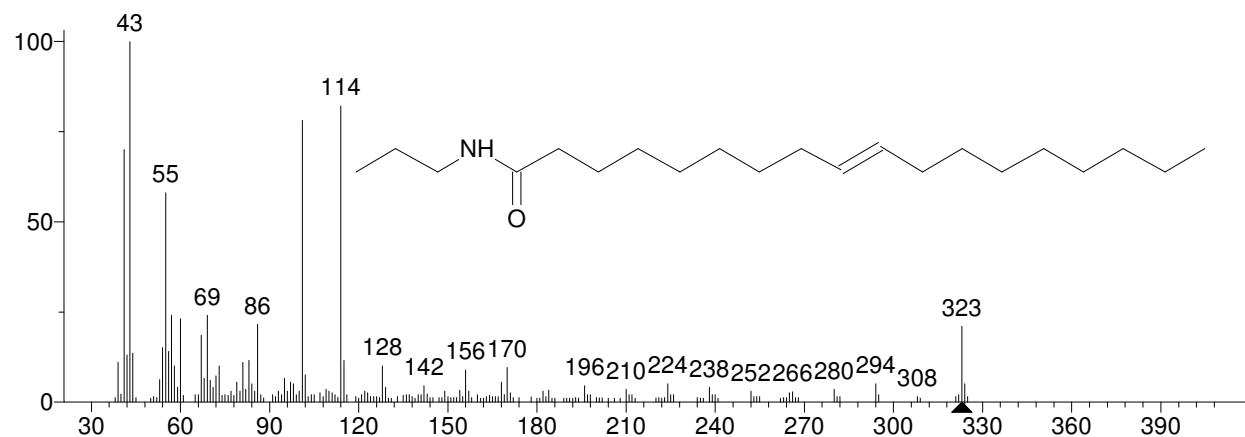
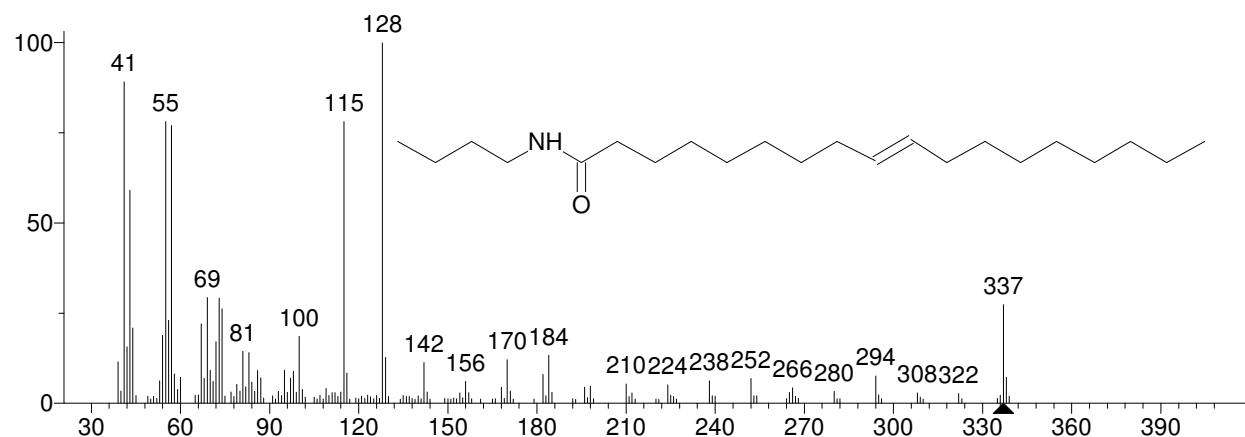


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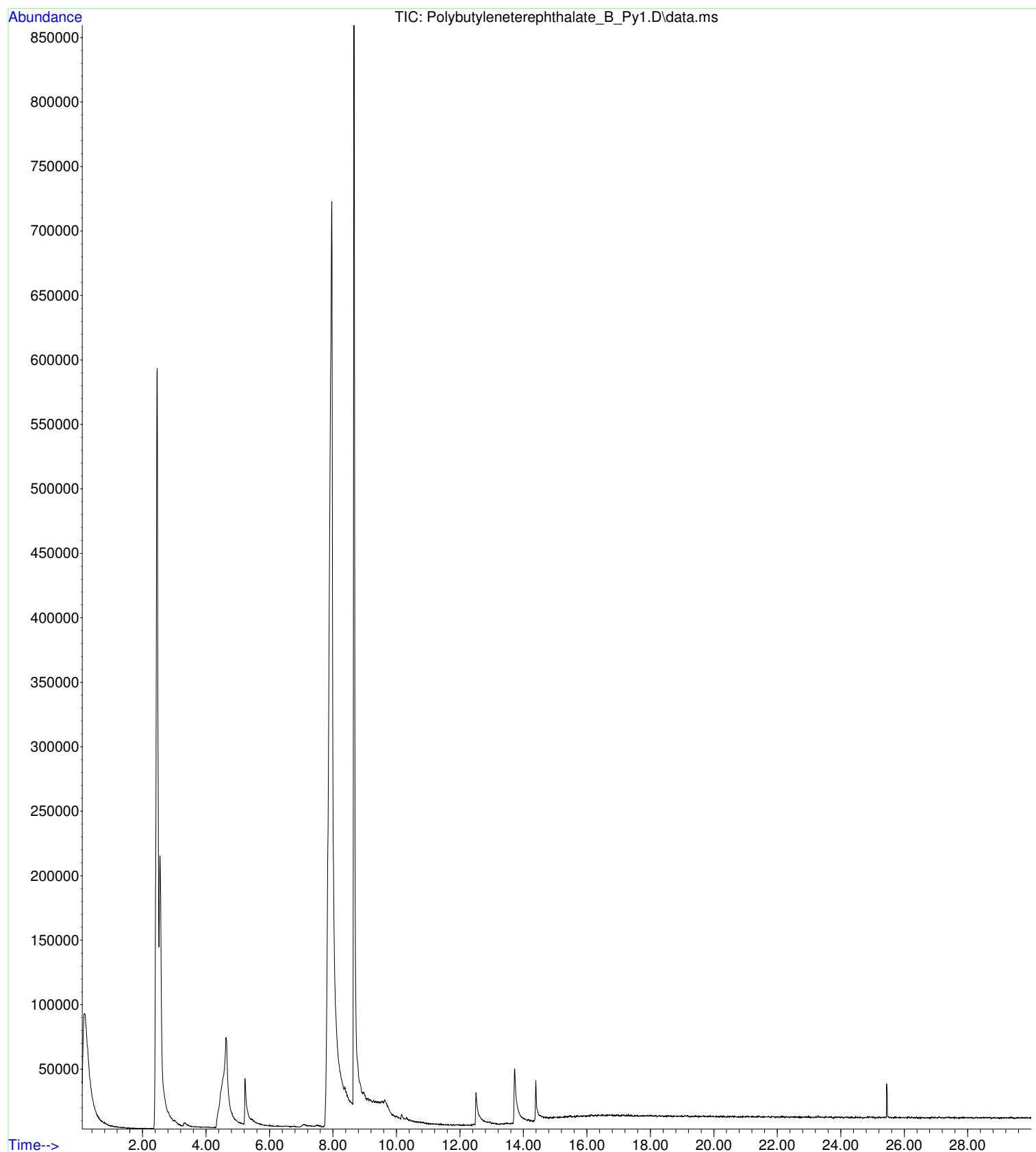
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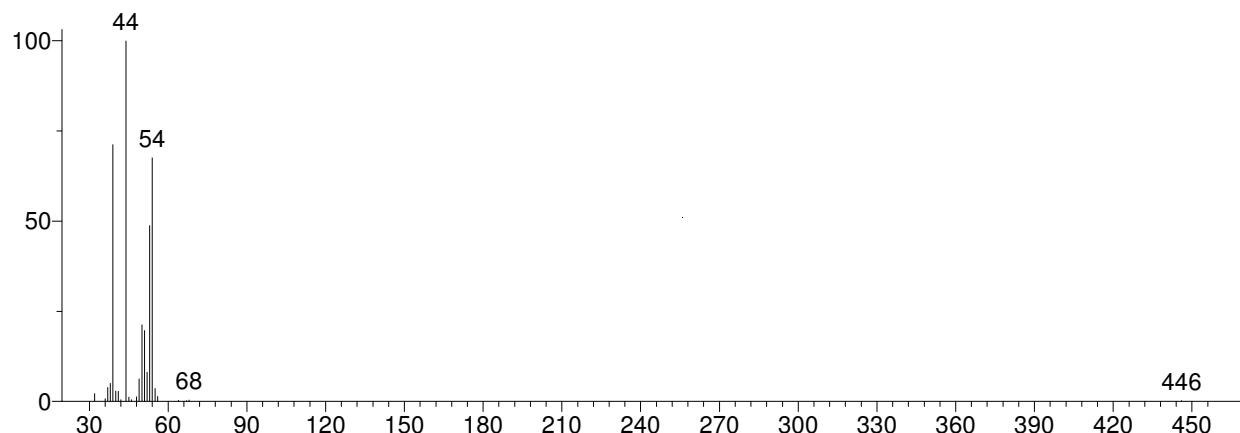


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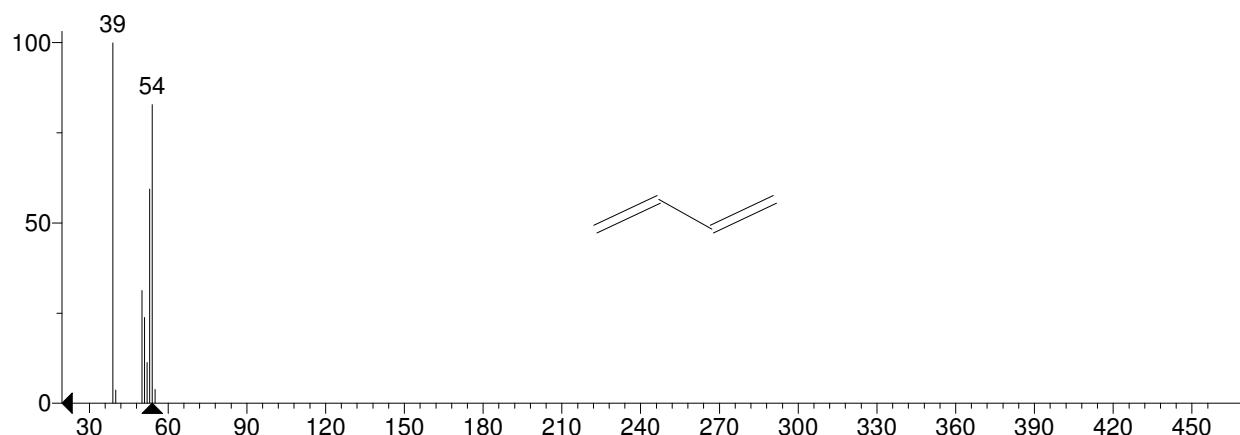


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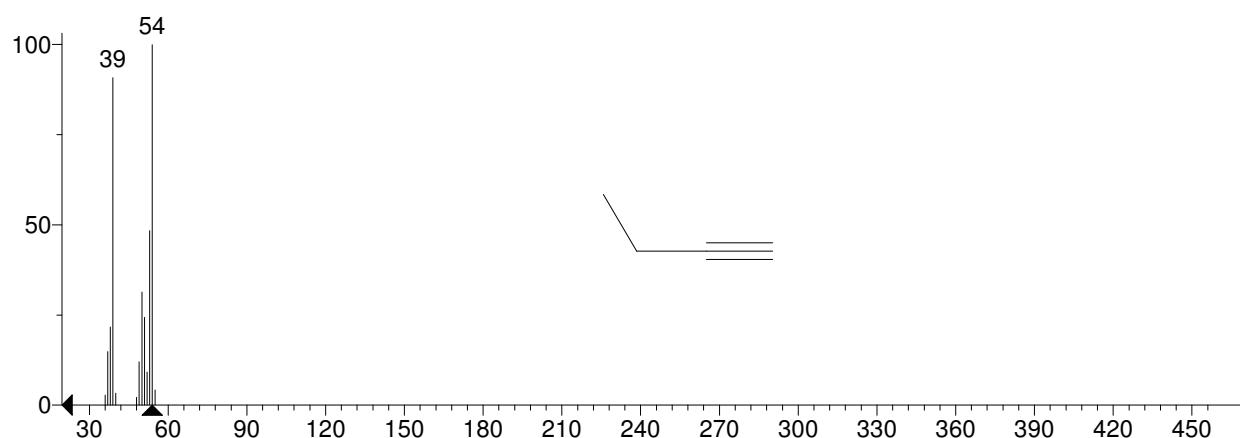
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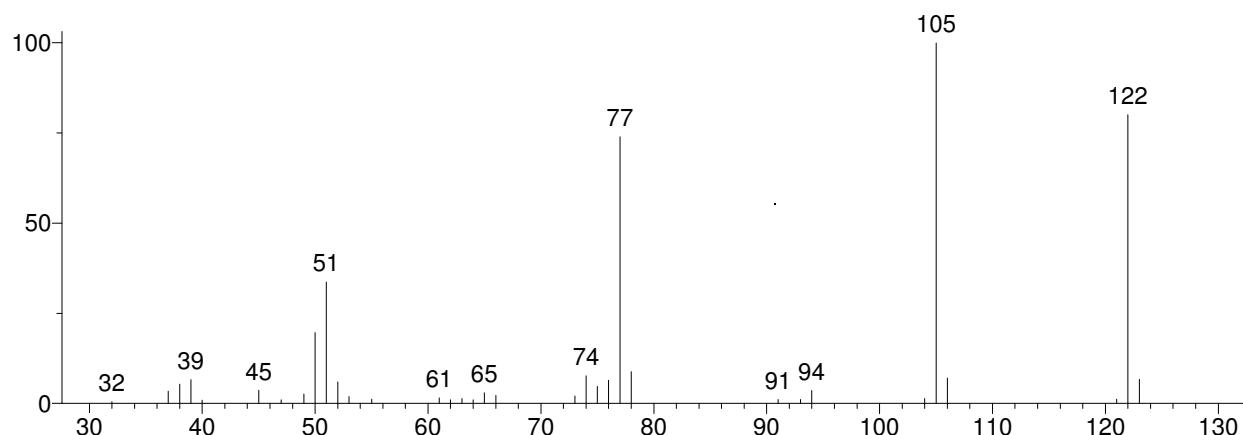


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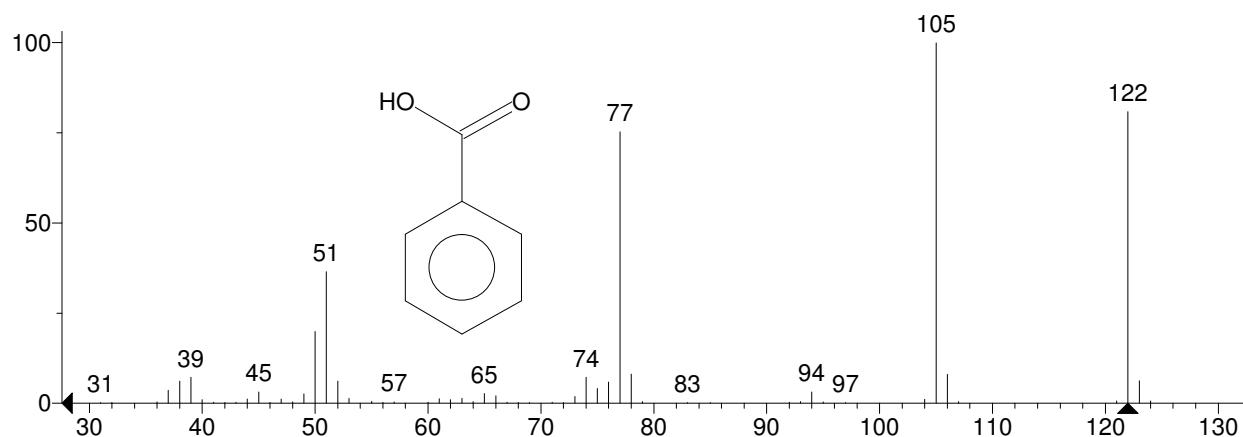


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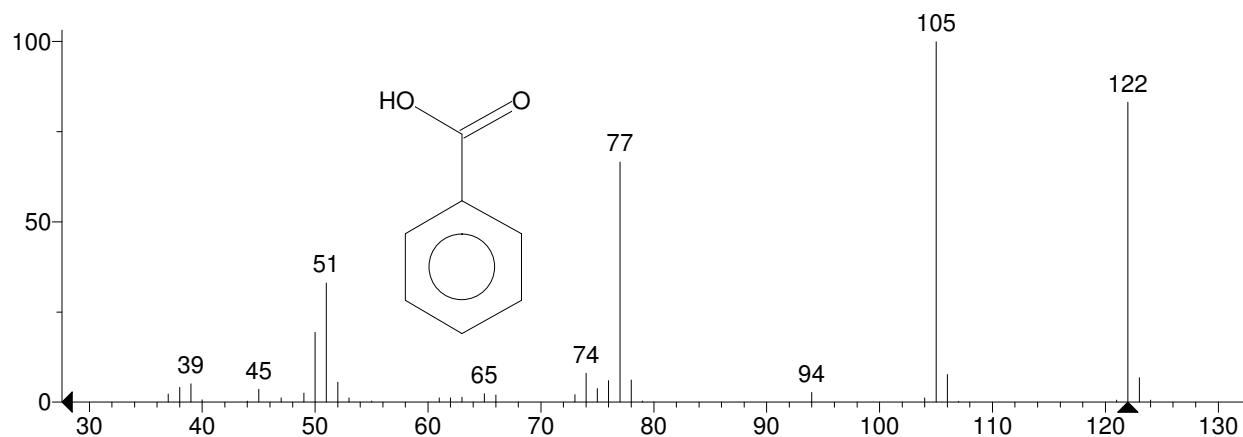
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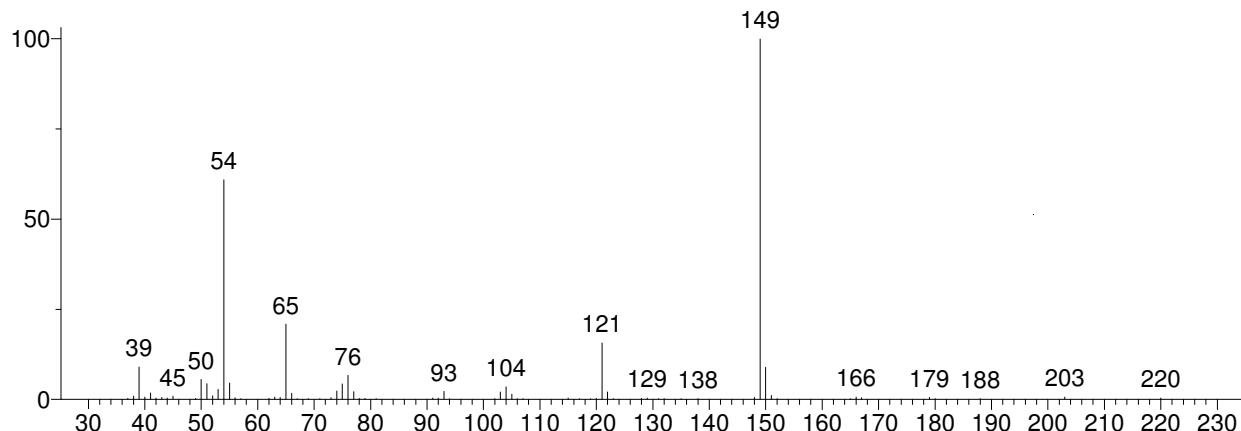


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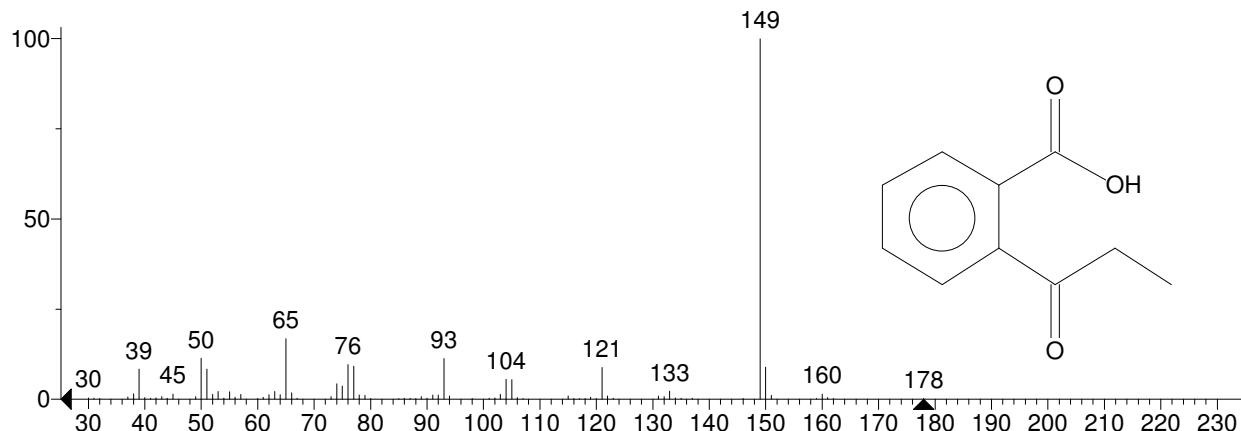


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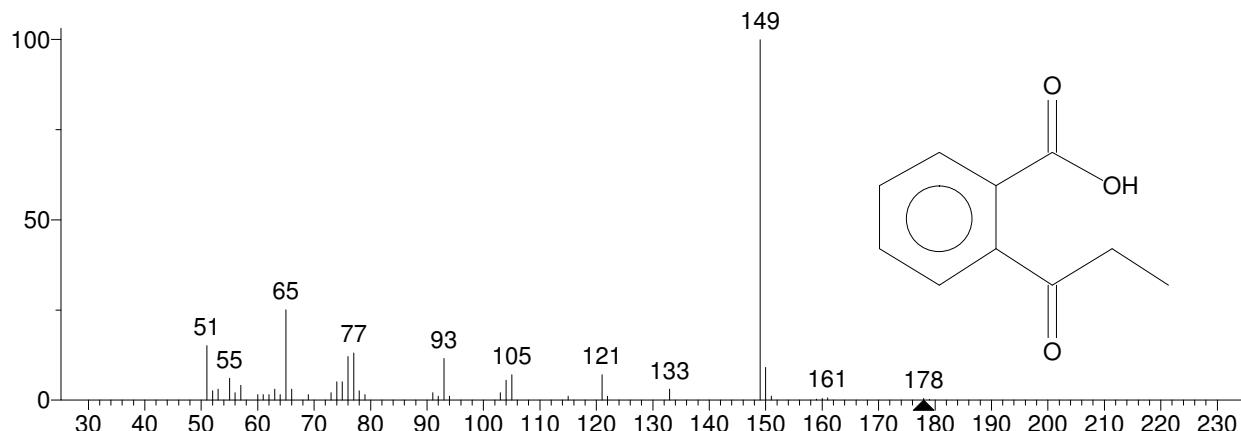
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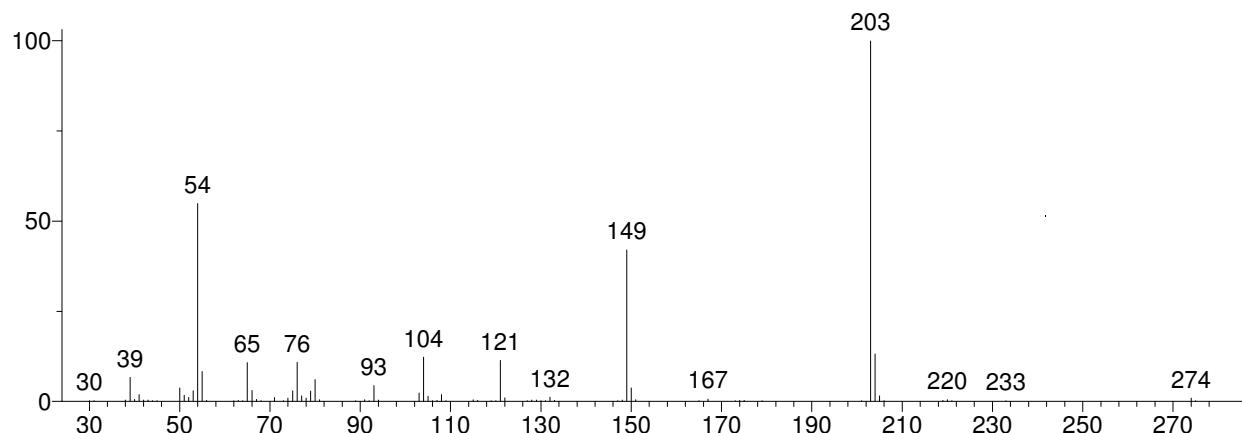


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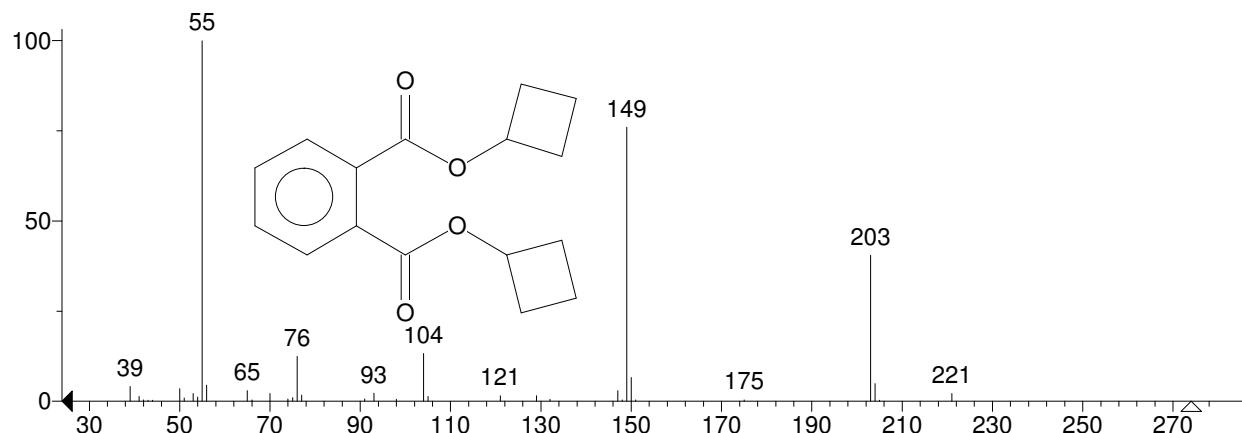


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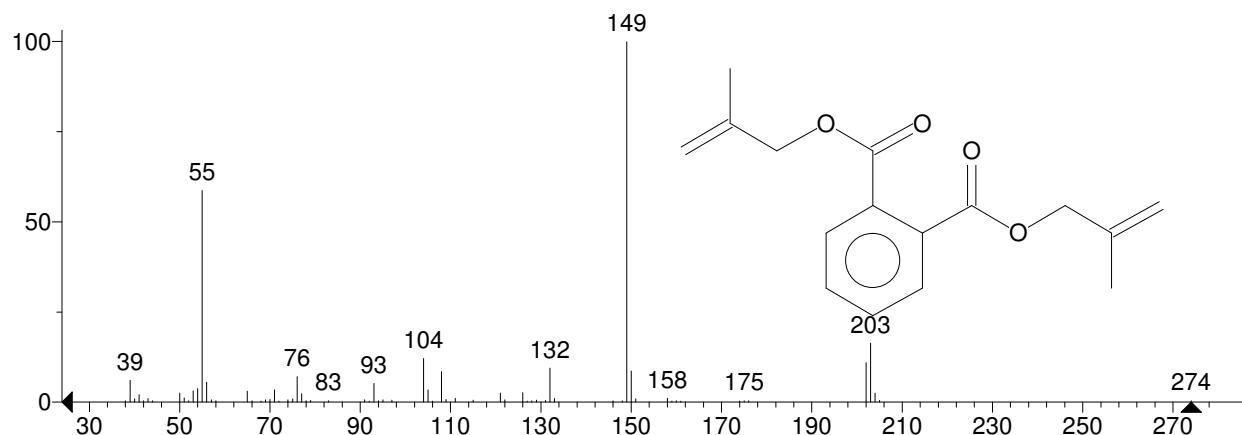
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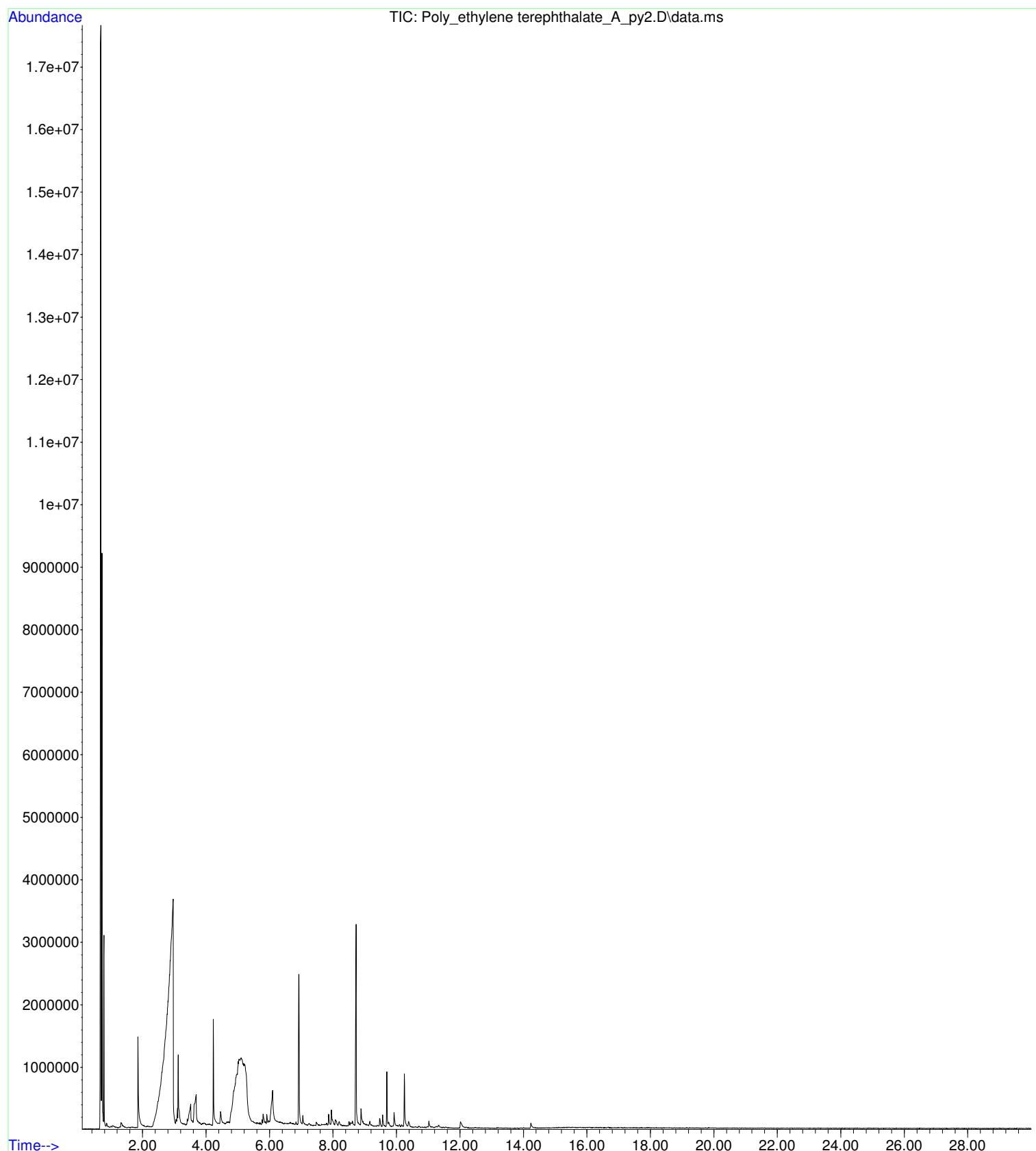
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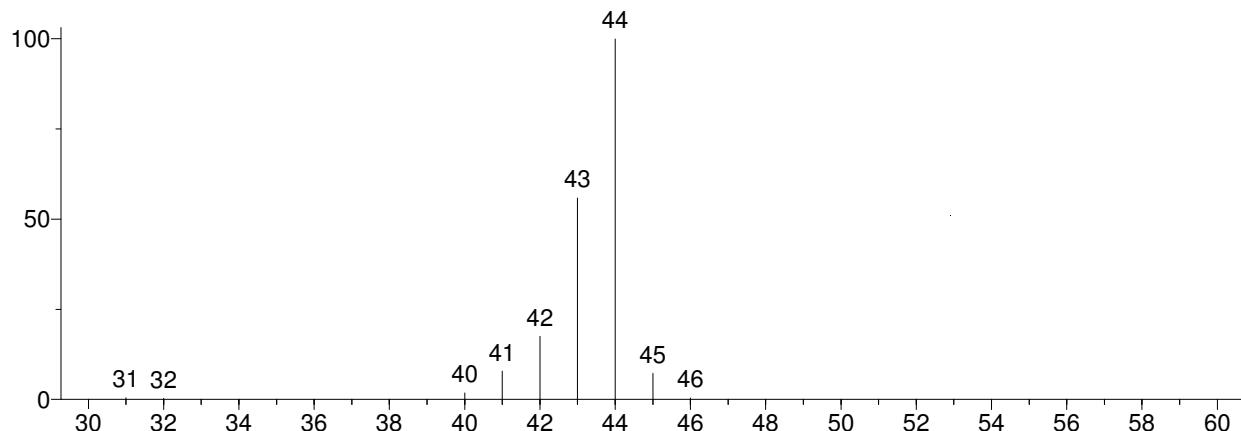


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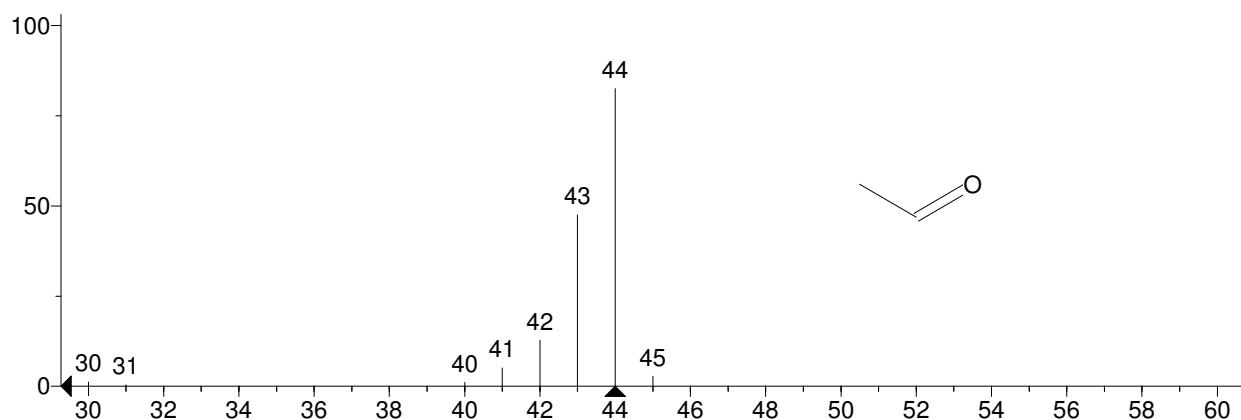


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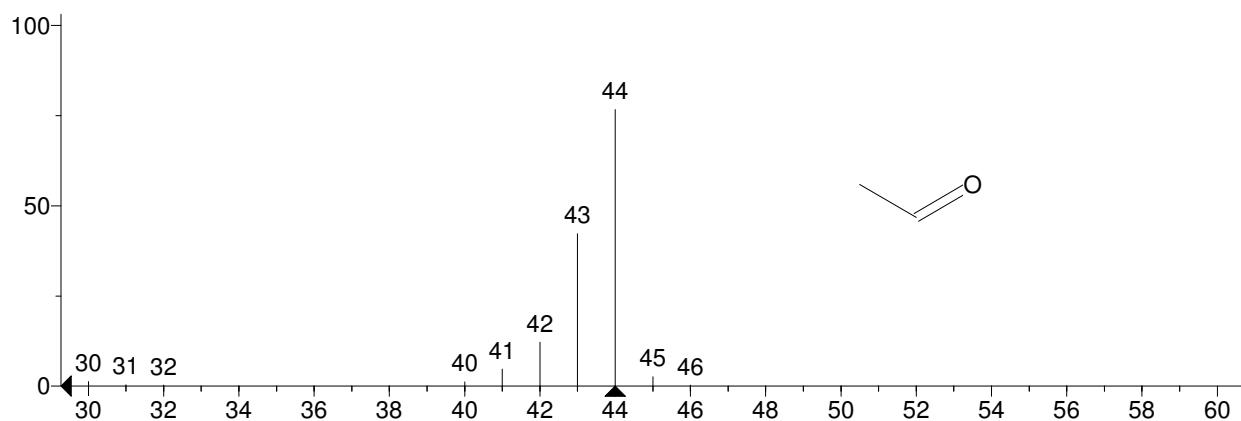
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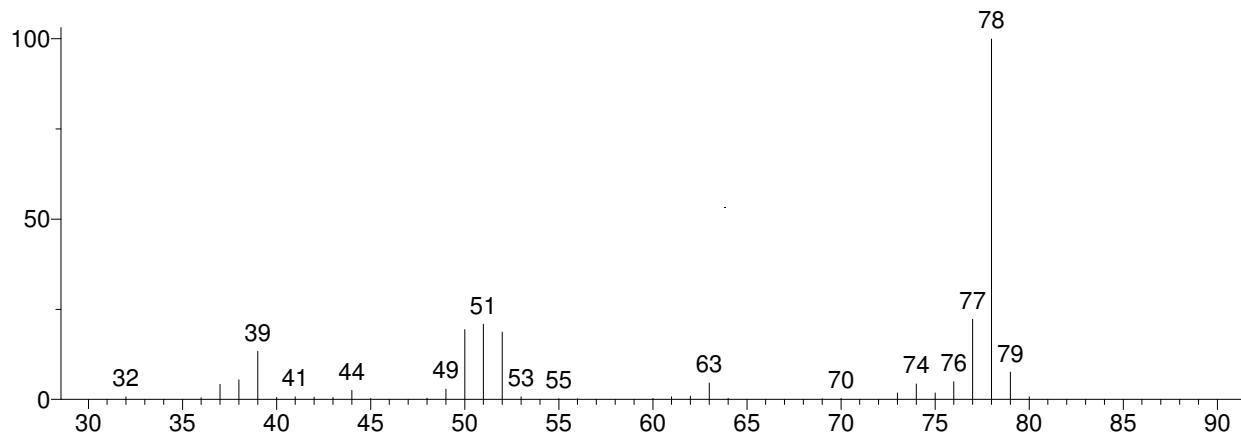


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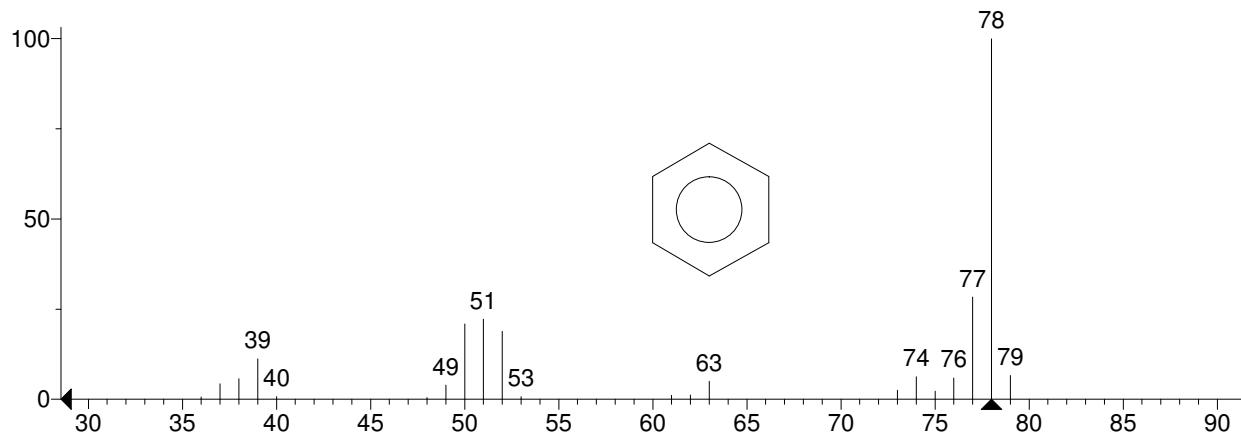


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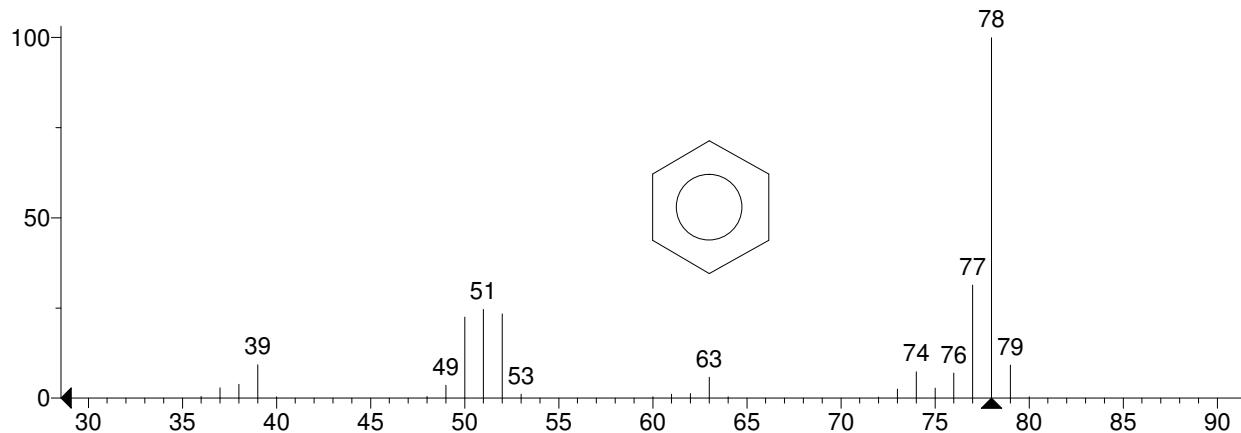
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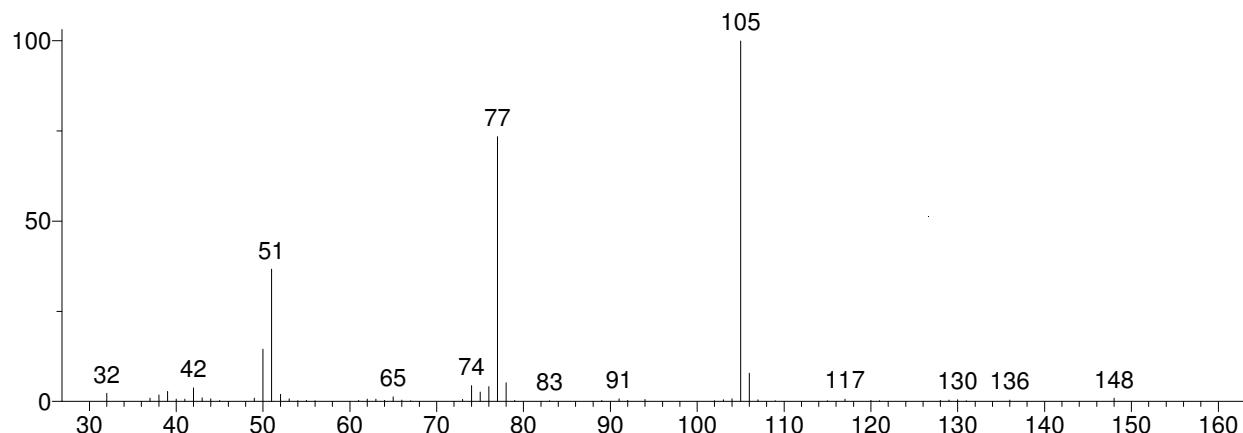


Hit 2 : Benzene
C6H6; MF: 950; RMF: 957; Prob 71.8%; CAS: 71-43-2; Lib: replib; ID: 9506.

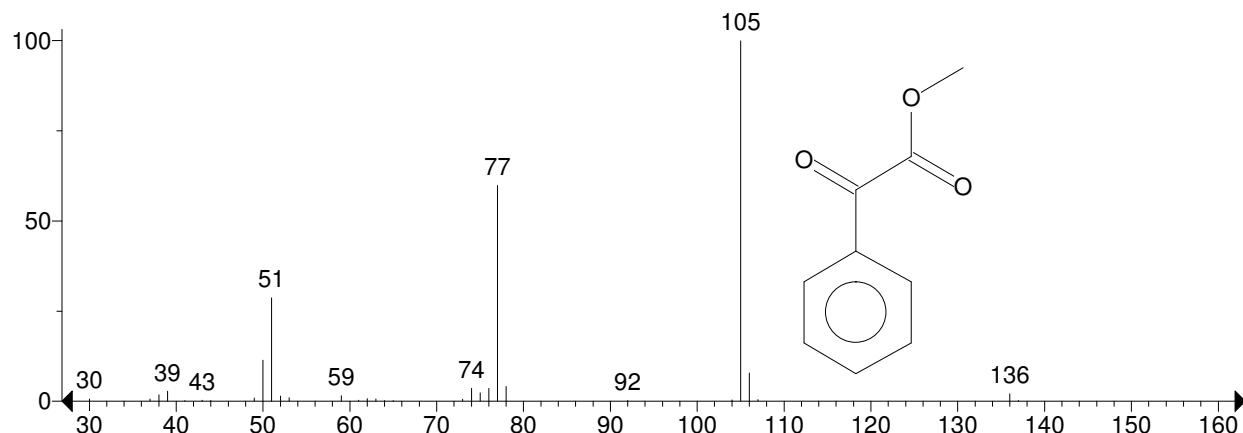


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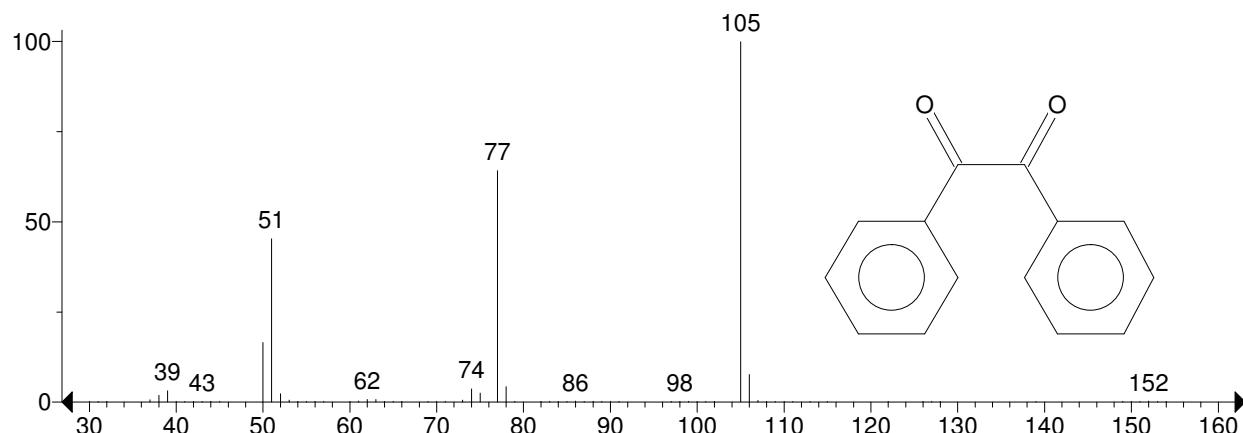
Unknown: Scan 234 (1.851 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -117



Hit 1 : Benzeneacetic acid, .alpha.-oxo-, methyl ester
 C9H8O3; MF: 927; RMF: 950; Prob 17.2%; CAS: 15206-55-0; Lib: mainlib; ID: 59819.

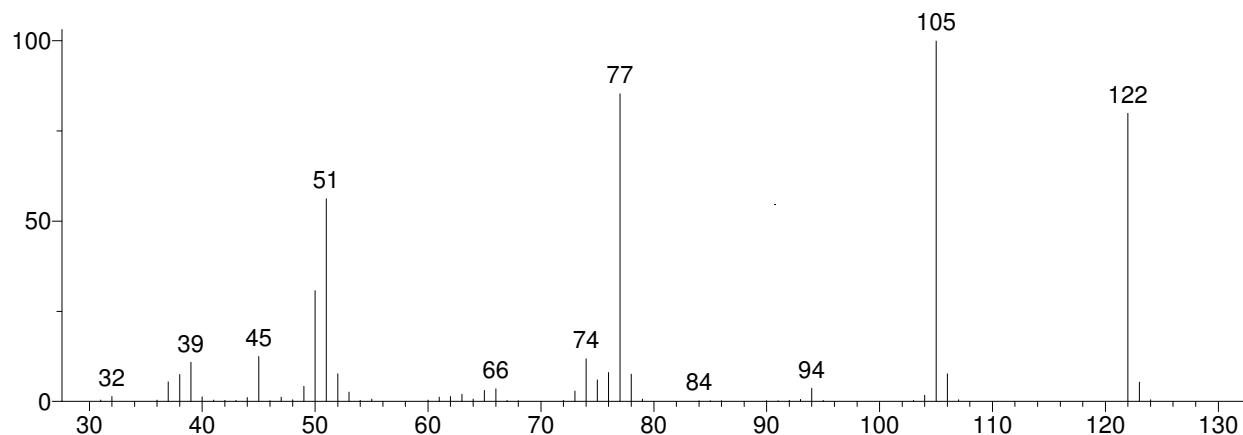


Hit 2 : Ethanedione, diphenyl-
 C14H10O2; MF: 911; RMF: 946; Prob 9.89%; CAS: 134-81-6; Lib: replib; ID: 13644.

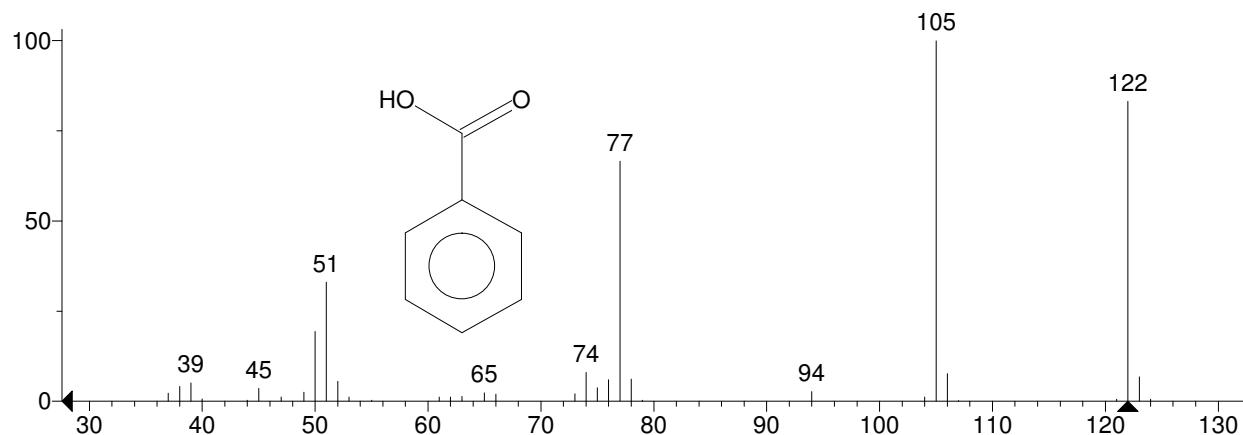


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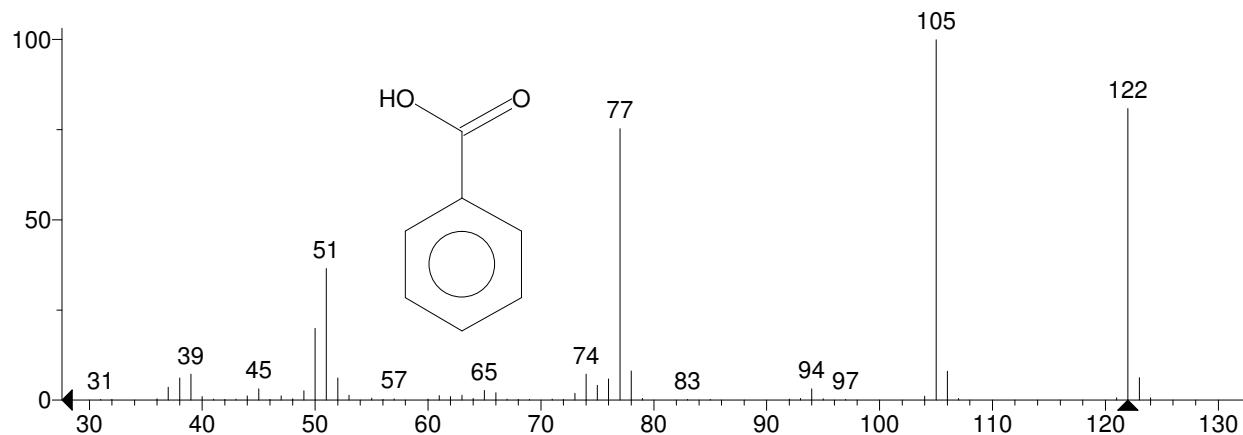
Unknown: Scan 382 (2.966 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = 138



Hit 1 : Benzenecarboxylic acid
 C7H6O2; MF: 933; RMF: 938; Prob 57.4%; CAS: 65-85-0; Lib: replib; ID: 13938.

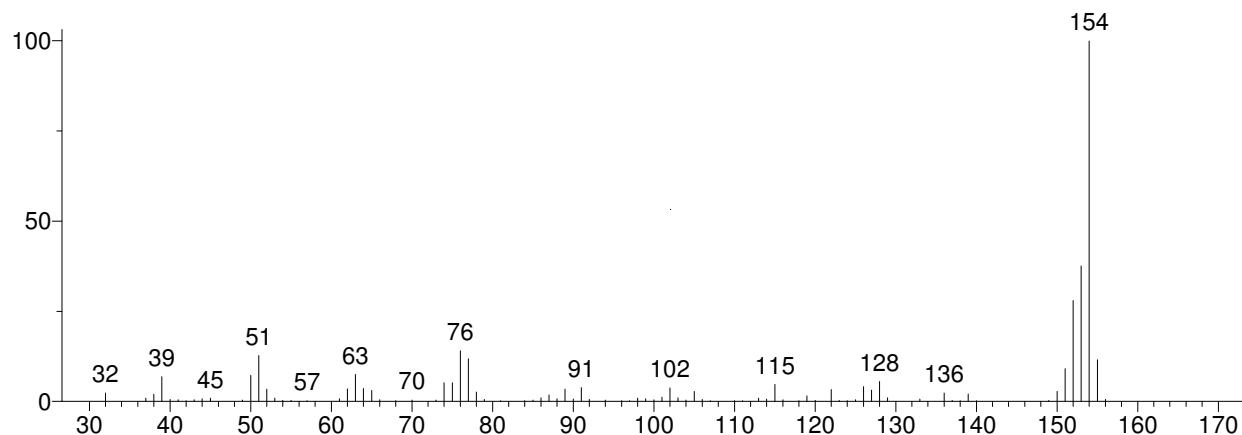


Hit 2 : Benzenecarboxylic acid
 C7H6O2; MF: 927; RMF: 928; Prob 57.4%; CAS: 65-85-0; Lib: replib; ID: 13937.

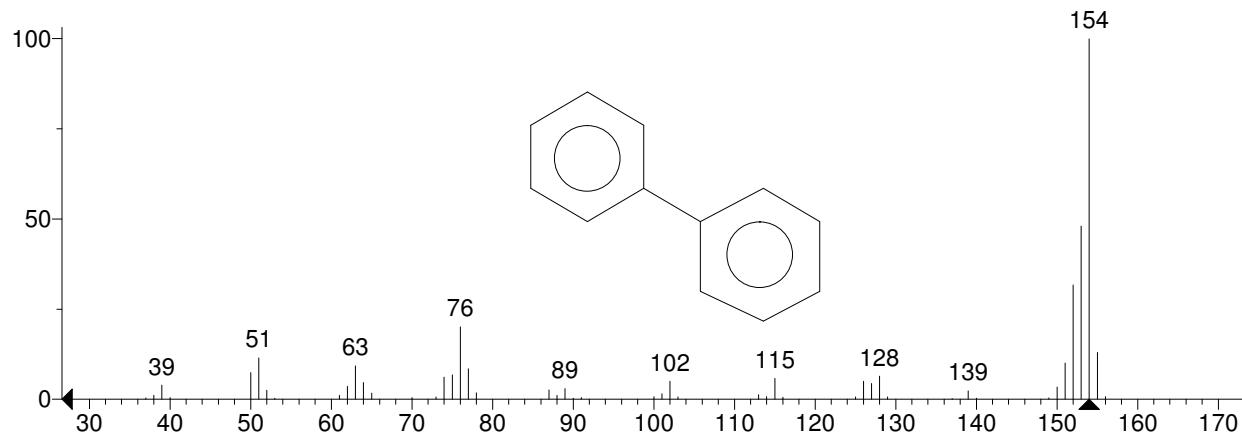


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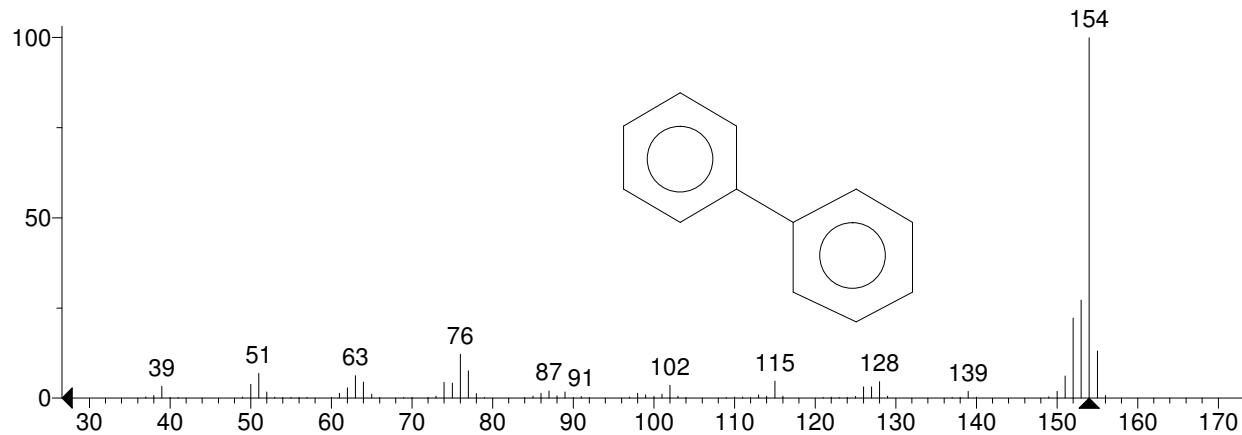
Unknown: Scan 403 (3.124 min): Poly_ethylene terephthalate_A_py2.D\data.ms
Compound in Library Factor = 116



Hit 1 : Biphenyl
C12H10; MF: 906; RMF: 933; Prob 74.4%; CAS: 92-52-4; Lib: mainlib; ID: 99714.

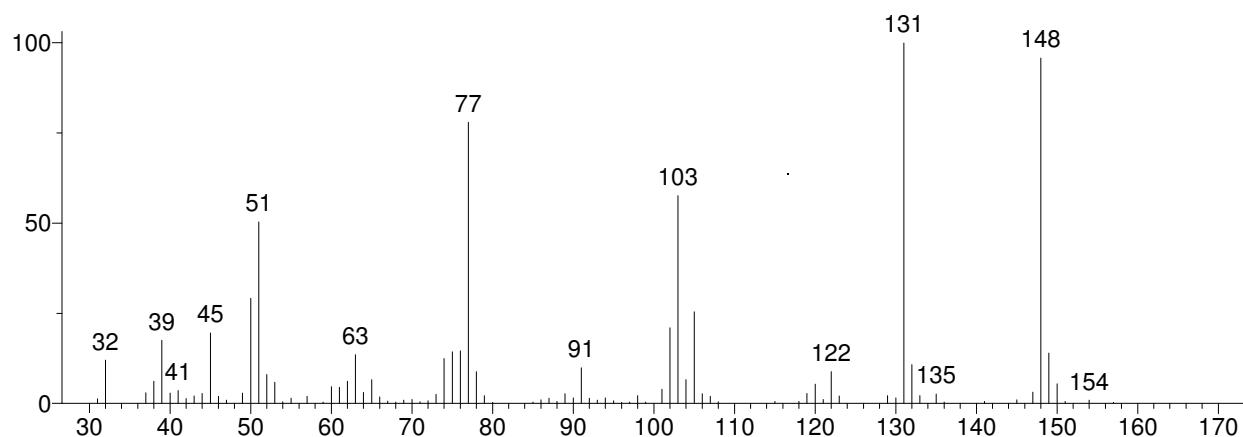


Hit 2 : Biphenyl
C12H10; MF: 899; RMF: 917; Prob 74.4%; CAS: 92-52-4; Lib: replib; ID: 20364.

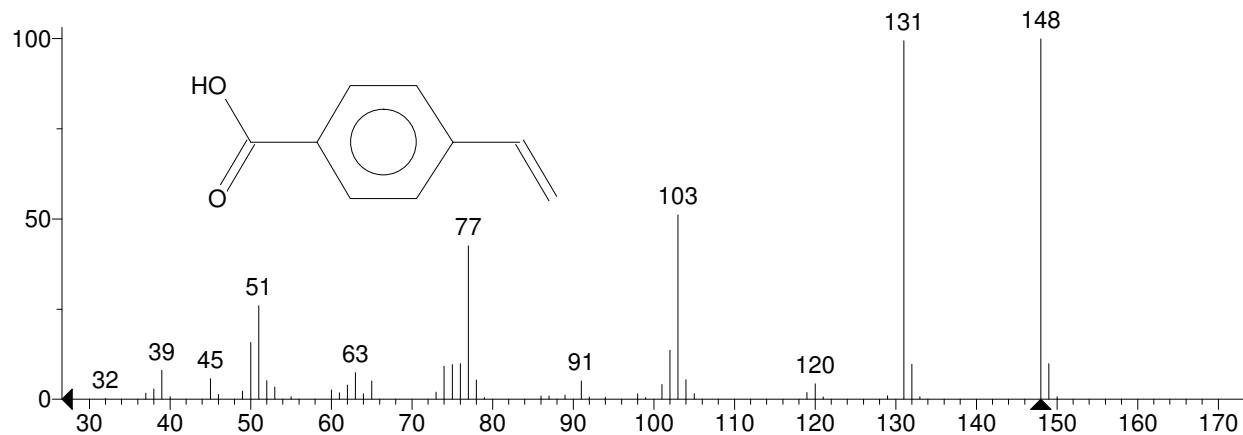


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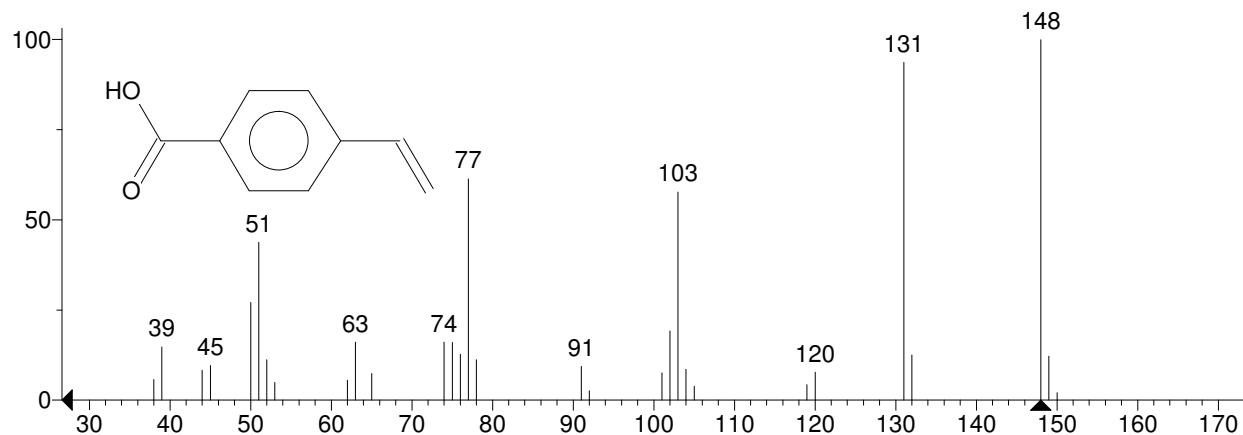
Unknown: Scan 478 (3.689 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -109



Hit 1 : 4-Vinylbenzoic acid
 C9H8O2; MF: 850; RMF: 888; Prob 83.3%; CAS: 1075-49-6; Lib: replib; ID: 19647.

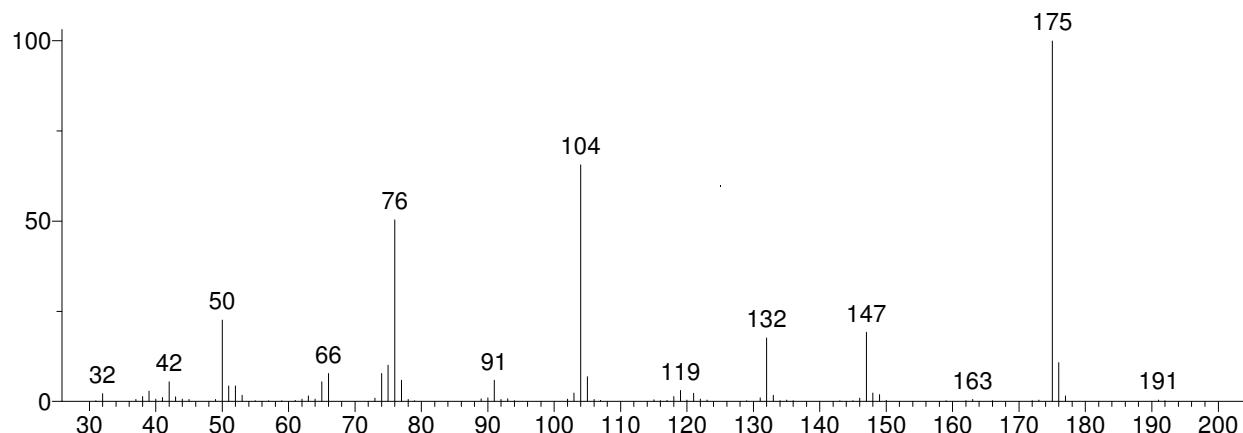


Hit 2 : 4-Vinylbenzoic acid
 C9H8O2; MF: 841; RMF: 909; Prob 83.3%; CAS: 1075-49-6; Lib: replib; ID: 19646.

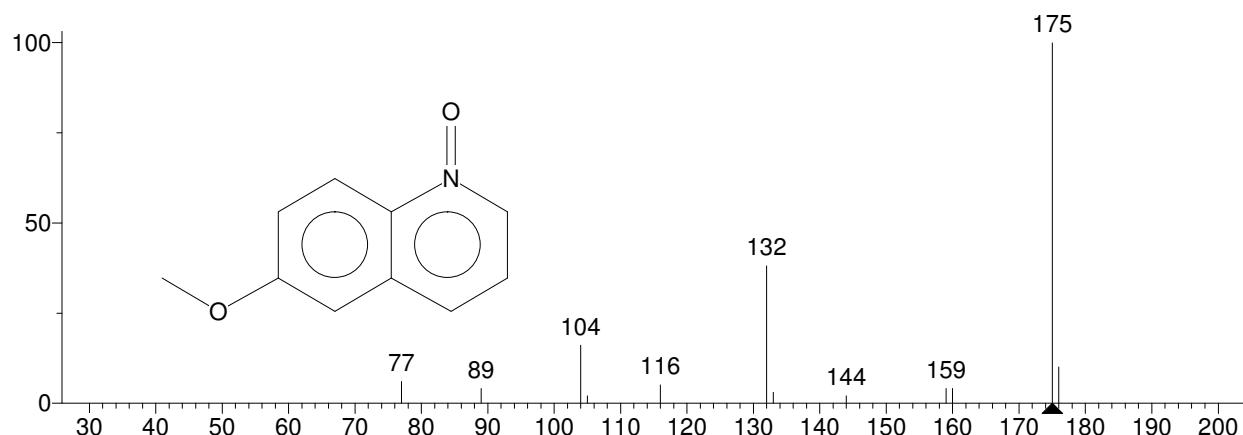


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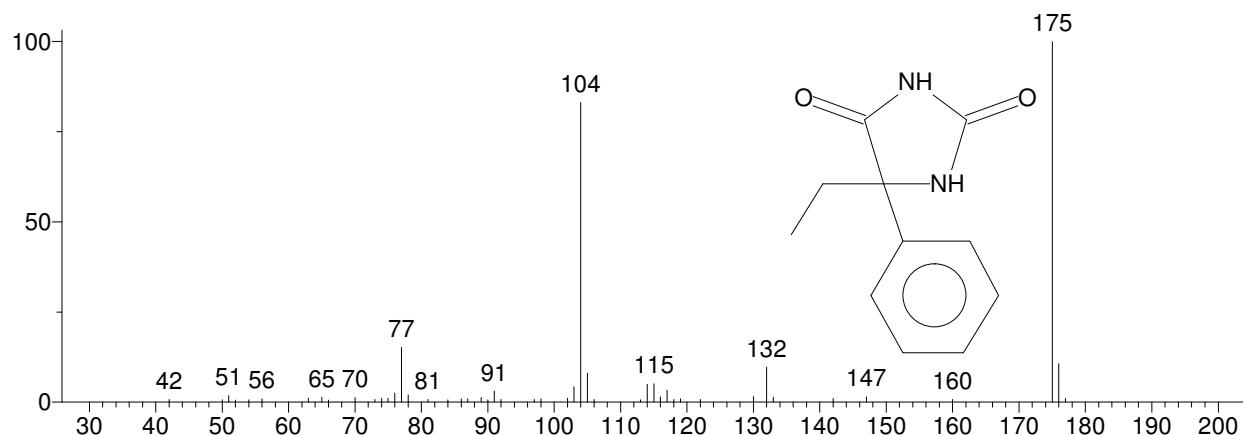
Unknown: Scan 549 (4.224 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -299



Hit 1 : Quinoline, 6-methoxy-, 1-oxide
 C10H9NO2; MF: 762; RMF: 877; Prob 40.1%; CAS: 6563-13-9; Lib: replib; ID: 22160.

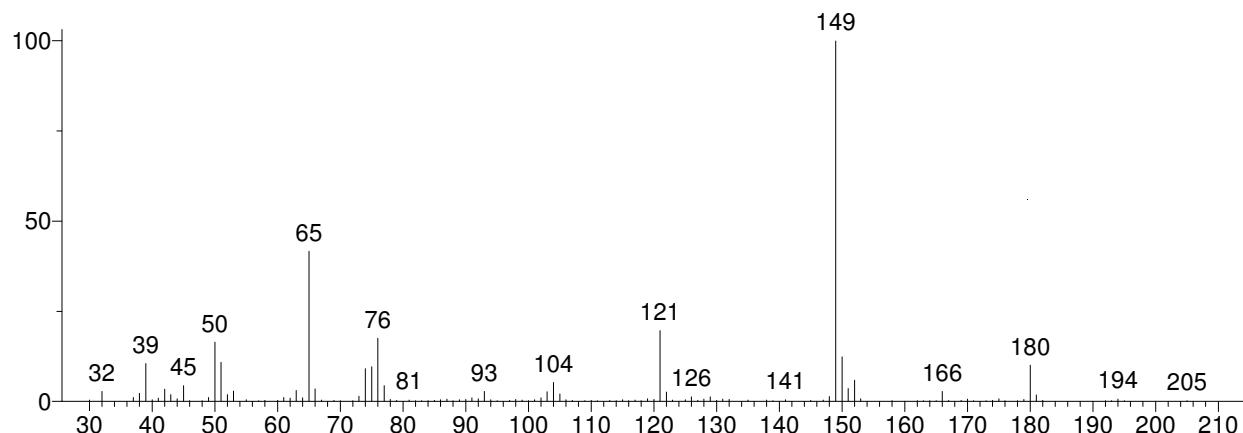


Hit 2 : Hydantoin, 5-ethyl-5-phenyl-, (+/-)-
 C11H12N2O2; MF: 754; RMF: 774; Prob 29.9%; CAS: 2216-93-5; Lib: mainlib; ID: 111540.

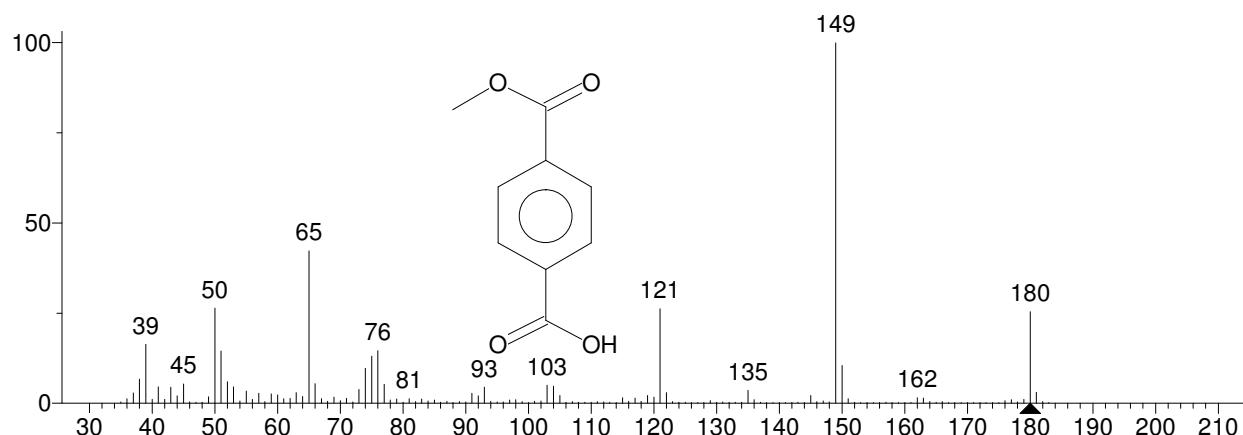


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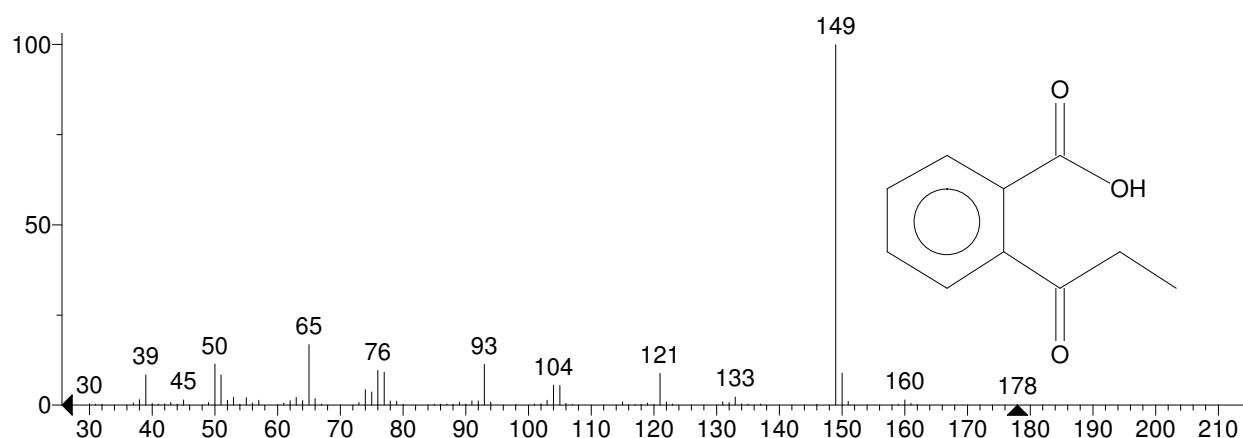
Unknown: Scan 657 (5.038 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -464



Hit 1 : 1,4-Benzenedicarboxylic acid, methyl ester
 C9H8O4; MF: 800; RMF: 802; Prob 51.0%; CAS: 39379-10-7; Lib: mainlib; ID: 95468.

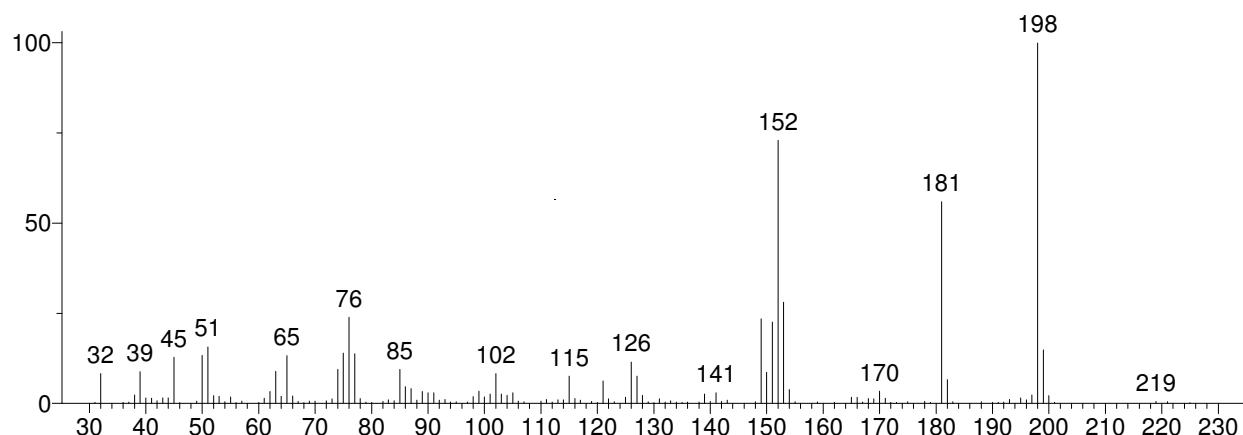


Hit 2 : Benzoic acid, 2-(1-oxopropyl)-
 C10H10O3; MF: 771; RMF: 847; Prob 14.4%; CAS: 2360-45-4; Lib: mainlib; ID: 95467.

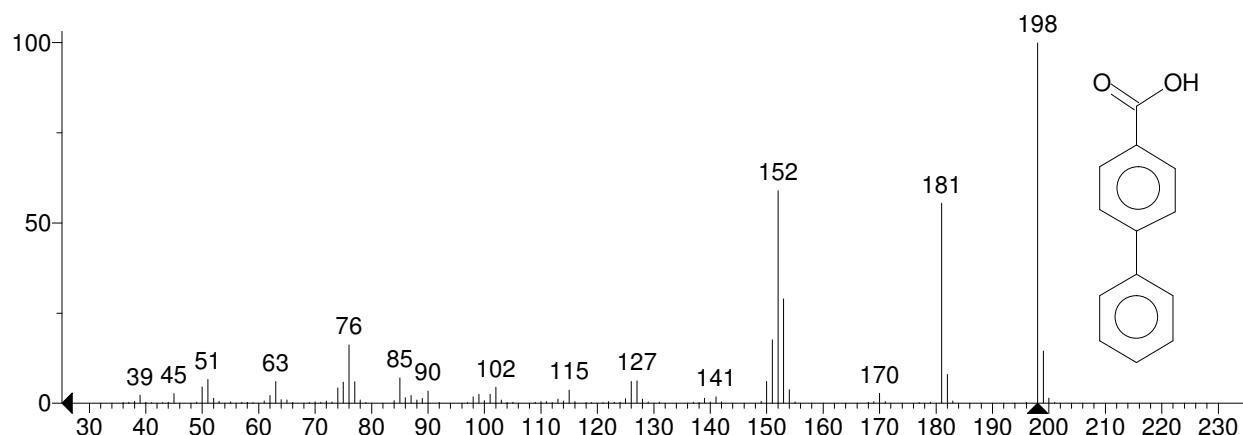


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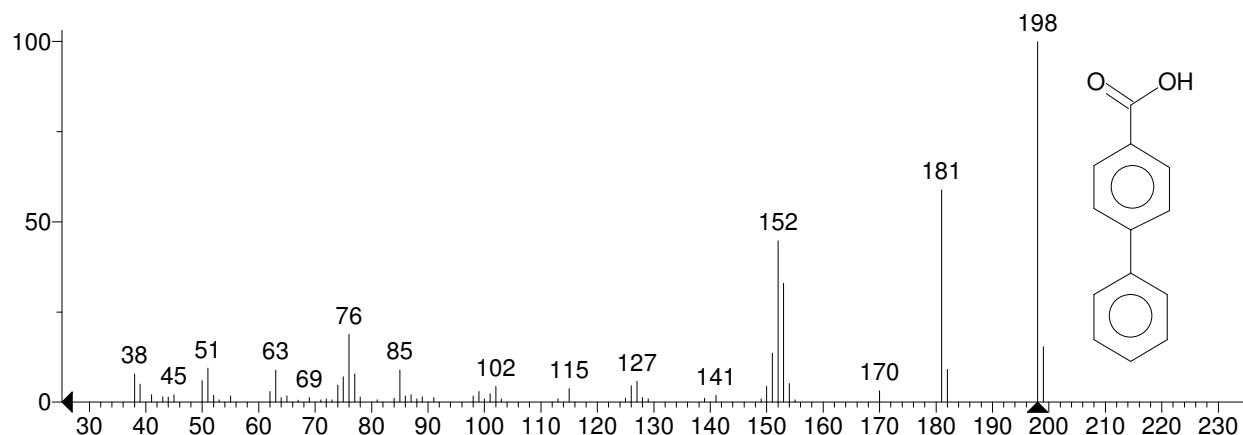
Unknown: Scan 798 (6.101 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -197



Hit 1 : Biphenyl-4-carboxylic acid
 C13H10O2; MF: 837; RMF: 860; Prob 74.4%; CAS: 92-92-2; Lib: replib; ID: 23783.

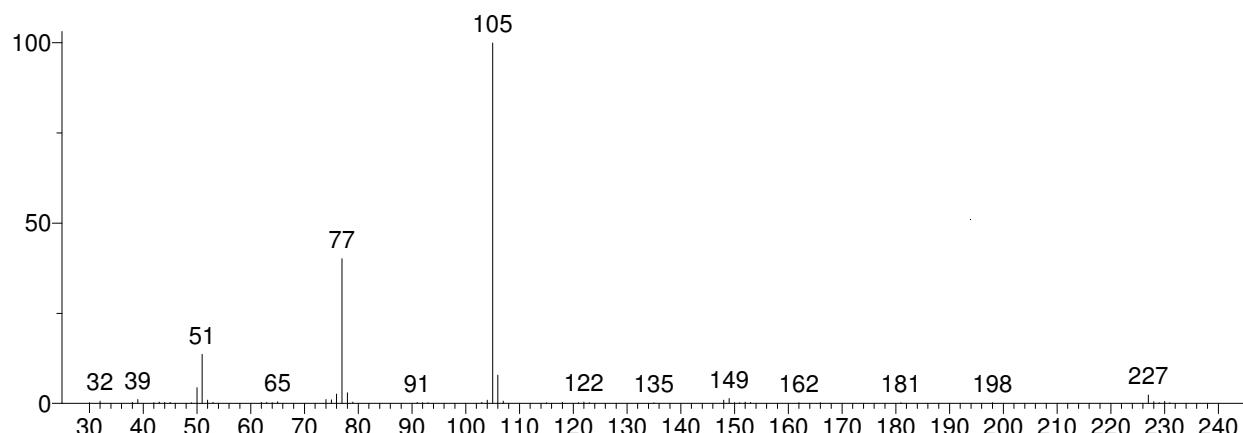


Hit 2 : Biphenyl-4-carboxylic acid
 C13H10O2; MF: 824; RMF: 877; Prob 74.4%; CAS: 92-92-2; Lib: replib; ID: 23792.

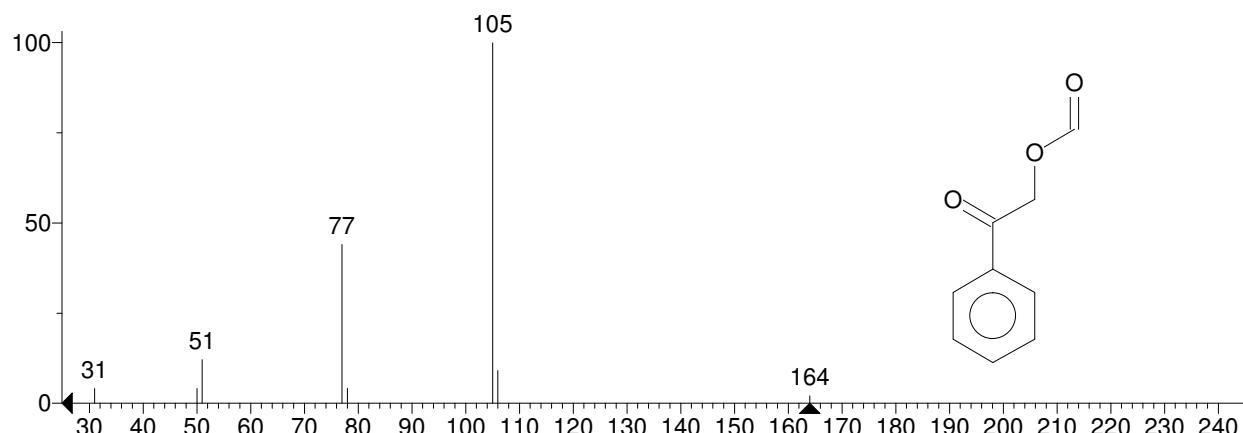


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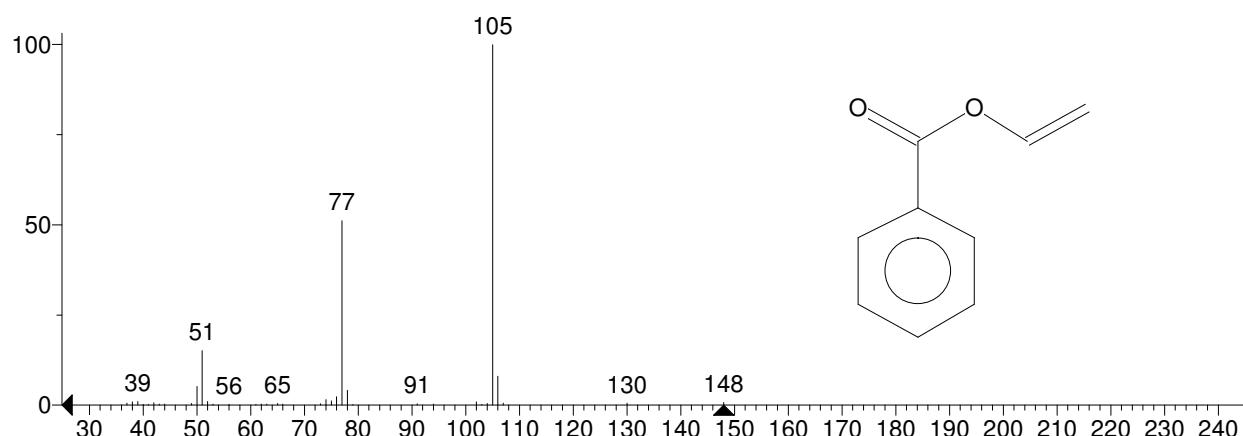
Unknown: Scan 907 (6.922 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -185



Hit 1 : Ethanone, 2-(formyloxy)-1-phenyl-
 C9H8O3; MF: 885; RMF: 956; Prob 9.29%; CAS: 55153-12-3; Lib: mainlib; ID: 59890.

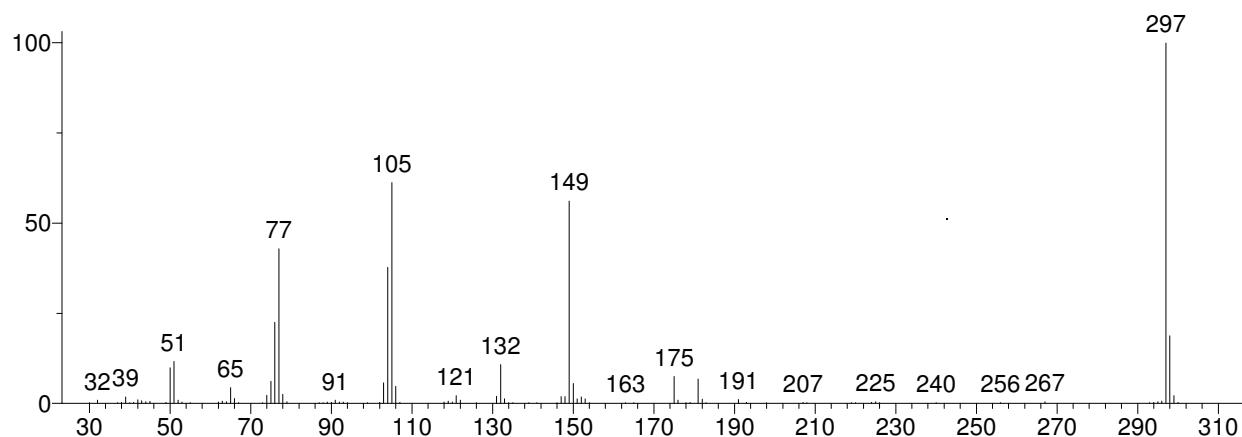


Hit 2 : Vinyl benzoate
 C9H8O2; MF: 873; RMF: 907; Prob 6.19%; CAS: 769-78-8; Lib: mainlib; ID: 59909.

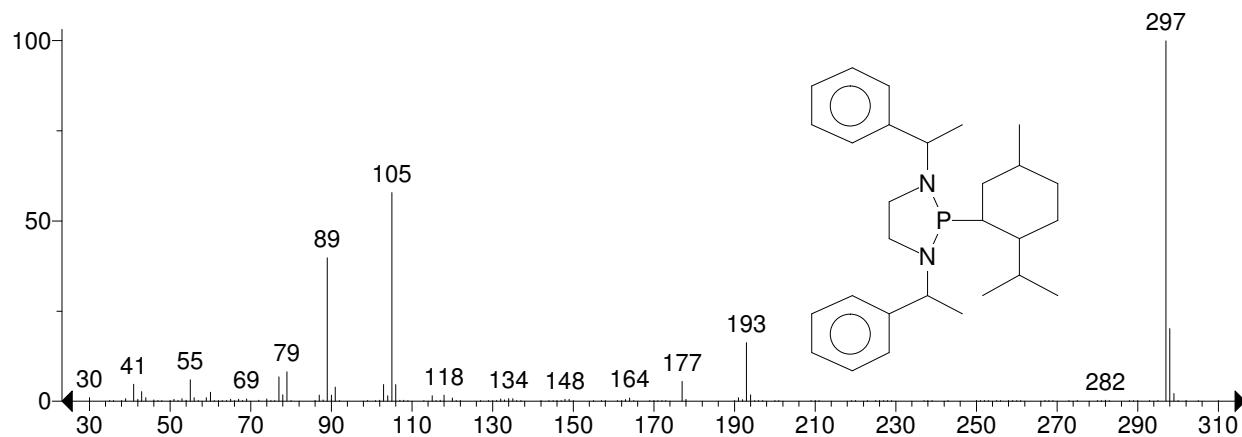


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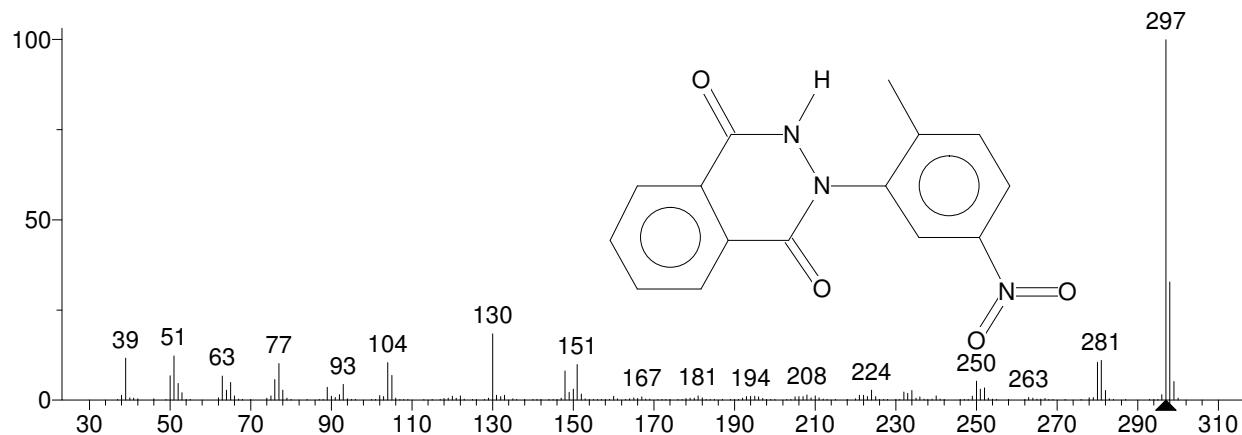
Unknown: Scan 1147 (8.730 min): Poly_ethylene terephthalate_A_py2.D\data.ms
 Compound in Library Factor = -1296



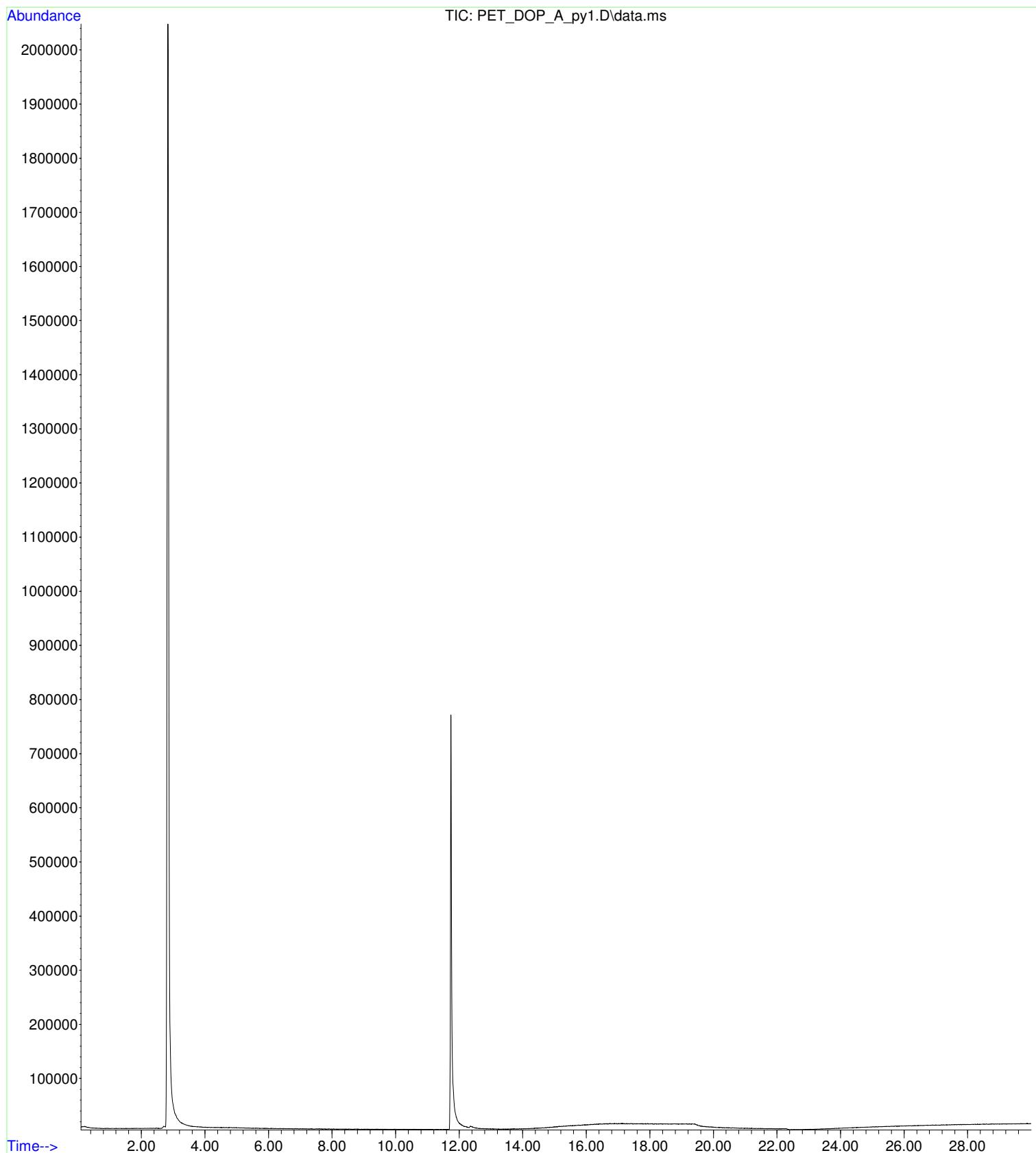
Hit 1 : 1,3,2-Diazaphospholidine, 2-methyl-1,3-bis(1-phenylethyl)-
 C₂₈H₄₁N₂P; MF: 592; RMF: 632; Prob 21.9%; Lib: mainlib; ID: 150647.



Hit 2 : Phthalazine-1,4(2H,3H)-dione, 2-(2-methyl-5-nitrophenyl)-
 C₁₅H₁₁N₃O₄; MF: 563; RMF: 571; Prob 6.20%; Lib: mainlib; ID: 150756.

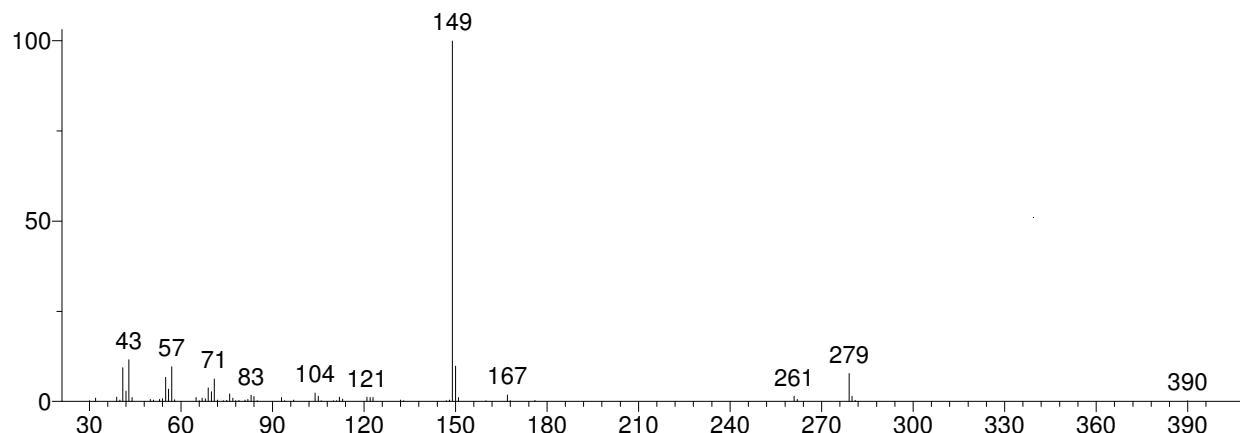


File : C:\msdchem\1\DATA\2010\Temp\091610\PET_DOP_A_py1.D
Operator : Mark Jordi
Acquired : 17 Sep 2010 18:11 using AcqMethod PYMS2A.M
Instrument : Instrument #1
Sample Name: PET DOP
Misc Info : PET DOP
Vial Number: 25

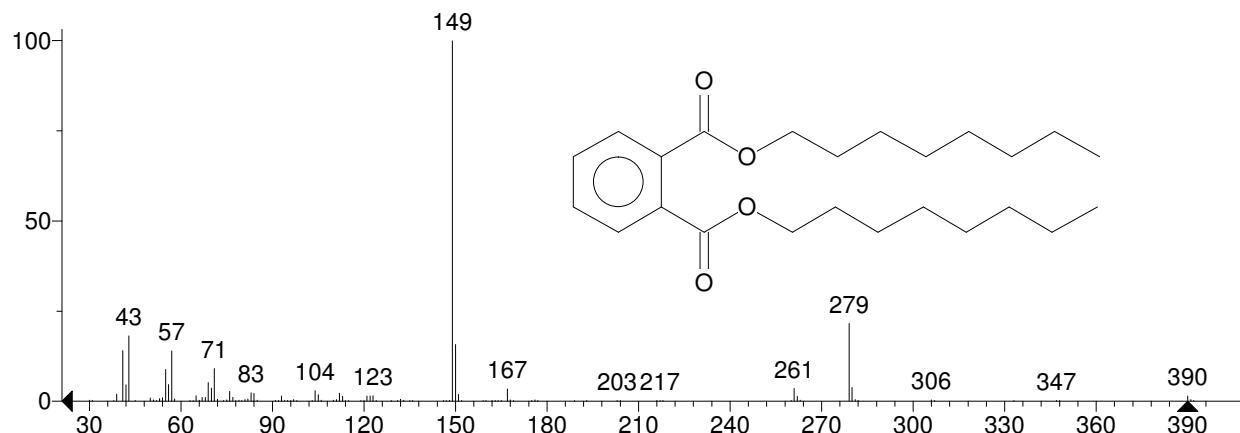


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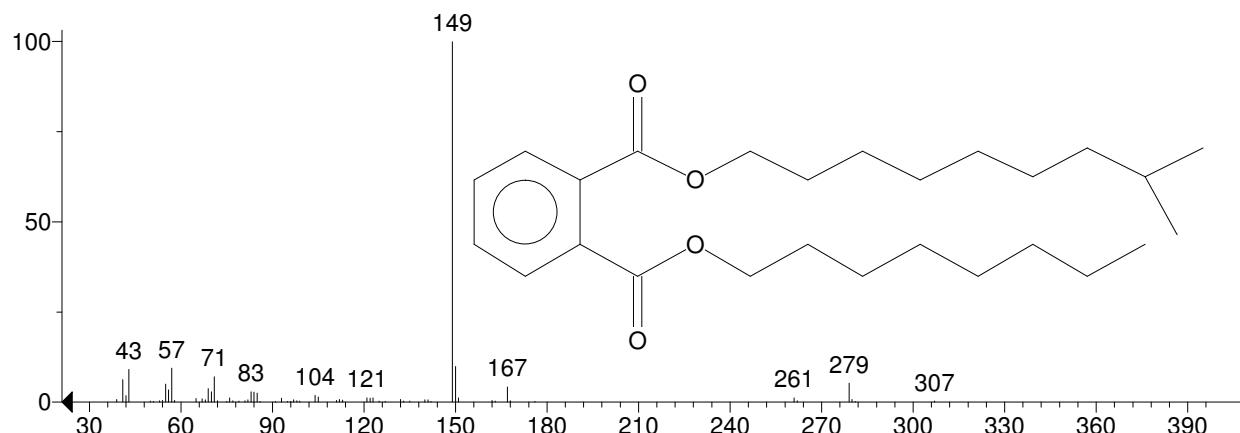
Unknown: Scan 1546 (11.737 min): PET_DOP_A_py1.D\data.ms
 Compound in Library Factor = 109



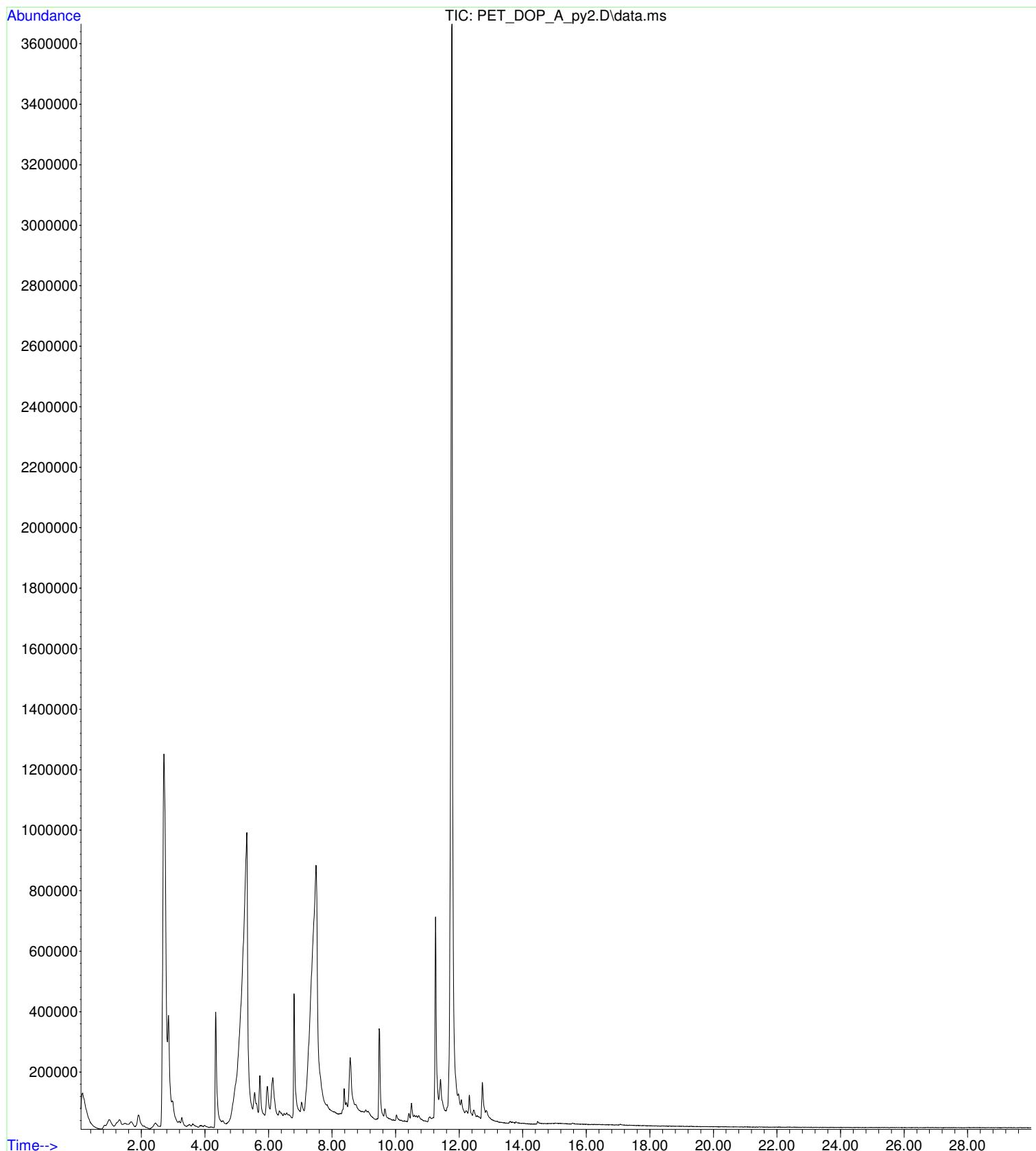
Hit 1 : Di-n-octyl phthalate
 C₂₄H₃₈O₄; MF: 923; RMF: 925; Prob 41.5%; CAS: 117-84-0; Lib: replib; ID: 19824.



Hit 2 : 1,2-Benzenedicarboxylic acid, isodecyl octyl ester
 C₂₆H₄₂O₄; MF: 903; RMF: 906; Prob 18.9%; CAS: 1330-96-7; Lib: mainlib; ID: 96124.

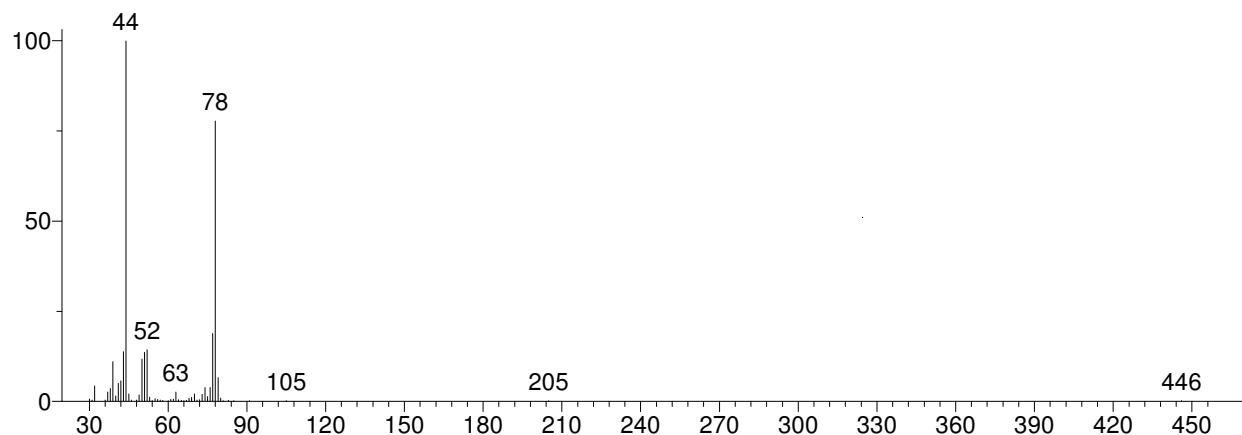


File : C:\msdchem\1\DATA\2010\Temp\091610\PET_DOP_A_py2.D
Operator : Mark Jordi
Acquired : 20 Sep 2010 8:39 using AcqMethod PYMS2A.M
Instrument : Instrument #1
Sample Name: PET DOP
Misc Info : PET DOP
Vial Number: 25

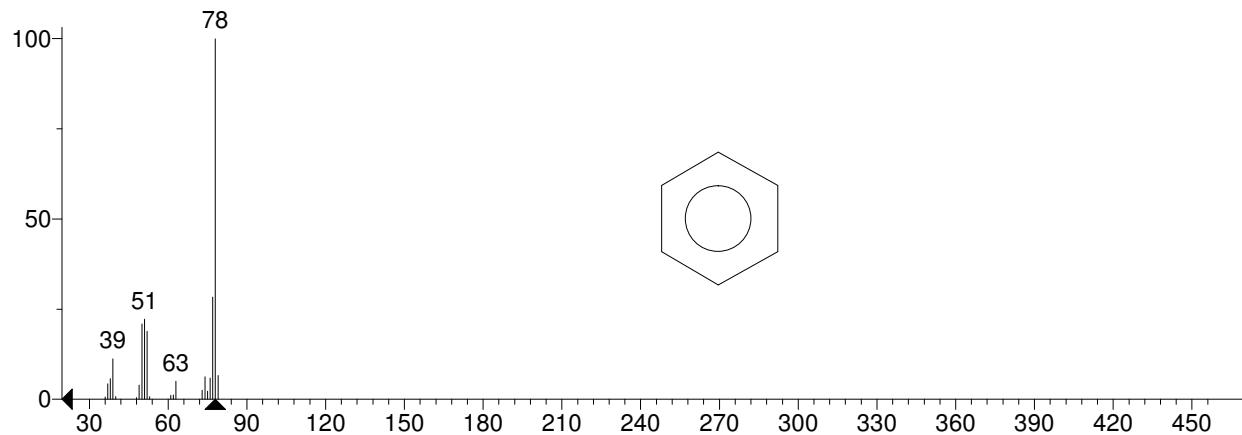


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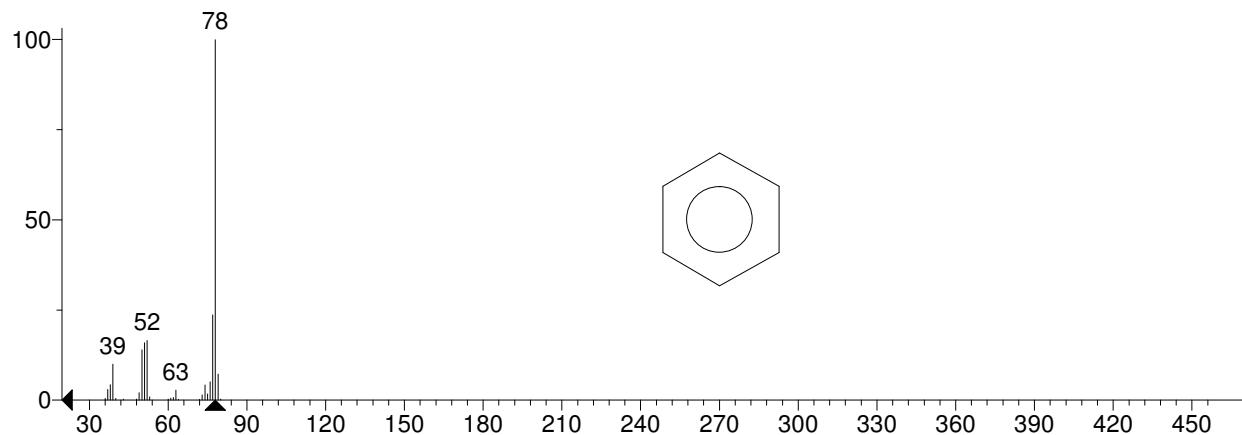
Unknown: Scan 367 (2.853 min): PET_DOP_A_py2.D\data.ms
Compound in Library Factor = -399



Hit 1 : Benzene
C6H6; MF: 762; RMF: 950; Prob 61.7%; CAS: 71-43-2; Lib: mainlib; ID: 37960.

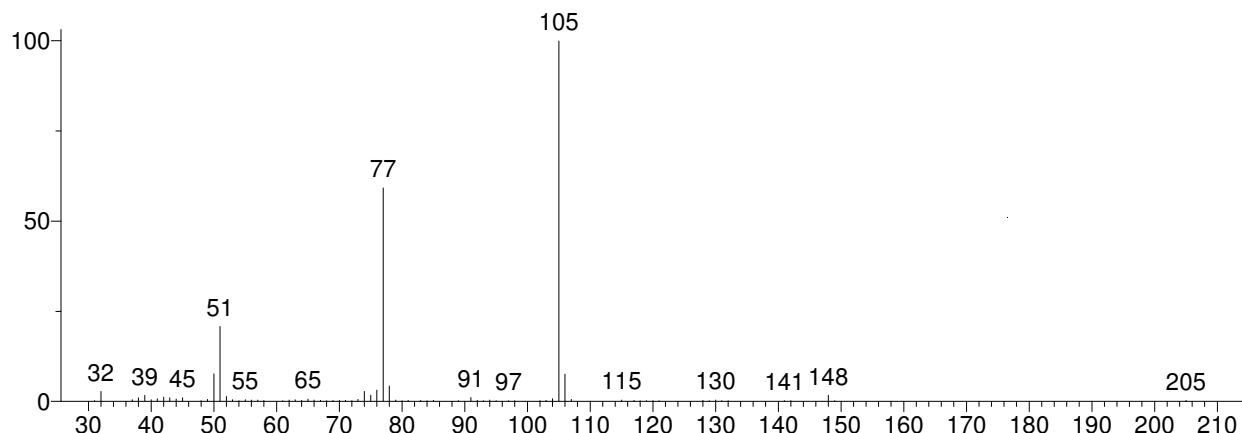


Hit 2 : Benzene
C6H6; MF: 741; RMF: 902; Prob 61.7%; CAS: 71-43-2; Lib: replib; ID: 9508.

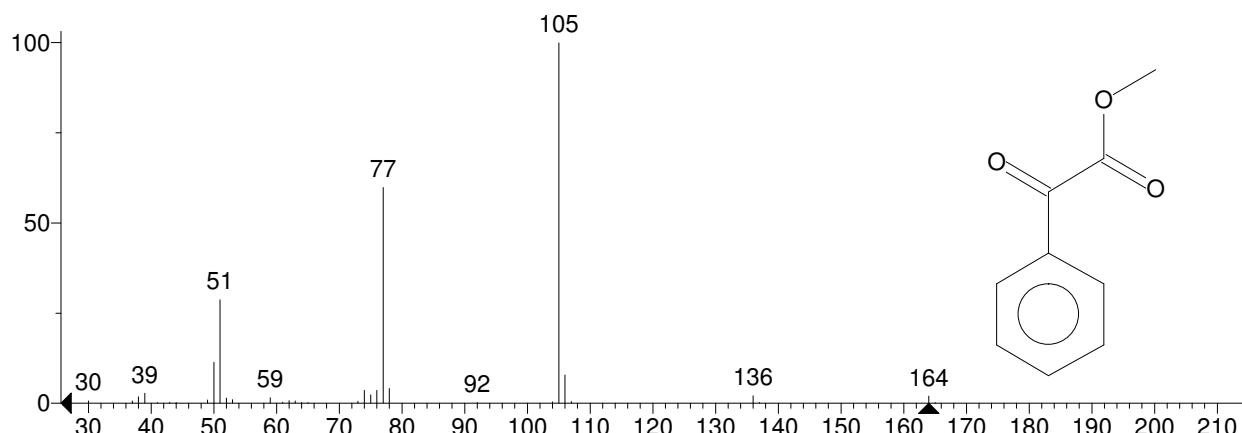


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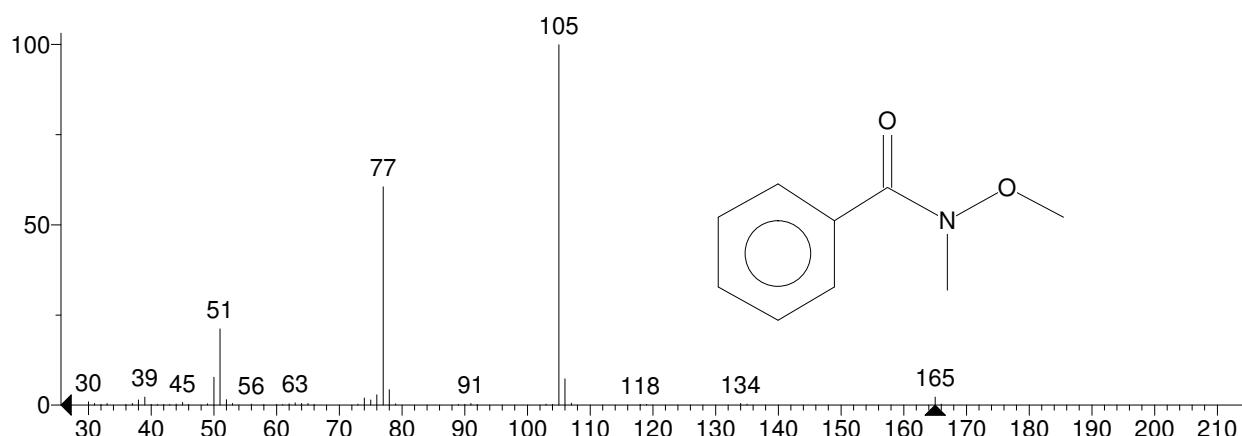
Unknown: Scan 564 (4.338 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -207



Hit 1 : Benzeneacetic acid, .alpha.-oxo-, methyl ester
 C9H8O3; MF: 900; RMF: 930; Prob 7.54%; CAS: 15206-55-0; Lib: mainlib; ID: 59819.

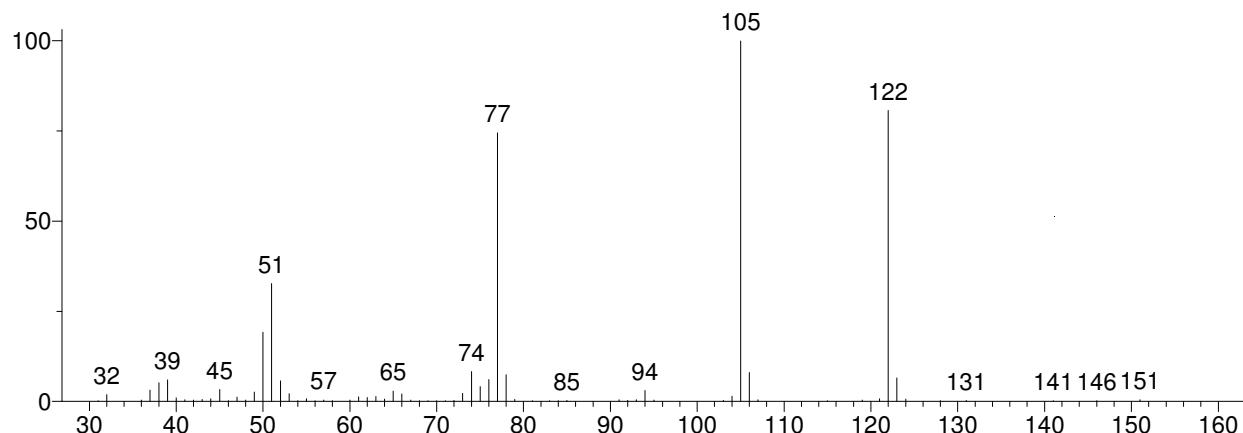


Hit 2 : N-Methoxy-N-methylbenzamide
 C9H11NO2; MF: 895; RMF: 914; Prob 6.07%; CAS: 6919-61-5; Lib: mainlib; ID: 59860.

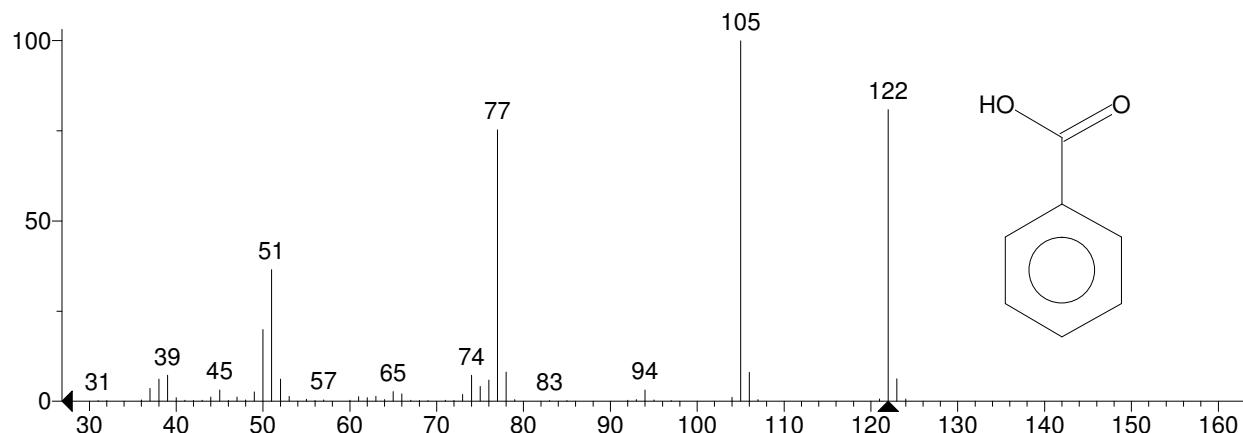


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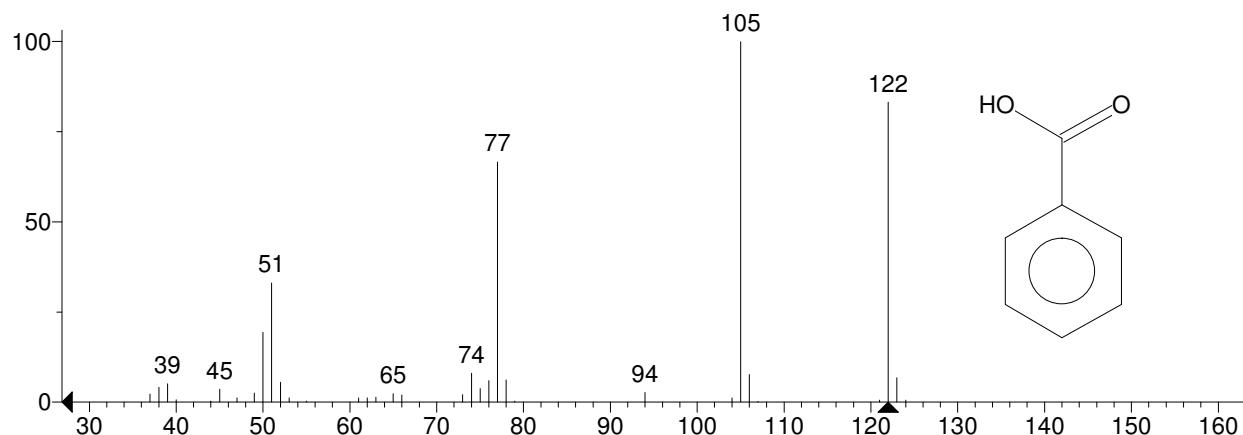
Unknown: Scan 694 (5.317 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = 141



Hit 1 : Benzenecarboxylic acid
 C7H6O2; MF: 943; RMF: 946; Prob 56.0%; CAS: 65-85-0; Lib: replib; ID: 13937.

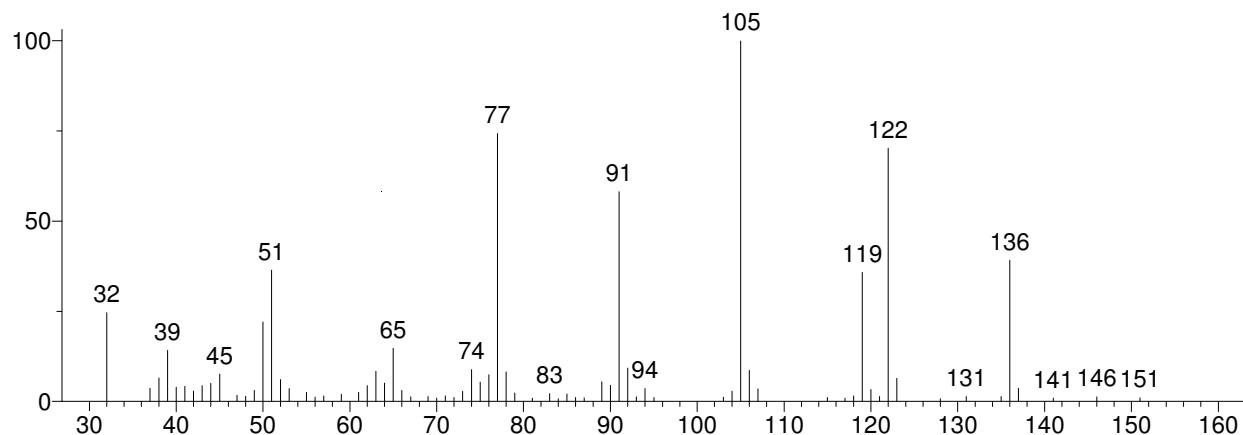


Hit 2 : Benzenecarboxylic acid
 C7H6O2; MF: 940; RMF: 948; Prob 56.0%; CAS: 65-85-0; Lib: replib; ID: 13938.

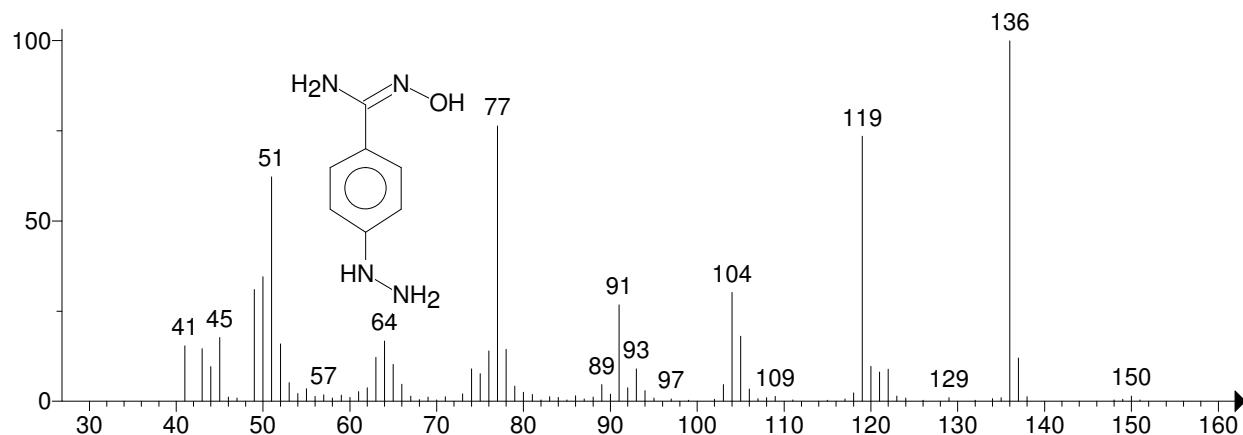


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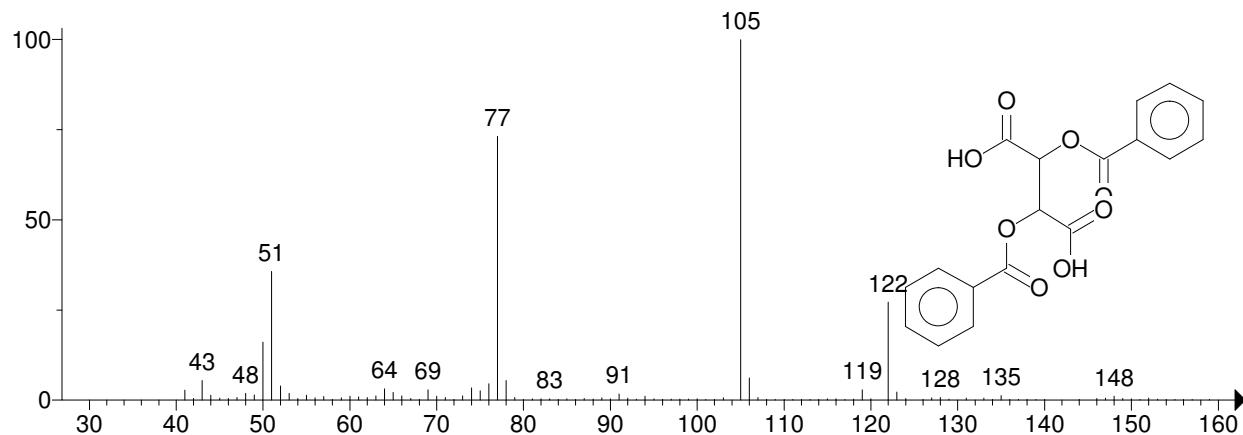
Unknown: Scan 726 (5.558 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -897



Hit 1 : p-Hydrazinobenzamidoxime
 C7H10N4O; MF: 702; RMF: 708; Prob 15.7%; Lib: mainlib; ID: 86816.

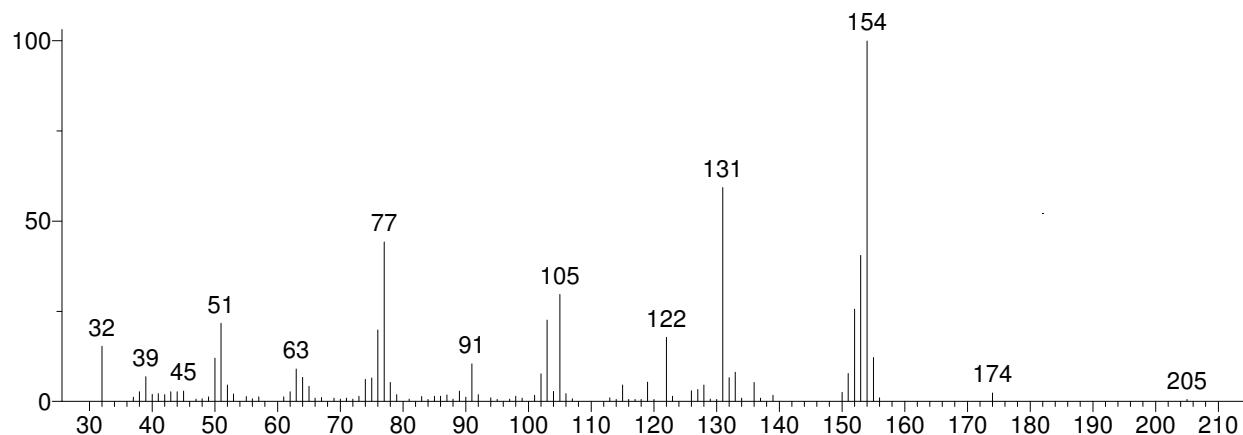


Hit 2 : (d)-(+)-(2R,3R)-2,3-Dibenzoyltartaric acid
 C18H14O8; MF: 681; RMF: 689; Prob 6.66%; CAS: 2743-38-6; Lib: replib; ID: 13613.

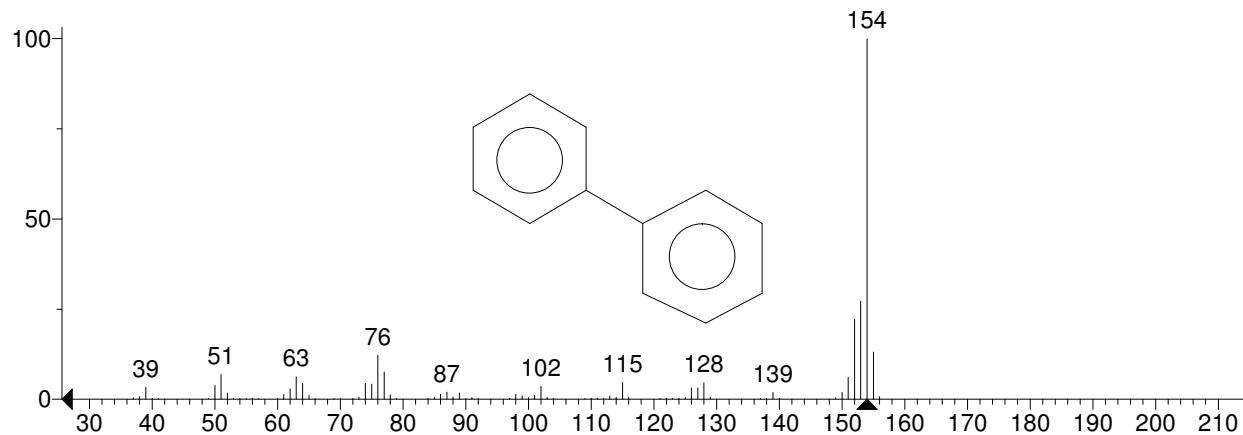


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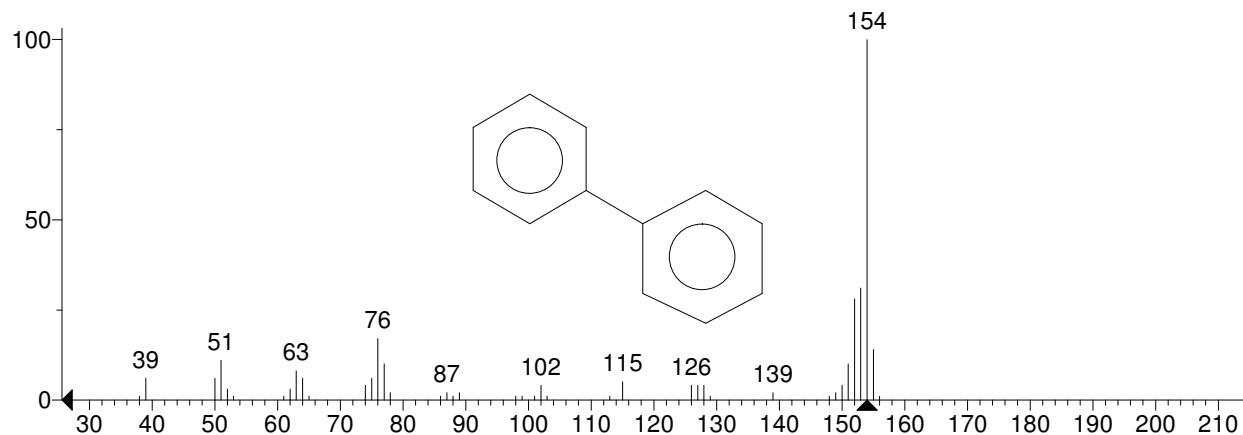
Unknown: Scan 748 (5.724 min): PET_DOP_A_py2.D\data.ms
Compound in Library Factor = -573



Hit 1 : Biphenyl
C12H10; MF: 718; RMF: 850; Prob 58.3%; CAS: 92-52-4; Lib: replib; ID: 20364.

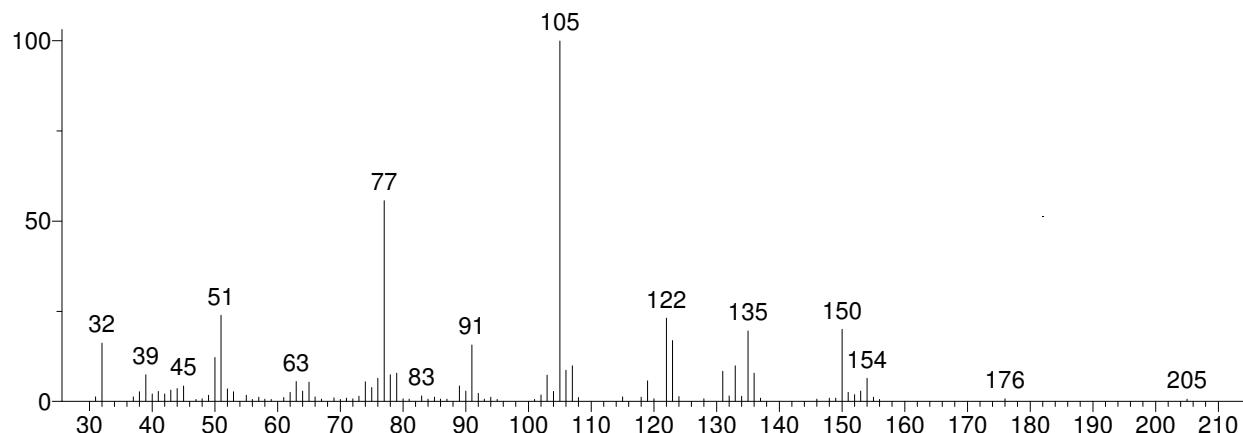


Hit 2 : Biphenyl
C12H10; MF: 706; RMF: 881; Prob 58.3%; CAS: 92-52-4; Lib: replib; ID: 20366.

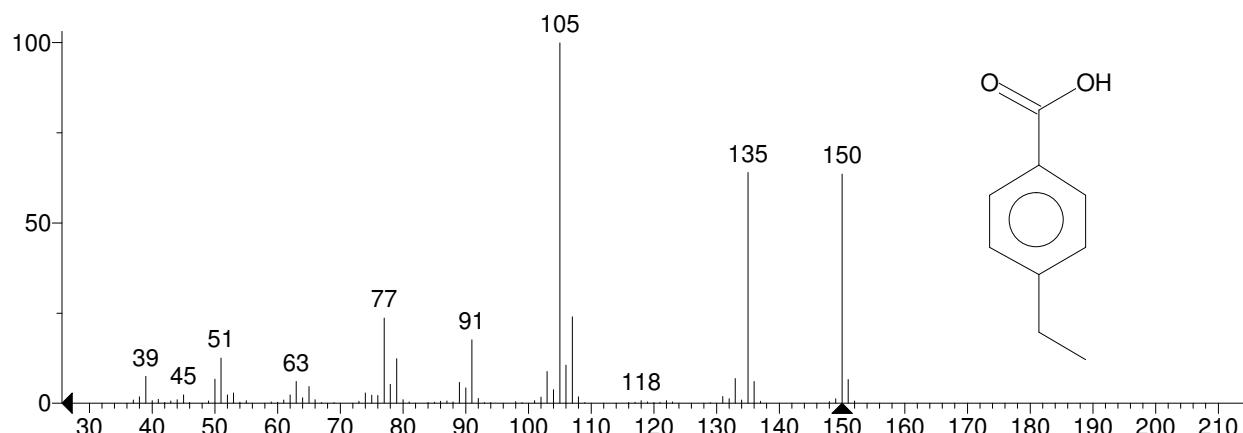


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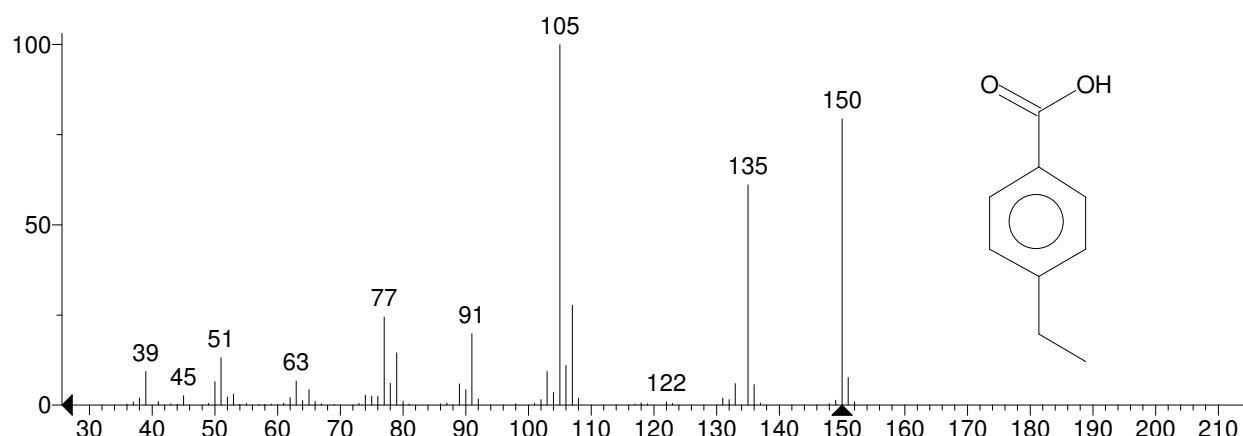
Unknown: Scan 779 (5.958 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -733



Hit 1 : 4-Ethylbenzoic acid
 C9H10O2; MF: 741; RMF: 773; Prob 36.7%; CAS: 619-64-7; Lib: mainlib; ID: 61731.

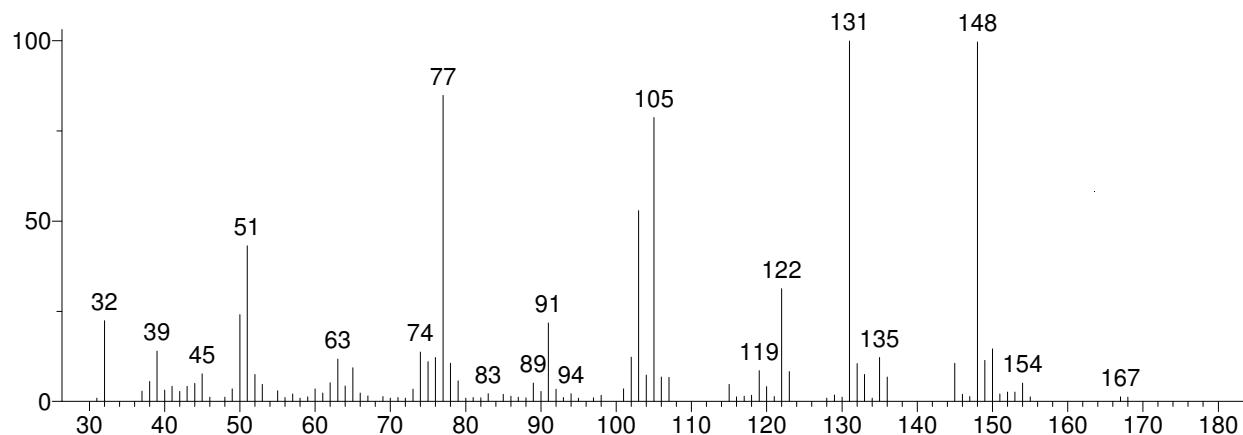


Hit 2 : 4-Ethylbenzoic acid
 C9H10O2; MF: 725; RMF: 763; Prob 36.7%; CAS: 619-64-7; Lib: replib; ID: 14004.

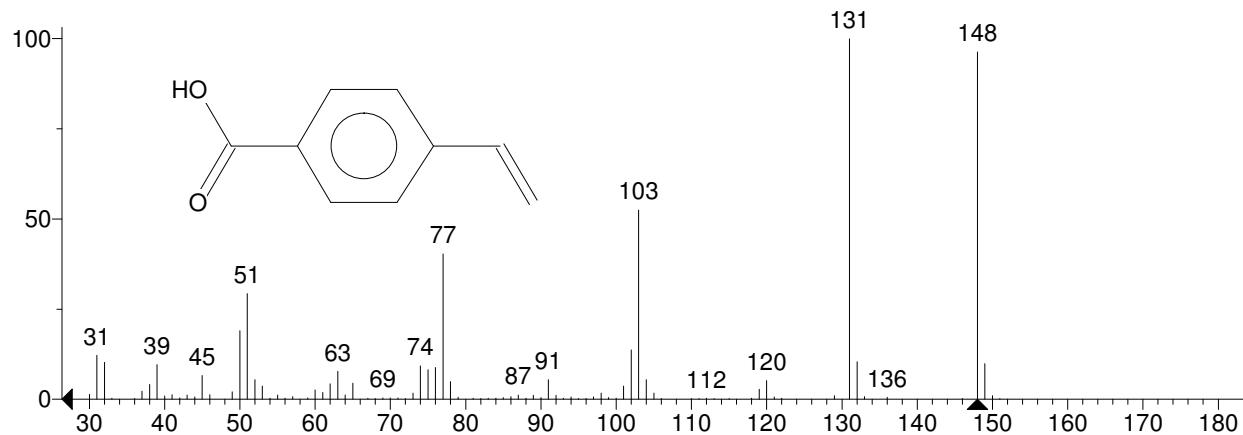


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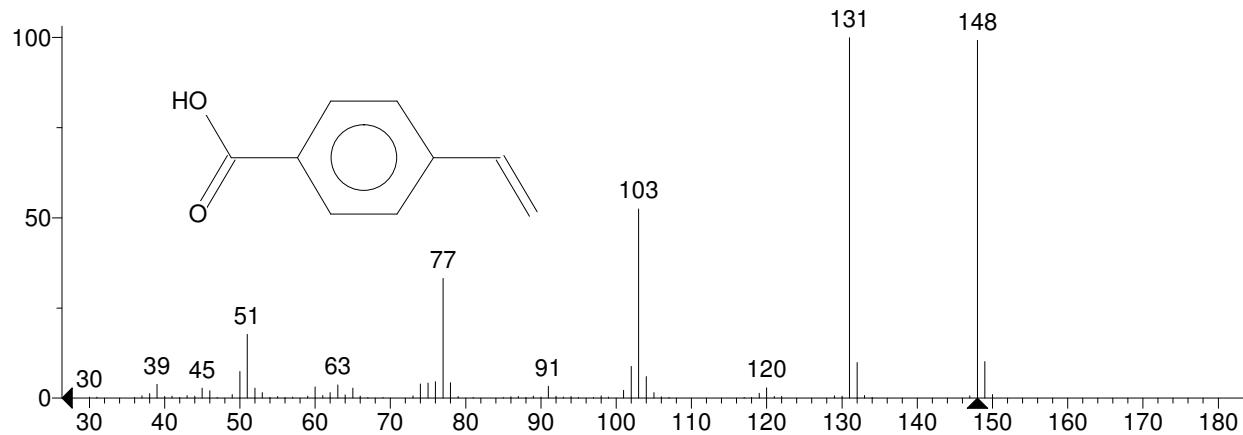
Unknown: Scan 802 (6.131 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -521



Hit 1 : 4-Vinylbenzoic acid
 C9H8O2; MF: 736; RMF: 776; Prob 54.4%; CAS: 1075-49-6; Lib: replib; ID: 17751.

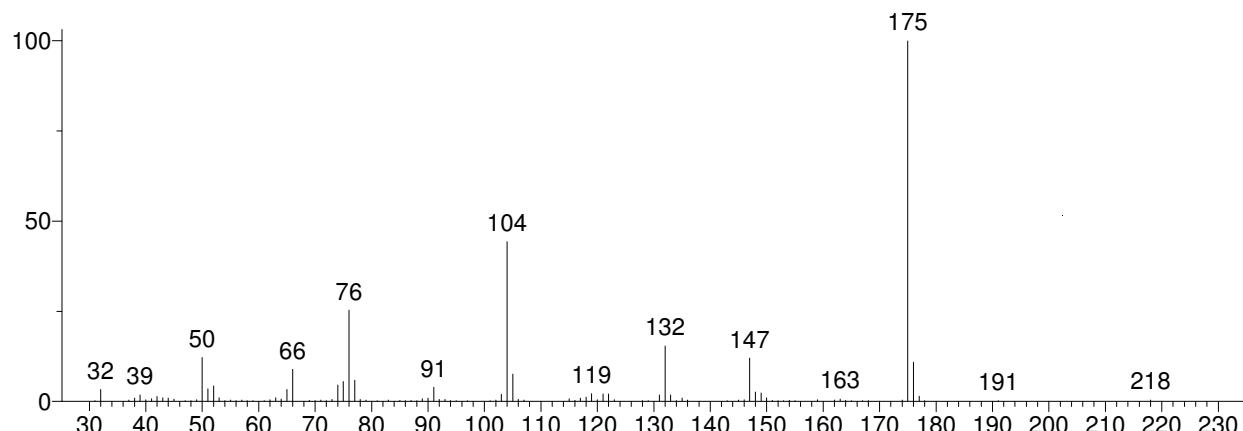


Hit 2 : 4-Vinylbenzoic acid
 C9H8O2; MF: 724; RMF: 771; Prob 54.4%; CAS: 1075-49-6; Lib: mainlib; ID: 82295.

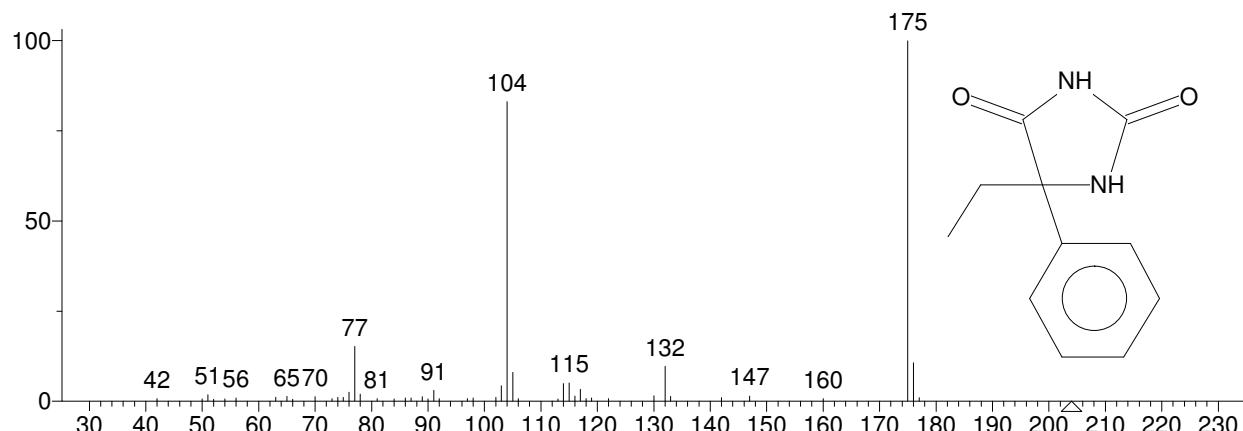


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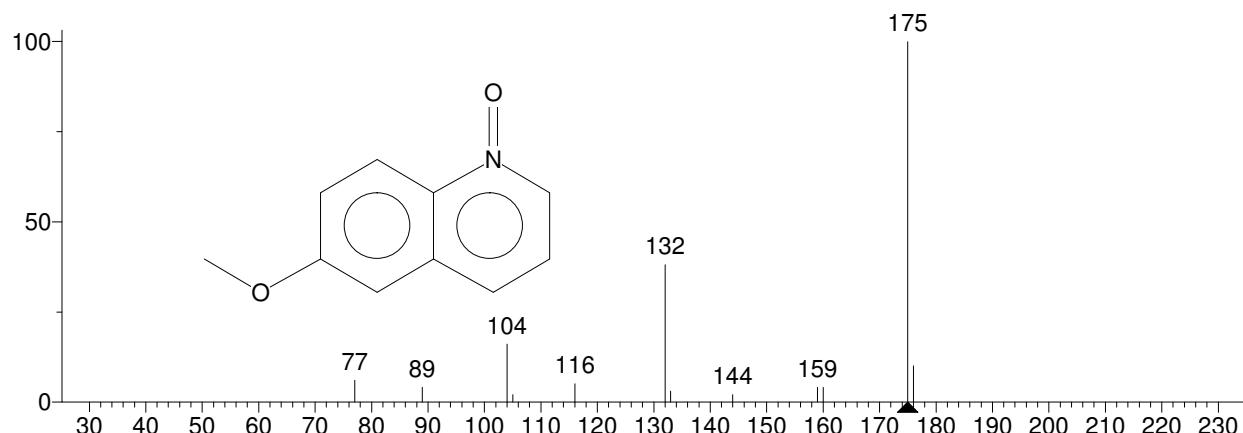
Unknown: Scan 891 (6.802 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -282



Hit 1 : Hydantoin, 5-ethyl-5-phenyl-, (+/-)-
 C11H12N2O2; MF: 777; RMF: 812; Prob 44.6%; CAS: 2216-93-5; Lib: mainlib; ID: 111540.

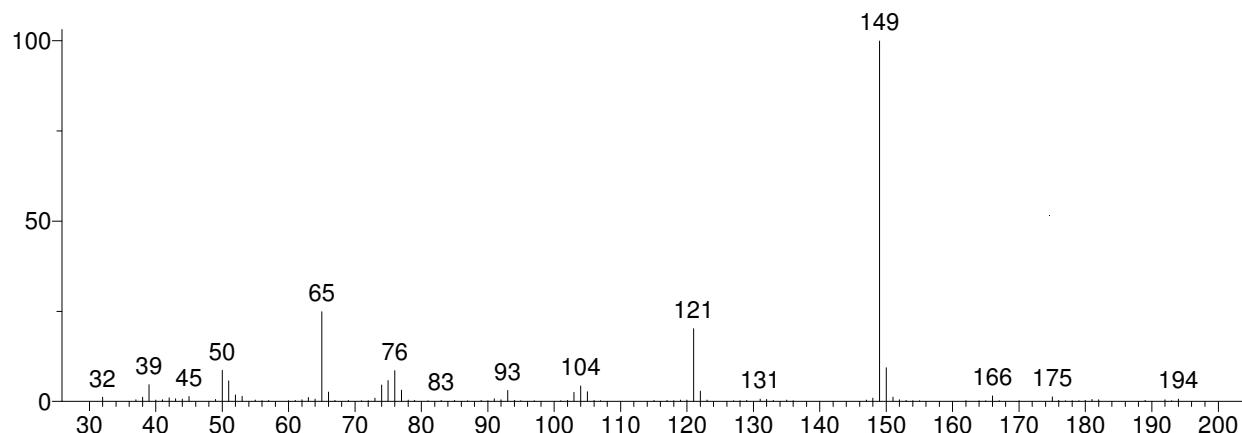


Hit 2 : Quinoline, 6-methoxy-, 1-oxide
 C10H9NO2; MF: 772; RMF: 890; Prob 36.0%; CAS: 6563-13-9; Lib: replib; ID: 22160.

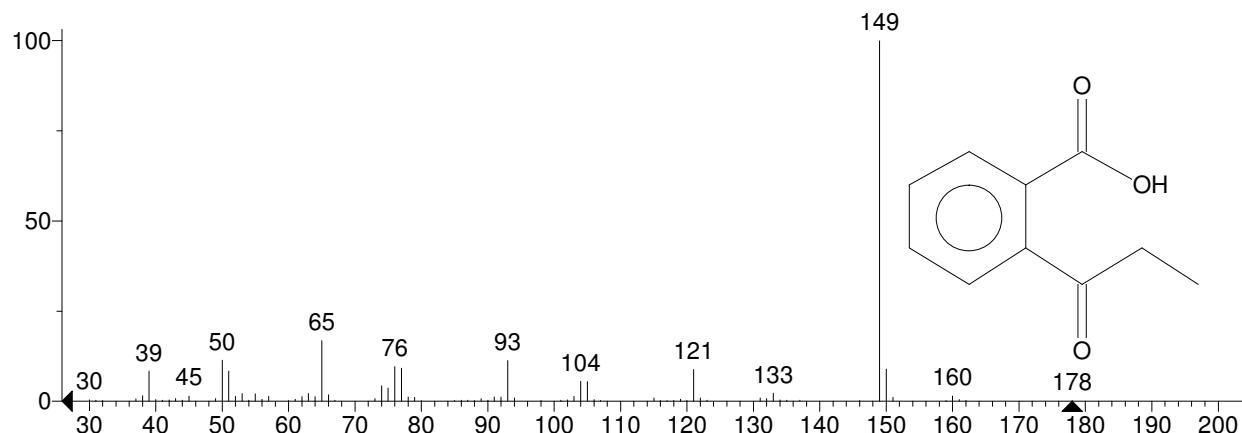


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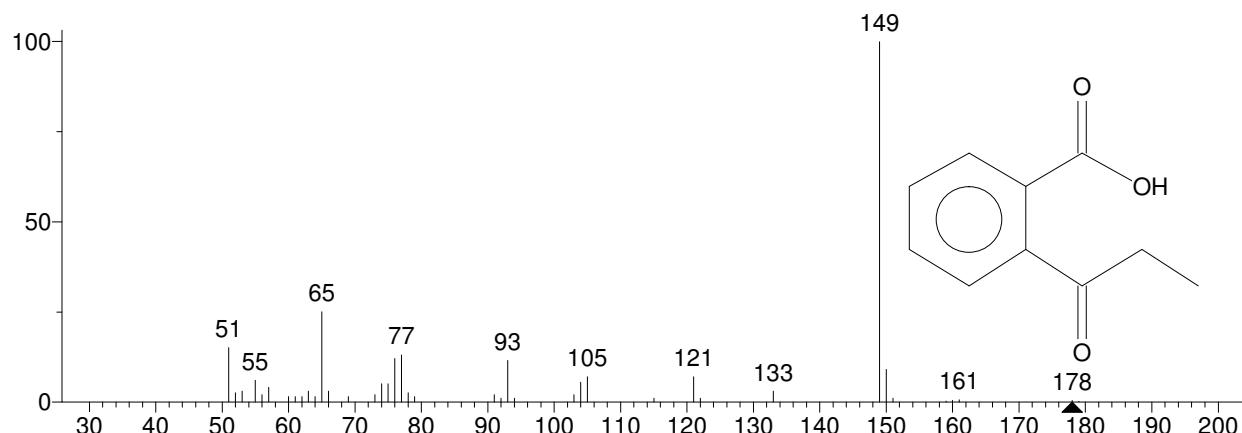
Unknown: Scan 983 (7.495 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -1.81



Hit 1 : Benzoic acid, 2-(1-oxopropyl)-
 C10H10O3; MF: 849; RMF: 874; Prob 50.9%; CAS: 2360-45-4; Lib: mainlib; ID: 95467.

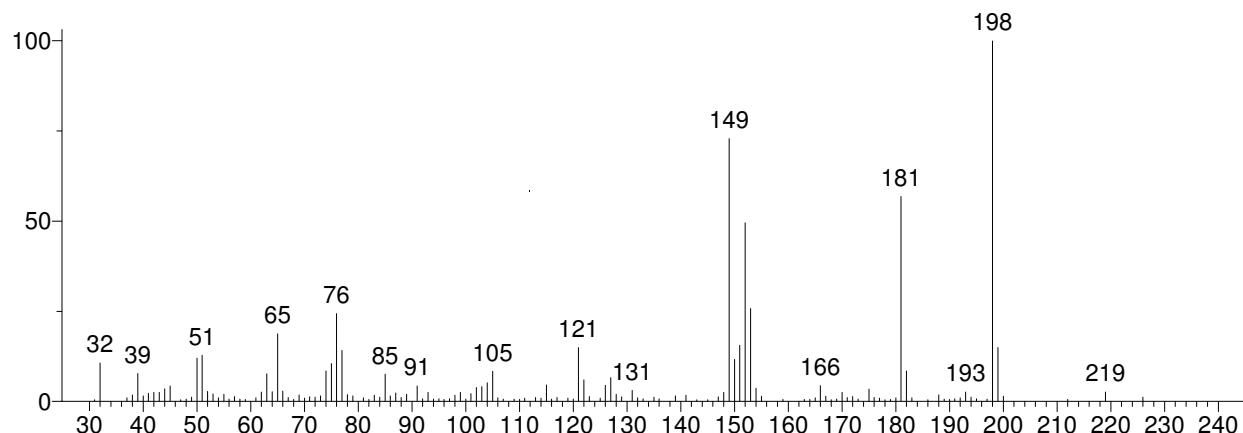


Hit 2 : Benzoic acid, 2-(1-oxopropyl)-
 C10H10O3; MF: 841; RMF: 873; Prob 50.9%; CAS: 2360-45-4; Lib: replib; ID: 19721.

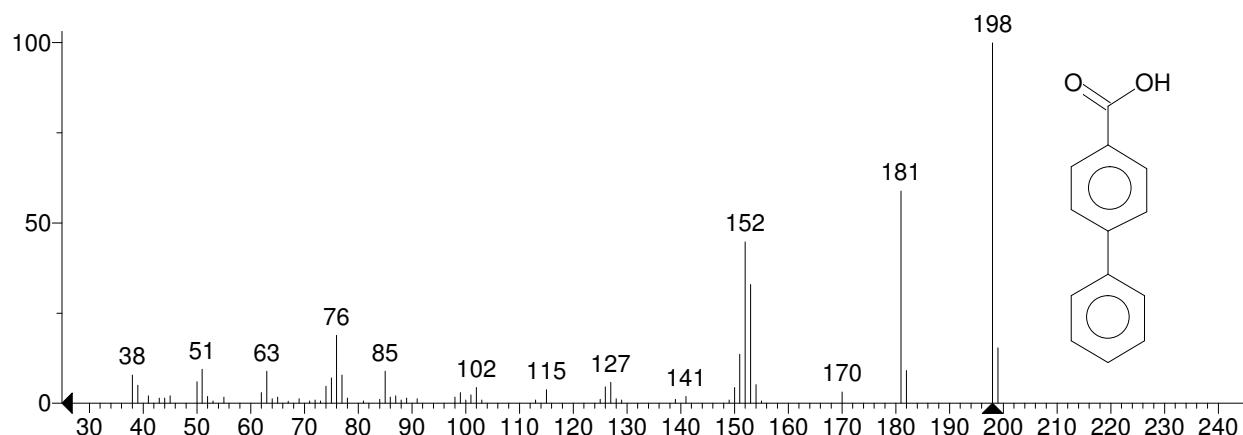


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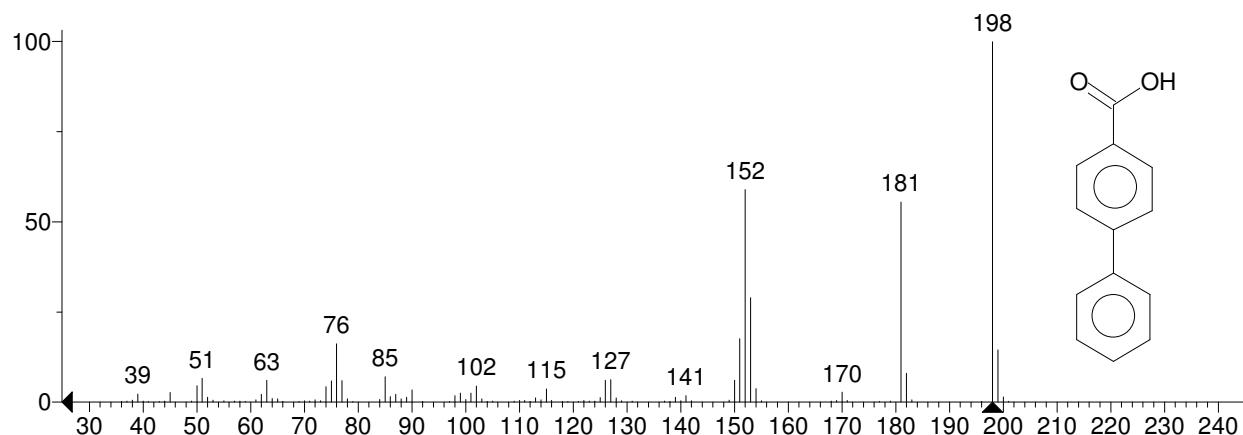
Unknown: Scan 1126 (8.572 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -281



Hit 1 : Biphenyl-4-carboxylic acid
 C13H10O2; MF: 764; RMF: 848; Prob 65.7%; CAS: 92-92-2; Lib: replib; ID: 23792.

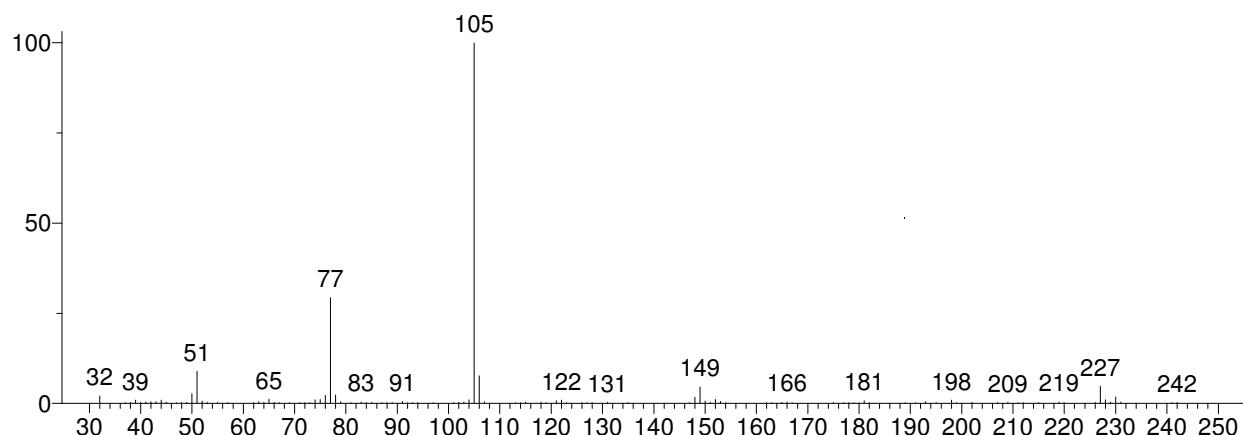


Hit 2 : Biphenyl-4-carboxylic acid
 C13H10O2; MF: 749; RMF: 792; Prob 65.7%; CAS: 92-92-2; Lib: replib; ID: 23783.

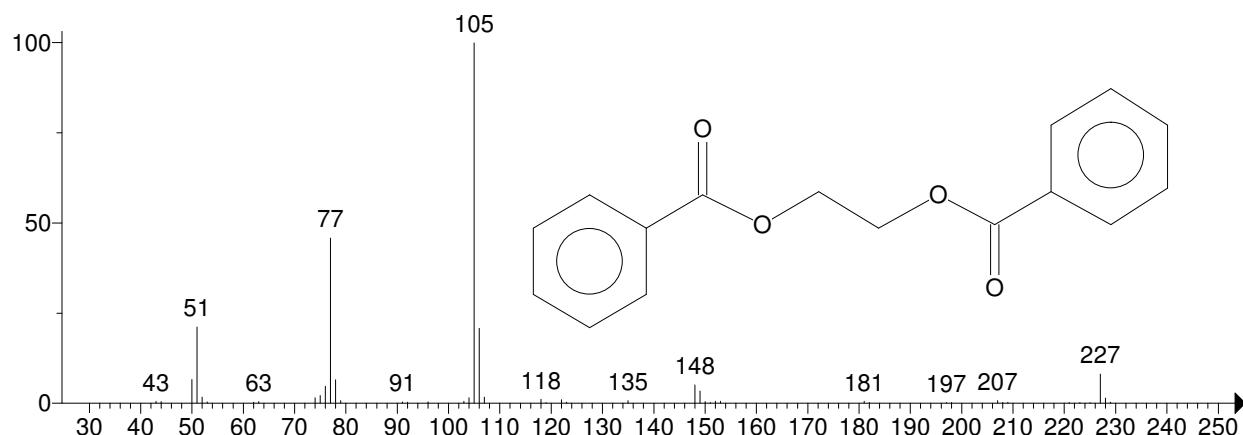


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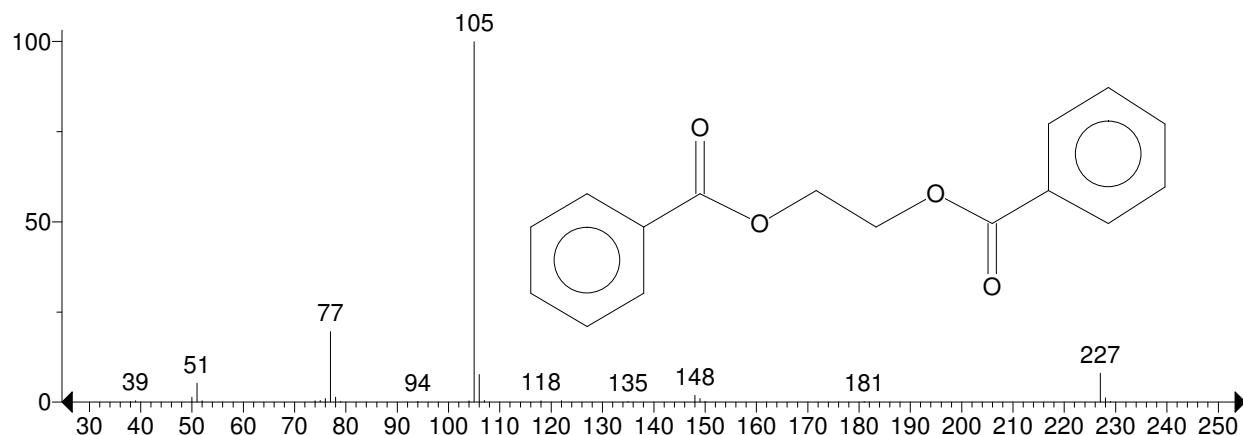
Unknown: Scan 1247 (9.484 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -229



Hit 1 : 1,2-Ethanediol, dibenzoate
 C16H14O4; MF: 839; RMF: 875; Prob 28.8%; CAS: 94-49-5; Lib: replib; ID: 13582.

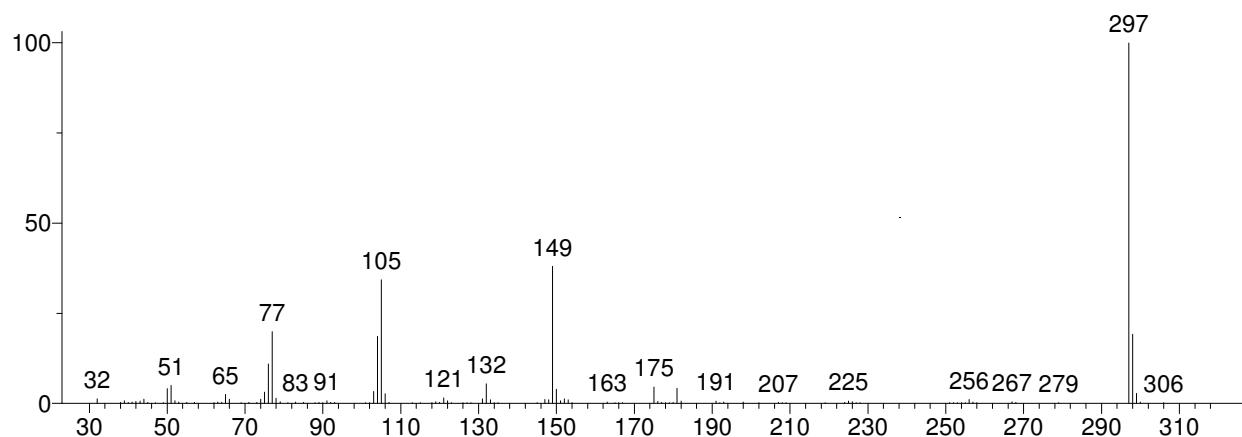


Hit 2 : 1,2-Ethanediol, dibenzoate
 C16H14O4; MF: 829; RMF: 888; Prob 28.8%; CAS: 94-49-5; Lib: mainlib; ID: 60720.

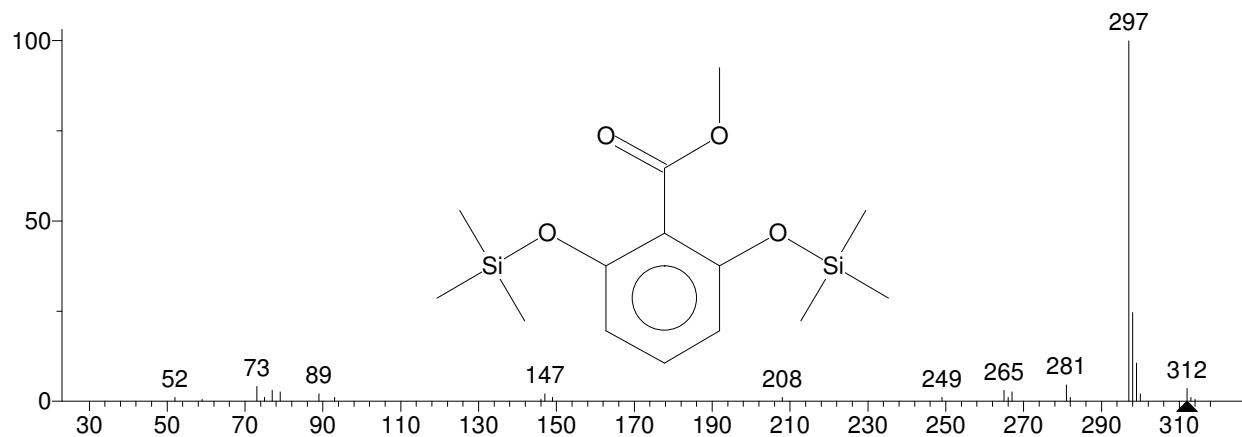


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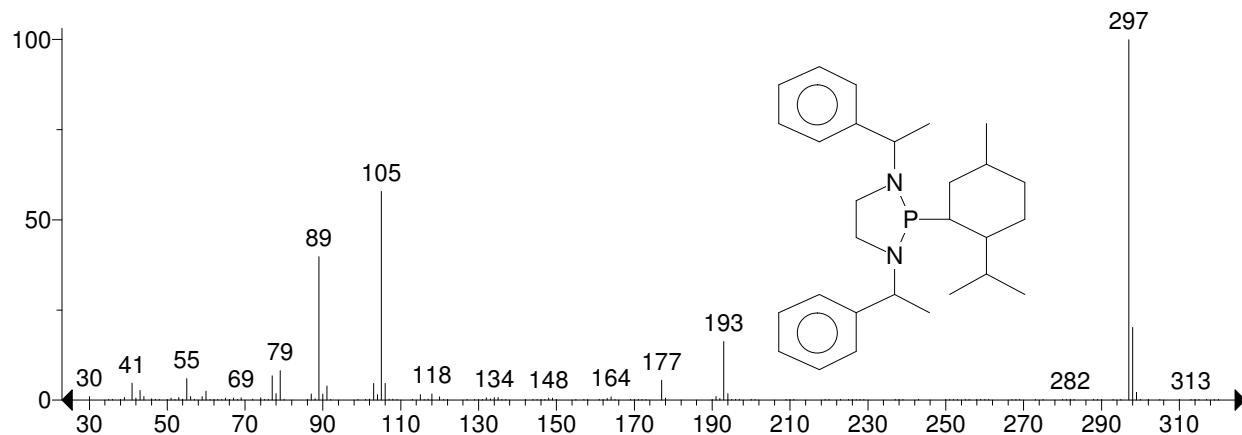
Unknown: Scan 1482 (11.255 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -1302



Hit 1 : Benzoic acid, 2,6-bis(trimethylsiloxy)-, methyl ester
 C₁₄H₂₄O₄Si₂; MF: 625; RMF: 771; Prob 11.4%; CAS: 27798-57-8; Lib: mainlib; ID: 150769.

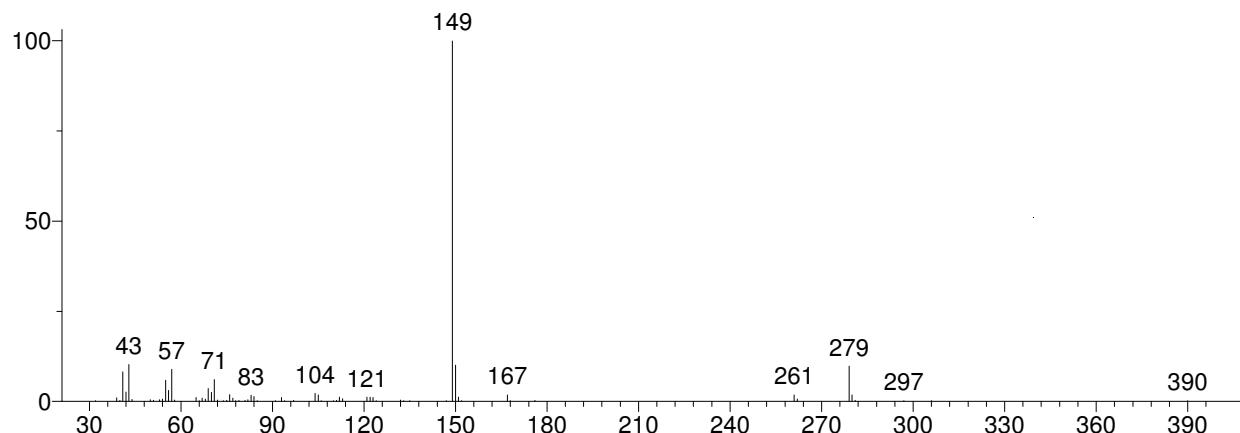


Hit 2 : 1,3,2-Diazaphospholidine, 2-menthyl-1,3-bis(1-phenylethyl)-
 C₂₈H₄₁N₂P; MF: 620; RMF: 658; Prob 9.17%; Lib: mainlib; ID: 150647.

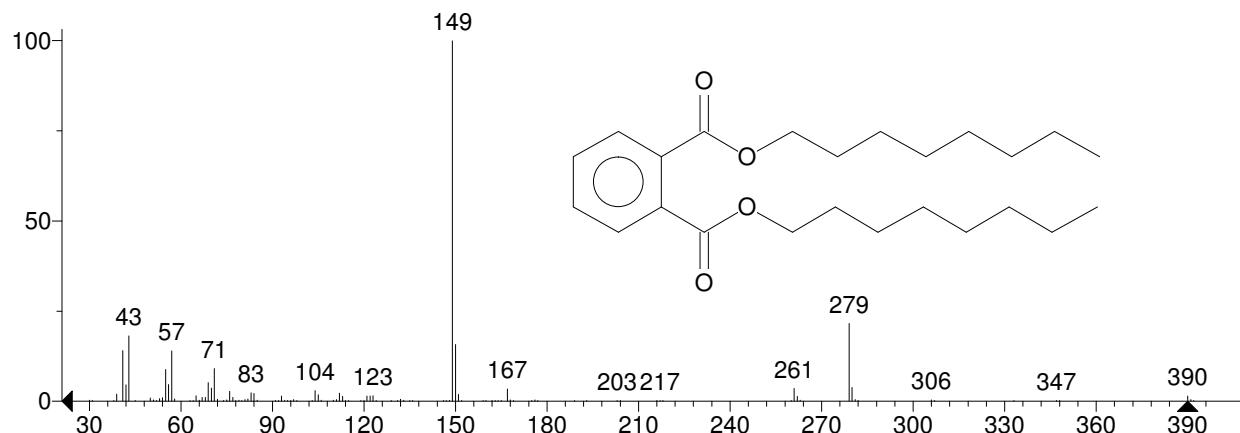


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Unknown: Scan 1551 (11.775 min): PET_DOP_A_py2.D\data.ms
 Compound in Library Factor = -113



Hit 1 : Di-n-octyl phthalate
 C₂₄H₃₈O₄; MF: 916; RMF: 916; Prob 37.3%; CAS: 117-84-0; Lib: replib; ID: 19824.



Hit 2 : 1,2-Benzenedicarboxylic acid, isodecyl octyl ester
 C₂₆H₄₂O₄; MF: 907; RMF: 908; Prob 27.1%; CAS: 1330-96-7; Lib: mainlib; ID: 96124.

