COMPLIANCE EVALUATION INSPECTION REPORT
U.S. ENVIRONMENTAL PROTECTION AGENCY, REGION 5

Purpose: NPDES Compliance Evaluation Inspection

Facility:
Cynamic Chemical Company
1472 Louis Bork Drive
Batavia, Illinois 60510

Date of Inspection: March 19, 2024

EPA Inspectors:
Val Dooling, Environmental Engineer, (312) 886-7167
Sophie Bazan, Physical Scientist, (312) 886-6068

IEPA Representatives:
Ricardo NG, Environmental Protection Engineer
Mohammed Saleem, Environmental Protection Engineer

City of Batavia Representatives:
Zac Bonesz, Superintendent, Wastewater Division

Cynamic Chemical Company Representatives:
Tim Daley, President, Owner
Lisa Johnson, Plant Manager

Report Prepared By:
Val Dooling, Environmental Engineer
EPA Inspector Signature and Date:

VALERIE DOOLING Digitally signed by VALERIE DOOLING Date: 2025.05.06 11:29:49 -05'00'

Approver Name and Title:
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Bahr, Ryan Digitally signed by Bahr, Ryan Date: 2025.05.06 11:49:07 -05'00'

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I. INTRODUCTION

The purpose of the report is to describe, evaluate and document Cynamic Chemical Company ("Cynamic")'s compliance with the Clean Water Act (CWA) and the National Pretreatment Categorical Effluent Guidelines.

II. BACKGROUND

On March 19, 2025, EPA conducted a Clean Water Act Compliance Evaluation Inspection at City of Batavia Wastewater Treatment Plant (WWTP) located at 400 S Shumway Avenue in Batavia, Illinois and at Cynamic Chemical Company ("Cynamic") located at 1472 Louis Bork Drive Batavia, Illinois 60510. Batavia WWTP does not have a federally approved pretreatment program and the State of Illinois is not approved for a pretreatment program, so EPA is the Control Authority and Approval Authority. Cynamic is an industrial user of Batavia, which holds NPDES Permit IL0022543, effective January 9, 2019, and expired December 31, 2023, and was administratively continued. Cynamic did not self-identify as a categorical industrial user that is subject to effluent standards.

III. OPENING CONFERENCE AND DISCUSSION AT BATAVIA WWTP

Inspector Sophie Bazan, Illinois Environmental Protection Agency (IEPA) Inspectors Ricardo NG and Mohammed Saleem and I arrived at Batavia WWTP at 10:15am. I presented my credentials to Zac Bonesz and began the opening conference. I requested whether any information that was discussed was confidential business information and he replied that it was not.

Mr. Bonesz described the current situation with its industrial user, Cynamic, in which the industry must hold all wastewater rather than sending it to the sewer since it is under a cease-and-desist letter from Batavia WWTP. The city has not physically severed the connection between the industry and sewer, but the facility is legally not allowed to discharge anything other than domestic wastewater. Mr. Bonesz stated the company is currently complying.

I asked him to describe what events took place that led to the WWTP upset in February 2025. Mr. Bonesz stated that he had produced a written narrative of events (Appendix C) and also described the following to me:

On Friday, February 21, 2025, WWTP Operators noted a "horrible, chemical-like, petrol-like" smell surrounding the WWTP. The aeration tanks, when operating normally, would have a crisp foam. At this time, operators noted there was no foam on the aeration tanks. The dissolved oxygen (DO) in these tanks had dropped to zero during the previous night. There are emergency blowers that start operating at 2ppm, and these revived the DO for a time, but eventually, the DO was at zero and continued to be at that same level (Appendix D). Samples collected from the nitrification basin indicated that the microbial activity had died and that no internal plant processes were active. Operators noted that all midge flies, leeches and snails that typically live under the roof in the covered final clarifiers had died.

Mr. Bonesz estimated that approximately 10-12 million gallons of untreated effluent went through the plant during the five-day time period from February 21 to 25 or 2.2 million gallons per day. At that time, the effluent was a milky color. Batavia WWTP has a UV disinfection system. During this time period, it was operating at maximum power; however, the ultraviolet transmittance (UVT) was around 4% compared to the typically operating range around 60%. The WWTP was operated to maximize wasting in order to flush out the contaminant that caused the upset. Operators had raised the level of digesters and would maximize centrifuging out. The sludge was not tested at this time.

Once the DO levels indicated that the contaminant has been flushed from the plant, approximately 150,000 gallons of seed was introduced to the WWTP on Tuesday February 25, 2025. The seed slug consisted of return activated sludge (RAS) from a nearby city that had similar profiles of industrial and residential percentages. Eleven days after the initial upset, Batavia WWTP was back online. Prior to this incident, the WWTP had been operating very well with no problem meeting NPDES Permit limits.

Mr. Bonesz told me that he had a portable combustible gas leak detector (Appendix E) at the WWTP which was used periodically to check for gas leaks. At the time of the upset and chemical like smell on February 21, 2025, the gas meter was activated at the highest level, indicating presence of combustible gas. Operators and staff were instructed to open all doors and vents in order to prevent a possible explosion. The WWTP has been under some construction and, as a result, the flows from east (across the Fox River) and from the west had been separated and operators could determine that the flow from the east had presence of the combustible gas whereas the west flow did not. Mr. Bonesz directed a team of public works staff from the WWTP and collection systems to move upstream on the east laterals and check each manhole upstream for the presence of the combustible gas. Appendix F shows a map of the manholes that indicated presence of combustible gas. The last manhole that indicated the presence of combustible gas was at an industrial park and all manholes upstream of that one did not. Mr. Bonesz stated that at that time, the manholes smelled violent, and many of his staff left the search early complaining of headaches. For the health of his staff, he discontinued the search for the source of the odor. Overall, five WWTP staff and seven water department staff, as well as some construction staff were exposed to the odor and many left early with headaches.

Mr. Bonesz continued that search on Tuesday, February 25, 2025. While the WWTP plant was reseeded, the public works staff noticed the same odor at the WWTP that occurred on Friday and therefore began a door-to-door search of the industrial park which discharges to the manhole where the combustible gas meter last was activated. On that day, the manhole was also checked for the same odor and staff noted the same pungent odor downstream of that manhole whereas staff noted no odor upstream.

At Cynamic, just prior to the point where process wastewater is discharged to the Batavia sewer is a triple-basin fats, oils and grease (FOG) and water separator (triple basin). When staff removed the lid of the triple basin, the WWTP staff identified the same pungent odor as had

been in the manholes and at the WWTP. The odor was noted to be stronger at the facility, and the combustible gas meter was activated at the highest level. WWTP staff took a grab sample of the residual wastewater that was sitting in the triple basin (Appendix G), but the facility was not discharging at the time. WWTP staff informed the Cynamic Plant Manager that the contents were potentially explosive and issued a cease-and-desist letter to Cynamic (Appendix H), citing the City of Batavia's sewer use ordinance (SUO) which prohibits discharges to the sewer that cause damage to the WWTP including viscous, flammable, explosive liquids, solids or gases such as gasoline, benzene, naphtha, or fuel oil.

Batavia staff allowed one batch discharge from Cynamic of a week's worth of their wastewater on March 6, 2025, and collected a sample from the discharge at that time which identified 10,900 mg/L of chemical oxygen demand (Appendix I). Batavia reiterated its cease and desist to Cynamic, citing prohibition of unusual chemical oxygen demand in such quantities as to constitute a significant load on the wastewater treatment works in the Batavia SUO. Staff noted that it took approximately four hours for the discharge to leave Cynamic and at that time, they observed a large amount of foam at the WWTP.

I asked Mr. Bonesz to describe the wastewater discharges from other industries neighboring Cynamic who discharge to the same spot as the manhole where the combustible gas meter last was active. He told me that one is a cleaning company that sends out cleaners and does no manufacturing onsite and another is a paperboard company that neutralizes its wastewater, but staff did not notice the distinct odor at either of those companies.

I asked Mr. Bonesz whether there had been previous incidents or past problems from industry at the WWTP. He told me that no survey of Batavia's industrial users had been done, but an industrial user and FOG survey had been planned for in the next year. He told me that operators had noted foaming or black wastewater passthrough the WWTP in the past, but never as bad as this upset.

After this discussion, IEPA and USEPA Inspectors left Batavia WWTP.

IV. OPENING CONFERENCE AND DISCUSSION AT CYNAMIC CHEMICAL COMPANY

Inspector Sophie Bazan, Illinois Environmental Protection Agency (IEPA) Inspectors Ricardo NG and Mohammed Saleem and I arrived at Cynamic Chemical Company at 11:50am. We met with Lisa Johnson, Plant Manager, who instructed us to call Tim Daley, President and Owner of Cynamic, who was not present locally. I was not able to present my credentials, as we spoke with Mr. Daley via phone. I asked him whether any information discussed was Confidential Business Information (CBI). He told me that chemical ingredients are not CBI but the exact percentages of ingredients in their products are CBI, which was beyond the scope of this inspection.

Mr. Daley described the processes at the facility as mixing raw ingredients to produce commercial and industrial cleanup products. The process is strictly mixing raw products and does not involve reactions via heating or cooling. Examples of cleanup products are janitorial

and kitchen dish detergents, rinse aids, floor cleaners or carpet cleaning aids. He told me that there are about 20 employees at the facility and the positions on site are usually two batch makers and a “gopher” on the liquid side and the rest are positions filling bottles and drums and shipping and receiving. The facility operates 6am – 4:30pm for 4 days per week.

I asked how often new products come to market, he told me that many products have not changed in 20 years and that it has been a while since any new products were developed. He told me there are five products that are made the most frequently: alkali dish detergent, rinse agent, laundry detergent, dish detergent and Pull-It-Out. The facility has been in the same location for the past 12 years and at first did not have any mixers. Between 2015 – 2018 mixers were slowly added to the facility and it has been operating in its current setup since 2019. At the time of inspection, there are 10 mixers that surround a wastewater pan which can process up to 500,000 gallons of varying products. A second mixer is located in a separate part of the building and is reserved for one product, labeled Pull it Out, which does not discharge to the wastewater pan.

I asked if there were floor drains in the facility and what the spill protocol is to prevent a slug discharge to the sewer. Mr. Daley told me that he is not aware of any floor drains that go to the sewer. All wastewater goes to the triple catch basin on the south side of the facility. If powder spills, it will be swept up and put in dumpster, if not hazardous. If liquid spills, it would be cleaned up with a floor scrubber and discharged to wastewater pan. I asked for a description of the chemicals that are stored onsite and how the facility purchases chemicals in bulk. Mr. Daley told me that raw materials are purchased based on how fast each is consumed and how quickly it can be replenished, but most things can be delivered in a few days. He told me that they are purchased in 50-pound bags, drums and totes by over 100 different vendors. Mr. Daley stated that there is generally no hazardous waste onsite, and if so, a contractor will remove any drums. I asked for the hazardous waste manifest for the last year, and Mr. Daley did not think that there was one in the last year since he told me that it has only occurred a few times in the last 12 years. He did not think that the laboratory would generate any hazardous waste either, or if so, it would not be a significant amount.

He described the process wastewater as rinse from the sides of mixing tank, the rinse from the filler lines and weekly floor cleaning scrubber. Wastewater is discharged into pans and then it is pumped into the wastetank. Mr. Daley described the pan as a raised 12- by 16-foot platform that holds 700 gallons and the wastetank is 2000-gallon mixer. The laboratory technician will collect a sample, and since the untreated wastewater will often have a high pH, it will be neutralized with acid until it is below 8. The 2000-gallon wastetank is discharged to a 6000-gallon tank. When this second tank is full, it is discharged through a surge tank and then through the triple basin FOG-water separator, then afterwards combined with domestic wastewater and discharged to the sewer. Generally, one batch discharge of 8000-gallons is discharged once a week. The surge tank was implemented because the discharge flow would be too large for the triple basin and would pool on the floor and bottom of valve.

When asked if the laboratory performs any other tests than pH, Mr. Daley told me that the lab will test products for quality control. I asked what happens to products and raw materials that are outside of the desired quality range. Mr. Daley told me that they never have anything out of quality control. If a product doesn't meet standards, then it would be adjusted and reworked into a new batch to meet standards.

Mr. Daley told me that wastewater is not recorded when it is discharged to the city and he does not know, prior to the city's cease and desist order on February 25, when the last discharge of wastewater to the city occurred. Other than pH neutralization, no other tests or samples are collected on the wastewater. Inspector Saleem indicated the results of the sampling at Batavia collected on February 25, 2025 (Appendix G) which identified the presence of various benzene containing organic chemicals and asked whether Mr. Daley was aware what or if any benzene containing products could have been discharged to the sewer. Mr. Daley replied that he did not know what would have been its source. Inspector Saleem then referenced the safety data sheets (SDS) for products "DSC" and "Cynamic Cleaner Degreaser" which list Alkyl dimethyl ethylbenzyl ammonium chlorides, alkyl dimethylbenzylammonium chloride and alkylbenzyldimethylammonium chloride as ingredients and questioned whether potential reactions could occur in the wastewater mixing tank which would result in these benzene containing compounds. Mr. Daley replied that he is not aware of any reactions but stated that there are over 500 chemicals and potentially tens of thousands of things could occur. Mr. Daley expressed that he did not believe that the February 25th sample collected from the triple basin by Batavia staff was representative of Cynamic's discharge because there was no discharge at the time of sample collection, and the basin is designed to separate FOG from water, and he was not sure whether the sample was collected from the oil or water side of the triple basin. I asked whether Cynamic has ever sampled its discharge for FOG, volatile or semi volatile organics, or anything other than pH and Mr. Daley replied that they had not. Mr. Daley told me that Cynamic's currently plan to come into compliance with the City of Batavia SUO is to reduce their wastewater chemical oxygen demand (COD) using enzymes until it reaches a level that is permitted by the SUO.

V. FACILITY SITE VISIT

On March 19, 2025 at 12:45 PM, EPA, IEPA Inspectors and Ms. Johnson began walking around the facility. Mr. Daley remained on the phone with us during our walkthrough of the facility. He informed us that we may not speak with staff other than Ms. Johnson and the laboratory technician. We started in the laboratory where the wastewater samples would be analyzed for pH. Then we walked the location of the ten mixers and wastewater pan (Photo 1). Bulk materials in IBC poly tanks and totes were stored on shelving along the walls, adjacent to the mixers and wastewater pan. Ms. Johnson informed us that this storage area is for the essential raw materials that were most frequently used. I noted totes stacked on the floor labeled as "blue" or "pink". Ms. Johnson told me that these were rinses from the mixers that will be incorporated into the next batch. The color coding is to group like materials into the same rinse. She provided me the documents that describe grouping products that contain floor finish, mineral spirits, disinfectant and sanitizer rinse water policy according to a color code system.

Each policy lists the chemical formulas or product lines that must be captured into the colored totes including rinses from mixing tanks, holding tanks, totes and filling lines and that no rinse water is permitted to flush down the sanitary sewer.

I observed the ten tanks which surround the wastewater pan (Photo 1). I observed some 50-gallon barrels and other pails sitting on top of the wastewater pan and Ms. Johnson explained that everything that was open was actively being used to make product. I asked whether each mixer has a dedicated tank. Mr. Daley told me that none of the main mixing tanks are dedicated, except tank 2, but they are trying to get better about mixing similar types of products back-to-back. Tank 2 is used as the wastewater collection tank. Mr. Daley told me that from the wastewater pan, wastewater is stored in mixer 3 until it is manually released about once a week.

From the mixing tank area, we walked past the filling line and more storage of bulk raw materials to the mixing tank for the Pull-it-out mixer (Photo 2). Near this mixer were stacked IBC totes labeled with the product name and a raised platform with a supersack on top.

We then walked to the triple basin (Photo 3). I observed that the lids were off, and the basins were exposed. There was some liquid sitting in each of the three basins (Photo 4). Mr. Daley told me that the triple basin is scheduled to be cleaned monthly. I did not observe any strong odors at the time of the inspection. Next to the basin was the white tote that Mr. Daley explained was the overflow tank. There was a white pipe and clear tubing which were disconnected. Mr. Daley explained that the white pipe is a vent, and the poly tubing would normally connect to the overflow tank which would then discharge to the triple basin, but both have been disconnected since Batavia issued its cease-and-desist letter. Nearby the triple basin was a floor drain (Photo 5). Mr. Daley explained anything that flowed through the drain would be discharged to the triple basin. Adjacent to the floor drain and triple basin was the storage area for empty mineral spirits totes waiting to be shipped back to the company from where it was purchased (Photo 6). I asked whether these totes were also rinsed before they were stored in this area, and Mr. Daley explained that they were not.

We walked to the manhole where Batavia collected its sample on March 6th (Photo 7) and Mr. Daley explained that this sample was of combined domestic and process wastewater while a discharge of process wastewater was occuring. We also walked to the loading docks. At the bottom of the loading docks was a floor drain (Photo 8). Mr. Daley explained that there was a sump pit with a pump that was operated automatically by float and would also drain to the triple basin.

We then concluded the site walkthrough at 1:20 PM.

VI. CLOSING CONFERENCE

I began a closing conference at 1:21PM. The following are the areas of concern discussed during the closing conference.

1. Prohibition against passthrough or interference

General prohibitions at 40 CFR that that a user may not introduce into a WWTP:

a. any pollutant(s) which cause Passthrough or Interference (40 CFR §403.5(a)(1)); or
b. petroleum oil, nonbiodegradable cutting oil, or products of mineral oil origin in amounts that will cause interference or pass through (40 CFR §403.5(b)(6)).

Batavia WWTP's suffered an upset where the dissolved oxygen in the aerated tank was at zero, the microbial activity in the nitrification basin had died, disinfection rate was insufficient and approximately 10-12 million gallons of untreated effluent went through the plant to the receiving waters.

Sampling taken at Cynamic's triple basin (Appendix G) and at Batavia WWTP (Appendix J) have overlapping presence of semi-volatiles: acetophenone, bis-(2-ethylhexyl) phthalate, diethyl phthalate, di-n-butyl phthalate, napthalene and overlapping absence of other semi-volatiles. Batavia WWTP staff noted the same odor at Cynamic triple basin as at Batavia WWTP and the combustible gas meter was activated at the highest level. Odors and combustible gas meter readings at manholes between Cynamic and Batavia WWTP indicate that the gases had been discharged to the manhole downstream from Cynamic.

Samples collected at Cynamic's triple basin indicates presence of substances prohibited by the City of Batavia's sewer use ordinance which prohibits discharges that contain:

(a) gasoline, benzene, naptha, fuel oil or other flammable or explosive liquid, solid or gas from being discharged to any sanitary sewer. It also prohibits
(b) wastes containing a toxic, radioactive or poisonous substance in sufficient quantity to injure or interfere with any sewage treatment process, constitute a hazard to humans or animals or create any hazard in the receiving waters of the sewage treatment plant.
(c) unusual chemical oxygen demand or chlorine requirements in such quantities as to constitute a significant load on the wastewater treatment works
(d) unusual volume or flow or concentration of wastes constituting slugs.
(e) waters or wastes containing substances which are not amenable to treatment or reduction by the wastewater treatment processes employed or are amenable to treatment only to such degree that the wastewater treatment plant effluent cannot meet the requirements of agencies having jurisdiction over discharge to the receiving waters.

2. Prohibition against discharge of toxic gases, vapor or fumes

Specific prohibitions listed at 40 CFR §403.5(b)(7) state that pollutants shall not be introduced into a WWTP which result in the presence of toxic gases, vapors, or fumes within the WWTP in a quantity that may cause acute worker health and safety problems.

Using EPA's Screening Technique to Identify Gas/Vapor Toxic Discharges, vapor concentrations collected February 25, 2025 by grab sample from Cynamic's triple basin exceeded screening levels of Napthalene, di-n-butyl phthalate, chloroform and xylenes (Appendix K). The screening technique references ACGIH threshold limit value-time weighted averages (TLV-TWA) which are the gas/vapor toxicity levels that workers may be repeatedly exposed, over a 8-hour workday and a 8-hour workweek without adverse effect. Discharges above the screening levels may warrant further investigation.

City of Batavia wastewater treatment employees reported insect and invertebrate die off events in enclosed space of final clarifier at the time of incident, possibly due to toxic vapors in the wastewater.

City of Batavia wastewater treatment employees reported negative health impacts, such as headaches, while performing their jobs both at the wastewater treatment facility and while servicing manholes in the collection system.

3. Prohibition against discharge of fire or explosion hazards

Specific prohibitions at 40 CFR §403.5(b)(1) states that pollutants shall not be introduced into a WWTP which create a fire or explosion hazard in the WWTP, including, but not limited to, wastestreams with a closed cup flashpoint of less than 140 degrees Fahrenheit or 60 degrees Centigrade using the test methods specified in 40 CFR §261.21.

Characteristic of ignitability at 40 CFR §261.21(a)(1) states that a solid waste exhibits the characteristic of ignitability if a representative sample of the waste is a liquid that has a flash point less than 60 °C (140 °F).

Five of the pollutants that were identified present at Cynamic's triple basin had flashpoints less than 60 °C (140 °F).

Pollutant	Concentration	Flashpoint
2-Chlorotoluene	3.75 mg/L	96°F
Acetone	3.27 mg/L	0°F
Ethylbenzene	0.195 mg/L	59°F
Xylene	0.385	85°F
Toluene	0.121	40°F

Using EPA's Screening Technique to Identify Flammable/Explosive Discharges, vapor concentrations collected February 25, 2025 by grab sample from Cynamic's triple basin approached screening levels for napthalene (Appendix L). The screening technique references 10% of the lower explosive limit (LEL). Discharges that exceed screening levels may warrant further investigation.

A gas detector identified presence of combustible gases at Cynamic's triple basin and in the manholes leading from Batavia water treatment facility directly to the manhole closest to Cynamic's discharge point. The gas detector identifies the presence of the vapor form of napthalene, phthalates, toluene, acetone, xylenes and benzene, among other gases at levels above 10ppm.

I concluded the inspection at 1:30 PM and EPA and IEPA Inspectors left the facility.

Appendix A: Inspection Photo Log

Cynamic Chemical Company
EPA Inspection: March 19, 2025
All photos taken by Sophie Bazan, Physical Scientist, U.S. EPA
Camera: Canon PowerShot SX230 HS

Note: All timestamps are one hour earlier than photos were taken.

1: IMG_0254
Description: Ten mixers, each of varying sizes surrounding the wastewater pan. Mixers have a valve with hose connection centered above the wastewater pan. The wastewater pan is the raised silver platform. Two drums are located on a pallet sitting atop the wastewater pan. Another drum and several pails are also sitting atop the wastewater pan. At least one drum is open and several hoses are attached to the open drum.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 12:57 AM

2: IMG_0255
Description: One mixer labeled “#25” is in center of frame. A valve attached to a hose is on the lower section of the mixer. To the left are six stacked IBC totes labeled as “Pull It Out”. To the right is a platform. A dry mixer is located below the platform in the process of filling several fiber drums. On top of the platform off the edge is a supersack. On the floor is a noticable white powder residue.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:01 PM

3: IMG_0256
Description: The triple basin FOG/water separator is located underneath a shelving system. Three open holes are against the wall and lids are propped up to the right of the holes. A white pipe is installed in three points into the ground adjacent to the triple basin and brown flexible tubing is located next to the pipe. Both the white pipe and brown tubing have open connections. A white tank used as a surge tank is located to the left of the triple basin.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:05 PM

4: IMG_0257
Description: A closer view of the open holes of the triple basin. Two open holes and the white pipe are visible. A liquid is visible in each of the open holes.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:05 PM

5: IMG_0258
Description: A floor drain is visible in foreground and the triple basin and surge tank are visible in the background. The shelving unit is visible with wrapped supplies stored above and to the right of the triple basin.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:06 PM

6: IMG_0259
Description: Totes of empty chemicals are stored three high to be picked up by the transport company. At front are several totes that are labeled “Mineral Oil”. The location of this photo is adjacent to the floor drain and triple basin from Photo 5.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:07 PM

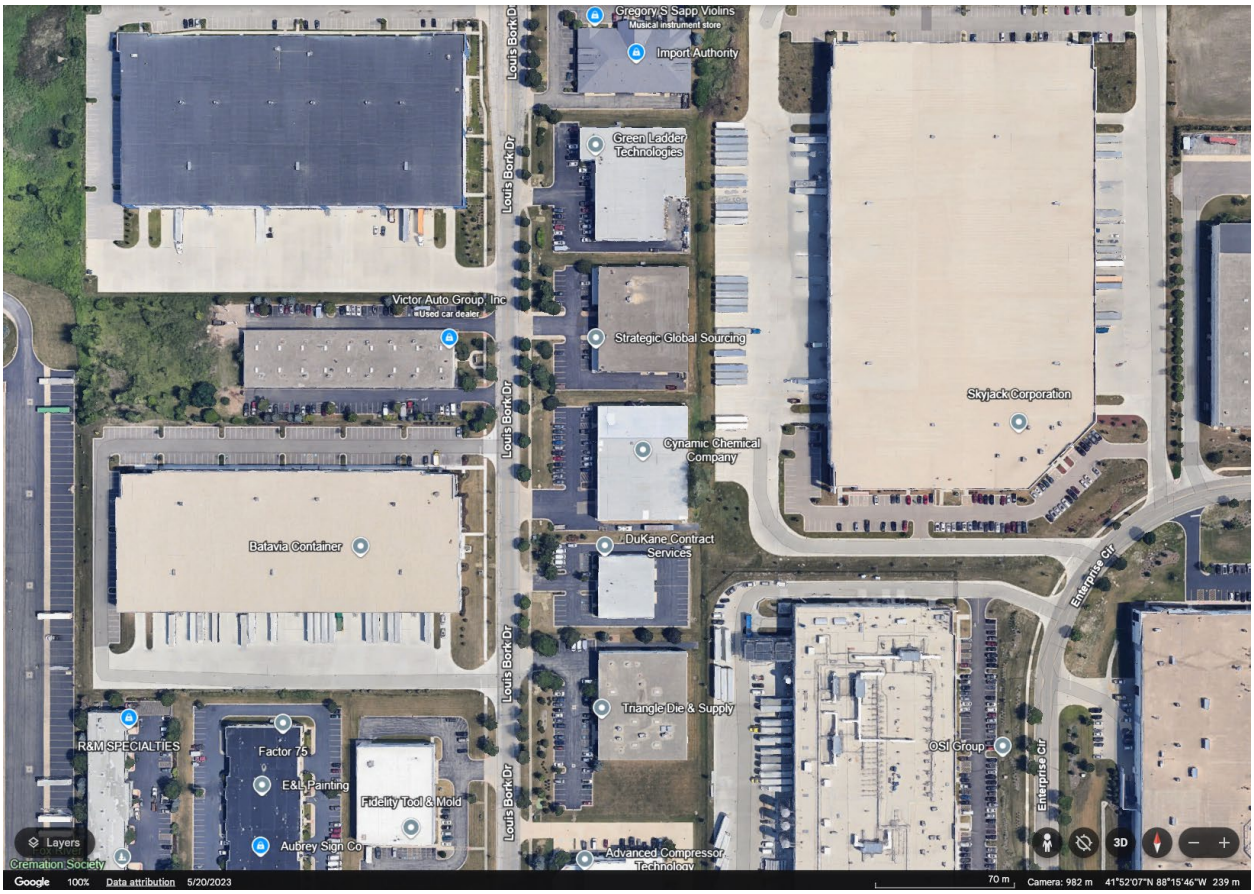
7: IMG_0260
Description: Manhole outside of Cynamic building where WWTP staff collected a sample of Cynamic's wastewater discharge consisting of combined process and domestic wastewaters on March 6, 2025.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:08 PM

8

8: IMG_0261
Description: Floor drain on center of two loading docks. The dock appears to be sloped to allow liquids to flow towards drain. A truck is parked at one of the docks. The ground under the truck and surrounding most of the drain is a darker color indicating presence of a liquid.
Location: Cynamic Chemical Company
Date/Time: March 19, 2025 1:19 PM

Appendix B: Aerial image of Cynamic Chemical Company

Cynamic Chemical Company and neighboring businesses have been identified according to Google Business.



Note: Aerial images obtained from Google Earth. Images do not represent conditions observed and are only to be used as reference.

Appendix C: Batavia WWTP memo

CITY OF BATAVIA
PUBLIC WORKS

City of Batavia- IL 0022543
400 S. Shumway Ave.
Batavia Il, 60510

To whom it may concern,

This narrative is to describe the bypass event that occurred during the period of 2/20/25-2/25/25 and the investigation that followed.

Upon arrival to the plant on Friday 2/21/25 Batavia's wastewater treatment plant operators noted a distinct chemical smell coming from the aeration basins. Inspection of SCADA monitoring trends indicated that dissolved oxygen (DO) levels had dropped to 1.2ppm around 7pm the previous night. Normal DO levels during that time range from 6 ppm to 9 ppm. When the lab technician arrived, they obtained samples from our Nitrification basin which showed no microbial activity. I (Zac Bonesz) notified the EPA shortly after with a Bypass notification form.

Vapors that were present were strong enough to alarm a combustible gas detector, so crews were advised to stay away from any structures that were enclosed and contained water. Wasting was dramatically increased to begin removal of dead biomass and prepare for reseeding efforts.

DO levels were monitored throughout the weekend with the DO remaining near 1ppm until it began to spike on 2/23/25 at approximately 2am, indicating that the chemical had left the plant. Wasting of the dead biomass continued until the plant was able to be reseeded.

Seed sludge was obtained from St. Charles WWTP on 2/25/25. Approximately 144,000 gallons of waste activated sludge from the St. Charles plant was to be delivered to the aeration basins at Batavia's WWTP using a total of 27 semi-tanker trucks.

At approximately 1:30 on Tuesday 2/25/25, during an ongoing search for an illicit discharge that caused an upset at the WWTP, I (Zac Bonesz) was contacted by Dan Gillespie from Trotter and Associates, Inc., Batavia's wastewater engineering consultant. Dan notified me about a suspected industry located upstream of the Hubbard lift station, Cynamic Chemical Company. Upon arrival, Dan and I opened Cynamic's exterior inspection manhole and recognized the distinct odor emanating from the manhole that was the same odor I smelled at the plant on 2/21/2025. I entered Cynamic's lobby and asked for the plant manager. I was directed to speak to Lisa (no last name given). During our conversation I explained the upset at the plant and asked if she would allow us to inspect the facility to determine if they were the cause of the upset. She agreed. During the inspection of the facility, which manufactures a variety of chemical agents, we discovered a large (approximately 350 gallon) tank connected to a triple trap basin. Opening the cover of the basin, we were overwhelmed by the same strong acrid odor that matched the smell in the manhole and the smell at the plant. It was immediately clear that this was the source of the discharge. (see photo, Triple 1.jpg)

We asked the plant manager if we could take samples to confirm or deny that this was the source of the upset at the treatment plant and she agreed. A combustible gas detector was used to further identify the substance. The detector immediately went to high alarm level when it was waved near the chemical tank. The plant manager was advised to stop draining the tank to the sewer system and that the contents were highly explosive.

Samples from the plant collected on 2/22/25, and samples collected from the triple tap basin, were sent off to Suburban Labs in Geneva Il for analysis.

While awaiting results, Cynamic provided us with batch tickets from their production runs from February 19th-24th. Numerous chemical violations of the city's Sewer Use Ordinance (SUO) were indicated on the batch tickets. The ticket on the 2/20 was particularly note-worthy, as the chemical listing showed 3,100 lbs of mineral spirits being used in the process. Benzene, along with other aromatic hydrocarbons (see photo Benzene Breakdown Chart.pdf), is a component of mineral spirits. This, along with the batch tickets description of appearance as an "opaque liquid", are consistent with the substance that appeared in our plant effluent.

The results from the Suburban Labs testing showed a strong correlation between the substance found in Cynamic's triple basin and our plant effluent, with the primary component being Benzene, which is explicitly prohibited in our SUO. Other hydrocarbon derivatives found in the samples indicated that the substance found at Cynamic was the chemical that caused the plant upset.

Cynamic was allowed to discharge 6,000 gallons of chemical on 3/6. Initial testing has shown this to contain a level of 343 ppm of phosphorous (see below). Approximately four hours after the chemical left their facility, which is the approximate time it takes for a sewer discharge from Cynamic to reach the plant, a large amount of foam began to develop at Batavia's WWTP (see photo, Foam6.jpg, Foam5.jpg, Foam11 -Day after effluent.jpg)

Strength of Concentration

Lbs = Concentration (ppm)x Flow(MGD)x 8.34 (weight of water)

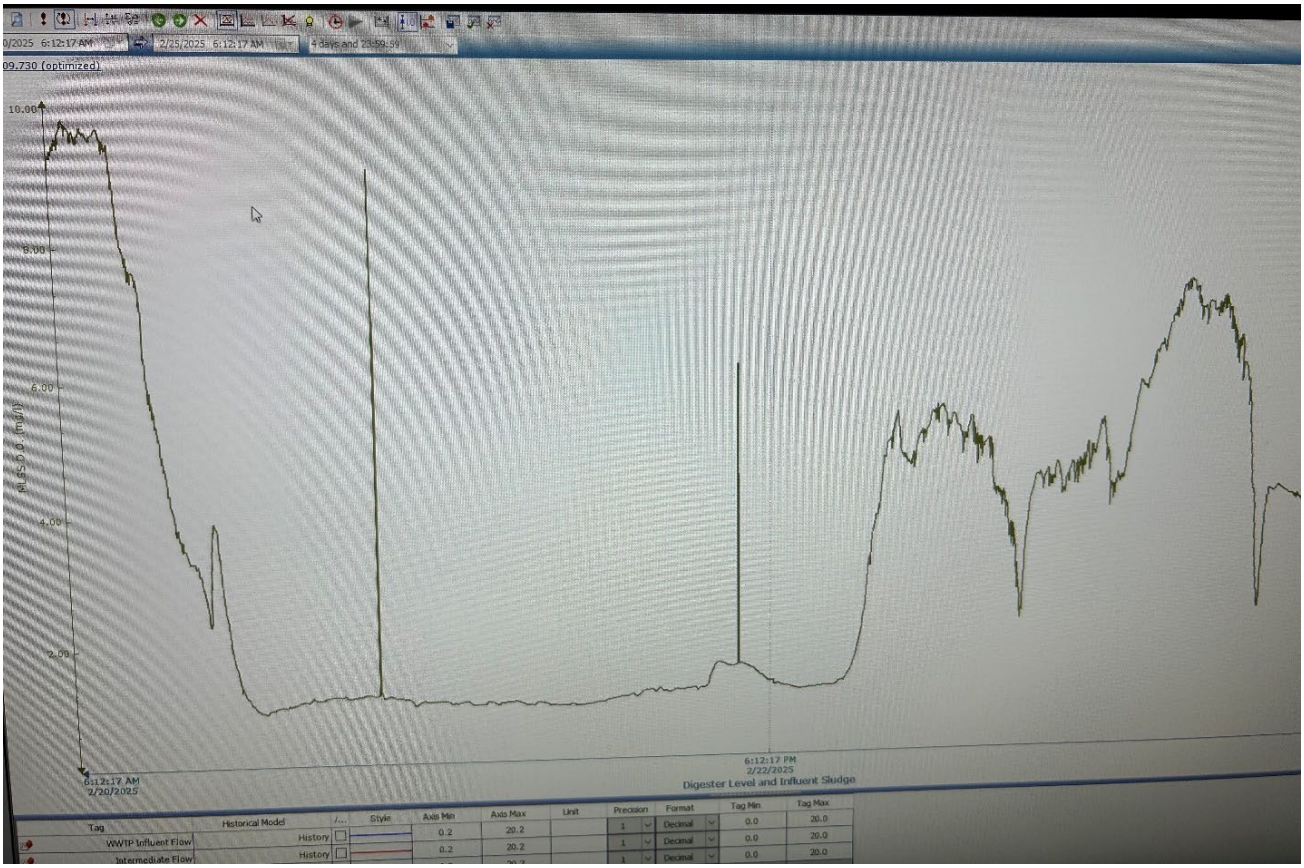
Cynamic

343 x 0.006 (six thousand gallons) x 8.34 = 17.16lbs

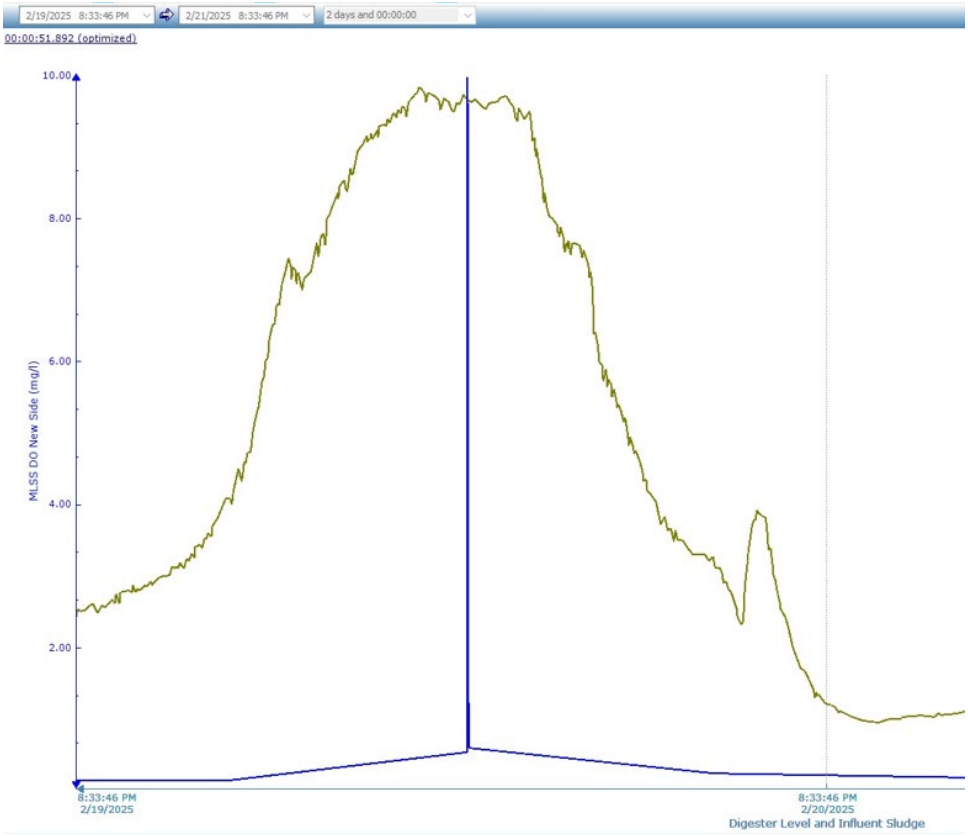
Plant Daily loading (ranges between 3-5ppm)

5 x 2.2 MGD (daily average flow) x 8.34 = 91 lbs (high average)

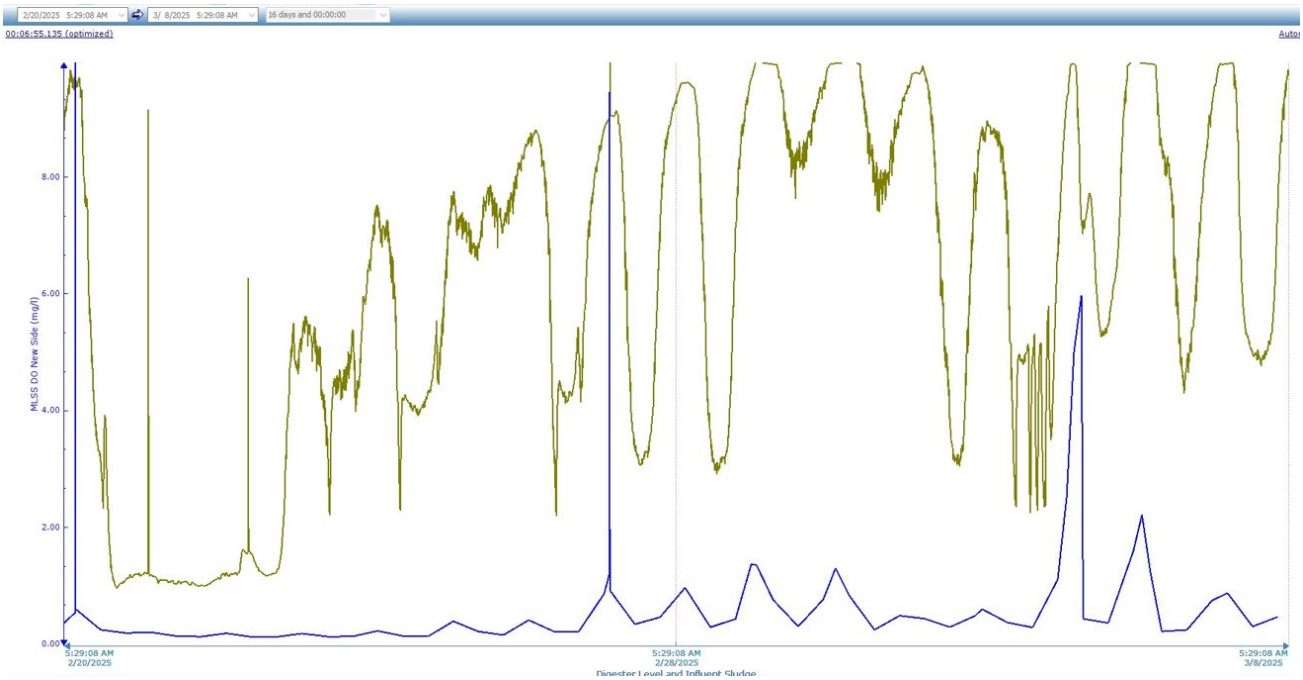
Appendix D: Dissolved Oxygen in Batavia WWTP Activated Sludge



Screenshot of Dissolved Oxygen in Digester Level and Influent Sludge at Batavia WWTP from February 20, 2025 at 6:00 am through February 22 at 6:00 PM as a midway point. The graph indicates a drop in DO after 6am on February 20, 2025 and beginning recovery after February 22, 2025.



Screenshot of Dissolved Oxygen in Digester Level and Influent Sludge at Batavia WWTP from February 19 at 8:30 PM to February 20, 2025 at 8:30 PM indicating a drop in DO after 6am on February 20, 2025. A smaller peak on the downward slope indicates when the backup blower was activated at DO of 2.0.



Screenshot of Dissolved Oxygen in Digester Level and Influent Sludge at Batavia WWTP from February 20 at 5:30 AM to March 8, 2025 at 5:30 AM with a midpoint at February 28, 2025 at 5:30 AM.

Appendix E: Gas detector used by WWTP staff with information on detection and sensitivity

GAS-Mate®

COMBUSTIBLE GAS LEAK DETECTOR

Safely detect combustible gas and flammable refrigerant leaks.

GAS-Mate is an intrinsically safe combustible gas leak detector that can safely and reliably detect leaks of combustible gases, flammable refrigerants, and hydrogen forming gas. It is a versatile tool for use in heating, air conditioning, refrigeration, and automotive applications. You can leak check with confidence knowing GAS-Mate is backed by an industry-best three-year warranty.

3 YEAR WARRANTY

MET HAZARDOUS LOCATION SAFETY

A3 CERTIFIED

CE UK CA 2xD

WATCH OUR VIDEO!

MADE IN USA

SPECIFICATIONS

Includes	GAS-Mate Combustible gas sensor Two D-size alkaline batteries Carrying case
Compatible refrigerants	Propane (R290), Isobutane (R600a), R441a, hydrogen forming gas (95/5), natural gas, methane, ammonia, and more
Sensitivity	5 ppm for methane, propane (R290), Isobutane (R600a), and hydrogen 1 ppm for gasoline
Power source	Two D-size alkaline batteries (use Duracell® MN1300 to maintain intrinsically safe approval)
Battery life	25 hours
Weight	1.54 lb. (700 g)
Certifications	Intrinsically safe for Class I, Division 1, Groups A - D, T4 and II 3G Ex nA nL IIC T4 X as per MET Laboratories Listing #E112145 CE, UKCA
Probe length	15 in. (38 cm)
Warranty	Three-year over-the-counter

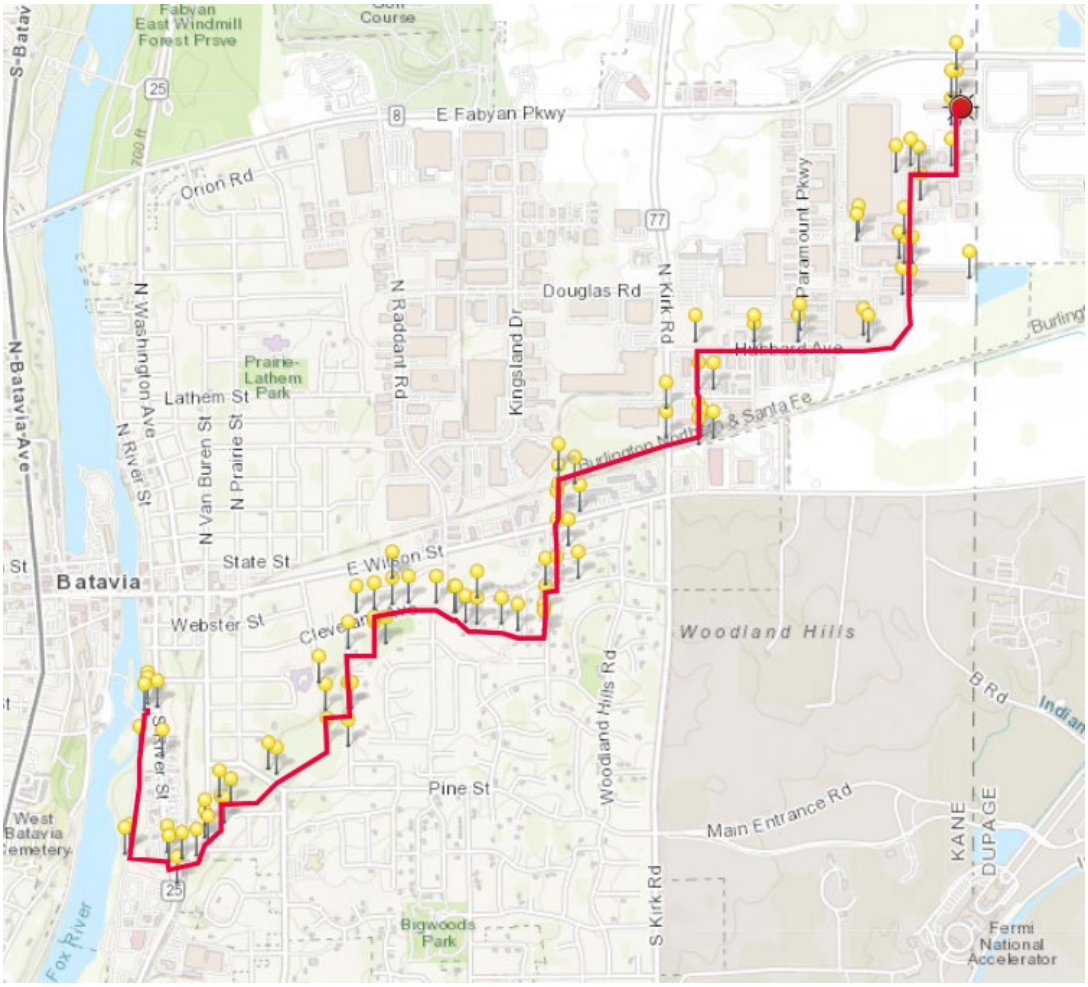
ORDERING INFORMATION

GAS-Mate	718-202-G1
Accessories and Replacement Parts	
Sensor	706-700-G1
Carrying case	718-701-G1

ADVANTAGES

- Detects natural gas, propane, isobutane, ammonia, hydrogen forming gas (95/5), and more
- Ultimate sensitivity of 5 ppm for methane, R290 (propane), and R600a (isobutane)
- Intrinsically safe for use in combustive/explosive environments
- Great for flammable refrigerants like R290, R600a, and R441a
- Runs on two D-cell batteries

Appendix F: Manholes tested in search with tracer line indicating positive reading from gas detector and close up of manholes on Louis Bork Drive.



Appendix G: Semivolatile, Volatile and Total Organic Carbon results from Cynamic from February 25, 2025

Analyte	Result /Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Semivolatile Organics									
Unknonw Ar, RT 5.660	27.6	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Ar, RT 4.932	19.7	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Ar, RT 5.461	53.6	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Ar, RT 5.537	21.7	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Ar, RT 5.847	17.5	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown AR, RT 5.893*	18.6	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Ar, RT 6.006	44.9	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 4.628	47.4	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 4.733	29.5	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 4.796	19.8	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 4.889	26.7	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.034	25.9	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.134	90.3	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.199	39.5	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.247	103	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.409	151	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.495	82.5	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.603	58.1	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.623	46.8	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010
Unknown Non Ar, RT 5.796	21.3	3.00	3.00	ug/L	02/25/25 14:00	03/04/25	1	625/625.1	BB02010

Analyte	Result /Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Semivolatile Organics - Prep EPA 625									
1,2-Dihydro-2,2,4-trimethylquinoline	ND	40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,3,4-Trimethylquinoline	ND	20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,4,6-Trichlorophenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,4,6-Trimethylquinoline	ND	20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,4-Dichlorophenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,4-Dimethylphenol	ND	200	200	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,4-Dimethylquinoline	ND	20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,4-Dinitrophenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,6-Dimethylquinoline	ND	20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2,6-Di-tert-butyl-4-methoxyphenol	ND S,	300	300	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2-Chlorophenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2-Methylnaphthalene	6040	40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2-Nitrophenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
2-Phenyl-2-propanol	ND	60.0	60.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
3,3-Dichlorobenzidine	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
4,6-Dinitro-2-methylphenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
4-Chloro-3-methylphenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
4-Nitrophenol	ND	100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
4-tert-Butylphenol	720	200	200	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Acenaphthene	ND	40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010

Analyte	Result	/Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Semivolatile Organics - Prep EPA 625 (Continued)										
Acenaphthylene	ND		40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Acetophenone	132000		60.0	60.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Anthracene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Benzo(a)anthracene	ND		40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Benzo(a)pyrene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Benzo(b)fluoranthene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Benzo(g,h,i)perylene	ND		60.0	60.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Benzo(k)fluoranthene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Benzothiazole	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
bis(2-Ethylhexyl)adipate	7280		50.0	50.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Bis(2-ethylhexyl)phthalate	1080		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Bisphenol-A	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Butyl benzyl phthalate	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Caprolactam	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Chrysene	ND		30.0	30.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Dibenzo(a,h)anthracene	ND		40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Diethyl phthalate	2520		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Dimethyl phthalate	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Di-n-butyl phthalate	514000		10000	10000	ug/L	02/25/25 14:00	03/04/25	5000	625/625.1	BB02010
Di-n-octyl phthalate	ND		110	110	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Fluoranthene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Fluorene	ND		40.0	40.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Indeno(1,2,3-cd)pyrene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Isophorone	ND		50.0	50.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
m,p-Cresol	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Naphthalene	207000		500	500	ug/L	02/25/25 14:00	03/04/25	1000	625/625.1	BB02010
N-Nitroso-di-n-butylamine	ND		70.0	70.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
N-Nitroso-di-n-propylamine	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
N-Nitrosodiphenylamine	ND		30.0	30.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
O-Cresol	ND		100	100	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Pentachlorophenol	ND		50.0	50.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Phenanthrene	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Phenol	ND		50.0	50.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Phenyl Sulfone	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Pyrene	ND		60.0	60.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Quinoline	ND		20.0	20.0	ug/L	02/25/25 14:00	03/03/25	100	625/625.1	BB02010
Surrogate: 2,4,6-Tribromophenol	*0%*	S,	*10-136*				*03/03/25*	*100*	*625/625.1*	
Surrogate: 2-Fluorobiphenyl	*72.00%*	S	*20-129*				*03/03/25*	*100*	*625/625.1*	
Surrogate: 2-Fluorophenol	*68.00%*	S	*10-106*				*03/03/25*	*100*	*625/625.1*	
Surrogate: 4-Terphenyl-d14	*0%*	S,	*18-160*				*03/03/25*	*100*	*625/625.1*	
Surrogate: Nitrobenzene-d5	*264.00%*	S	*13-150*				*03/03/25*	*100*	*625/625.1*	
Surrogate: Phenol-d5	*110.00%*	S	*10-105*				*03/03/25*	*100*	*625/625.1*	

Analyte	Result /Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Volatile Organics									
Ethyl Dimethyl Benzene Isomer, RT:10.057	16700	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Ethyl Dimethyl Benzene Isomer, RT:10.079	16300	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Ethyl Dimethyl Benzene Isomer, RT:10.152	39200	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Methyl Indan Isomer, RT:10.835	11200	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Methyl Indan Isomer, RT:11.022	15100	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Methyl Propyl Toluene Isomer, RT:9.703	11400	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Tetramethyl Benzene Isomer, RT:10.575	18600	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Tetramethyl Benzene Isomer, RT:10.631	26600	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Unknown, NoAr, HC, RT:8.158	71600	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Unknown, NoAr, HC, RT:8.587	15300	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887

Analyte	Result /Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Volatile Organics (Continued)									
Unknown, NoAr, HC, RT:8.872	10400	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Unknown, NoAr, HC, RT:8.938	65300	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887
Unknown, NoAr, HC, RT:9.630	53800	1000	1000	ug/L	02/25/25 14:00	02/28/25	1000	*** DEFAULT SPECIFIC METHOD ***	BB01887

Analyte	Result	/Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Volatile Organics										
1,1,1-Trichloroethane	ND	S,	0.0159	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,1,2,2-Tetrachloroethane	ND		0.0355	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,1,2-Trichloroethane	ND		0.0224	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,1-Dichloroethane	ND		0.0527	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,1-Dichloroethene	ND		0.0311	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,2,4-Trimethylbenzene	16.2		0.409	1.00	mg/L	02/25/25 14:00	02/26/25	1000	8260B	BB01887
1,2-Dichloroethane	ND		0.0185	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,2-Dichloropropane	ND		0.0210	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
1,3,5-Trimethylbenzene	2.21		0.0360	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
2-Butanone	ND		0.361	1.00	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
2-Chlorotoluene	0.738		0.0289	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
2-Hexanone	ND		0.493	2.50	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
4-Isopropyltoluene	3.75		0.0441	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
4-Methyl-2-pentanone	ND		0.213	2.50	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Acetone	3.27		0.668	2.50	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Benzene	ND		0.00850	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Bromoform	ND		0.0746	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Bromomethane	ND	S,	0.0862	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Carbon disulfide	ND		0.0674	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Carbon tetrachloride	ND		0.0393	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Chlorobenzene	ND		0.0146	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Chloroethane	ND		0.0950	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Chloroform	2.56		0.0161	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Chloromethane	ND		0.0428	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
cis-1,2-Dichloroethene	ND		0.0241	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
cis-1,3-dichloropropene	ND		0.0343	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Dibromochloromethane	ND		0.0237	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Ethylbenzene	0.105		0.0160	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
m,p-Xylene	0.385		0.0513	0.200	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Methyl acrylonitrile	0.909		0.0842	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Methyl tert-butyl ether	ND		0.0434	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Methylene chloride	ND		0.0620	0.500	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
n-Butylbenzene	45.4		0.573	1.00	mg/L	02/25/25 14:00	02/26/25	1000	8260B	BB01887
n-Propylbenzene	0.504		0.0277	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Naphthalene	5.91	S	0.147	0.200	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
o-Xylene	0.191		0.0227	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
sec-Butylbenzene	1.99		0.0308	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Styrene	ND		0.0310	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Tetrachloroethene	ND		0.0849	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Toluene	0.121		0.0220	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
trans-1,2-Dichloroethene	ND		0.0183	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
trans-1,3-dichloropropene	ND		0.0582	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Trichloroethene	ND		0.0246	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Vinyl chloride	ND		0.0346	0.100	mg/L	02/25/25 14:00	02/26/25	100	8260B	BB01887
Surrogate: 4-Bromofluorobenzene		*114%*		*76-119*			*02/26/25*	*100*	*8260B*	

Analyte	Result	/Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Volatile Organics (Continued)										
Surrogate: Dibromofluoromethane		*101%*		*66-137*			*02/26/25*	*100*	*8260B*	
Surrogate: Toluene-d8		*108%*		*80-120*			*02/26/25*	*100*	*8260B*	

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Unknown
HC, NoAr MW≥156

Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

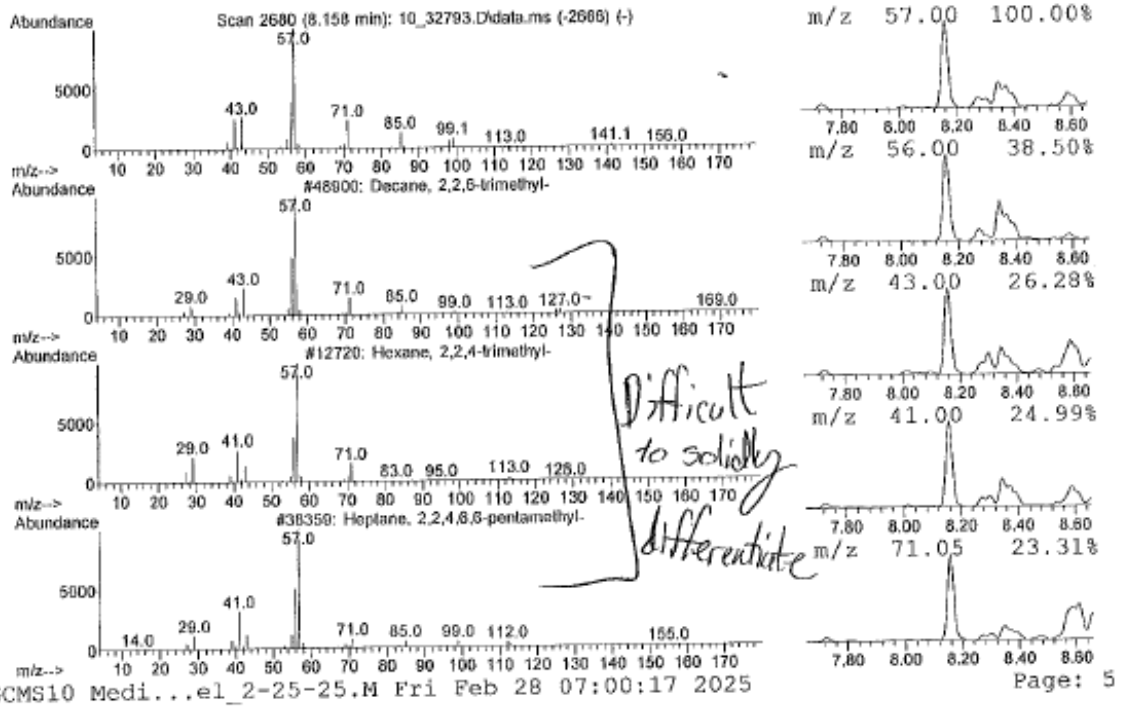
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 1 Decane, 2,2,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	71.62 ug/L	4330030	CHLOROBENZENE-d5	7.201

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	64
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
3	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
4	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
5	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64



Difficult to solidly differentiate

** Substructure Report Page 1 **

Search Pattern: Scan 2680 (8.158 min): 10_32793.D\data.ms (-2694)

Structures present:

Number	Probability	Short Name And Description
1	99	RDB0, rings + double bonds count = 0
2	99	-CH2/3-1, exactly one methylene or methyl group (chain)
3	99	HCSAT, saturated hydrocarbon
4	99	-CH2-, methylene group (chain)
5	99	-CH2/3-, methylene or methyl group (chain)
6	99	CCH3, methyl bonded to carbon
7	99	sat, saturated compound (no unsaturated bonds)
8	99	CH3, methyl
9	99	HC, hydrocarbon (C and H atoms only)
10	99	CH2/3, primary or secondary saturated carbon
11	99	nocycle, no rings
12	99	C3+-alkyl, methylene attached to saturated C-atoms (chain)
13	99	NoAr, no aromatic rings
14	98	CH2, methylene group
15	98	C2H5/CH2CH2, primary or secondary ethyl linkage
16	98	CH2-CH2/3, ethyl or dimethylene group (chain)
17	93	CH-alk, tertiary carbon attached to alkyl
18	90	Ctert, tertiary carbon (>CH-)
19	88	Ctert-chain, tertiary carbon (>CH-), chain
20	88	CH-alk-chain, carbon attached to alkyl (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	N-C, nitrogen-carbon single bond
4	99	ph, phenyl group (C6H5)
5	99	ArOR, alkyl-aryl ether
6	99	cond, condensed ring structure (1,2-overlap)
7	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
8	99	Ar-O, aromatic ring-oxygen atom bond (chain)
9	99	.N., any nitrogen atom in ring
10	99	noAr_cy, rings present, but not aromatic

MW(Nominal Mass)Information:

Number	MW	Probability
1	156	73
2	170	14
3	184	1
4	171	1

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Unknown NoAr, HC

MW ≥198

Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

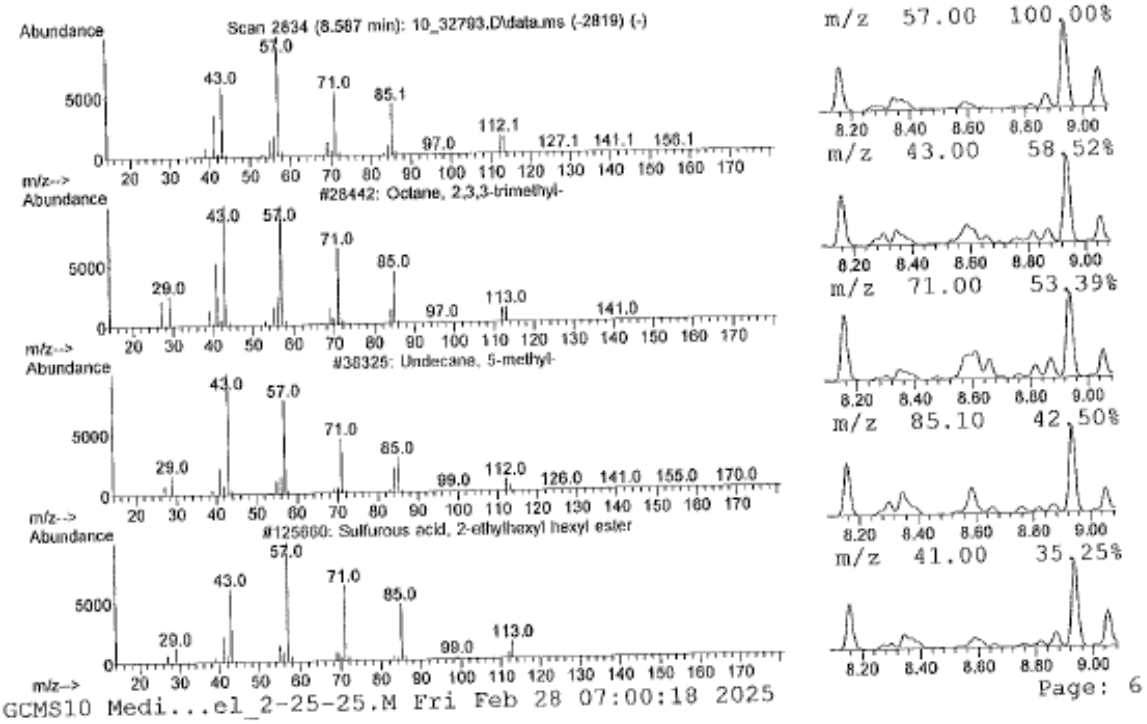
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 2 Octane, 2,3,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.587	15.26 ug/L	1888030	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	90
2	Undecane, 5-methyl-	170	C12H26	001632-70-8	78
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	78
4	Heneicosane	296	C21H44	000629-94-7	72
5	Tetradecane	198	C14H30	000629-59-4	64



GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:00:18 2025

** Substructure Report Page 1 **

Search Pattern: Scan 2834 (8.587 min): 10_32793.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	97	RDB0, rings + double bonds count = 0
2	96	HCSAT, saturated hydrocarbon
3	96	nocycle, no rings
4	96	CH2/3, primary or secondary saturated carbon
5	95	-CH2-, methylene group (chain)
6	95	-CH2/3-, methylene or methyl group (chain)
7	95	-CH2/3-1, exactly one methylene or methyl group (chain)
8	95	CH2, methylene group
9	95	CH3, methyl
10	95	CCH3, methyl bonded to carbon
11	95	C2H5/CH2CH2, primary or secondary ethyl linkage
12	94	sat, saturated compound (no unsaturated bonds)
13	94	HC, hydrocarbon (C and H atoms only)
14	94	CH2-CH2/3, ethyl or dimethylene group (chain)
15	94	NoAr, no aromatic rings
16	93	C3+-alkyl, methylene attached to saturated C-atoms (chain)
17	92	(CH2)3-ch, trimethylene linkage
18	91	CH2-CH2-CH2/3, trimethylene group (chain)
19	89	CH-alk, tertiary carbon attached to alkyl
20	86	Ctert, tertiary carbon (>CH-)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
4	99	ArOR, alkyl-aryl ether
5	99	O1, contains 1 oxygen atom
6	99	PhCO, phenyl carbonyl
7	99	PhCsat, phenyl attached to saturated carbon atom
8	99	O, contains oxygen
9	99	RDB1, rings + double bonds count = 1
10	99	N, contains nitrogen

MW(Nominal Mass)Information:

Number	MW	Probability
1	198	27
2	170	24
3	184	21
4	156	11

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Unknown
NoAr, HC MW≥170

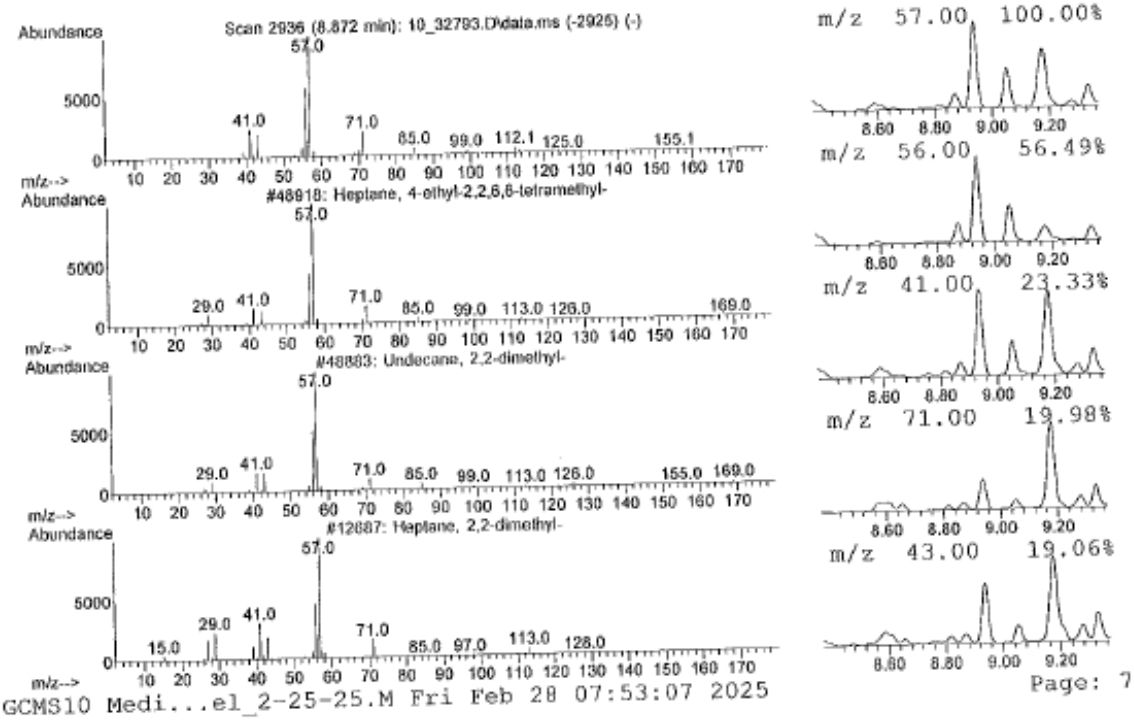
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptane, 4-ethyl-2,2,6,6-te... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.872	10.35 ug/L	1280080	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	78
2	Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	64
3	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64
4	Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	59
5	Decane, 2,2,4-trimethyl-	184	C13H28	062237-98-3	59



** Substructure Report Page 1 **

Search Pattern: Scan 2936 (8.872 min): 10_32793.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB0, rings + double bonds count = 0
2	99	-CH2/3-1, exactly one methylene or methyl group (chain)
3	99	HCSAT, saturated hydrocarbon
4	99	CCH3, methyl bonded to carbon
5	99	sat, saturated compound (no unsaturated bonds)
6	99	-CH2/3-, methylene or methyl group (chain)
7	99	>C<, quaternary carbon
8	99	HC, hydrocarbon (C and H atoms only)
9	99	CH3, methyl
10	99	NoAr, no aromatic rings
11	99	nocycle, no rings
12	99	CH2/3, primary or secondary saturated carbon
13	98	>C<, alk quaternary carbon attached to alkyl
14	98	>C<, chain quaternary carbon (chain)
15	92	CH2, methylene group
16	92	-CH2-, methylene group (chain)
17	91	C(CH3)3, tertiary butyl
18	91	R-C(CH3)3, alkyl tertiary butyl
19	91	SatC(CH3)3, tertiary butyl (no double, triple, or aromatic bond)
20	90	C3+-alkyl, methylene attached to saturated C-atoms (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
2	99	RDB5_PLUS, rings + double bonds count >= 5
3	99	RDB10_PLUS, rings + double bonds count >= 10
4	99	PhOCH3, substituted anisole (methoxyphenyl)
5	99	Ctert-ring, tertiary carbon (>CH-), in ring
6	99	CH-alk-ring, carbon attached to alkyl (ring)
7	99	ArOR, alkyl-aryl ether
8	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
9	99	-O-, contains oxygen atom in chain (non-ring)
10	99	het_ring, ring containing non-carbon atom(s)

MW(Nominal Mass)Information:

Number	MW	Probability
1	170	71
2	128	10
3	156	7
4	142	2

Clorine and/or Bromine information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

2nd Library suggests 12-Carbon Hydrocarbon as highest likelyhood

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm Unknown
Operator : ES
Sample : ABB1619-01 1000X N2Ar, HC MW170
Misc :
ALS Vial : 57 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

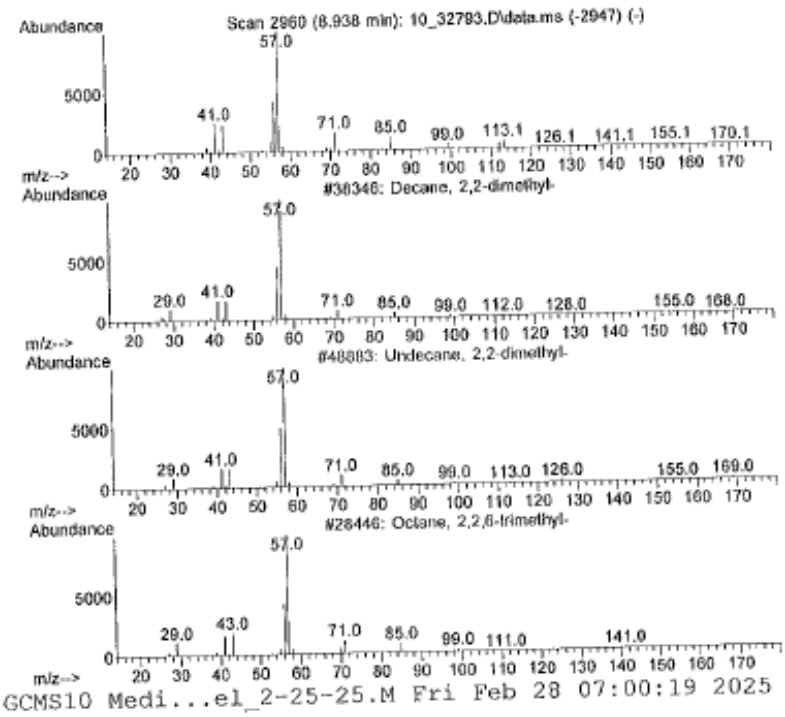
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

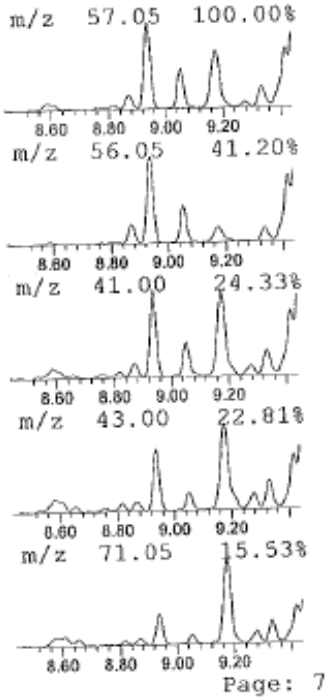
****

Peak Number 3 Decane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.938	65.30 ug/L	8076600	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	78
2	Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	72
3	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
4	Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72
5	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72





GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:00:19 2025 Page: 7

** Substructure Report Page 1 **

Search Pattern: Scan 2960 (8.938 min): 10_32793.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	C(CH3)3, tertiary butyl
2	99	C-(CH3)2, quaternary (no-H) carbon attached to 2 methyl groups
3	99	R-C(CH3)3, alkyl tertiary butyl
4	99	SatC(CH3)3, tertiary butyl (no double, triple, or aromatic bond)
5	99	>C<, alk-chain quaternary carbon (chain)
6	98	HCSAT, saturated hydrocarbon
7	97	RDB0, rings + double bonds count = 0
8	97	HC, hydrocarbon (C and H atoms only)
9	96	sat, saturated compound (no unsaturated bonds)
10	96	C3+-alkyl, methylene attached to saturated C-atoms (chain)
11	96	nocycle, no rings - No Rings = Non-Aromatic
12	96	CH2/3, primary or secondary saturated carbon
13	95	CH2, methylene group
14	95	CCH3, methyl bonded to carbon
15	95	>C<, alk quaternary carbon attached to alkyl
16	95	CH3, methyl
17	95	>C<, quaternary carbon
18	95	-CH2/3-, methylene or methyl group (chain)
19	95	-CH2-, methylene group (chain)
20	95	-CH2/3-1, exactly one methylene or methyl group (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
2	99	RDB5_PLUS, rings + double bonds count >= 5
3	99	RDB10_PLUS, rings + double bonds count >= 10
4	99	PhOCH3, substituted anisole (methoxyphenyl)
5	99	Ctert-ring, tertiary carbon (>CH-), in ring
6	99	CH-alk-ring, carbon attached to alkyl (ring)
7	99	ArOR, alkyl-aryl ether
8	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
9	99	-O-, contains oxygen atom in chain (non-ring)
10	99	het_ring, ring containing non-carbon atom(s)

MW(Nominal Mass)Information:

Number	MW	Probability
1	170	90
2	212	0
3	184	0

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Library Search Compound Report

Unknown
HC, NoAr MW≥184

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

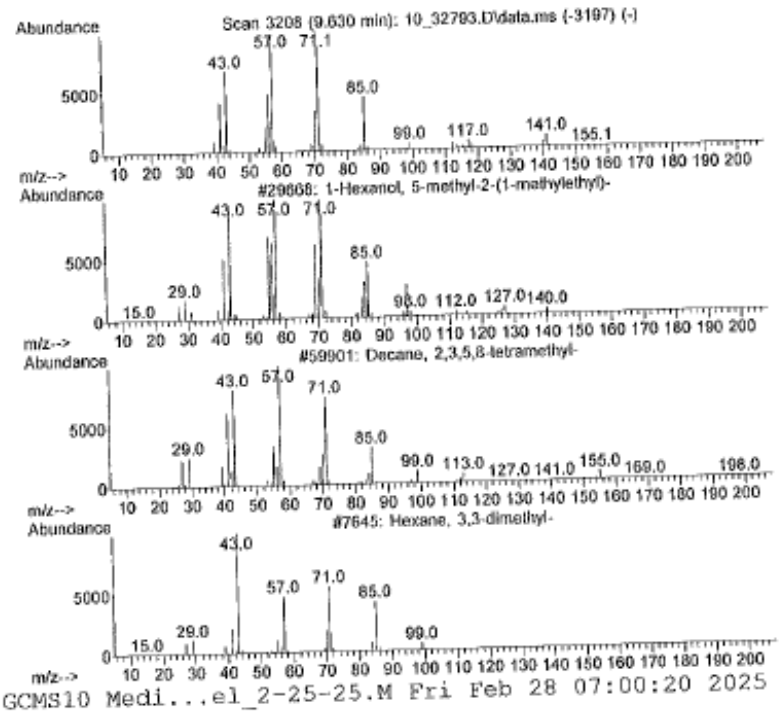
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

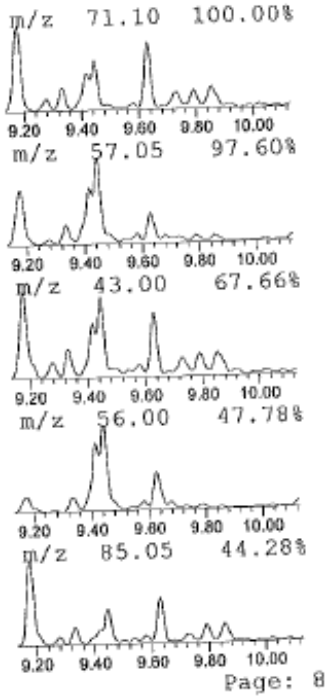
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 5-methyl-2-(1-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.630	53.78 ug/L	6652380	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	78
2	Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	59
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
4	Undecane, 3-methyl-	170	C12H26	001002-43-3	43
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43





GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:00:20 2025 Page: 8

** Substructure Report Page 1 **

Search Pattern: Scan 3208 (9.630 min): 10_32793.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	HCSAT, saturated hydrocarbon
2	99	NoAr, no aromatic rings
3	99	CCH3, methyl bonded to carbon
4	99	-CH2-, methylene group (chain)
5	99	-CH2/3-, methylene or methyl group (chain)
6	99	sat, saturated compound (no unsaturated bonds)
7	99	RDB0, rings + double bonds count = 0
8	99	CH3, methyl
9	99	HC, hydrocarbon (C and H atoms only)
10	99	C3+-alkyl, methylene attached to saturated C-atoms (chain)
11	99	nocycle, no rings
12	99	CH2/3, primary or secondary saturated carbon
13	98	CH2, methylene group
14	98	C2H5/CH2CH2, primary or secondary ethyl linkage
15	98	CH2-CH2/3, ethyl or dimethylene group (chain)
16	98	CH2-CH2-CH2/3, trimethylene group (chain)
17	96	(CH2)3-ch, trimethylene linkage
18	91	-CH2/3-1, exactly one methylene or methyl group (chain)
19	89	CH-alk, tertiary carbon attached to alkyl
20	86	Ctert, tertiary carbon (>CH-)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB10_PLUS, rings + double bonds count >= 10
2	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
3	99	ArOR, alkyl-aryl ether
4	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
5	99	-O-, contains oxygen atom in chain (non-ring)
6	99	O1, contains 1 oxygen atom
7	99	PhCO, phenyl carbonyl
8	99	PhCsat, phenyl attached to saturated carbon atom
9	99	RDB1, rings + double bonds count = 1
10	99	O, contains oxygen

MW(Nominal Mass)Information:

Number	MW	Probability
1	184	50
2	170	10
3	212	8
4	198	7

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Library Search Compound Report

Methyl Propyl Toluene
Isomers MW = 134

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

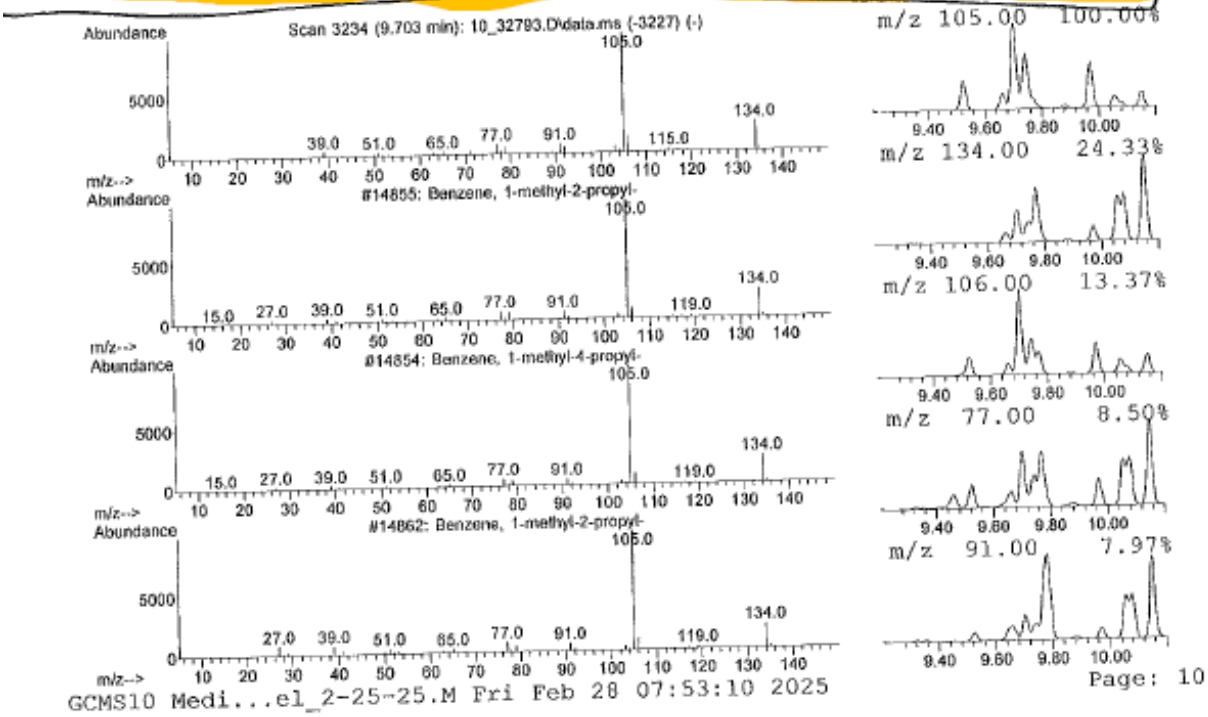
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-methyl-2-propyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.703	11.40 ug/L	1410360	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	91
2	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	91
3	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	91
4	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	91
5	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	90



GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:53:10 2025 Page: 10

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Ethyl, Dimethyl Benzene
Isomer
MW = 134

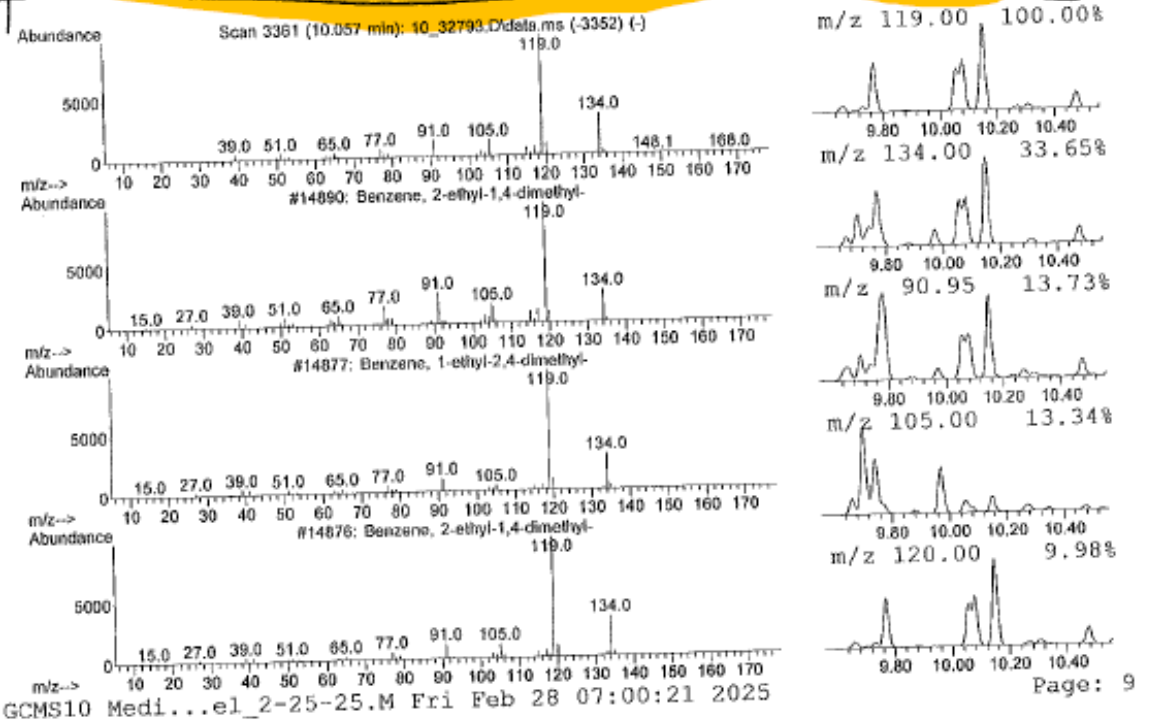
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.057	16.69 ug/L	2064590	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Library Search Compound Report

Ethyl Dimethyl Benzene
Isomer MW = 134

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

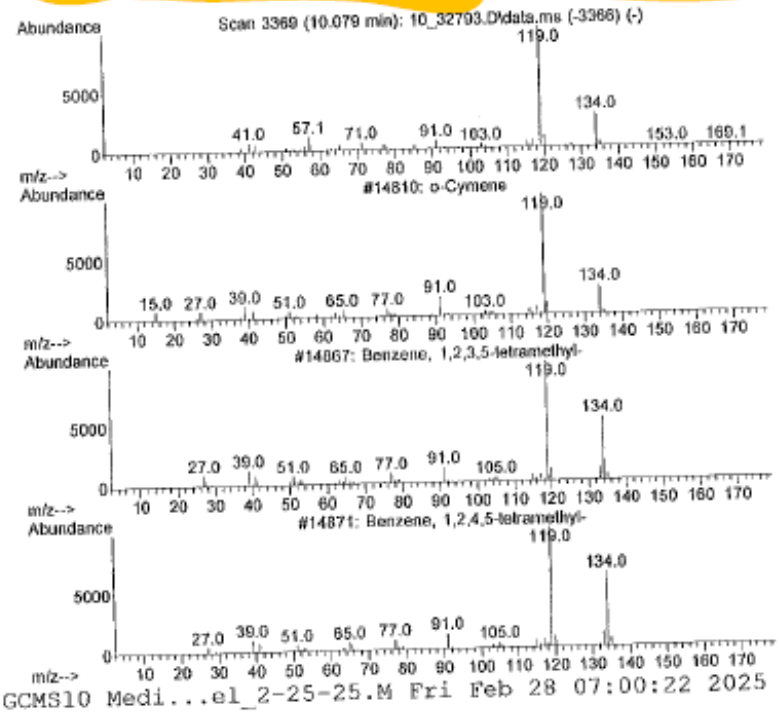
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

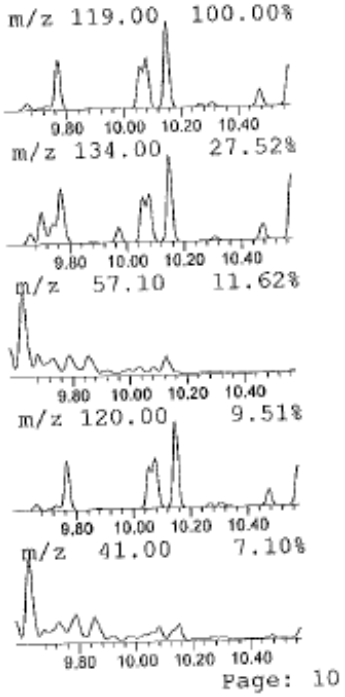
****

Peak Number 6 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.079	16.27 ug/L	2012550	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	87
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	87
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87





GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:00:22 2025 Page: 10

Library Search Compound Report

Ethyl Dimethyl Benzene
Isomer MW=134

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

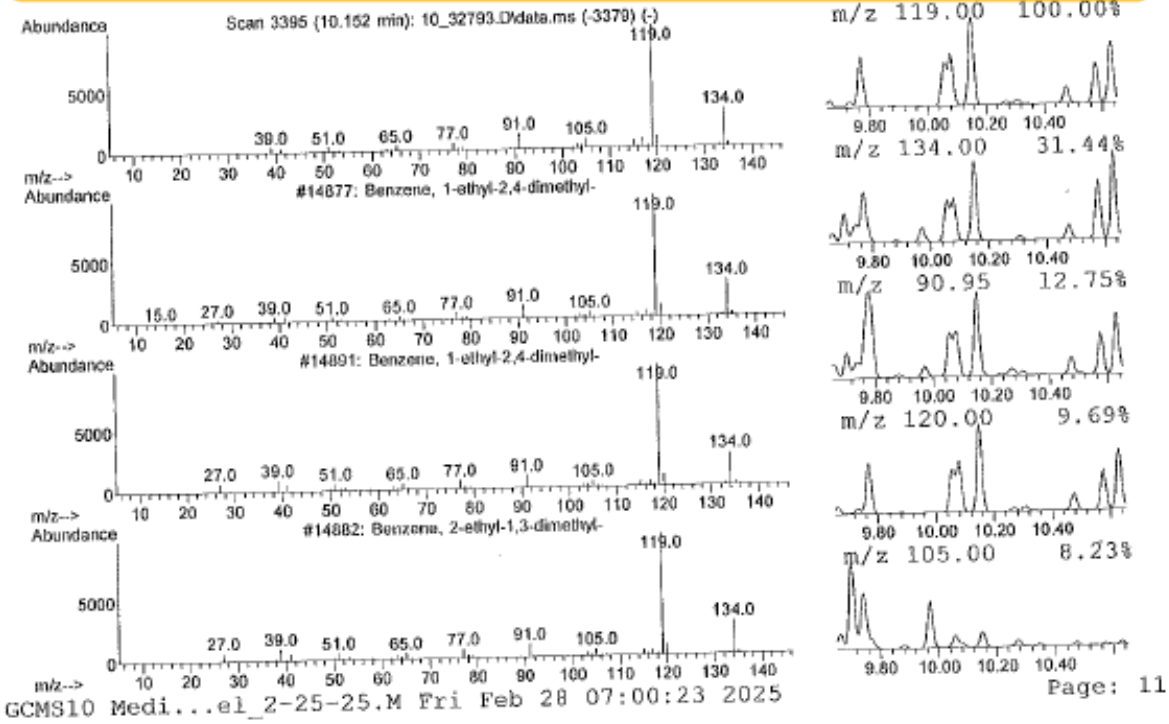
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.152	39.22 ug/L	4851120	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:00:23 2025 Page: 11

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Tetramethyl Benzene
Isomer MW = 134

Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

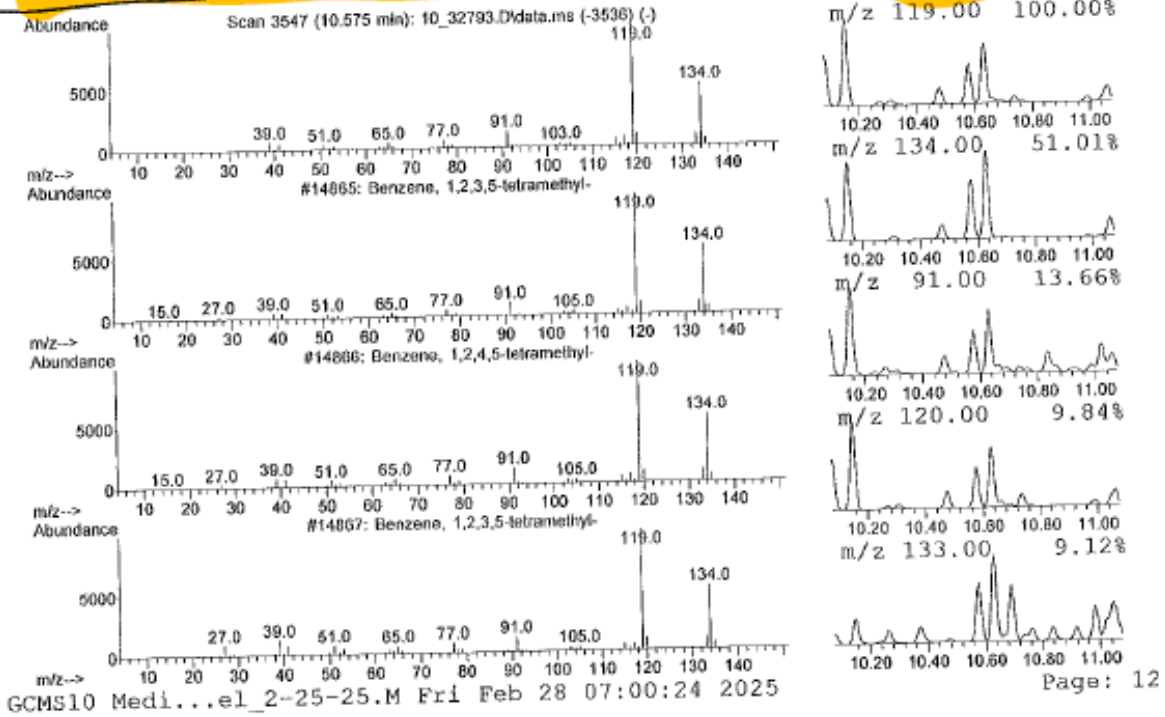
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.575	18.65 ug/L	2306690	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95



Library Search Compound Report

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Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Tetramethyl Benzene Isomer MW = 134

Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

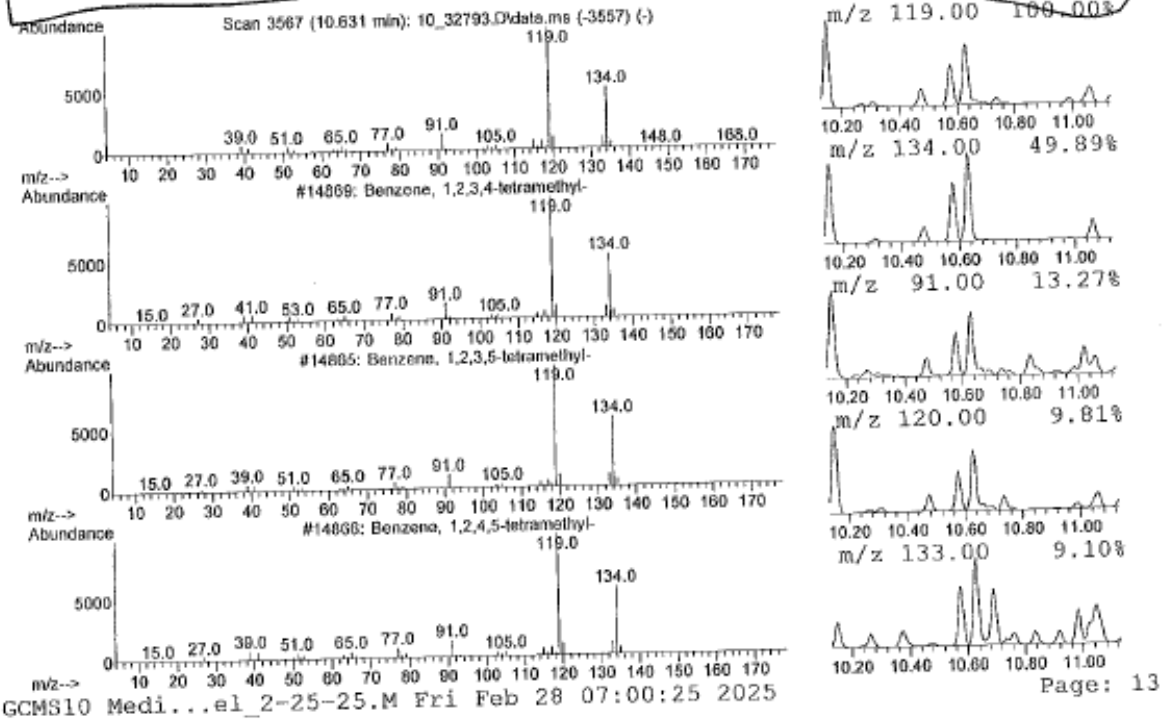
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.631	26.60 ug/L	3289820	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95



Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Methyl Indan
Isomer MW=132

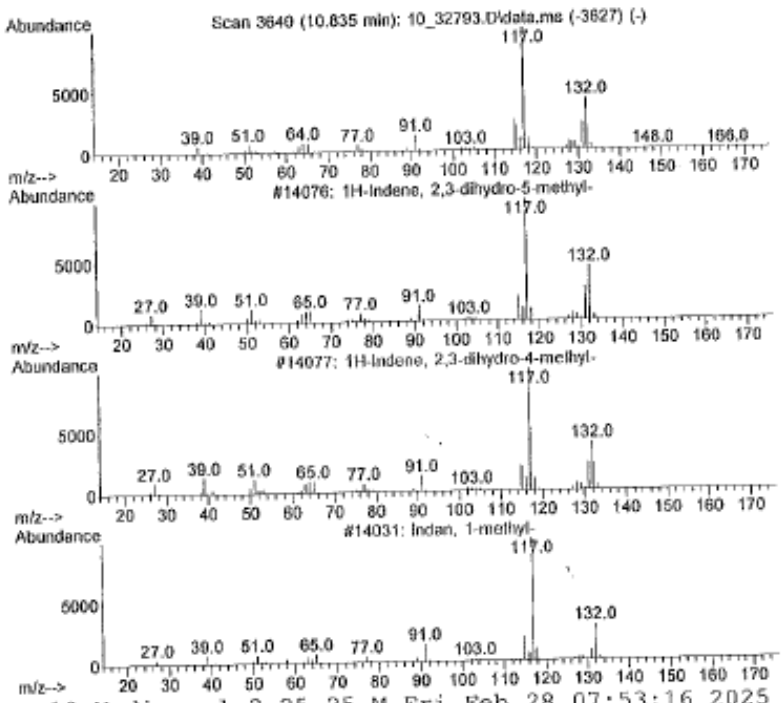
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

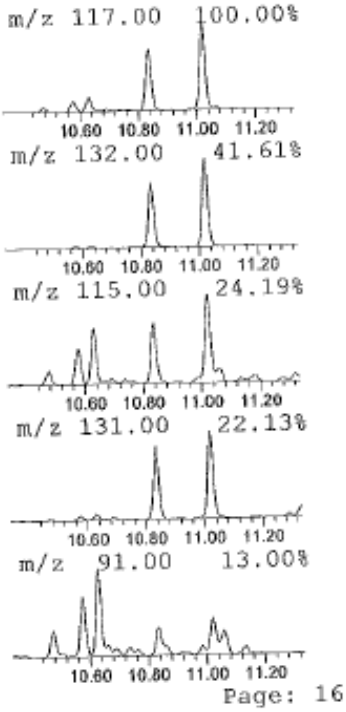
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.835	11.21 ug/L	1386870	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 1-ethenyl-4-ethyl	132	C10H12	003454-07-7	87
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83





GCMS10 Medi...el_2-25-25.M Fri Feb 28 07:53:16 2025

Library Search Compound Report

Data Path : C:\msdchem\1\data\250227\
Data File : 10_32793.D
Acq On : 27 Feb 2025 1:39 pm
Operator : ES
Sample : ABB1619-01 1000X
Misc :
ALS Vial : 57 Sample Multiplier: 1

Methyl Indan Isomer
MW = 132

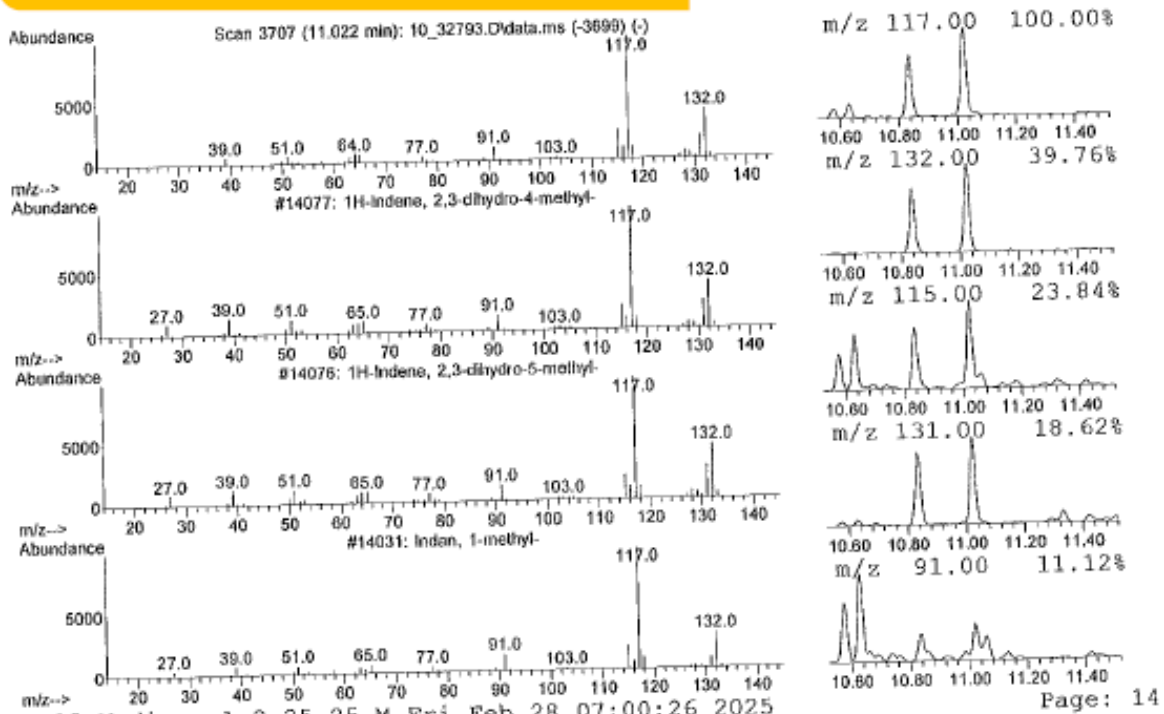
Quant Method : C:\msdchem\1\methods\GCMS10 Medium_Level_2-25-25.M
Quant Title : 8260 Medium Level GCMS10 2/25/2025

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.022	15.09 ug/L	1866730	1,4-DICHLOROBENZENE-d4	9.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3	Indan, 1-methyl-	132	C10H12	000767-58-8	91
4	Indan, 1-methyl-	132	C10H12	000767-58-8	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86



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Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : D2-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

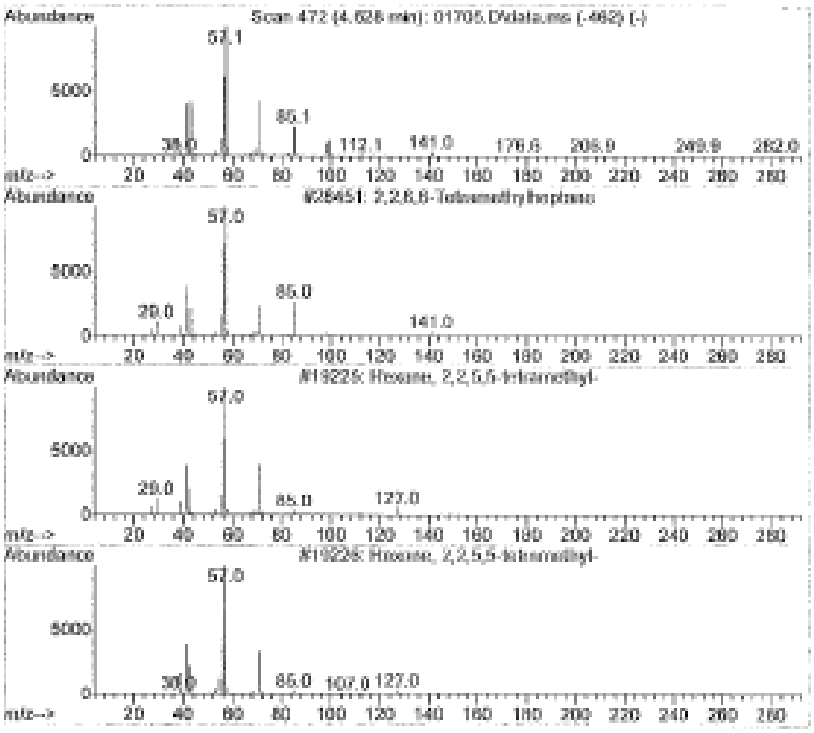
NO#, MW=156

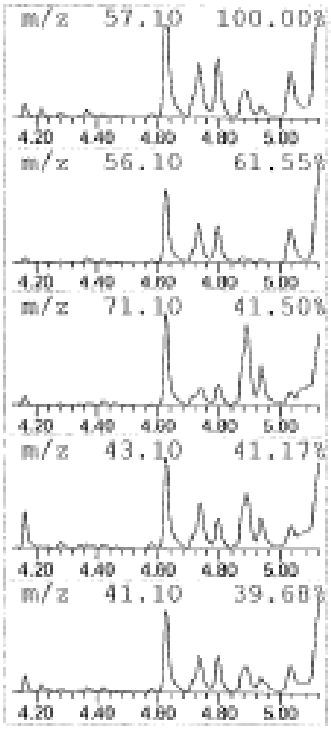
****

Peak Number 1 2,2,6,6-Tetramethylheptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.628	47.37 ug/mL	51529100	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	53
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50
3	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50
4	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	47
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	47





** Substructure Report Page 1 **

Search Pattern: Scan 472 (4.628 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	98	HCSAT, saturated hydrocarbon
2	97	RDB0, rings + double bonds count = 0
3	97	HC, hydrocarbon (C and H atoms only)
4	96	sat, saturated compound (no unsaturated bonds)
5	96	CH2/3, primary or secondary saturated carbon
6	96	nocycle, no rings
7	95	-CH2/3-1, exactly one methylene or methyl group (chain)
8	95	-CH2/3-, methylene or methyl group (chain)
9	95	CCH3, methyl bonded to carbon
10	95	CH3, methyl
11	94	NoAr, no aromatic rings
12	93	C3+-alkyl, methylene attached to saturated C-atoms (chain)
13	92	-CH2-, methylene group (chain)
14	92	CH2, methylene group
15	89	CH-alk, tertiary carbon attached to alkyl
16	86	C2H5/CH2CH2, primary or secondary ethyl linkage
17	86	Ctert, tertiary carbon (>CH-)
18	85	CH2-CH2/3, ethyl or dimethylene group (chain)
19	83	Ctert-chain, tertiary carbon (>CH-), chain
20	83	CH-alk-chain, carbon attached to alkyl (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	N-C, nitrogen-carbon single bond
4	99	ph, phenyl group (C6H5)
5	99	ArOR, alkyl-aryl ether
6	99	cond, condensed ring structure (1,2-overlap)
7	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
8	99	Ar-O, aromatic ring-oxygen atom bond (chain)
9	99	.N., any nitrogen atom in ring
10	99	noAr_cy, rings present, but not aromatic

MW(Nominal Mass)Information:

Number	MW	Probability
1	156	77
2	170	10
3	184	2
4	198	1

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of C

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

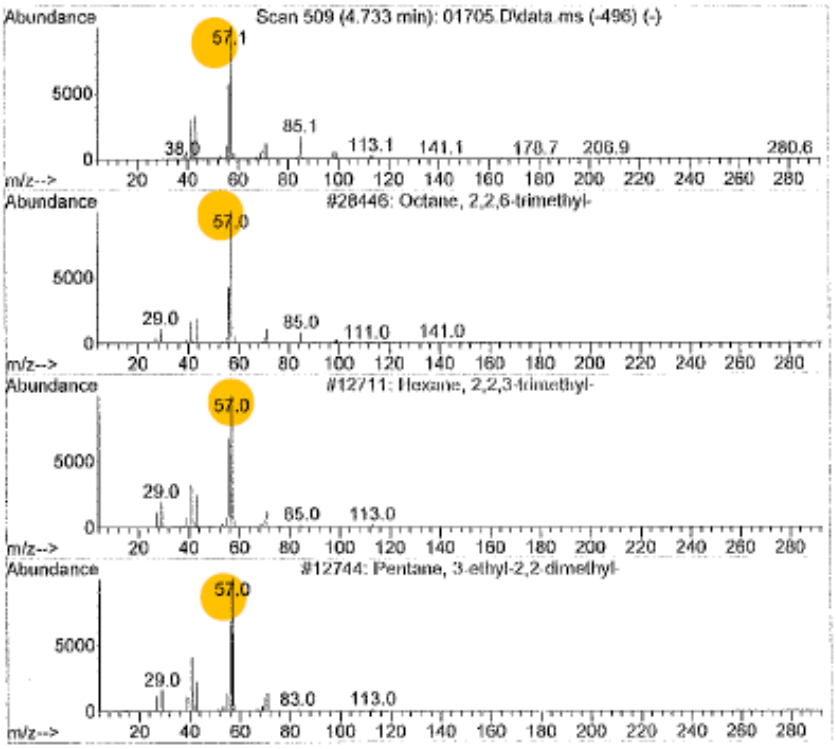
No AR MW 156

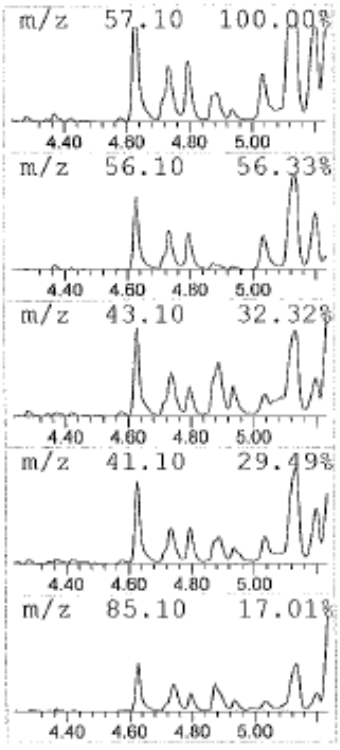
****

Peak Number 2 Octane, 2,2,6-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.733	29.49 ug/mL	32083500	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	59
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	53
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	43





** Substructure Report Page 1 **

Search Pattern: Scan 509 (4.733 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB0, rings + double bonds count = 0
2	99	-CH2/3-1, exactly one methylene or methyl group (chain)
3	99	HCSAT, saturated hydrocarbon
4	99	-CH2/3-, methylene or methyl group (chain)
5	99	CCH3, methyl bonded to carbon
6	99	CH3, methyl
7	99	sat, saturated compound (no unsaturated bonds)
8	99	CH2/3, primary or secondary saturated carbon
9	99	nocycle, no rings
10	99	NoAr, no aromatic rings
11	99	HC, hydrocarbon (C and H atoms only)
12	93	CH-alk, tertiary carbon attached to alkyl
13	90	Ctert, tertiary carbon (>CH-)
14	90	C3+-alkyl, methylene attached to saturated C-atoms (chain)
15	88	CH2, methylene group
16	88	Ctert-chain, tertiary carbon (>CH-), chain
17	88	-CH2-, methylene group (chain)
18	88	CH-alk-chain, carbon attached to alkyl (chain)
19	86	C2H5/CH2CH2, primary or secondary ethyl linkage
20	85	CH2-CH2/3, ethyl or dimethylene group (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	N-C, nitrogen-carbon single bond
4	99	ph, phenyl group (C6H5)
5	99	ArOR, alkyl-aryl ether
6	99	cond, condensed ring structure (1,2-overlap)
7	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
8	99	Ar-O, aromatic ring-oxygen atom bond (chain)
9	99	.N., any nitrogen atom in ring
10	99	noAr_cy, rings present, but not aromatic

MW(Nominal Mass)Information:

Number	MW	Probability
1	156	58
2	170	22
3	142	6
4	184	4

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Cont

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

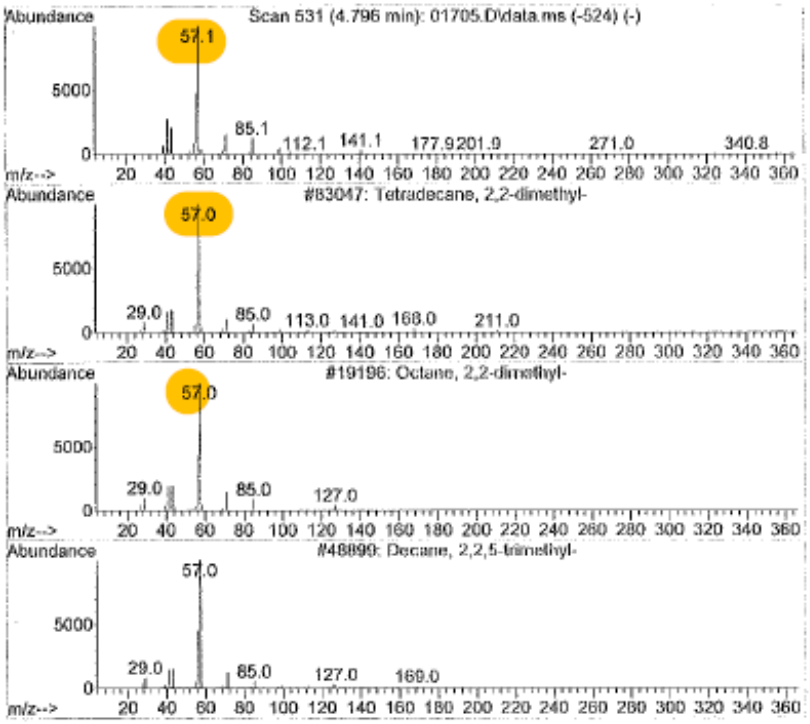
No Ar, MW 198

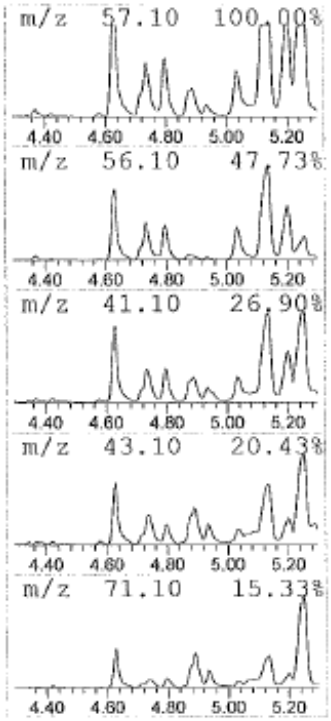
****

Peak Number 3 Tetradecane, 2,2-dimethyl- Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.796	19.85 ug/mL	21596300	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72
2	Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	64
3	Decane, 2,2,5-trimethyl-	184	C13H28	062237-96-1	64
4	Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	64
5	2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	56





** Substructure Report Page 1 **

Search Pattern: Scan 531 (4.796 min): 01706.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	98	HCSAT, saturated hydrocarbon
2	97	RDB0, rings + double bonds count = 0
3	97	HC, hydrocarbon (C and H atoms only)
4	96	C3+-alkyl, methylene attached to saturated C-atoms (chain)
5	96	nocycle, no rings
6	96	CH2/3, primary or secondary saturated carbon
7	96	sat, saturated compound (no unsaturated bonds)
8	95	CH2, methylene group
9	95	CH3, methyl
10	95	CCH3, methyl bonded to carbon
11	95	-CH2/3-, methylene or methyl group (chain)
12	95	-CH2-, methylene group (chain)
13	95	-CH2/3-1, exactly one methylene or methyl group (chain)
14	94	NoAr, no aromatic rings
15	82	C2H5/CH2CH2, primary or secondary ethyl linkage
16	82	C(CH3)3, tertiary butyl
17	81	>C<, quaternary carbon
18	81	CH2-CH2/3, ethyl or dimethylene group (chain)
19	80	>C<, alk quaternary carbon attached to alkyl
20	80	C-(CH3)2, quaternary (no-H) carbon attached to 2 methyl groups

Structures absent:

Number	Probability	Short Name And Description
1	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
2	99	RDB5_PLUS, rings + double bonds count >= 5
3	99	RDB10_PLUS, rings + double bonds count >= 10
4	99	PhOCH3, substituted anisole (methoxyphenyl)
5	99	Cterl-ring, tertiary carbon (>CH-), in ring
6	99	CH-alk-ring, carbon attached to alkyl (ring)
7	99	ArOR, alkyl-aryl ether
8	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
9	99	-O-, contains oxygen atom in chain (non-ring)
10	99	het_ring, ring containing non-carbon atom(s)

MW(Nominal Mass)Information:

Number	MW	Probability
1	156	72
2	198	7
3	170	6
4	184	2

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Cor

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

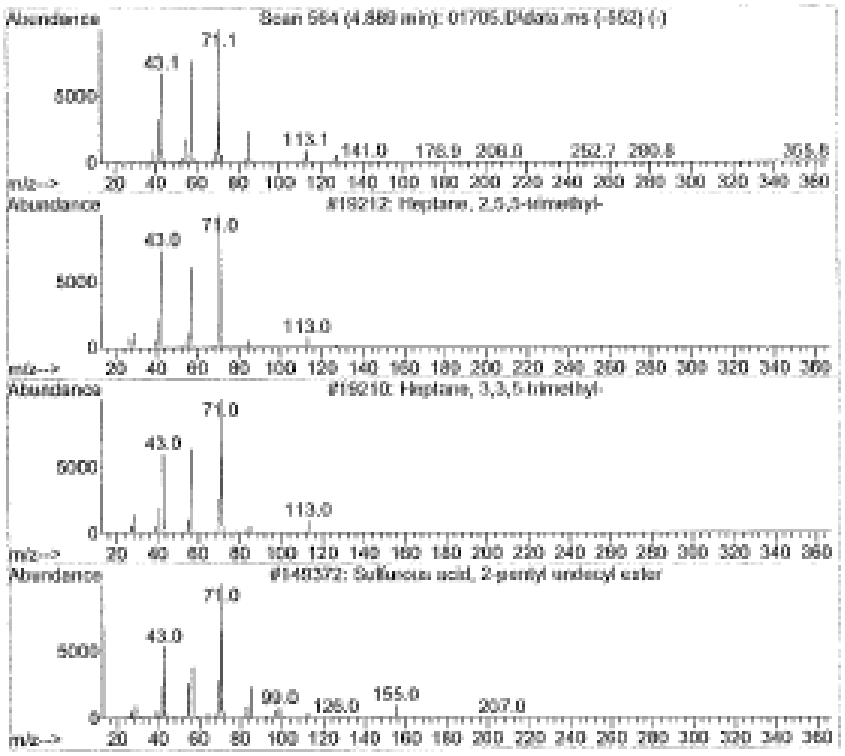
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

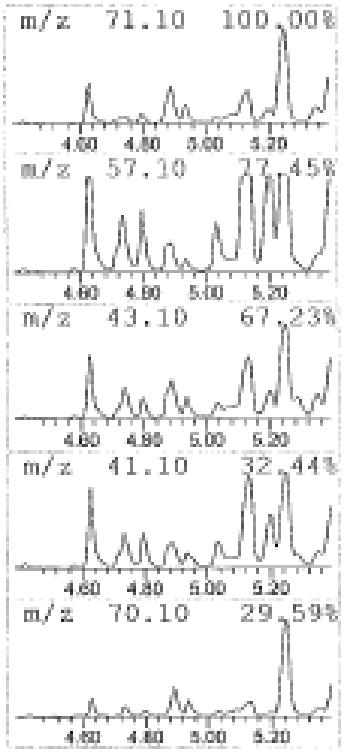
****

Peak Number 4 Heptane, 2,5,5-trimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.889	26.71 ug/mL	29053100	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	72
2	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	64
3	Sulfurous acid, 2-pentyl undecyl...	306	C16H34O3S	1000309-16-0	64
4	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64
5	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	59





** Substructure Report Page 1 **

Search Pattern: Scan 664 (4.889 min): 01706.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB0, rings + double bonds count = 0
2	99	-CH2/3-1, exactly one methylene or methyl group (chain)
3	99	HCSAT, saturated hydrocarbon
4	99	-CH2-, methylene group (chain)
5	99	-CH2/3-, methylene or methyl group (chain)
6	99	CCH3, methyl bonded to carbon
7	99	sat, saturated compound (no unsaturated bonds)
8	99	CH3, methyl
9	99	HC, hydrocarbon (C and H atoms only)
10	99	noAr, no aromatic rings
11	99	C3+-alkyl, methylene attached to saturated C-atoms (chain)
12	99	nocyde, no rings
13	99	CH2/3, primary or secondary saturated carbon
14	98	CH2, methylene group
15	98	C2H5/CH2CH2, primary or secondary ethyl linkage
16	98	CH2-CH2/3, ethyl or dimethylene group (chain)
17	80	CH-alk, tertiary carbon attached to alkyl
18	77	Ctert, tertiary carbon (>CH-)
19	75	CH-alk-chain, carbon attached to alkyl (chain)
20	74	Ctert-chain, tertiary carbon (>CH-), chain

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	N-C, nitrogen-carbon single bond
4	99	ph, phenyl group (C6H5)
5	99	ArOR, alkyl-aryl ether
6	99	cond, condensed ring structure (1,2-overlap)
7	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
8	99	Ar-O, aromatic ring-oxygen atom bond (chain)
9	99	.N., any nitrogen atom in ring
10	99	noAr_cy, rings present, but not aromatic

MW(Nominal Mass)Information:

Number	MW	Probability
1	198	27
2	155	23
3	212	17
4	184	13

Clorine and/or Bromine Information:

Cl=2, Br=0 Probability=6%
There is a peak (m/z=113 ab=9%) above highest possible ClBr cluster

Table of Con

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

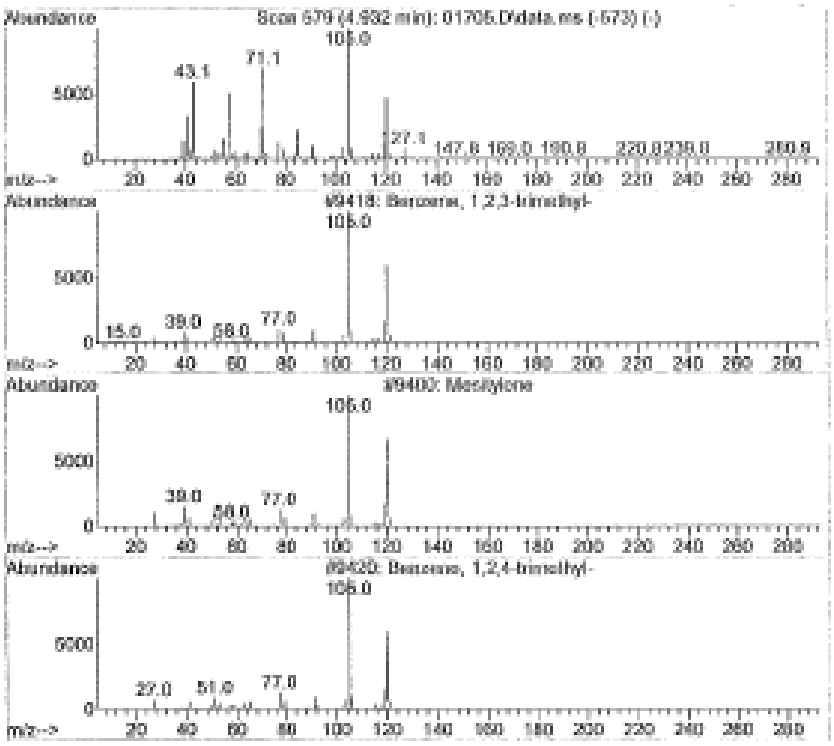
DW, MW 2/12

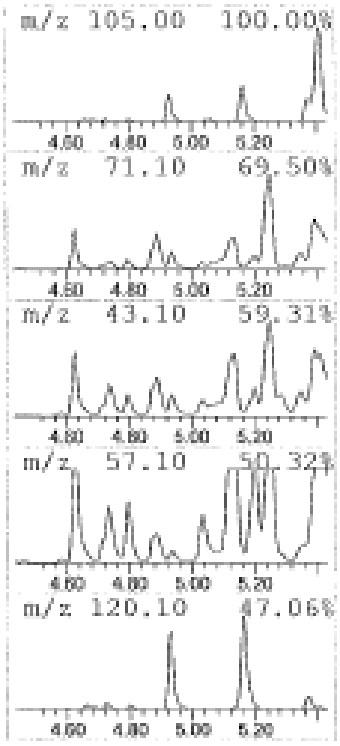
****

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.932	19.73 ug/mL	21446100	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
2	Mesitylene	120	C9H12	000108-67-8	83
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	83
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	64
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	64





** Substructure Report Page 1 **

Search Pattern: Scan 579 (4.932 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	97	HC, hydrocarbon (C and H atoms only)
2	96	CH2/3, primary or secondary saturated carbon
3	96	PhCsat, phenyl attached to saturated carbon atom
4	96	-CH2/3-, methylene or methyl group (chain)
5	96	CH3, methyl
6	96	Ph-all, isolated benzenoid (6-membered) ring
7	95	AR, aromatic ring
8	94	RDB4, rings + double bonds count = 4
9	94	Ar-C, aromatic ring-saturated carbon atom bond (chain)
10	93	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
11	93	ArC, aromatic carbon attached to carbon
12	91	-CH2/3-1, exactly one methylene or methyl group (chain)
13	90	HCUNS, unsaturated hydrocarbon
14	89	PhCH3, phenyl methyl (toluene)
15	85	Ph-2+sub, phenyl with 2 or more substituents
16	84	ArCH3, aryl methane group
17	84	Ar-CH2,3, aromatic bond to methyl or methylene group
18	55	Ph-3sub, trisubstituted phenyl
19	32	CCH3, methyl bonded to carbon
20	26	CH2-CH2/3, ethyl or dimethylene group (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	Si(CH3)3, trimethyl silyl
2	99	RDB1, rings + double bonds count = 1
3	99	ArOR, alkyl-aryl ether
4	99	ArO, aromatic carbon-oxygen bond
5	99	O1, contains 1 oxygen atom
6	99	Ar-O, aromatic ring-oxygen atom bond (chain)
7	99	ether, divalent oxygen
8	99	:N:, any nitrogen atom in ring
9	99	-O-, contains oxygen atom in chain (non-ring)
10	99	Cter-ring, tertiary carbon (>CH-), in ring

MW(Nominal Mass)Information:

Number	MW	Probability
1	142	37
2	144	13
3	143	6
4	146	5

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Contents

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

NO HR, MW 2-170

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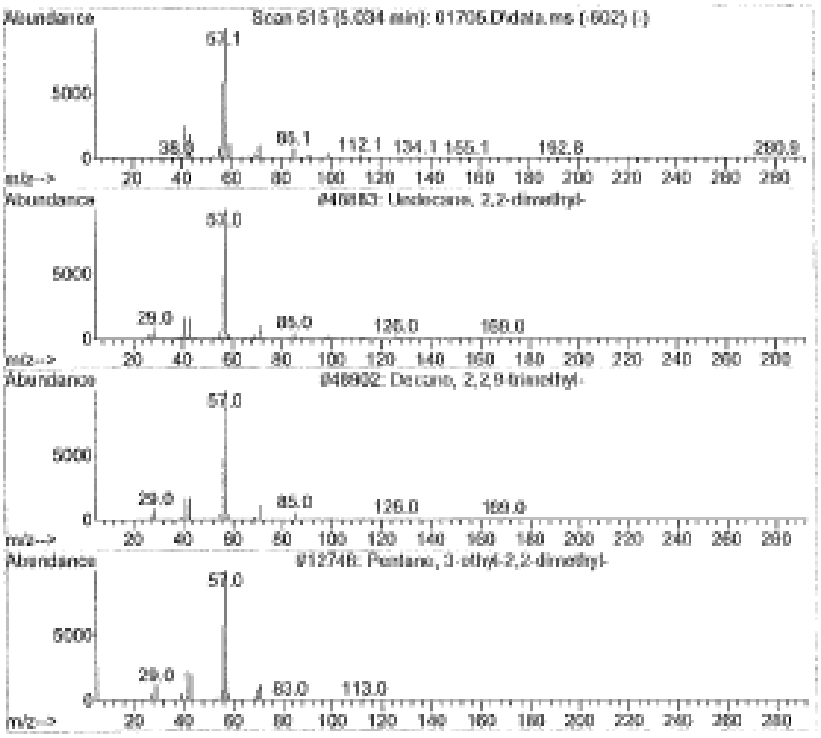
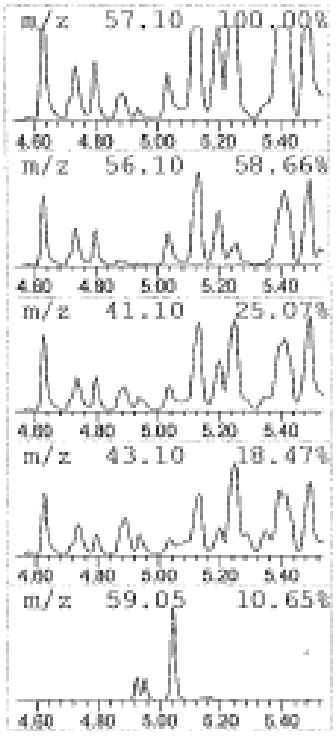
Peak Number 6 Undecane, 2,2-dimethyl- Concentration Rank 17

R.T.	EstConc		Area	Relative to ISTD	R.T.
5.034	25.90	ug/mL	28170200	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	59
2	Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	59
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50
4	Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	50
5	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	47





** Substructure Report Page 1 **

Search Pattern: Scan 815 (5.034 min): 01706.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	>C<, alk-chain quaternary carbon (chain)
2	99	C-(CH3)2, quaternary (no-H) carbon attached to 2 methyl groups
3	99	R-C(CH3)3, alkyl tertiary butyl
4	99	>C<, chain quaternary carbon (chain)
5	99	SatC(CH3)3, tertiary butyl (no double, triple, or aromatic bond)
6	99	C(CH3)3, tertiary butyl
7	98	HCSAT, saturated hydrocarbon
8	98	>C<, quaternary carbon
9	97	>C<, alk quaternary carbon attached to alkyl
10	97	RDB0, rings + double bonds count = 0
11	97	HC, hydrocarbon (C and H atoms only)
12	96	nocycle, no rings
13	96	CH2/3, primary or secondary saturated carbon
14	96	sat, saturated compound (no unsaturated bonds)
15	95	CH3, methyl
16	95	-CH2/3-1, exactly one methylene or methyl group (chain)
17	95	-CH2/3-, methylene or methyl group (chain)
18	95	CCH3, methyl bonded to carbon
19	94	NoAr, no aromatic rings
20	92	-CH2-, methylene group (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB1, rings + double bonds count = 1
2	99	N-C, nitrogen-carbon single bond
3	99	C-O, carbon-oxygen single bond
4	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
5	99	Si, contains silicon
6	99	ArOR, alkyl-aryl ether
7	99	het_ring, ring containing non-carbon atom(s)
8	99	CH-alk-ring, carbon attached to alkyl (ring)
9	98	Cter-ring, tertiary carbon (>CH-), in ring
10	99	ether, divalent oxygen

MW(Nominal Mass)Information:

Number	MW	Probability
1	170	85
2	184	11
3	156	5
4	142	3

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Cont

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

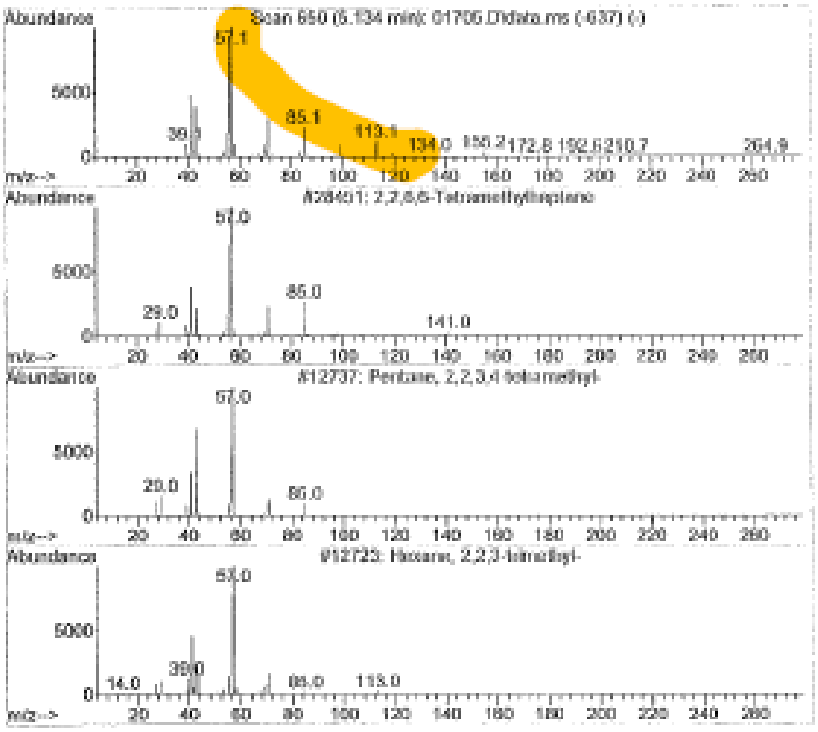
No Ar, MW ≥ 170

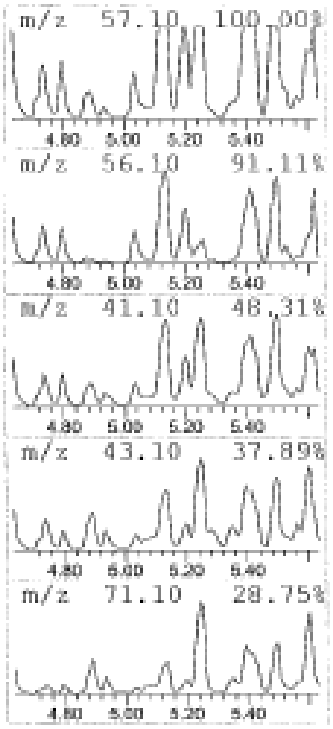
****

Peak Number 7 2,2,6,6-Tetramethylheptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	90.33 ug/mL	982588D0	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,6,6-Tetramethylheptane	156	C11H24	04D117-45-1	64
2	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50





** Substructure Report Page 1 **

Search Pattern: Scan 550 (5.134 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB0, rings + double bonds count = 0
2	99	CCH3, methyl bonded to carbon
3	99	NoAr, no aromatic rings
4	99	Isocycle, no rings
5	99	CH2/3, primary or secondary saturated carbon
6	99	CH3, methyl
7	99	-CH2/3-, methylene or methyl group (chain)
8	99	-CH2/3-1, exactly one methylene or methyl group (chain)
9	96	HCSAT, saturated hydrocarbon
10	94	HC, hydrocarbon (C and H atoms only)
11	94	sat, saturated compound (no unsaturated bonds)
12	92	-CH2-, methylene group (chain)
13	92	CH2, methylene group
14	90	C3+-alkyl, methylene attached to saturated C-atoms (chain)
15	81	>C<, quaternary carbon
16	80	C-(CH3)2, quaternary (no-H) carbon attached to 2 methyl groups
17	80	>C<, alk-quaternary carbon attached to alkyl
18	80	CH-alk, tertiary carbon attached to alkyl
19	77	>C<, alk-chain quaternary carbon (chain)
20	77	Ctert, tertiary carbon (>CH-)

Structures absent:

Number	Probability	Short Name And Description
1	99	ArOR, alkyl-aryl ether
2	99	cond, condensed ring structure (1,2-overlap)
3	99	noAr_cy, rings present, but not aromatic
4	99	C17-ring, 17 carbon atoms ring, usually steroid
5	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
6	99	RDB1, rings + double bonds count = 1
7	99	Ph-all, isolated benzenoid (6-membered) ring
8	99	PhOCH3, substituted anisole (methoxyphenyl)
9	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
10	99	O1, contains 1 oxygen atom

MW(Nominal Mass)Information:

Number	MW	Probability
1	170	66
2	212	3
3	184	3
4	198	1

Cloxine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Conte

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : D2-24-25 625 SV-12 LOW LEVEL ICAL

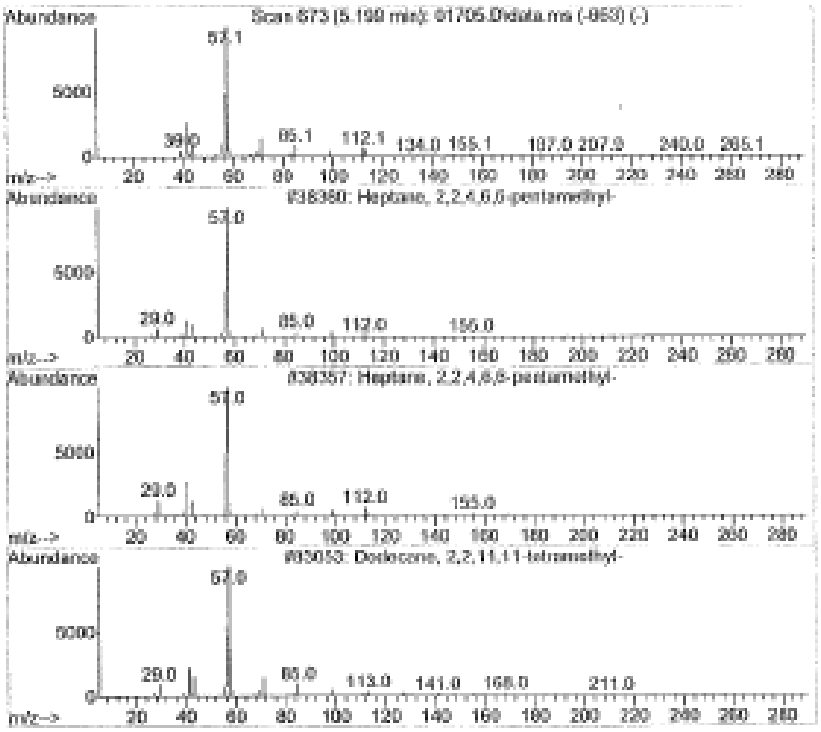
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

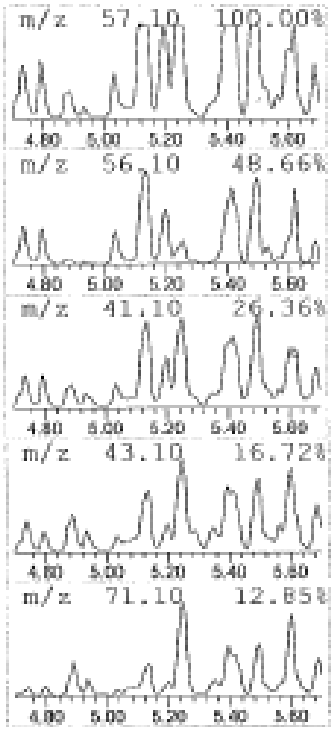
****

Peak Number 8 Heptane, 2,2,4,6,6-pentamet... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	39.46 ug/mL	42927200	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	78
2	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	78
3	Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	78
4	Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	72
5	Decane, 2,2,5-trimethyl-	184	C13H28	062237-96-1	72





** Substructure Report Page 1 **

Search Pattern: Scan 673 (5.199 min): 01705.Didata.ms

Structures present:

Number	Probability	Short Name And Description
1	99	>C<, alk-chain quaternary carbon (chain)
2	99	C-(CH3)2, quaternary (no-H) carbon attached to 2 methyl groups
3	99	R-C(CH3)3, alkyl tertiary butyl
4	99	>C<, chain quaternary carbon (chain)
5	99	SatC(CH3)3, tertiary butyl (no double, triple, or aromatic bond)
6	99	C(CH3)3, tertiary butyl
7	99	nocycle, no rings
8	99	RDB0, rings + double bonds count = 0
9	99	HCSAT, saturated hydrocarbon
10	99	NoAr, no aromatic rings
11	99	CCH3, methyl bonded to carbon
12	99	CH2/3, primary or secondary saturated carbon
13	99	sat, saturated compound (no unsaturated bonds)
14	99	CH3, methyl
15	99	-CH2/3-1, exactly one methylene or methyl group (chain)
16	99	HC, hydrocarbon (C and H atoms only)
17	99	-CH2-, methylene group (chain)
18	99	-CH2/3-, methylene or methyl group (chain)
19	98	>C<, quaternary carbon
20	98	CH2, methylene group

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB1, rings + double bonds count = 1
2	99	N-C, nitrogen-carbon single bond
3	99	C-O, carbon-oxygen single bond
4	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
5	99	Si, contains silicon
6	99	ArOR, alkyl-aryl ether
7	99	het_ring, ring containing non-carbon atom(s)
8	99	CH-alk-ring, carbon attached to alkyl (ring)
9	99	Ctert-ring, tertiary carbon (>CH-), in ring
10	99	ether, divalent oxygen

MW(Nominal Mass)Information:

Number	MW	Probability
1	170	83
2	212	1
3	171	0
4	184	0

Chlorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Conti

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown
Quant Method : C:\msdchem\1\methods\Processing\RQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

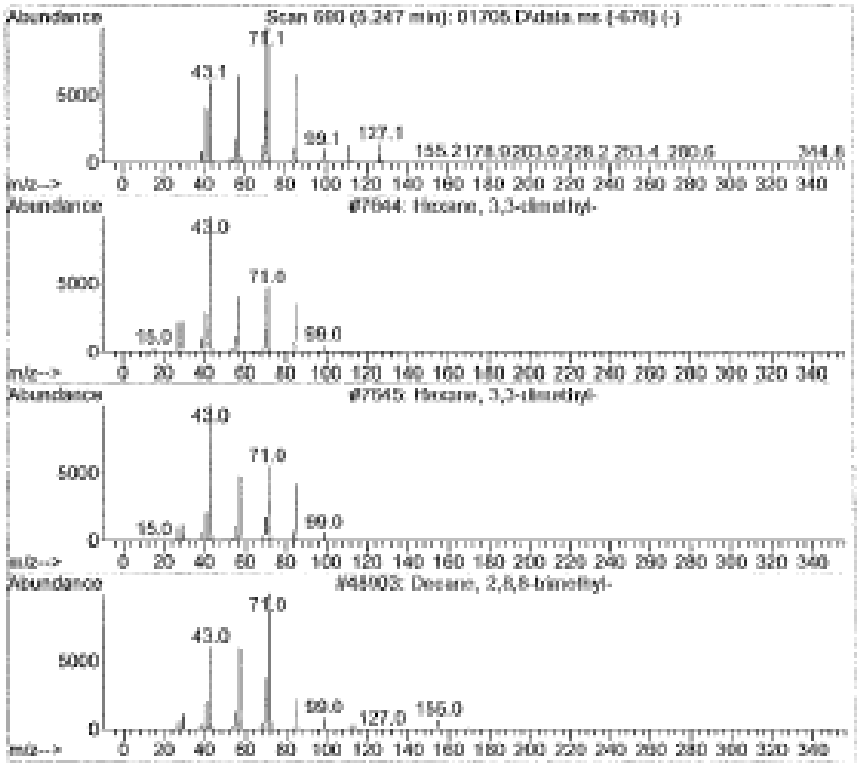
Note, MW = 212

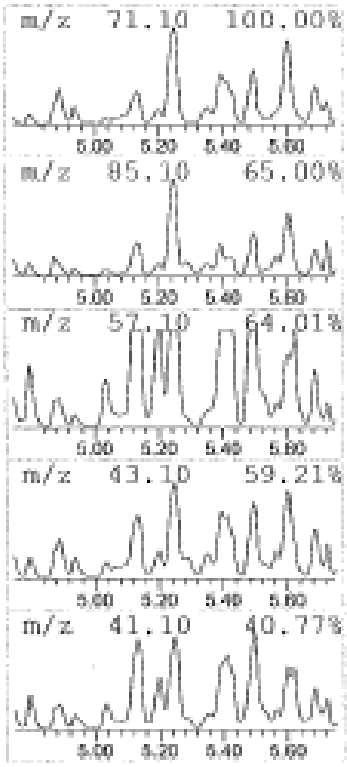
****

Peak Number 9 Hexane, 3,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.247	102.99 ug/mL	111994000	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3	Decane, 2,8,8-trimethyl-	184	C13H28	1000060-81-2	53
4	Undecane, 3,3-dimethyl-	184	C13H28	017312-65-1	50
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50





** Substructure Report Page 1 **

Search Pattern: Scan 690 (5.247 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	CCH3, methyl bonded to carbon
2	99	-CH2-, methylene group (chain)
3	99	-CH2/3-, methylene or methyl group (chain)
4	99	CH3, methyl
5	99	NoAr, no aromatic rings
6	99	C3+-alkyl, methylene attached to saturated C atoms (chain)
7	99	CH2/3, primary or secondary saturated carbon
8	99	nocycle, no rings
9	98	CH2, methylene group
10	97	RDB0, rings + double bonds count = 0
11	97	HC, hydrocarbon (C and H atoms only)
12	96	HCSAT, saturated hydrocarbon
13	96	sat, saturated compound (no unsaturated bonds)
14	95	C2H5/CH2CH2, primary or secondary ethyl linkage
15	94	CH2-CH2/3, ethyl or dimethylene group (chain)
16	88	(CH2)3-ch, trimethylene linkage
17	87	CH2-CH2-CH2/3, trimethylene group (chain)
18	88	-CH2/3-1, exactly one methylene or methyl group (chain)
19	85	CH-alk, tertiary carbon attached to alkyl
20	83	Ctert, tertiary carbon (>CH-)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB10_PLUS, rings + double bonds count >= 10
2	99	PhOCH3, substituted anisole (methoxyphenyl)
3	99	ArOR, alkyl-aryl ether
4	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
5	99	-O-, contains oxygen atom in chain (non-ring)
6	99	O1, contains 1 oxygen atom
7	99	PhCO, phenyl carbonyl
8	99	PhCsat, phenyl attached to saturated carbon atom
9	99	RDB1, rings + double bonds count = 1
10	99	O, contains oxygen

MW(Nominal Mass)Information:

Number	MW	Probability
1	212	40
2	198	25
3	184	14
4	170	4

Clorine and/or Bromine Information:

Cl=1, Br=0 Probability=6%
Cl/Br Match factor (809) is too small (<850)

Table of Conter

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 0170D5.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

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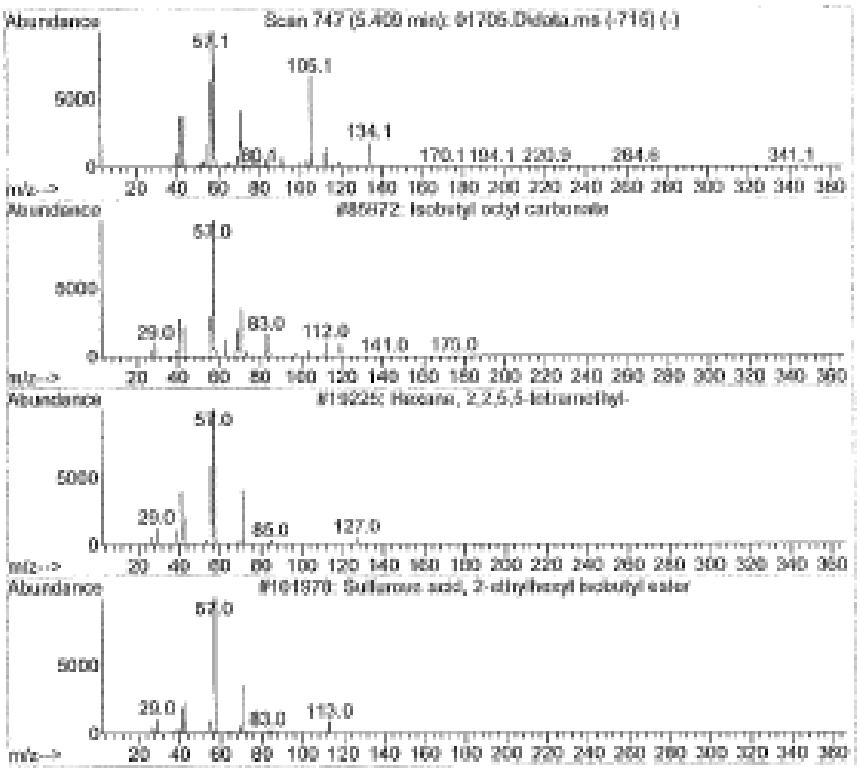
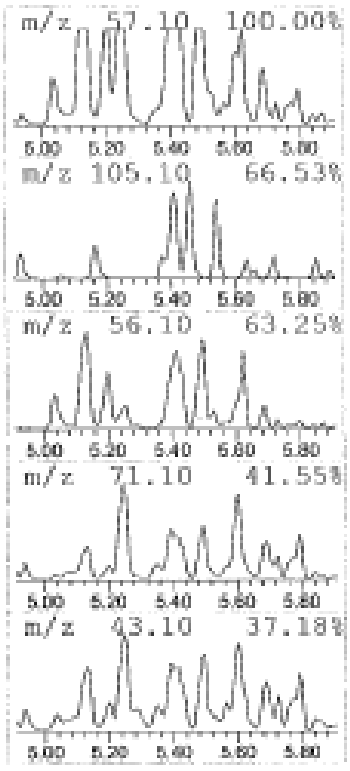
Peak Number 10 Isobutyl octyl carbonate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.409	150.60 ug/mL	163822000	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl octyl carbonate	230	C13H26O3	1000372-74-6	53
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47
3	Sulfurous acid, 2-ethylhexyl iso...	250	C12H26O3S	1000309-18-7	38
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	38
5	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	38





" Substructure Report Page 1 "

Search Pattern: Scan 747 (8.409 min): 01706.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	98	HCSAT, saturated hydrocarbon
2	97	RD00, rings + double bonds count = 0
3	97	CH-alk, tertiary carbon attached to alkyl
4	97	HC, hydrocarbon (C and H atoms only)
5	96	sat, saturated compound (no unsaturated bonds)
6	96	CH2/3, primary or secondary saturated carbon
7	96	nocycle, no rings
8	95	-CH2/3-1, exactly one methylene or methyl group (chain)
9	95	CCH3, methyl bonded to carbon
10	95	-CH2/3-, methylene or methyl group (chain)
11	95	CH3, methyl
12	95	Ctert, tertiary carbon (>CH-)
13	94	NoAr, no aromatic rings
14	93	Csec-chain, tertiary carbon (>CH-), chain
15	93	CH-alk-chain, carbon attached to alkyl (chain)
16	92	-CH2-, methylene group (chain)
17	92	CH2, methylene group
18	88	C3+-alkyl, methylene attached to saturated C-atoms (chain)
19	88	C2H6/CH2CH2, primary or secondary ethyl linkage
20	85	CH2-CH2/3, ethyl or dimethylene group (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	N-C, nitrogen-carbon single bond
4	99	ph, phenyl group (C6H5)
5	99	ArOR, alkyl-aryl ether
6	99	cond, condensed ring structure (1,2-overlap)
7	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
8	99	Ar-O, aromatic ring-oxygen atom bond (chain)
9	99	.N., any nitrogen atom in ring
10	99	noAr_cy, rings present, but not aromatic

MW(Nominal Mass)Information:

Number	MW	Probability
1	177	15
2	190	12
3	176	11
4	163	11

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=98%
Possible Cl,Br cluster(s) found

Table of Conter

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

Pr, MW2 134

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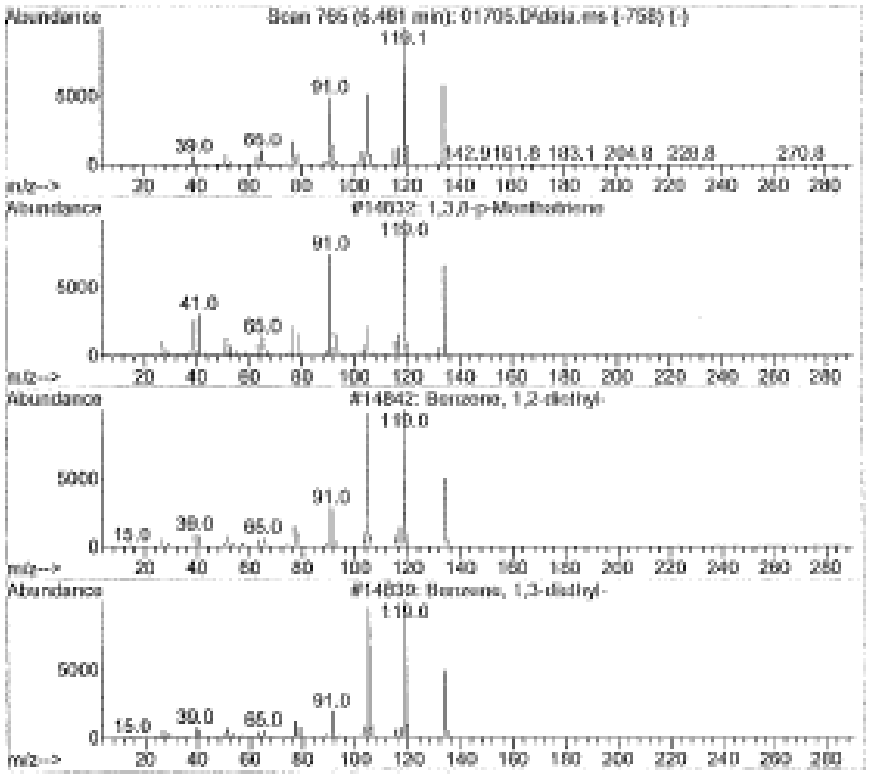
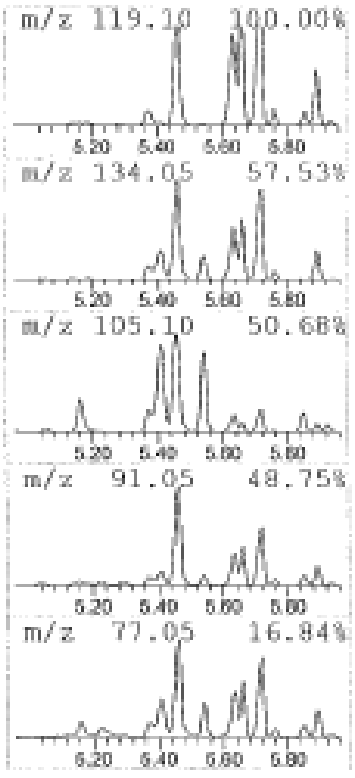
Peak Number 11 1,3,8-p-Menthatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.461	53.63 ug/mL	58340300	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,8-p-Menthatriene	134	C10H14	018368-95-1	91
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	90
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	87
4	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	87
5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	86





** Substructure Report Page 1 **

Search Pattern: Scan 795 (5.461 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB4, rings + double bonds count = 4
2	99	CH2G, primary or secondary saturated carbon
3	99	HC, hydrocarbon (C and H atoms only)
4	99	-CH2/3-, methylene or methyl group (chain)
5	99	CH3, methyl
6	99	PhCH2, phenyl with methylene substituent
7	99	HCUNS, unsaturated hydrocarbon
8	98	Ar-CH2, aryl methylene bond (chain)
9	98	Ar-C, aromatic ring-saturated carbon atom bond (chain)
10	98	PhCsat, phenyl attached to saturated carbon atom
11	98	Ph-all, isolated benzenoid (6-membered) ring
12	98	C2alk, ethyl group
13	98	AR, aromatic ring
14	97	Ph-2+sub, phenyl with 2 or more substituents
15	97	ArC, aromatic carbon attached to carbon
16	97	Ar-CH2,3, aromatic bond to methyl or methylene group
17	97	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
18	96	-CH2-CH2/3-1, exactly one ethyl or dimethylene group (chain)
19	96	CH2, methylene group
20	96	C2H5/CH2CH2, primary or secondary ethyl linkage

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB10_PLUS, rings + double bonds count >= 10
2	99	noAr_cy, rings present, but not aromatic
3	99	ArOR, alkyl-aryl ether
4	99	C17-ring, 17 carbon atoms ring, usually steroid
5	99	PhOCH3, substituted anisole (methoxyphenyl)
6	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
7	99	RDB1, rings + double bonds count = 1
8	99	PhCO, phenyl carbonyl
9	99	-O-, contains oxygen atom in chain (non-ring)
10	99	O1, contains 1 oxygen atom

MW(Nominal Mass)Information:

Number	MW	Probability
1	134	99
2	135	0

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Co

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

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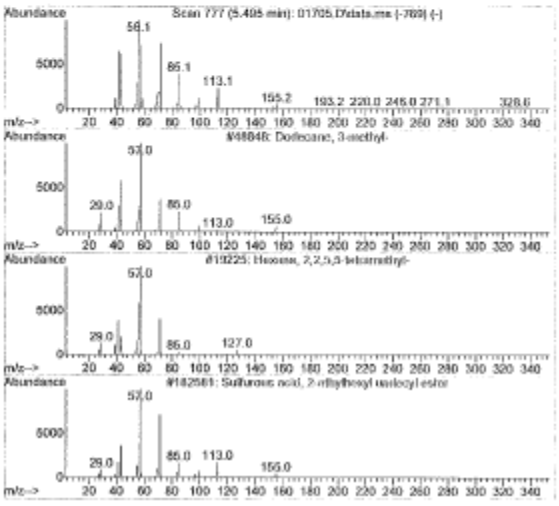
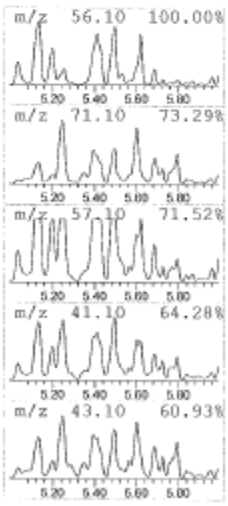
Peak Number 12 Dodecane, 3-methyl- Concentration Rank 4

R.T.	EstConc		Area	Relative to ISTD	R.T.
5.495	82.51	ug/mL	89756700	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 3-methyl-	184	C13H28	017312-57-1	53
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50
3	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	43
4	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	43
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	38





** Substructure Report Page 1 **

Search Pattern: Scan 777 (5.495 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	NoAr, no aromatic rings
2	99	CH2/3, primary or secondary saturated carbon
3	99	nocycle, no rings
4	99	CCH3, methyl bonded to carbon
5	99	CH3, methyl
6	99	RDB0, rings + double bonds count = 0
7	99	-CH2/3-, methylene or methyl group (chain)
8	99	-CH2/3-1, exactly one methylene or methyl group (chain)
9	96	C3+-alkyl, methylene attached to saturated C-atoms (chain)
10	95	CH2, methylene group
11	95	-CH2-, methylene group (chain)
12	93	HCSAT, saturated hydrocarbon
13	92	C2H5/CH2CH2, primary or secondary ethyl linkage
14	91	CH2-CH2/3, ethyl or dimethylene group (chain)
15	91	sat, saturated compound (no unsaturated bonds)
16	90	HC, hydrocarbon (C and H atoms only)
17	89	CH-alk, tertiary carbon attached to alkyl
18	86	Ctert, tertiary carbon (>CH-)
19	83	Ctert-chain, tertiary carbon (>CH-), chain
20	83	CH-alk-chain, carbon attached to alkyl (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
2	99	RDB5_PLUS, rings + double bonds count >= 5
3	99	RDB10_PLUS, rings + double bonds count >= 10
4	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
5	99	ArOR, alkyl-aryl ether
6	99	O1, contains 1 oxygen atom
7	99	PhCO, phenyl carbonyl
8	99	PhCsat, phenyl attached to saturated carbon atom
9	99	O, contains oxygen
10	99	N, contains nitrogen

MW(Nominal Mass)information:

Number	MW	Probability
1	184	21
2	212	18
3	198	17
4	170	12

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Cont

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

Unknown

Or MW = 148

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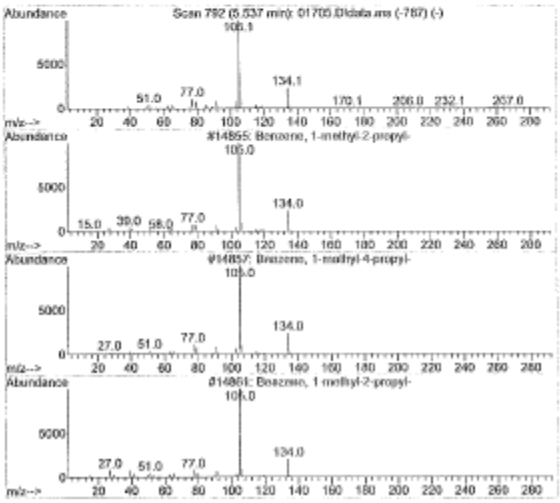
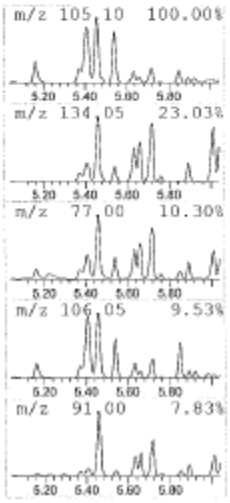
Peak Number 13 Benzene, 1-methyl-2-propyl- Concentration Rank 21

R.T.	EstConc		Area	Relative to ISTD	R.T.
5.537	21.6	ug/mL	23594000	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	93
2	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	93
3	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	90
4	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	90
5	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	90





** Substructure Report Page 1 **

Search Pattern: Scan 792 (5.537 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	CH2/3, primary or secondary saturated carbon
2	99	AR, aromatic ring
3	98	Ph-all, isolated benzenoid (6-membered) ring
4	97	PhCsat, phenyl attached to saturated carbon atom
5	97	ArC, aromatic carbon attached to carbon
6	96	Ar-C, aromatic ring-saturated carbon atom bond (chain)
7	95	-CH2/3-, methylene or methyl group (chain)
8	93	Ar-CH, aromatic-saturated C bond with 1 or more hydrogen atoms
9	91	-CH2/3-1, exactly one methylene or methyl group (chain)
10	91	CH3, methyl
11	87	CCH3, methyl bonded to carbon
12	84	CH2, methylene group
13	77	RDB4, rings + double bonds count = 4
14	76	-CH2-, methylene group (chain)
15	71	PhCH2, phenyl with methylene substituent
16	70	Ar-CH2, aryl methylene bond (chain)
17	68	Ph-2sub, disubstituted phenyl
18	68	C2H5/CH2CH2, primary or secondary ethyl linkage
19	68	CH2-CH2/3, ethyl or dimethylene group (chain)
20	67	Ar-CH2,3, aromatic bond to methyl or methylene group

Structures absent:

Number	Probability	Short Name And Description
1	99	4-brid, 4 bridging atoms in ring cluster
2	99	Si, contains silicon
3	99	ArOR, alkyl-aryl ether
4	99	OCH2/OCH3, ether oxygen attached to methyl or methylene
5	99	Ar-O, aromatic ring-oxygen atom bond (chain)
6	99	NoAr, no aromatic rings
7	99	cond, condensed ring structure (1,2-overlap)
8	99	RDB1, rings + double bonds count = 1
9	99	CH-alk-ring, carbon attached to alkyl (ring)
10	99	-O-, contains oxygen atom in chain (non-ring)

MW(Nominal Mass)Information:

Number	MW	Probability
1	148	20
2	162	12
3	147	10
4	163	10

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=98%
Possible Cl,Br cluster(s) found

Table of Conte

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

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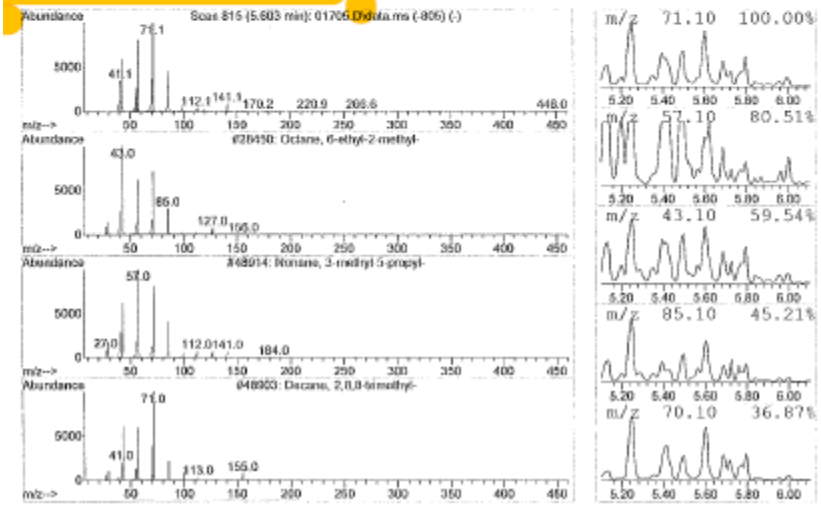
Peak Number 14 Octane, 6-ethyl-2-methyl- Concentration Rank 5

R.T.	FnlConc	Area	Relative to ISTD	R.T.
5.603	58.06 ug/mL	63157600	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	72
2	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	64
3	Decane, 2,8,8-trimethyl-	184	C13H28	1000060-81-2	50
4	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	50
5	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	50



** Substructure Report Page 1 **

Search Pattern: Scan 815 (5.803 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	98	HCSAT, saturated hydrocarbon
2	97	RDB0, rings + double bonds count = 0
3	97	HC, hydrocarbon (C and H atoms only)
4	96	sat, saturated compound (no unsaturated bonds)
5	96	C3+-alkyl, methylene attached to saturated C-atoms (chain)
6	96	nocycle, no rings
7	96	(CH2)3-ch, trimethylene linkage
8	96	CH2/3, primary or secondary saturated carbon
9	95	CH3, methyl
10	95	C2H5/CH2CH2, primary or secondary ethyl linkage
11	95	-CH2/3-, methylene or methyl group (chain)
12	95	-CH2-, methylene group (chain)
13	95	CH2-CH2-CH2/3, trimethylene group (chain)
14	95	CH2, methylene group
15	95	CCH3, methyl bonded to carbon
16	94	NoAr, no aromatic rings
17	94	CH2-CH2/3, ethyl or dimethylene group (chain)
18	60	CH-alk, tertiary carbon attached to alkyl
19	57	Ctert, tertiary carbon (>CH-)
20	57	CH-alk-chain, carbon attached to alkyl (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	98	C-O, carbon-oxygen single bond
4	99	N-C, nitrogen-carbon single bond
5	99	cond, condensed ring structure (1,2-overlap)
6	99	ArOR, alkyl-aryl ether
7	99	ph, phenyl group (C6H5)
8	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
9	99	noAr_cy, rings present, but not aromatic
10	99	C17-ring, 17 carbon atoms ring, usually steroid

MW(Nominal Mass)Information:

Number	MW	Probability
1	184	49
2	212	16
3	198	15
4	170	7

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Conte

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-D1 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

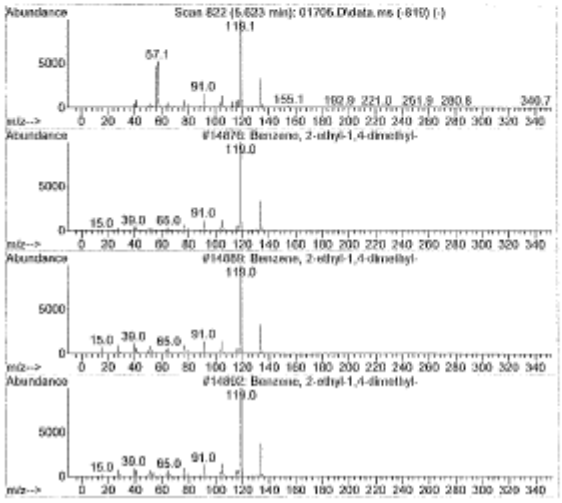
No Qv, MW = 150

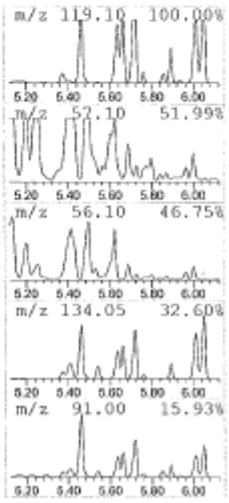
****

Peak Number 15 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	46.81 ug/mL	50926600	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	92





** Substructure Report Page 1 **

Search Pattern: Scan 822 (5.023 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	>C<, alk-chain quaternary carbon (chain)
2	98	HCSAT, saturated hydrocarbon
3	97	RDB0, rings + double bonds count = 0
4	97	HC, hydrocarbon (C and H atoms only)
5	96	nocycle, no rings
6	96	CH2/3, primary or secondary saturated carbon
7	96	sat, saturated compound (no unsaturated bonds)
8	95	CH3, methyl
9	95	CCH3, methyl bonded to carbon
10	95	-CH2/3-, methylene or methyl group (chain)
11	95	-CH2/3-1, exactly one methylene or methyl group (chain)
12	94	NoAr, no aromatic rings
13	92	-CH2-, methylene group (chain)
14	92	CH2, methylene group
15	90	C-(CH3)2, quaternary (no-H) carbon attached to 2 methyl groups
16	89	R-C(CH3)3, alkyl tertiary butyl
17	88	>C<, quaternary carbon
18	87	C(CH3)3, tertiary butyl
19	87	>C<, alk quaternary carbon attached to alkyl
20	84	CH-alk, tertiary carbon attached to alkyl

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB5_PLUS, rings + double bonds count >= 5
2	99	RDB10_PLUS, rings + double bonds count >= 10
3	99	N-C, nitrogen-carbon single bond
4	99	ph, phenyl group (C6H5)
5	99	ArOR, alkyl-aryl ether
6	99	cond, condensed ring structure (1,2-overlap)
7	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
8	99	Ar-O, aromatic ring-oxygen atom bond (chain)
9	99	.N., any nitrogen atom in ring
10	99	noAr_cy, rings present, but not aromatic

MW(Nominal Mass)Information:

Number	MW	Probability
1	190	29
2	191	16
3	204	13
4	177	6

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=98%
Possible Cl,Br cluster(s) found

Table of Content

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

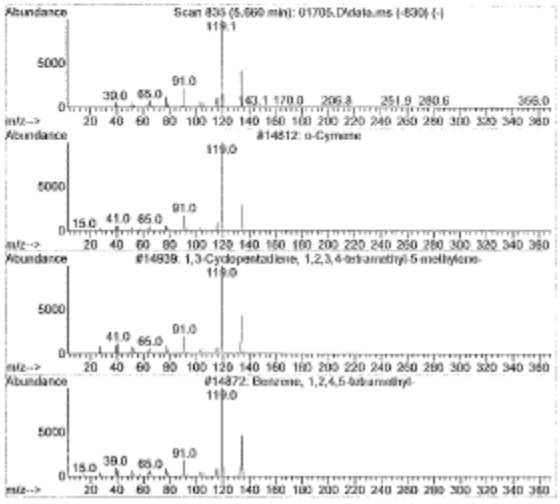
Ar, MW 134

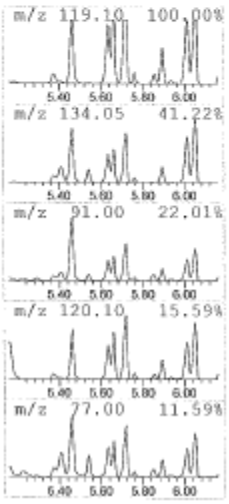
****

Peak Number 16 o-Cymene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.660	27.56 ug/mL	29976100	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	94
2	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	93
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





** Substructure Report Page 1 **

Search Pattern: Scan 835 (5.660 min): 01705.Ddata.ms

Structures present:

Number	Probability	Short Name And Description
1	99	PhCH3, phenyl methyl (toluene)
2	99	RDB4, rings + double bonds count = 4
3	98	AR, aromatic ring
4	98	ArCH3, aryl methane group
5	98	Ph-all, isolated benzenoid (6-membered) ring
6	98	Ar-C, aromatic ring-saturated carbon atom bond (chain)
7	98	PhCsat, phenyl attached to saturated carbon atom
8	97	ArC, aromatic carbon attached to carbon
9	97	HCUNS, unsaturated hydrocarbon
10	97	Ar-CH2,3, aromatic bond to methyl or methylene group
11	97	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
12	97	HC, hydrocarbon (C and H atoms only)
13	97	Ph-2+sub, phenyl with 2 or more substituents
14	96	CH2/3, primary or secondary saturated carbon
15	95	CH3, methyl
16	95	-CH2/3-1, exactly one methylene or methyl group (chain)
17	95	-CH2/3-, methylene or methyl group (chain)
18	83	CCH3, methyl bonded to carbon
19	71	PhCH2, phenyl with methylene substituent
20	70	Ar-CH2, aryl methylene bond (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB10_PLUS, rings + double bonds count >= 10
2	99	noAr_cy, rings present, but not aromatic
3	99	ArOR, alkyl-aryl ether
4	99	C17-ring, 17 carbon atoms ring, usually steroid
5	99	PhOCH3, substituted anisole (methoxyphenyl)
6	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
7	99	RDB1, rings + double bonds count = 1
8	99	PhCO, phenyl carbonyl
9	99	-O-, contains oxygen atom in chain (non-ring)
10	99	O1, contains 1 oxygen atom

MW(Nominal Mass)Information:

Number	MW	Probability
1	134	98
2	495	0

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Cont

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Unknown

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

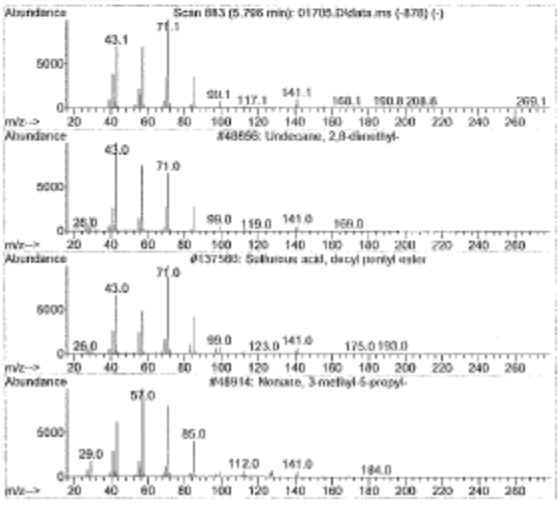
NOAA, MW ≥ 191

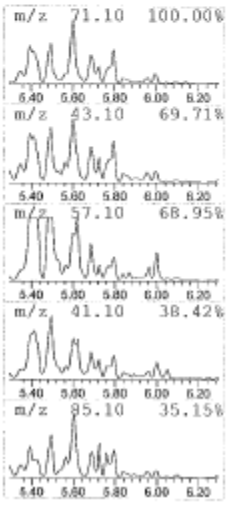
****

Peak Number 17 Undecane, 2,8-dimethyl- Concentration Rank 22

R.T.	EstConc		Area	Relative to ISTD	R.T.
5.796	21.29	ug/mL	23158200	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	86
2	Sulfurous acid, decyl pentyl ester	292	C15H32O3S	1000309-14-3	78
3	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	72
5	Decane, 4-methyl-	156	C11H24	002847-72-5	64





** Substructure Report Page 1 **

Search Pattern: Scan 883 (5.796 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	98	HCSAT, saturated hydrocarbon
2	97	HC, hydrocarbon (C and H atoms only)
3	97	RDB0, rings + double bonds count = 0
4	96	CH2/3, primary or secondary saturated carbon
5	96	sat, saturated compound (no unsaturated bonds)
6	96	nocycle, no rings
7	96	C3+-alkyl, methylene attached to saturated C-atoms (chain)
8	95	-CH2-, methylene group (chain)
9	95	-CH2/3-, methylene or methyl group (chain)
10	95	CH2, methylene group
11	95	CH3, methyl
12	95	CCH3, methyl bonded to carbon
13	95	C2H5/CH2CH2, primary or secondary ethyl linkage
14	94	CH2-CH2/3, ethyl or dimethylene group (chain)
15	94	NoAr, no aromatic rings
16	92	(CH2)3-CH, trimethylene linkage
17	91	CH2-CH2-CH2/3, trimethylene group (chain)
18	57	C5+-alkyl, n-alkyl with 5 or more carbon atoms
19	55	CH-alk, tertiary carbon attached to alkyl
20	53	CH-alk-chain, carbon attached to alkyl (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	RDB10_PLUS, rings + double bonds count >= 10
2	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
3	99	ArOR, alkyl-aryl ether
4	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
5	99	-O-, contains oxygen atom in chain (non-ring)
6	99	O1, contains 1 oxygen atom
7	99	PhCO, phenyl carbonyl
8	99	PhCsat, phenyl attached to saturated carbon atom
9	99	RDB1, rings + double bonds count = 1
10	99	O, contains oxygen

MW(Nominal Mass)Information:

Number	MW	Probability
1	198	32
2	184	29
3	212	18
4	170	5

Clorine and/or Bromine Infonnation:

Cl=0, Br=0 Probability=99%
Probability of presence of Cl=0%, of Br=0%

Table of Cont

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : 02-24-25 625 SV-12 LOW LEVEL ICAL

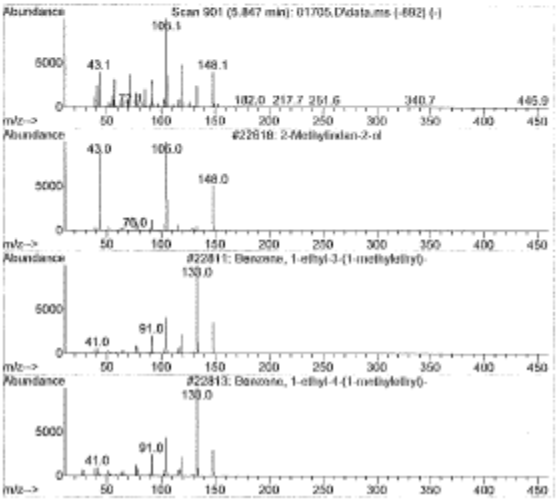
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

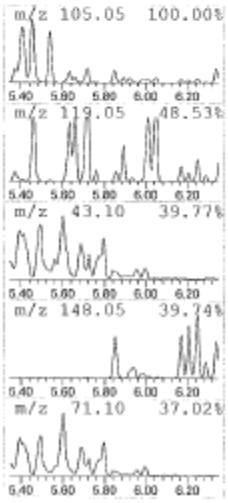
****

Peak Number 18 2-Methylindan-2-ol Concentration Rank 27

R.T.	EstConc		Area	Relative to ISTD	R.T.
5.847	17.51	ug/mL	19044800	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindan-2-ol	148	C10H12O	033223-84-6	46
2	Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	38
3	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	38
4	2-Butanone, 4-phenyl-	148	C10H12O	002550-26-7	38
5	2-Butanone, 3-phenyl-	148	C10H12O	000769-59-5	30





** Substructure Report Page 1 **

Search Pattern: Scan 901 (5.847 min): 01706.Dldata.ms

Structures present:

Number	Probability	Short Name And Description
1	99	-CH2/3-1, exactly one methylene or methyl group (chain)
2	98	CH2/3, primary or secondary saturated carbon
3	98	-CH2/3-, methylene or methyl group (chain)
4	96	CH3, methyl
5	92	CH2, methylene group
6	92	RDB4, rings + double bonds count = 4
7	86	HCUNS, unsaturated hydrocarbon
8	82	C2H5/CH2CH2, primary or secondary ethyl linkage
9	79	HC, hydrocarbon (C and H atoms only)
10	72	Ctert, tertiary carbon (>CH-)
11	67	AR, aromatic ring
12	61	CCH3, methyl bonded to carbon
13	61	Ph-all, isolated benzenoid (6-membered) ring
14	56	PhCsat, phenyl attached to saturated carbon atom
15	52	Ar-C, aromatic ring-saturated carbon atom bond (chain)
16	49	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
17	49	ArC, aromatic carbon attached to carbon
18	46	C3+-alkyl, methylene attached to saturated C-atoms (chain)
19	45	cy-C=C<, monosubstituted interior double bond (ring)
20	45	-CH2-, methylene group (chain)

Structures absent:

Number	Probability	Short Name And Description
1	99	OCH2/OCH3, ether oxygen attached to methyl or methylene
2	99	RDB1, rings + double bonds count = 1
3	99	Ar-CO, aromatic-carbonyl bond in chain (non-ring)
4	99	ether, divalent oxygen
5	99	-O-, contains oxygen atom in chain (non-ring)
6	99	4+brid, 4 bridging atoms in ring cluster
7	99	het_ring, ring containing non-carbon atom(s)
8	99	Si, contains silicon
9	99	RDB10_PLUS, rings + double bonds count >= 10
10	99	ArOR, alkyl-aryl ether

MW(Nominal Mass)Information:

Number	MW	Probability
1	162	45
2	163	13
3	176	6
4	188	4

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=98%
Probability of presence of Cl=0%, of Br=0%

Table of Contents

Library Search Compound Report

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Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On    :  3 Mar 2025    8:07 pm
Operator  : YS
Sample    : ABB1619-01 100X
Misc      : DL due to matrix, final volume=40ml
ALS Vial  : 14   Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\MQA250224.M
Quant Title  : 02-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library   : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p
```

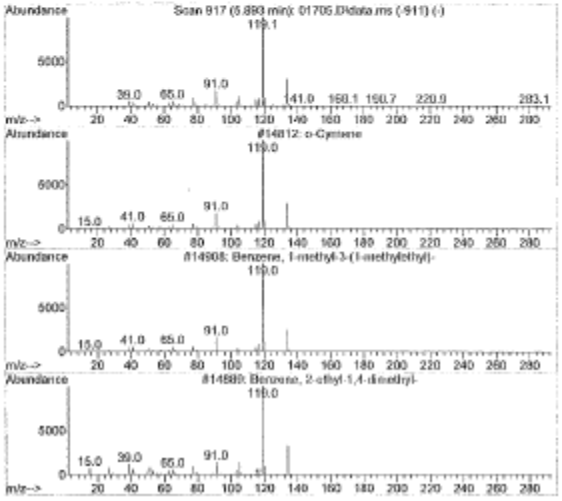
AK, MW 2/25

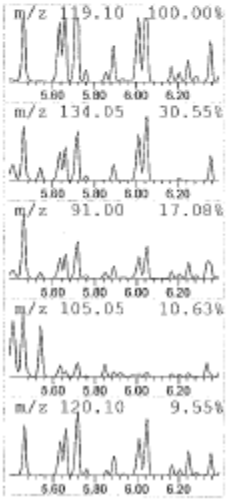
****

Peak Number 19 o-Cymene Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.893	18.55 ug/mL	20180400	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	94
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





** Substructure Report Page 1 **

Search Pattern: Scan 917 (5.893 min): 01705.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB4, rings + double bonds count = 4
2	99	AR, aromatic ring
3	99	HCUNS, unsaturated hydrocarbon
4	99	Ph-all, isolated benzenoid (6-membered) ring
5	99	ArC, aromatic carbon attached to carbon
6	99	PhCsat, phenyl attached to saturated carbon atom
7	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
8	99	HC, hydrocarbon (C and H atoms only)
9	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
10	99	CH3, methyl
11	99	CH2/3, primary or secondary saturated carbon
12	99	-CH2/3-, methylene or methyl group (chain)
13	99	-CH2/3-1, exactly one methylene or methyl group (chain)
14	98	Ar-CH2,3, aromatic bond to methyl or methylene group
15	98	Ph-2+sub, phenyl with 2 or more substituents
16	98	ArCH3, aryl methane group
17	91	CCH3, methyl bonded to carbon
18	86	PhCH2, phenyl with methylene substituent
19	86	Ar-CH2, aryl methylene bond (chain)
20	83	Ph-3sub, trisubstituted phenyl

Structures absent:

Number	Probability	Short Name And Description
1	99	-O-, contains oxygen atom in chain (non-ring)
2	99	RDB5_PLUS, rings + double bonds count >= 5
3	99	RDB10_PLUS, rings + double bonds count >= 10
4	99	ArOR, alkyl-aryl ether
5	99	O1, contains 1 oxygen atom
6	99	sat, saturated compound (no unsaturated bonds)
7	99	.N., any nitrogen atom in ring
8	99	O, contains oxygen
9	99	N, contains nitrogen
10	99	hetcyc, ring containing at least one heteroatom

MW(Nominal Mass)Information:

Number	MW	Probability
1	135	48
2	148	17
3	149	7
4	136	5

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=98%
Possible Cl,Br cluster(s) found

Table of Conte

Library Search Compound Report

Data Path : C:\msdchem\1\data\250303\
Data File : 01705.D
Acq On : 3 Mar 2025 8:07 pm
Operator : YS
Sample : ABB1619-01 100X
Misc : DL due to matrix, final volume=40ml
ALS Vial : 14 Sample Multiplier: 1

Quant Method : C:\msdchem\1\methods\Processing\WQA250224.M
Quant Title : D2-24-25 625 SV-12 LOW LEVEL ICAL

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: Lscint.p

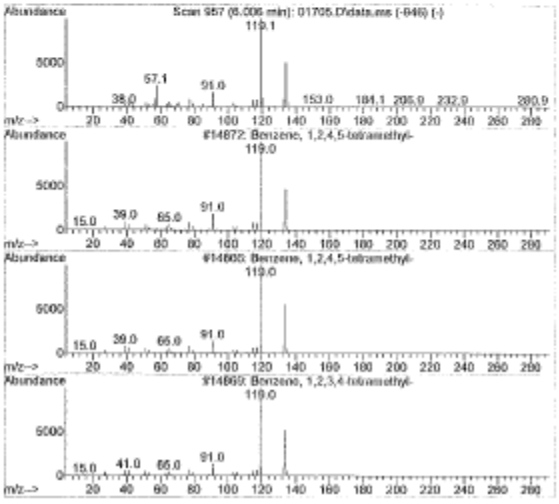
MW 3,163

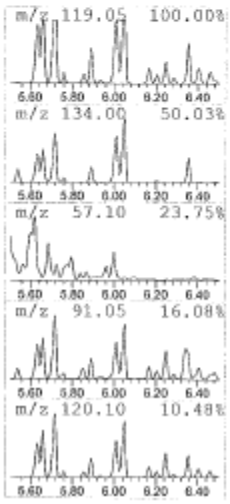
****

Peak Number 20 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.006	44.87 ug/mL	48811100	Naphthalene-d8	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	93
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93





** Substructure Report Page 1 **

Search Pattern: Scan 957 (8.008 min): 01706.D\data.ms

Structures present:

Number	Probability	Short Name And Description
1	99	RDB4, rings + double bonds count = 4
2	99	PhCH3, phenyl methyl (toluene)
3	99	HC, hydrocarbon (C and H atoms only)
4	99	HCUNS, unsaturated hydrocarbon
5	98	CH2/3, primary or secondary saturated carbon
6	99	CH3, methyl
7	99	-CH2/3-, methylene or methyl group (chain)
8	99	-CH2/3-1, exactly one methylene or methyl group (chain)
9	97	ArCH3, aryl methane group
10	97	PhCsat, phenyl attached to saturated carbon atom
11	96	Ph-all, isolated benzenoid (6-membered) ring
12	96	Ph-2+sub, phenyl with 2 or more substituents
13	96	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
14	96	Ar-C, aromatic ring-saturated carbon atom bond (chain)
15	96	Ar-CH2,3, aromatic bond to methyl or methylene group
16	95	AR, aromatic ring
17	95	ArC, aromatic carbon attached to carbon
18	47	Ph-4sub, tetrasubstituted phenyl
19	37	CCH3, methyl bonded to carbon
20	28	Ph-3sub, trisubstituted phenyl

Structures absent:

Number	Probability	Short Name And Description
1	99	-O-, contains oxygen atom in chain (non-ring)
2	99	RDB5_PLUS, rings + double bonds count >= 5
3	99	RDB10_PLUS, rings + double bonds count >= 10
4	99	O1, contains 1 oxygen atom
5	99	ArOR, alkyl-aryl ether
6	99	sat, saturated compound (no unsaturated bonds)
7	99	.N., any nitrogen atom in ring
8	99	O, contains oxygen
9	99	N, contains nitrogen
10	99	hetcyc, ring containing at least one heteroatom

MW(Nominal Mass)Information:

Number	MW	Probability
1	163	8
2	176	7
3	164	6
4	168	5

Clorine and/or Bromine Information:

Cl=0, Br=0 Probability=98%
Possible Cl,Br cluster(s) found

Appendix H: Cease and Desist Letter to Cynamic

DRENDEL & JANSONS Law Group

ATTORNEYS AT LAW
Kevin G. Drendel (kgd@batavialaw.com)
Carolyn D. Jansons (cdj@batavialaw.com)
Roman J. Seckel (rjs@batavialaw.com)
Mark D. Brent (mdb@batavialaw.com)
Edward J. Boula, III (ejb@batavialaw.com)

OF COUNSEL
Gilbert X. Drendel, Jr.

February 27, 2025

Via Certified, First Class Mail, and email:
Seamus.d@cynamicchem.com
Cynamic Chemical Company
Attention: Seamus Daley
1472 Louis Bork Dr. #1511
Batavia, IL 60510

RE: Cynamic Chemical Company – Cease & Desist

Dear Mr. Daley:

I am general legal counsel for the City of Batavia, and I am sending you this Cease and Desist letter/notice following an occurrence of a prohibited discharge that reached the City's wastewater treatment plant on February 20, 2025, resulting in an emergency response and the killing of biological organisms that are a critical component of the treatment process. As of today, the biological processes within the plant are still not viable. City workers have had to replace all the biological sludge in the system and rebalance it to safe and effective operating conditions.

Using combustible gas detection, City workers traced the source of the prohibited discharge that damaged the plant from manhole to manhole through the sewer system to the last manhole where the odor could be detected, just downstream from 1472 Louis Bork Drive, Batavia, IL 60510, the Cynamic Chemical Company building. Staff followed up by obtaining permission to perform an inspection of the premises. Staff obtained batch ticket reports for February 19 – February 25. The samples of the substance that Staff believes caused the killing of biological organisms at the plant, and they have been sent off for lab testing along with samples taken from the Cynamic Chemical Company site.

Based on the batch tickets obtained from Cynamic, staff have identified substances that are prohibited to be discharged, regardless of confirmation of the source of the discharge that caused the damage to the plant. Staff have determined that many of the products being manufactured at Cynamic Chemical Company contain substances that are prohibited from being discharged into the sanitary sewer system as provided in the Batavia Municipal Code Section 8-3-10-3 (a copy of which Code Section is included with this letter).

Based on the information the City has obtained, it is clear that Cynamic Chemical Company has been discharging prohibited substances into the City sanitary sewer system. Further, based on information collected to date, the City is confident in its assertion that Cynamic discharged prohibited waste that was the source of the slug that damaged the City's wastewater treatment plant.

Home Office
111 Flinn Street
Batavia, IL 60510
Phone: 630.406.5440
Fax: 630.406.6179

www.batavialaw.com
www.ilfamilylaw.com

Satellite Office
2000 W. Galena Blvd., Ste 204
Aurora, IL 60506
Phone: 630.897.5957

Therefore, I am sending this letter/notice to demand that Cynamic Chemical Company ***cease and desist from discharging any prohibited substances into the sanitary sewer system immediately***.

The City has also notified the Illinois Environmental Protection Agency of the occurrence of the discharge, and the City will be cooperating with the IEPA with the investigation and follow up. I should note to you that the IEPA representative who inspected the wastewater treatment plant after the occurrence has never witnessed a more significant occurrence. The City had to haul in twenty-five (25) semi-truckloads of new biological sludge and is still in the process of getting the plant back into operation. The City is, therefore, treating this matter as a matter of the highest importance and seeks your immediate cooperation in minimizing the damage that has been done and in avoiding any future occurrences.

Sincerely,

DRENDEL & JANSONS LAW GROUP

Kevin G. Drendel

KGD/lf

R:\Secretary\Clients - Municipal\City of Batavia\Ordinance Enforcement\Cynamic Chemical Co. Sewer Discharge\2025-2-27 Cease & Desist Letter.docx

Appendix I: Chemical Oxygen Demand Results from Cynamic from March 6, 2025

Sample Results
(Continued)

Sample: COB 710 - Cyniamic
ABC0658-02 (Water)

Analyte	Result /Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
Wet Chemistry									
Chemical Oxygen Demand	10900	726	800	mg/L	03/06/25 14:30	03/13/25	20	HACH 8000	BB02462

Appendix J Semi Volatile Organics at Batavia WWTP from February 22, 2025

Semivolatile Organics - Prep EPA 625

1,2-Dihydro-2,2,4-trimethylquinoline	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,3,4-Trimethylquinoline	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,4,6-Trichlorophenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,4,6-Trimethylquinoline	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,4-Dichlorophenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,4-Dimethylphenol	ND	2.00	2.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,4-Dimethylquinoline	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,4-Dinitrophenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,6-Dimethylquinoline	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2,6-Di-tert-butyl-4-methoxyphenol	ND	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2-Chlorophenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2-Methylnaphthalene	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2-Nitrophenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2-Phenyl-2-propanol	ND	0.600	0.600	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
3,3-Dichlorobenzidine	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
4,6-Dinitro-2-methylphenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
4-Chloro-3-methylphenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
4-Nitrophenol	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
4-tert-Butylphenol	2.09	2.00	2.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Acenaphthene	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Acenaphthylene	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Acetophenone	2.53	0.600	0.600	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Anthracene	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzo(a)anthracene	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzo(a)pyrene	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzo(b)fluoranthene	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzo(g,h,i)perylene	ND	0.600	0.600	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzo(k)fluoranthene	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzothiazole	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
bis(2-Ethylhexyl)adipate	ND	0.500	0.500	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Bis(2-ethylhexyl)phthalate	6.03	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Bisphenol-A	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Butyl benzyl phthalate	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Caprolactam	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Chrysene	ND	0.300	0.300	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Dibenzo(a,h)anthracene	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Diethyl phthalate	11.2	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Dimethyl phthalate	ND	1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Di-n-butyl phthalate	69.6	10.0	10.0	ug/L	02/22/25 12:00	02/26/25	5	625/625.1	BB01704
Di-n-octyl phthalate	ND	1.10	1.10	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Fluoranthene	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Fluorene	ND	0.400	0.400	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Indeno(1,2,3-cd)pyrene	ND	0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Isophorone	ND	0.500	0.500	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704

Analyte	Result	/Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
GC/MS Peak Search (SVOC) - Tentatively Identified Compounds										
1,6-Octadien-3-ol, 3,7-dimethyl-	46.2	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	4.26	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
2-Propanol, 1,1`-oxybis-	5.74	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
4-tert-octylphenol Diethoxylate	44.5	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Benzeneethanol, .alpha., alpha.-dimethyl-	11.2	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Cyclohexanol, 4-(1,1-dimethyl)-, cis-	10.0	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Cyclohexanone, 4-(1,1-dimethylethyl)-	39.7	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Ethanol, 2-butoxy-, phosphate (3:1)	16.6	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Hexanoic acid, 3,5,5-trimethyl-	8.08	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Octoxynol 3	34.1	N, J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown Ar, O, RT 11.601	7.05	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown N, O, RT 15.542	11.5	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown Non Ar, O, RT 11.408	4.41	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown Non Ar, RT 7.046	38.7	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Semivolatile Organics - Prep EPA 625 (Continued)										
m,p-Cresol	ND		1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Naphthalene	9.47		0.500	0.500	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
N-Nitroso-di-n-butylamine	ND		0.700	0.700	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
N-Nitroso-di-n-propylamine	ND		1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
N-Nitrosodiphenylamine	ND		0.300	0.300	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
O-Cresol	ND		1.00	1.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Pentachlorophenol	ND		0.500	0.500	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Phenanthrene	ND		0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Phenol	ND		0.500	0.500	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Phenyl Sulfone	ND		0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Pyrene	ND		0.600	0.600	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Quinoline	ND		0.200	0.200	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Surrogate: 2,4,6-Tribromophenol	*81%*		*10-136*				*02/26/25*	*1*	*625/625.1*	
Surrogate: 2-Fluorobiphenyl	*74%*		*20-129*				*02/26/25*	*1*	*625/625.1*	
Surrogate: 2-Fluorophenol	*40%*		*10-106*				*02/26/25*	*1*	*625/625.1*	
Surrogate: 4-Terphenyl-d14	*35%*		*18-160*				*02/26/25*	*1*	*625/625.1*	
Surrogate: Nitrobenzene-d5	*82%*		*13-150*				*02/26/25*	*1*	*625/625.1*	
Surrogate: Phenol-d5	*34%*		*10-105*				*02/26/25*	*1*	*625/625.1*	

Analyte	Result	/Qual	DL	RL	Units	Date Sampled	Date Analyzed	DF	Method	Prep Batch
GC/MS Peak Search (SVOC) - Tentatively Identified Compounds (Continued)										
Unknown O, N, RT 16.798	6.92	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown, Ar, ether, RT:18.960	44.4	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown, Ar, ether, Si, RT:18.480	4.10	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown, Ar, HC, RT:6.336	5.65	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown, Ar, O, RT:13.687	6.54	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704
Unknown, NoAr, N, O, RT:5.279	5.65	J	3.00	3.00	ug/L	02/22/25 12:00	02/26/25	1	625/625.1	BB01704

Appendix K: Screening Technique to Identify Gas/Vapor Toxic Discharges for Pollutants Identified in February 25, 2025 sample collected at Cynamic's Triple Basin (Appendix G)

Adapted from June 1992 United States Environmental Protection Agency Guidance to Protect WWTP Workers from Toxic and Reactive Gases and Vapors, Appendix B

The screening technique entails (1) identifying gas/vapor toxicity criteria; (2) conversion of gas/vapor toxicity criteria into corresponding IU discharge screening levels; (3) comparison of these screening levels with actual IU discharge levels. Discharges above the specified screening level may warrant further investigation.

The toxicity criteria reference the American Conference of Governmental Industrial Hygienists (ACGIH) threshold limit value-time weighted averages (TLV-TWA) which are the gas/vapor toxicity levels are the vapor phase concentrations of volatile organic compounds to which nearly all workers may be repeatedly exposed, over a 8-hour workday and a 8 hour workweek without adverse effect.

Cvap from ACGIH.org; HA from pubchem.ncbi.nlm.nih.gov

Compound	Cdiscahrge = Concentration in Discharged Wastewater (mg/L)	HA = Henry's Law Constant (atm*m^3)/mol	R = Ideal Gas Constant (atm/mol K)	T = Temperature (K)	Cvap = ACGIH TLV-TWA (mg/m^3)	HC = Henry's Law Constant (mg/m^3)/(mg/L)	Clvl = Discharge Screening Level (mg/L)	Cvapor = Equilibrium Vapor Phase of Discharge (mg/M^3)	Fraction of TLV-TWA
Naphthalene	207	4.04E-04	0.08206	298	52	16.52	3.15	3419.64	**65.76**
Di-n-butyl phthalate	514	1.81E-06	0.08206	298	5	0.07	71.43	35.98	**7.2**
Chloroform	2.56	3.67E-03	0.08206	298	49	150.08	0.33	384.2	**7.84**
Bis(2-ethylhexyl)phthalate	1.08	2.70E-07	0.08206	298	0.1	0.01	10	0.01	0.1
Diethyl phthalate	2.52		0.08206	298	n/a	-	-	-	-
2-Chlorotoluene	3.75		0.08206	298	n/a	-	-	-	-
Acetone	3.27	3.97E-05	0.08206	298	594	1.62	366.67	5.3	0.01
Ethylbenzene	0.105	7.88E-03	0.08206	298	87	322.24	0.27	33.84	0.39
Assuming m-p xylene is 100% m-xylene	0.385	7.18E-03	0.08206	298	87	293.61	0.3	113.04	**1.3**
Assuming m-p xylene is 100% p-xylene	0.385	6.90E-03	0.08206	298	87	282.16	0.31	108.63	**1.25**
o-xylene	0.191	5.18E-03	0.08206	298	87	211.83	0.41	40.46	0.47
Toluene	0.121	6.64E-03	0.08206	298	75	271.53	0.28	32.86	0.44

Appendix L: Screening Technique to Identify Flammable/Explosive Discharges for Pollutants Identified in February 25, 2025 sample collected at Cynamic's Triple Basin (Appendix G)

Adapted from June 1992 United States Environmental Protection Agency Guidance to Protect WWTP Workers from Toxic and Reactive Gases and Vapors, Appendix C

The screening technique describes a procedure that will (1) Convert lower explosive limit (LEL) data into corresponding IU discharge screening levels, and (2) compare the screening levels to actual IU discharge levels. Discharges that exceed screening levels may warrant further investigation.

MW, LEL and Flash Point from pubchem.ncbi.nlm.nih.gov

Compound	HA=Henry's Law Constant	MW= Molecular W	R=Ideal Gas Constant	T=Temperature	LEL = Lower Explosive Limit	Closed Cup flash point	Cvap= 10% of LEL expressed in conc.	HB=Henry's Law Constant	CM=Discharge Screening Level	Cdiscahrge = Concentration in Discharged Wastewater
	(atm m^3)/mol	g/mol	atm 1/mol K	K	%	°C	mol/m^3	(mol/m^3)/(mg/l)	mg/l	(mg/L)
Naphthalene	4.04E-04	128.7	0.08206	298	0.9	79	0.037	0.00013	284.6	**207**
Di-n-butyl phthalate	1.81E-06	278.34	0.08206	298	0.5	157	0.02	0.00000266	75188.0	514
Chloroform	3.67E-03	119.37	0.08206	298	none	none	-	-	-	-
Bis(2-ethylhexyl)phthalate	2.70E-07	390.6	0.08206	298	0.3	215	0.012	0.00000028	428571.4	1.08
Diethyl phthalate	6.10E-07	222.24	0.08206	298	0.7	161	0.029	0.000000112	258928.6	2.52
2-Chlorotoluene	3.57E-03	126.58	0.08206	298	1.36	43	0.056	0.00115	48.7	3.75
Acetone	3.97E-05	58.08	0.08206	298	2.5	-17.8	0.102	0.000028	3642.9	3.27
Ethylbenzene	7.88E-03	106.16	0.08206	298	0.8	15	0.033	0.00304	10.9	0.11
(HA for m-xylene)	7.18E-03	106.16	0.08206	298	1.1	25	0.045	0.00277	16.2	0.39
m,p-xylene (HA for p-xylene)	6.90E-03	106.16	0.08206	298	1.1	25	0.045	0.00266	16.9	0.39
o-xylene	5.18E-03	106.16	0.08206	298	0.9	31	0.037	0.001995	18.5	0.19
Toluene	6.64E-03	92.14	0.08206	298	7.1	4	0.29	0.00295	98.3	0.12