CERTIFICATION OF APPROVAL

Effect of solution pH and initial solute concentration of organic compound on the adsorption by *Pentace triptera*.

by

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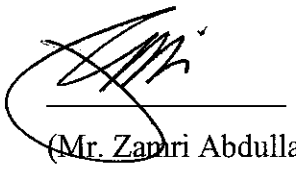

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the reference and acknowledgements, and that the original work contained herein have not been taken or done by unspecified sources or persons.

ABDUL MALIK BIN NIK ZAID

ABSTRACT

The project is to examine the effect of solution pH and initial concentration on the adsorption of organic compound by *Pentace triptera*. In this project *Pentace triptera* is used as adsorbent to remove benzene and toluene in wastewater. Adsorption concept is applied in this project. Fix size of grinding Pentace tripera used as adsorbent and various of concentration and pH of benzene and toluene are prepared. Samples shake with adsorbent using rotary shaker. After adsorption, samples are tested by using UV-vis spectrophotometer. Result show that the concentration of benzene and toluene after adsorption higher than before adsorption. First hypothesis was desorption of benzene and toluene occurs by *Pentace triptera*. Project continues by using Gas Chromatography Mass Spectrometer. Qualitative result show benzene and toluene concentration at different pH sample are zero. Separation of component sample has been show on chromatogram. Samples contain many components after adsorption based on peak appearance on chromatogram. Most of the samples were found to contain carbamic acid. Hypothesis from GCMS result were the carcinogenic compound shown by benzene and toluene. Different between GCMS and UV-vis explaining the qualitative measurement by Uv-vis may contribute to error in measurement of benzene and toluene concentration. Benzene and toluene were adsorbed by pentace triptera and at the same time benzene and toluene extract and digest Pentace Triptera leaves. Leaves normally contain chlorophyll and many other organic compounds such as amine group. Carbamic acid is the component that identifies to be mostly extracted from Pentace triptera leaves where toluene gives more formation of carbamic acid in sample.

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CHAPTER 1
INTRODUCTION

1.1. BACKGROUND OF STUDY

The project is to examine the effect of solution pH and initial concentration on the adsorption of organic compound by *Pentace triptera*. In this project *Pentace triptera* is used as adsorbent to remove benzene and toluene in wastewater. Benzene and toluene are organic compounds that are hazardous and harmful to human being. In petroleum refinery and other petrochemical industries, high amount of benzene and toluene are released into the water stream. The concept of adsorption is applied to remove components present in low concentration in nonadsorbing solvent and to separate the components in liquid mixtures by selective adsorption on solid adsorbent. In this project, *Pentace triptera* leaves will be used as an adsorbent to determine the optimum pH and initial concentration for the adsorption process to occur.

1.2. PROBLEM STATEMENT

The primary products of the petroleum refining industry fall into three major categories: fuels, finished non-fuel products and chemical industry feedstock. Many refineries unintentionally released liquid pollutants including benzene and toluene into ground and surface water. Accidentally discharge of large quantities of pollutants can occur as a result of abnormal operations in a refinery and potentially pose a major local environmental hazard. Adsorption is employed to remove the hazardous material and study effect of solution pH and initial concentration are important.

1.2.1 Problem Identification

1.2.1.1 *Pentace Triptera* as adsorbent

Pentace triptera is one of abundant plant in Malaysian tropical rainforest. Since Malaysian tropical rainforest is very rich with this plant, we would like to make use of this plant by using its leave as an adsorbent. In previous practice, as in the adsorption technology we are using the activated carbon as an adsorbent to adsorb the hazardous materials which are benzene and toluene.

Activated carbon also has been used in the treatment of waste water and drinking water. Based on study by Journal by Gullon, M and Front, R. (2000) about dynamic pesticide removal with activated carbon fiber, usually, the drinking water treatment ends in adsorption with granular activated carbon beds removes taste, odor and other micro pollutants. Although the odor and taste levels are apparently removed by granular activated carbon, it is still not effective in removing the micro pollutant in the water. Then, they conduct a research to develop a new carbon adsorbent which more effective for micro pollutant which is Activated Carbon Fiber because fiber structure is an ideal adsorbent where pores are slit-shaped, uniform in size and oriented along the fiber axis. By crossed-linked fiber structure which presence of micro pores that directly accessible from the external surface fiber provides much higher adsorption capacity and adsorption kinetic. *Pentace triptera* leaves used in this project have a fiber structure characteristic. By having this characteristic on the leaves, it could replace the Activated Carbon Fiber for a better adsorption process.

Other characteristic of *Pentace triptera* leave is organic compound. Organic compound can be obtained from natural resource that contain carbon compound. Journal by Franz, M. Arafat, H. and Pinto, N. (1999) about chemical surface heterogeneity on the adsorption mechanism of dissolved aromatics on activated carbon, it is found that water

adsorption, dispersion/repulsive interactions, and hydrogen-bonding were main mechanisms by which surface oxygen groups influence the adsorption capacity, while donor-acceptor interaction were found not to be significant. The adsorption mechanism also found to be influenced by the properties of functional group on the aromatic adsorbate. *Pentace triptera leaves* which naturally organic compound substance is one of alternative adsorbent to replace activated carbon as adsorbent to adsorb toluene and benzene.

1.2.1.2 Toxicity of benzene/toluene.

Benzene and toluene is an aromatic chemical compound. Both of the chemical are in liquid form and contain in refinery effluent. It is important to remove this type of chemical because it is hazardous for human. Based on the material safety data sheet, benzene and toluene can cause respiratory tract irritation, skin irritation, eye irritation, central nervous system depression, and a cancer hazard to human being. There are many ways human can be affected from these materials whether through inhale, skin contact, eye contact and ingestion. Higher dose of benzene and toluene exposure may result in illness for our health.

Benzene and toluene can be affected by ingestion in which resulting in vomiting. Breathing of benzene and toluene into the lungs must be avoided since small quantities may result in pneumonitis. Small amounts of this product aspirated into the respiratory system during ingestion or vomiting may cause mild to severe pulmonary injury, possibly progressing to death.

Inhalation may also cause difficulty in seeing in bright light. High vapor/aerosol concentrations (greater than approximately 1000 ppm) are irritating to the eyes and the respiratory tract may cause headaches, dizziness anesthesia, drowsiness, unconsciousness, central nervous system effects, brain damage and possibly death.

Skin contact with benzene and toluene could cause irritation of the skin. Peculiar skin sensations may be produced such as a "pins and needles feeling" or numbness. Occasional brief contact with the liquid will not result in significant irritation unless evaporation is impeded. Skin contact may aggravate an existing dermatitis condition.

The Summary of Chronic Health Hazards from Toluene and benzene vapor causes narcosis health effect. Early to moderate central nervous system depression may be evidenced by giddiness, headache, dizziness and nausea; in extreme cases, unconsciousness and death may occur. Aspiration pneumonitis may be evidenced by coughing, labored breathing and cyanosis (bluish skin); in severe cases death may result. Repeated or prolonged exposure to liquid toluene may cause drying and cracking of the skin. Prolonged intentional Toluene abuse may lead to brain damage characterized by disturbances in gait, personality changes and loss of memory. Comparable central nervous system effects have not been shown to result from occupational exposure to Toluene. Toluene may be harmful to the human fetus based on positive test results with laboratory animals. Case studies reveal that prolonged intentional abuse of Toluene during pregnancy may cause birth defects in humans. (Hill Brother Chemical Corporation, 2001 and Matheson Tri-gas Inc., 2003)

1.2.1.3 Important of pH and initial concentration

Solution pH and initial concentration of solutes play a major role in adsorption of organic compound. Solution pH and initial concentration set a medium for adsorption to takes place where different pH and initial concentration will result in different adsorption process. If the solution pH were higher than the pKa of the organic compound, adsorption would be insignificant since dissociation of the organic would occur. If the solution pH is too low, it would denature the biomass and effectiveness would be affected.

Initial concentration of the solute relate to the uptake capacity of biomass. In a fixed biomass size and mass, it is believe that increasing the initial concentration of solute would reduce the uptake capacity since available adsorption site is less. Regarding the effect of pH and initial concentration towards the solution, it is important to find optimum pH solution and initial concentration for best adsorption to occur. In this project, initial solute concentration is varies from 1-100 ppm which under the range of benzene discharges by Petroleum Refinery. There are also varying in pH of the solution which is at two acidic solution, two alkaline solutions and neutral.

1.2.2 Significant of the project

In this project, optimum pH and initial solute concentration for adsorption of organic compound is to be determined. In conventional wastewater treatment system, hazardous organic compound are removed using activated carbon which is the cost for activated carbon is too high. As an alternative, cheap and easy to get *Pentace triptera* could be used to replace activated carbon. Significantly from this project, a new alternative of using *Pentace triptera* leaves replacing activated carbon in wastewater treatment technology.

1.3 OBJECTIVE AND SCOPE OF STUDY

Objectives of the project:

1. To study the effect of regulating the solution pH and its effect on adsorption of toluene and benzene in a batch adsorption system.
2. To study the effect of changing the initial concentration of solute and its effect on adsorption of toluene and benzene in a batch adsorption system.

Referring to the objective of the project, it is relevant to study the effect of solution pH and initial concentration of solute since pH and initial concentration is important for adsorption to take place. Since, *Pentace triptera* is an abundant plant in Malaysia, so why not it is been used as adsorbent.

This present study is to examine the feasibility of using *Pentace triptera* which is grown abundantly in country for adsorption of toluene and benzene from wastewater that contain these hazardous organic compounds. This study could provide a wider option for using of biomass and optimum condition for a generation of new technology of absorbing hazardous material from refinery effluent.

CHAPTER 2
LITERATURE REVIEW

2.1 BIOSORPTION STUDY

Biosorption is a property of certain types of inactive, dead, microbial biomass to bind and concentrate heavy metals from even very dilute aqueous solutions. Biomass exhibits this property, acting just as a chemical substance as an ion exchanger of biological origin. It is particularly the cell wall structure of certain algae, fungi and bacteria which was found responsible for this phenomenon. Opposite to biosorption is metabolically driven active bioaccumulation by living cells. That is an altogether different phenomenon requiring a different approach for its exploration.(Volesky, 2004)

Mining activities, agricultural run off, industrial and domestic effluents are mainly responsible for the increase of the metallic species released into the environment. Contrary to toxic organics, that in many cases can be degraded, the metallic species that are released into the environment tend to persist indefinitely, accumulating in living tissues throughout the food chain. A complete understanding about noxious effects caused by the release of toxic metals into the environment and the emergence of more severe environmental protection laws, have encouraged studies about removal/recovery of heavy metals from aqueous solutions using biosorption. (Cossich, 2002)

The mechanisms by which microorganisms remove metals from solutions are:

(i) Extracellular accumulation/precipitation.

(ii) Cell-surface sorption or complexation

(iii) Intracellular accumulation.

Among these mechanisms, process (i) may be facilitated by using viable microorganisms, process (ii) can occur with alive or dead microorganisms, while the process (iii) requires microbial activity. Although living and dead cells are capable of metal accumulation, there are differences in the mechanisms involved, depending on the extent of metabolic dependence. (Cossich, 2002)

The physiological state of the organism, the age of the cells, the availability of micronutrients during their growth and the environmental conditions during the biosorption process (such as pH, temperature, and presence of certain co-ions), are important parameters that affect the performance of a living biosorbent. The efficiency of metal concentration on the biosorbent is also influenced by metal solution chemical features. (Cossich, 2002)

Biosorption uses biomass as the raw materials which are either abundant (seaweeds) or from the wastes of other industrial operations (fermentation wastes). The metal-sorbing performance of certain types of biomass can be more or less selective for heavy metals. It will depend on the type of biomass, the mixture in the solution, types of biomass preparation and the physico-chemical environment. Biosorption process for metal removal is as high performance as commercially used competitors, namely the ion exchange treatment. Effluent qualities in the order of only ppm (mg/L) of residual metal(s) can be achieved. While commercial ion exchange resins are rather costly, the price tag of biosorbents can be an order of magnitude cheaper (1/10 the ion exchange resin cost). The main attraction of biosorption is its cost effectiveness. (Volesky, 2004)

While ongoing research is essential for improving and optimizing metal biosorption effectiveness, wastewater purification applications of the biosorption process are ready for pilot testing of this alternative new technology. Optimization of specific biosorption process applications has to be done in conjunction with industrial users/clients and requires specific process engineering expertise and a serious development capital commitment.

2.2 BIOMASS

Most of biomass materials are from bacteria (e.g. *Spherotilus natans*), sludge bacterium (*Zoogloea ramigera*), fungi (e.g. *Phellinus badius*), algae and also plant materials such as *Medicago sativa* (Alfalfa). The biomass adsorptive capacities for heavy metals under the same physical and chemical environment are vary depending on the amount and type of biomass used. Even within a single biomass species, there is a noticeable variation in the adsorption capacity. In order to obtain an optimum potential biosorptive capacity, a single source or species of biomass may not be successful. A heterogeneous mixture of different microbial species may give better results. Biomass can be used in either living or nonliving state. (Elsevier, 2004)

Some of the biomass types come as a waste by-product of large-scale industrial fermentations (the mold Rhizopus or the bacterium Bacillus subtilis). Other metal-binding biomass types, certain abundant seaweeds (particularly brown algae e.g. Sargassum, Ecklonia), can be readily collected from the oceans. These biomass types, serving as a basis for metal biosorption processes, can accumulate in excess of 25% of their dry weight in deposited heavy metals: Pb, Cd, U, Cu, Zn, even Cr and others. Research on biosorption is revealing that it is sometimes a complex phenomenon where the metallic species could be deposited in the solid biosorbent through different sorption processes of ion exchange, complication, chelating, micro precipitation, etc. (Volesky, 2004)

There are potent biosorbents easily available in all the three groups: algae, fungi and bacteria. A source of low cost biomass produced in great quantities, are marine macroalgae. Recent studies about biosorption of toxic metals by algae are focused on toxicological aspects, metal accumulation, and pollution indicators by living (metabolically active) biomass. (Cossich, 2002)

2.3 ADSORPTION

Adsorption phenomena are operative in most natural physical, biological and chemical system, and its operations employing solids such as activated carbon and synthetic resins for industrial application and purification of wastewater. The adsorption process involves separation of a substance from one phase accompanied by its accumulation or concentration at the surface of another. The adsorbing phase is the adsorbent and the material concentrated or adsorbed at the surface is the adsorbates. Adsorption at the surface or interface is largely the result of the binding forces between the individual atoms, ions or molecules of an adsorbate and the surface, all of these forces having their origin in electromagnetic interactions. (Henly, 1998)

Adsorption, the binding of molecules or particles to a surface, must be distinguished from absorption, the filling of pores in a solid. The binding to the surface is usually weak and reversible. Just about anything including the fluid that dissolves or suspends the material of interest is bound, but compounds with color and those that have taste or odor tend to bind strongly. Compounds that contain chromogenic groups (atomic arrangements that vibrate at frequencies in the visible spectrum) very often are strongly adsorbed on activated carbon. Decolorization can be wonderfully efficient by adsorption and with negligible loss of other materials. (Bungay, 2004)

The most common industrial adsorbents are activated carbon, silica gel, and alumina, which has enormous surface areas per unit weight. Activated carbon is produced by roasting organic material to decompose it to granules of carbon such as coconut shell, wood, and bone are common sources. Silica gel is a matrix of hydrated silicon dioxide. Alumina is mined or precipitated aluminum oxide and hydroxide. Although activated carbon is a magnificent material for adsorption, its black color persists and adds a grey tinge if even trace amounts are left after treatment; however filter materials with fine pores remove carbon quite well. (Bungay, 2004)

A surface already heavily contaminated by adsorbates is not likely to have much capacity for additional binding. Freshly prepared activated carbon has a clean surface. Charcoal made from roasting wood differs from activated carbon in that its surface is contaminated by other products, but further heating will drive off these compounds to produce a surface with high adsorptive capacity. Although the carbon atoms and linked carbons are most important for adsorption, the mineral structure contributes to shape and to mechanical strength. Spent activated carbon is regenerated by roasting, but the thermal expansion and contraction eventually disintegrate the structure so some carbon is lost or oxidized. (Bungay, 2004)

2.4 ADSORBENT

The adsorbent is the separating agent used to express the difference between molecules in a mixture: adsorption equilibrium or kinetics (Baron, 2004). The most common industrial adsorbents are activated carbon, silica gel, and alumina, because they present enormous surface areas per unit weight. Activated carbon is produced by roasting organic material to decompose it to granules of carbon - coconut shell, wood, and bone are common sources. Silica gel is a matrix of hydrated silicon dioxide. Alumina is mined or precipitated aluminum oxide and hydroxide. Although activated carbon is a magnificent material for adsorption, its black color persists and adds a grey tinge if even trace amounts are left after treatment; however filter materials with fine pores remove carbon quite well. (Bungay, 2004)

2.4.1 Organic Material

A wide variety of organic materials have been used as for "sorption", besides activated carbon or charcoal. Some might function as solid adsorbent rather than adsorbent. Among these are cellose (the most abundant biopolymer in nature), chitin (the second abundant biopolymer in nature), collagen, wool, starch-polyacrylamide gels (which absorb many times their own weight of water at ambient temperature, but release most of it by gently heating), polysaccharides derive from corn and miscellaneous forms of biomass. (Kneabel, 1995)

2.4.2 Activated Carbon

The base materials that comprise activated carbon include: wool, coal, peat, coconut shell, saran, recycle tires, and others. The final adsorbents all look, to the casual observer, pretty much the same example granular or pellets but appearance can be deceptive. Acticavated produces a distribution of internal pores and affects the carbon surface example graphite versus oxidized, generally to enhance its adsorptive capacity. Thus by varying activation conditions, difference that varies depending on the nature of the base material which ash content that of course inorganic. Alkali ash near or at the surface can be removed by acid washing. The microscopic structure (pore size and surface area), surface qualities, and chemical composition all strongly affect adsorption characteristics and they therefore affect the performance parameter (capacity, selectivity, regeneralibility, kinetics, compatibility, and cost). (Kneabel, 1995)

2.5 ION EXCHANGE

Exchange adsorption or ion exchange involve electrostatic attachment of ionic species to sites of opposite charge at the surface of an adsorbent, with subsequent displacement of these species by other ionic adsorbates of greater electrostatic affinity, which are comprised of both London dispersion force and classical electrostatic force.

Chemical adsorption involves a reaction between an adsorbate and an adsorbent resulting in a change in the chemical form of the adsorbate. The resulting chemisorptive bond is usually stronger than that derive from physical Van Der Waals forces. Attachment of adsorbate molecules at functional groups on adsorbent surfaces can also result from specific interaction which does not result in adsorbate transformation. While for physical adsorption there is intermolecular attractive force between molecule of adsorbates and adsorbent. (Shuib, 2002)

An organic ion exchange resin is composed of high-molecular-weight polyelectrolyte that can exchange their mobile ions for ions of similar charge from the surrounding medium. Each resin has a distinct number of mobile ion sites that set the maximum quantity of exchanges per unit of resin. (Remco Engineering, 1981)

2.6 CHEMISORPTION AND PHYSISORPTION

Chemisorptions (or chemical adsorption) are adsorption in which the forces involved are valence forces of the same kind as those operating in the formation of chemical compounds. The problem of distinguishing between chemisorptions and physisorption is basically the same as that of distinguishing between chemical and physical interaction in general. No absolutely sharp distinction can be made and intermediate cases exist, for example, adsorption involving strong hydrogen bonds or weak charge transfer. (Everett, 2001)

Some features which are useful in recognizing chemisorptions include:

a. The phenomenon is characterized by chemical specificity

b. Changes in the electronic state may be detectable by suitable physical means

c. The chemical nature of the adsorptive may be altered by surface dissociation or reaction in such a way that on desorption the original species cannot be recovered; in this sense chemisorptions may not be reversible;

d. The energy of chemisorptions is of the same order of magnitude as the energy change in a chemical reaction between a solid and a fluid: thus chemisorptions, like chemical reactions in general, may be exothermic or endothermic and the magnitudes of the energy changes may range from very small to very large;

e. Elementary step in chemisorptions often involves an activation energy where the activation energy for adsorption and desorption is extremely large, true equilibrium may be achieved slowly or in practice not at all. For example in the adsorption of gases by solids the observed extent of adsorption, at a constant gas pressure after a fixed time, may in certain ranges of temperature increase with rise in temperature. Removal of the chemisorbed species from the surface may be possible only under extreme conditions of temperature or high vacuum, or by some suitable chemical treatment of the surface; (Everett, 2001)

Physisorption (or physical adsorption) is adsorption in which the forces involved are intermolecular forces (van der Waals forces) of the same kind as those responsible for the imperfection of real gases and the condensation of vapors, and which do not involve a significant change in the electronic orbital patterns of the species involved. The term van der Waals adsorption is synonymous with physical adsorption, but its use is not recommended. (Everett, 2001)

Some features which are useful in recognizing physisorption include:

a. The phenomenon is a general one and occurs in any solid/fluid system, although certain specific molecular interactions may occur, arising from particular geometrical or electronic properties of the adsorbent and/or adsorptive;

b. The adsorbed species are chemically identical with those in the fluid phase, so that the chemical nature of the fluid is not altered by adsorption and subsequent desorption;

d. The energy of interaction between the molecules of adsorbate and the adsorbent is of the same order of magnitude as, but is usually greater than, the energy of condensation of the adsorptive;

e. The elementary step in physical adsorption from a gas phase does not involve activation energy. Slow, temperature dependent, equilibration may however result from rate-determining transport processes;

f In physical adsorption, equilibrium is established between the adsorbate and the fluid phase. (Everett, 2001)

2.7 EFFECT OF CONCENTRATION ON BIOSORPTION

Each of the test metal ions was separately adsorbed by the *Nocardia* biomass. Several metal ion concentrations are used at constant pH 6.0. The adsorption of metal ions occurs rapidly, the equilibrium values of adsorption being reach after 4-hours contact with the biomass.

The best adsorption capacity of *Nocardia* cells was observed for Pb^{2+} ions. The electrostatic interaction of metal ions with the negatively charged functional groups on the microorganism surface is probably the primary mechanism of biosorption.

From the experiment of *Biosorption of Heavy Metals by Zoogloea Ramigera*, the initial biosorption rates of metal ions by *Z. Ramigera* increased with increasing metal ion concentrations up to 100 – 200 mg/l. Maximum initial biosorption rates for lead (II), nickel (II), copper (II) and iron (II) ions were determined as 10.4 mg/g.min, 7.5 mg/g.min, 3.3 mg/g.min and 3.8 mg/g.min at 150-200 mg/l, 200 mg/l, 125 mg/l and 100 mg/l, initial metal ion concentrations respectively at 25°C. (Kutsal, 1995)

The biosorption was reached equilibrium in 5 – 15 min. In order to determine the isotherms, initial metal ion concentrations were varied between 25 to 200 mg/l while dry cell weight in each sample was constant at 1.0 g/l.

2.8 EFFECT OF pH ON BIOSORPTION

Normally, heavy metals are taken up from water predominantly by ion exchange. Carboxyl and sulphate groups have been identified as the main metal-sequestering sites in seaweed and, as these groups are acids; its availability is pH dependent. At pH in the range 3.5-5.5 these groups generate a negatively charged surface, and electrostatic interactions between cationic species and this surface can be responsible for metal biosorption.

pH is an important parameter for the sorption process, especially in the temperature range from 30°C to 40°C. The chromium biosorption capacity was at all temperatures higher at pH 4.0 (at pH 5.0 a chromium precipitate was observed).This pH dependence suggests a competition of metallic ions and protons by the same binding sites, since in this pH range chromium ion is present as a cation.

The effect of pH on metal biosorption have been studied by many researches, and the results demonstrated the increasing cation uptake with increasing pH values, as fungi biomass as algae biomass.

After a certain contact time, a pH increase was observed during the flask experiments. After the first hour the pH decreased in those experiments at high values of initial chromium concentrations (> 200 mg/L).

Similar effects were observed when studying cobalt biosorption using several types of marine algae, including the brown alga *Sargassum natans*. An increase of pH could be the result of dissolution of some cytoplasmic components or ions, such as carbonates, released into the solution.

The hypothesis of dissolution of cell components seems to be viable for the present study, because of some difficulties of filtration at pH 4.0 and for solutions which showed an increase of pH. (Cossich, 2002)

2.9 PETROLEUM REFINERY WASTEWATER CHARACTERISTIC

Petroleum refineries units generate wastewaters from process operation such as vapor condensation, cooling tower blow down and storm water runoff. The quantity of wastewater and their characteristic depend on the process configuration.

Table 2.1: Sources of Pollutant in Petroleum Refinery

(Lenntech Water treatment and air purification Holding, 2004)

Pollution	Approximate Quantities
Cooling systems	3.5-5 m3 of wastewater generated per ton of crude
Polluted wastewater	BOD 150-250 mg/l COD 300-600 mg/l benzene 1-100 mg/l heavy metals 0.1-100 mg/l
Solid waste and sludge	3 to 5 kg per ton of crude (80 % should be considered as hazardous waste because of the heavy metals and toxic organic presence)
VOC emissions	0.5 to 6 kg/ton of crude
Others emissions	BTX (Benzene, Toluene and Xylene) 0.75 to 6 g/ton of crude Sulfur oxides 0.2-0.6 kg/ton of crude Nitrogen oxides 0.006-0.5 kg/ton of crude

The liquid effluent for direct discharge to offside surface water should meet outlined specification by local Environmental Protection Agency (EPA)

Table 2.2: Effluent Requirement from Petroleum Refinery

(U.S Environmental Protection Agency, 2004)

Parameter	Maximum Level
pH	6-9
BOD	30mg/l
COD	150mg/l
Phenol	0.5mg/l
Benzene	0.05mg/l
Heavy metals	0.7mg/l

CHAPTER 3
METHODOLOGY

3.1 PROCEDURE IDENTIFICATION

3.1.1 ADSORBENT PREPARATION

Adsorbent type used in this project are dry leaves and in powder form. There are several steps that need to be taken in adsorbent preparation. The method was proposed by *Abraham, (2002)* that used chemically modified biomass. The fresh *Pentace triptera* leaves were collected around UTP campus especially at chemical engineering program building. Selecting of *Pentace triptera* leaves must be taken into consideration because in conducting the experiment we need to find the best adsorbent for adsorption. Only leaves in a good condition without any flaw to be collected. Then, in second step leaves were washed with tap water to remove any dust and dirt to ensure all unwanted materials will not be contained in adsorbent. Step followed by rinse the leaves with deionizer water in order to give an acidic pH for the leaves and then leaves are dried in oven for 25 hours at 80°C. After 25 hours drying, dry leaves were grinded using lab mortar grinder, (Model Fritsch, 1800001807). Grinding is one of the methods to grind the sample into smaller component. After grinding process complete, last step is sieving the grinding adsorbent into desired adsorbent size range from 0.5 to 1mm. Equipment used in sieving is Sieving Machine with sieve type is 1mm and 500um and sieve setting is 60 Amplitude for 5minutes.

3.1.2 INITIAL CONCENTRATION PREPARATION

Preparation of 700ppm Benzene:

Solubility of Benzene: 0.07%

Density of Benzene: 0.873g/cm^3

In preparing standard sample, 700 ppm of benzene need to be prepared so that all benzene prepare will be dissolve in water.

1. Take about 0.802ml of Benzene and pour into 1000ml volumetric flask.
2. Mark up to 1000ml of volumetric flask with distilled water.

Preparation of 500ppm Toluene:

Solubility of Toluene: 0.05%

Density of Toluene: 0.864g/cm^3

In preparing standard sample, 500 ppm of toluene so that all toluene prepare will be dissolve in water.

1. Take about 0.578ml of Benzene and pour into 1000ml volumetric flask.
2. Mark up to 1000ml of volumetric flask with distilled water.

Preparation of 700ppm of benzene and 500ppm of Toluene will be used as the Standard Solution to prepare for other concentration of benzene and toluene. Since in varying the concentration within the range of benzene and toluene discharge from Petroleum Refinery which is 1-100ppm, I've prepare about 8 sample for different concentration of benzene and toluene.

The samples concentrations to be prepared are 1, 5, 10, 20, 40, 60, 80, 100 ppm using equation 1.

$m_1v_1 = m_2 v_2$ .....(Eq 1)

For Benzene:

700ppm (v_1) = (m_2) 100ml .....(Eq 2)

Substitute varying concentration into Eq 2 and calculate how much amount of benzene need to taken from standard solution to be pour in 100ml volumetric flask.

For Toluene:

500ppm (v_1) = (m_2) 100ml .....(Eq 3)

Substitute varying concentration into Eq 3 and calculate how much amount of Toluene need to taken from standard solution to be pour in 100ml volumetric flask.

Concentration Varies For Benzene

Table 3.1: Volume of benzene added for varies of concentration preparation

Concentration, m_2 (ppm)	1	5	10	20	40	60	80	100
Volume, v_1 ml	0.143	0.714	1.429	2.857	5.714	8.571	11.428	14.286

Concentration Varies For Toluene

Table 3.2: Volume of toluene added for varies of concentration preparation

Concentration, m_2 (ppm)	1	5	10	20	40	60	80	100
Volume, v_1 ml	0.200	1.000	2.000	4.000	8.000	12.000	16.000	20.000

3.1.3 pH SAMPLE PREPARATION

For pH preparation sample, we need to prepare at five different pH samples in order for us to study the effect of pH sample solution towards the adsorption on the *pentace triptera* leaves. Sample prepare at two acidic sample, two alkaline samples, neutral sample and control sample. For acidic sample, we prepare sample at low pH sample which is at pH 2 and at high pH sample which is at pH 5. For alkaline sample, we prepare sample at low alkaline sample which is at pH 9 and at high alkaline sample which is at pH 12. Then, sample prepare for neutral sample which is at pH 7 and the control sample which is at benzene and toluene pH solution. In preparing the acidic sample, Hydrochloric acid will be used to give the acidic solution for the sample and for alkaline sample; Sodium Hydroxide will be used to give the alkaline solution for the sample.

Equipment: pH meter (Model Hach sension)

Preparing acidic sample:

For preparation of acidic sample, sample at pH 2 and 5 are to be prepared using Hydrochloric acid. From calculation, to prepare sample at pH 2, aqueous hydrochloric acid of 0.01M prepared by diluting 0.244ml of Hydrochloric acid, HCl in 1000ml of distilled water. Actual sample pH were measured by using pH meter indicate sample at pH 1.99. The reading was recorded. For sample at pH 5, aqueous hydrochloric acid of 0.00001M needs to be prepared. 1ml from 0.01M aqueous hydrochloric acid were taken and diluted with 1000ml distilled water. Actual sample pH was 5.01.

Preparing alkaline sample:

For preparation of alkaline sample, sample at pH 9 and 12 are to be prepared using Sodium Hydroxide. 0.01M of aqueous sodium hydroxide need to be prepared where 0.4g of Sodium Hydroxide, NaOH was diluted in 1000ml of distilled water. Actual sample pH is 8.99. The reading was recorded. For sample at pH 12, 0.00001M of aqueous sodium hydroxide need to be prepared by diluting 1ml of 0.01M aqueous sodium hydroxide in 1000ml of distilled water. Recorded of actual pH were 12.01.

Prepare Neutral Sample:

Neutral sample at pH 7 was prepared by adding 50ml of 0.00001 M HCl with 50ml of 0.00001 M NaOH. Actual sample pH recorded at pH 7.01.

Prepare Control Sample:

Control sample are sample with initial concentration of 5ppm benzene and toluene. pH of the sample were measured and recorded where for pH for 5 ppm benzene is 5.39 and for 5ppm toluene is 5.80.

Take about 10ml of the prepared sample and then mix with 50ml of 5ppm benzene and 5pp toluene. pH sample of the mixture are recorded.

Benzene

Table 3.3: pH of benzene sample mixture before adsorption

pH sample solution	pH of 5ppm benzene	pH of mixture
Acidic Sample		
1.99	5.39	**2.66**
5.02	5.39	**5.44**
Alkaline Sample		
8.99	5.39	**7.46**
12.01	5.39	**11.38**
Neutral Sample		
7.01	5.39	**6.65**
Control Sample		
5.39	-	**5.39**

Toluene

Table 3.4: pH of toluene sample mixture before adsorption

pH sample solution	pH of 5ppm Toluene	pH of mixture
Acidic Sample		
1.99	5.80	**2.67**
5.02	5.80	**5.46**
Alkaline Sample		
8.99	5.80	**7.79**
12.01	5.80	**11.46**
Neutral Sample		
7.01	5.80	**6.67**
Control Sample		
5.80	-	**5.80**

3.1.4 Adsorption Process

50ml of each different concentration samples and 60ml of different pH were pour into 100ml Erlenmeyer flask. 0.5g of adsorbent were weighed and added into Erlenmeyer flask. Samples are shaken using Chemistry Lab Shaker (Model Platform) for 24hours at 130rpm.

3.2 TOOLS

To analyze the concentration of benzene and toluene in the solution after adsorption takes place, student used the equipment known as UV-VIS Spectrophotometer. Under the supervision of the Analytical Laboratory Technician, 30 sample were tested and the results printed and to be discussed.

1.2.1 Ultraviolet-visible Spectrophotometer (UV-Vis)

Ultraviolet-visible molecular spectrochemical method utilize in the ultraviolet and visible regions of the electromagnetic spectrum to analyze laboratory samples for molecular compound and complex ion. Basically, in spectrochemical analysis procedure, the degree to which light is absorbed, or the intensity of the light that is emitted, is related to the amount of an analyte present in the sample tested. Thus, the degree of light absorption and the intensity of light emission are the critical measurement. Qualitative analysis (identification of unknown and detection of impurities in known) is accomplished by comparing adsorption or transmission spectra (molecular finger prints) with known spectra. Qualitative analysis is accomplished with the use of Beer's Law. In UV-VIS instrumentation, a light source which frequently used is ultraviolet light from deuterium lamp directly passed through the sample solution held in cuvette and then proceeds to the detector. There are several procedures that need to be taken in order to do analysis to the sample using UV VIS Spectrophotometer.

UV-VIS Analysis Procedure:

1 Calibration Curve Preparation:

a. Prepare Standard Sample at 1 ppm, 20 ppm, 60 ppm and 100 ppm solution except with variation in pH prepared standard solution of 1 ppm, 3 ppm and 5 ppm.

b. Set up UV-VIS equipment and UV Probe software.

c. Calibrate the point of the concentration.

2. Based on calibration curve, put sample into UV-VIS sample slot and analyst the concentration of sample after adsorption process takes place.

4.2.2 Gas Chromatography Mass Spectrometer (GCMS)

Chromatography instruments used to separate and quantitate samples of complex mixtures with surprising ease and accuracy in a very short time. The separation occurs in a column, which is a tube that contains a stationary material phase that selectively impedes the progress of mixture components as they move through it. This forward movement occurs because a second phase, a moving gas or liquid phase called mobile phase, is passing through the column and also influence the rate of movement of the mixture components. Mixture components then emerge from end of the column one at a time are electronically detected and measured one at a time which mass spectrometer used as the detector system. Mobile phase used in GCMS is a gas usually helium. Separation of mixture components are based on the relative vapor pressure of component. Vapor pressure is the pressure exerted by molecules of a gas in equilibrium with its liquid present in same seal container. It measures the tendency of liquid molecule to escape from liquids phase and become gaseous. In GCMS, substance with high vapor pressure will strongly influenced by the moving gaseous mobile phase and will emerge from the column quickly (short retention time) if the solubility in the stationary phase are low. If their vapor pressure is high, but their solubility in the stationary phase are also high, then they will emerge more slowly (intermediate retention time). If their vapor pressure is low, but have high solubility in stationary phase, the required time for emergence from column will be long (high retention time).

CHAPTER 4
RESULT AND DISCUSSION

4.1 Effect of Varying Concentration

Appearance: The entire samples for both benzene and toluene at different concentration turn into brownish color after adsorption. (Refer Appendices)

Benzene

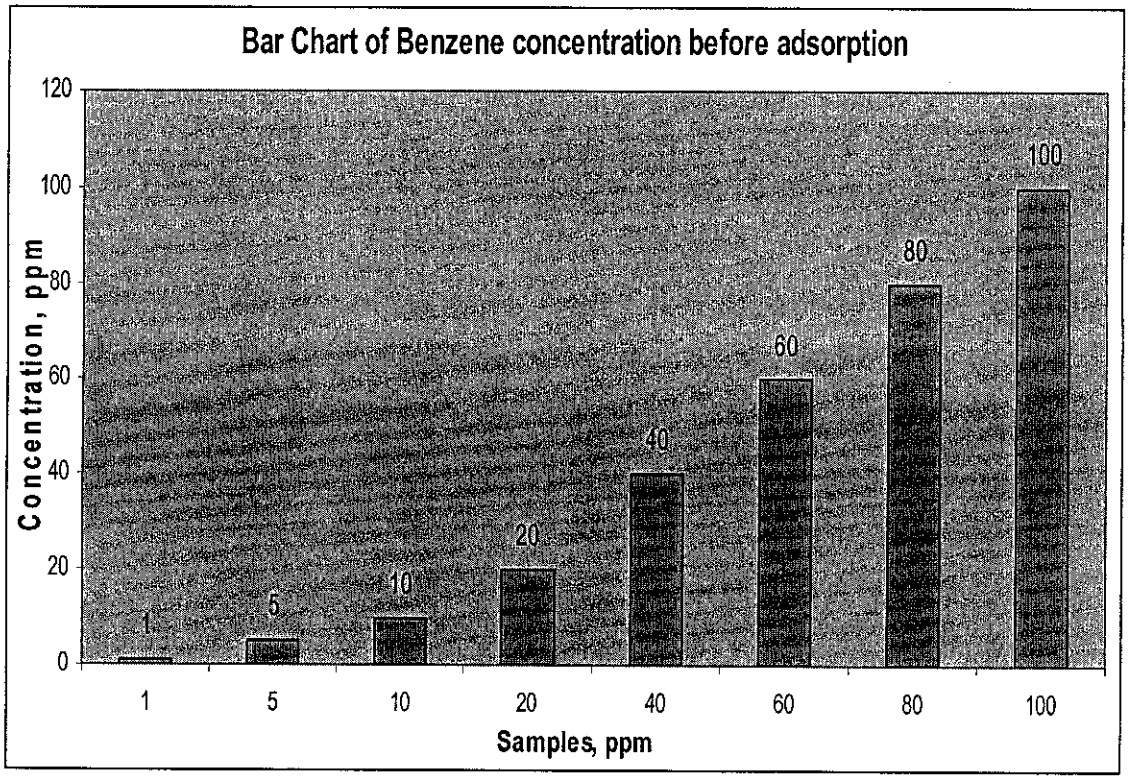

Figure 4.1: Bar Chart for Benzene concentration before adsorption

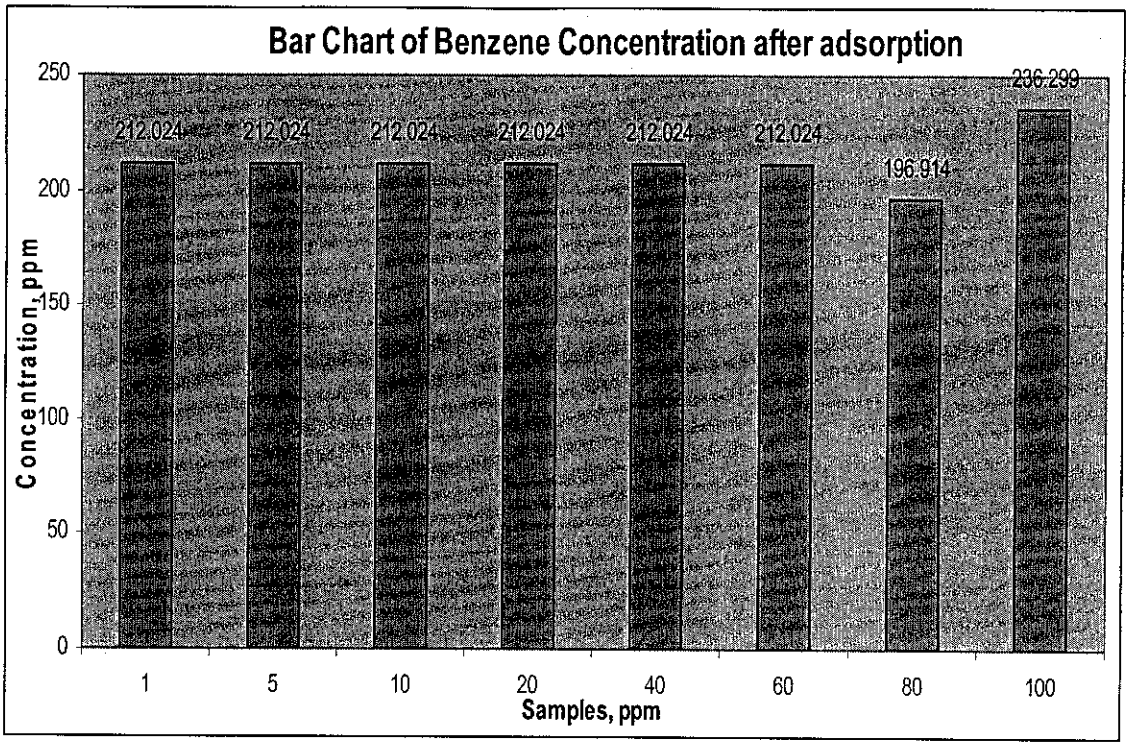

Figure 4.2: Bar Chart for Benzene concentration after adsorption

Toluene

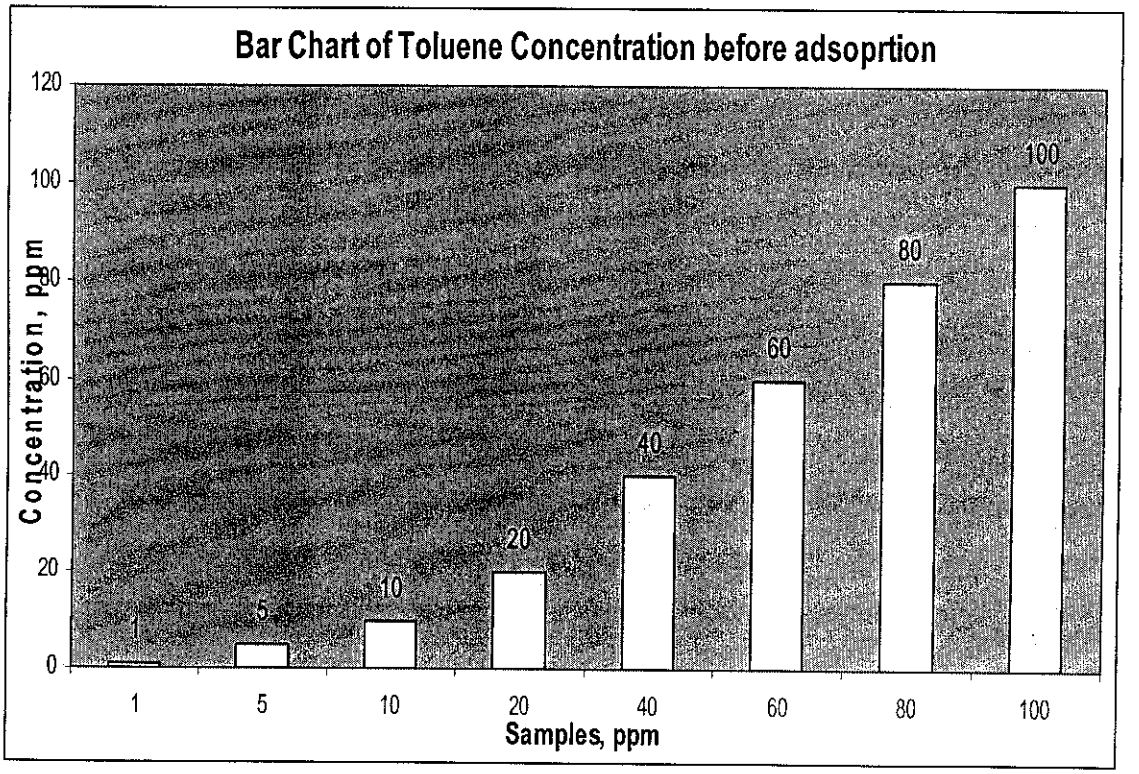

Figure 4.3: Bar Chart for Toluene concentration before adsorption

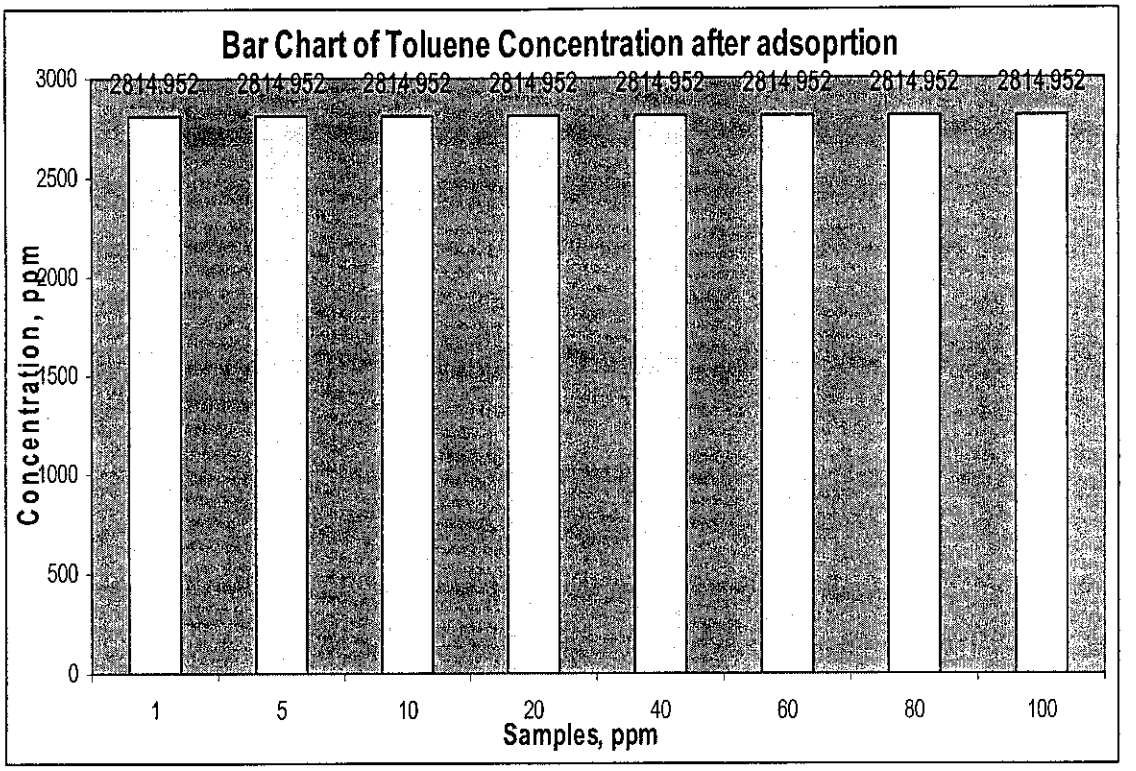

Figure 4.4: Bar Chart for toluene concentration after adsorption

In UV-vis Spectrophotometer, qualitative method analysis has been applied for testing sample concentration. Before any sample to be tested, calibration curves of standard sample need to be conducted. As shown in appendices (calibration curve varies in concentration), a calibration curve of benzene and toluene were conducted at four standard concentration (1ppm, 20ppm, 60ppm and 100ppm). From the calibration curve, the concentration of tested sample could be qualitatively determined. There are about 8 samples each for different of benzene concentration and toluene concentration. Figure 4.1 show a bar chart for benzene concentration before adsorption which concentration varies from 1 ppm to 100 ppm. Result of adsorption of benzene shown in Figure 4.2. Benzene samples concentration after adsorption are same for sample concentration of 1ppm, 5ppm, 10ppm, 20ppm, 40ppm and 60ppm ppm which is at 212.024ppm. While the result for sample at concentration of 80 ppm gives concentration after adsorption slightly lower at 196.914 ppm and for 100 ppm of benzene, the result of sample concentration after adsorption is 236.3 ppm which is slightly higher that other concentration.

The result had shown totally different from the adsorption concept of this project. Primary objective was to determine the optimum initial solute concentration for higher uptake of organic compound by Pentace triptera. As referring to the UV-vis result, the first hypothesis from the result are desorption of benzene occur which mean that the *Pentace triptera* desorp benzene in the sample rather than adsorption takes place.

Another analysis use in UV-vis Spectrophotometer is the spectrum analysis where samples are analyze in certain range of wavelength (190 – 300 nm). Analysis was conducted at several sample varies in benzene concentration. From the spectrum analysis in appendices B3, the result shown absorbance value forms a straight line at 4.516 Absorb in a range of wavelength from 190nm to 300nm. This mean that at every wavelength in that range the result will shown same absorptivity and no peak shown in result. Light at any wavelength pass through and striking the sample will result at same absorptivity. Other different concentrations also give the same behavior. Figure 4.3 show toluene varies of concentration from 1 ppm to 100 ppm before adsorption. In figure 4.4 shown a tested sample of toluene varies in concentration after adsorptions. From the figure, we can see that the concentration of samples after adsorption is at same concentration of 2814.9 ppm. The concentration of sample is measure dependence on the absorptivity at specified wavelength which is 260.9nm. Since, as spectrum analysis conducted on several sample varies in toluene concentration, the absorptivity of sample concentration will give a straight line of absorptivity at 5 Absorb meaning that at each wavelength the concentration interpolated from calibration curve will result in same concentration. Same hypothesis from UV-vis for varies in toluene concentration that *Pentace triptera* leaves desorp toluene compound rather that adsorb.

4.2 Effect of Varying pH

Appearance: Different color shown after adsorption process takes placed.

pH: pH of solution after adsorption are measured and recorded for each sample.

Benzene:

Table 4.1: pH and color appearance of benzene after adsorption

Sample	Color	pH	
		pH before	pH after
PB1	White-Brown	2.66	4.69
PB2	Brownish	5.44	6.50
PB3	Brownish	7.46	6.61
PB4	Brownish	11.36	6.96
PB5	High Brownish	6.62	7.31
PB6	Brownish	5.39	6.98

Toluene:

Table 4.2: pH and color appearance of benzene after adsorption

Sample	Color	pH	
		pH before	pH after
PT1	White-Brown	2.67	4.02
PT2	Brownish	5.46	6.46
PT3	Brownish	7.79	6.58
PT4	Brownish	11.46	6.78
PT5	High Brownish	6.67	7.23
PT6	Brownish	5.80	6.79

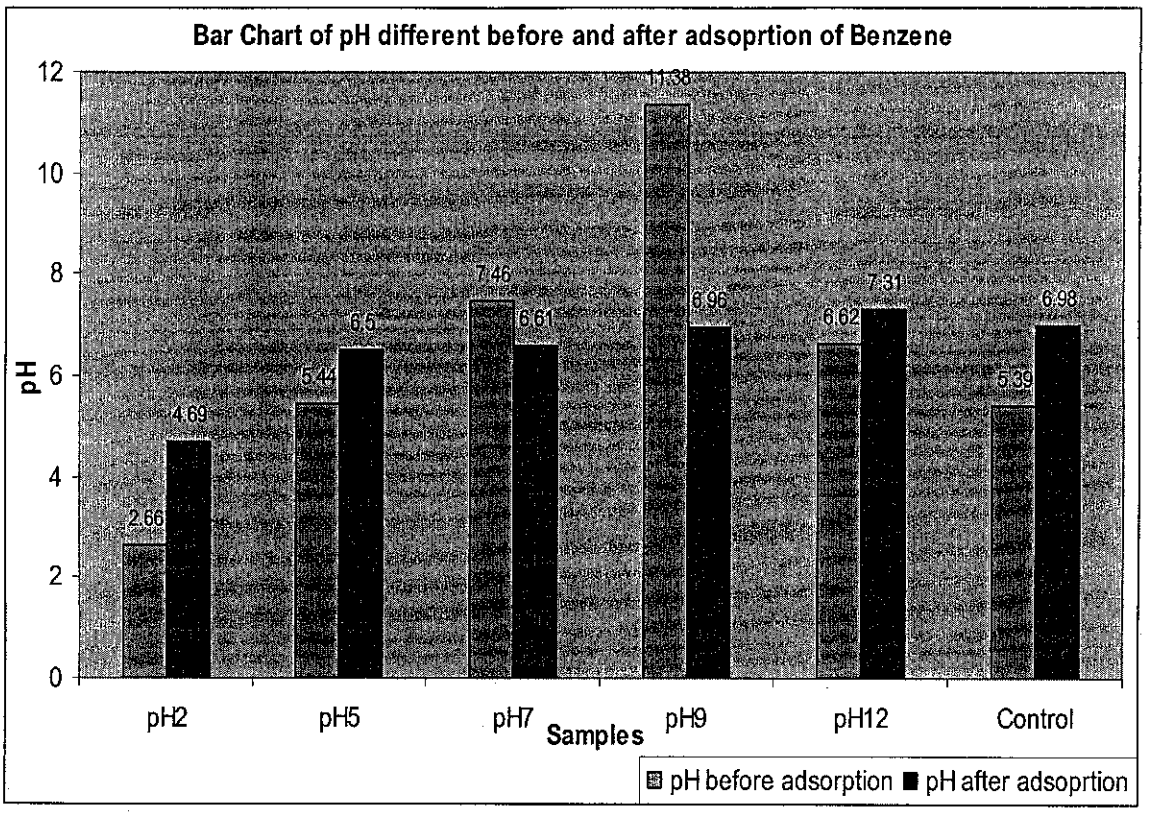

Figure 4.5: Bar Chart for pH different before and after adsorption of benzene

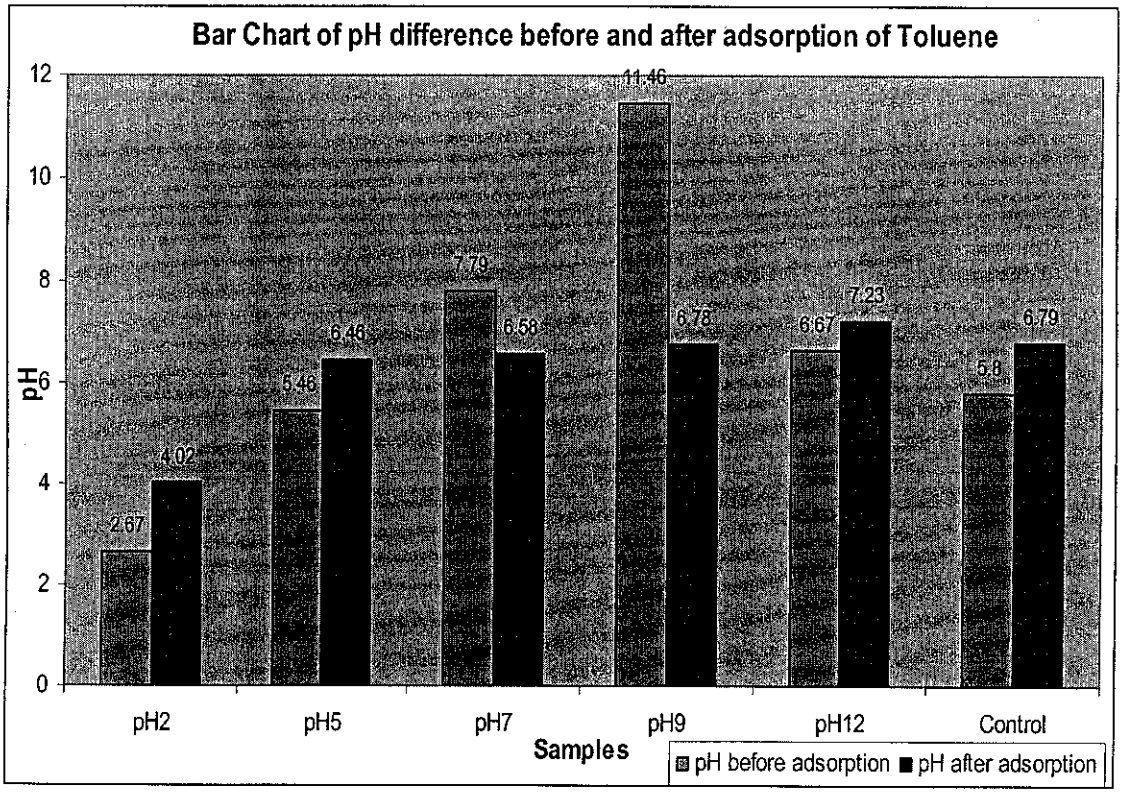

Figure 4.6: Bar Chart pH different before and after adsorption of benzene

In second experiment, pH is varies at two acidic solution, two alkaline solution, neutral sample and control sample in order to study the effect of pH sample toward adsorption of organic material on *Pentace triptera*. pH sample varies at same concentration of benzene and toluene which is at 5ppm. Appearance of the sample color and the pH of sample after adsorption take into account to show the result of adsorption. The appearance of sample for benzene and toluene seem to be at same color different which is at pH 2, the sample is white-brownish, pH 5, 7 and 9 are same which is brownish and at pH 12, the color is high brownish. So, based on the result, we can say that at low pH which is acidic sample will try to protect from color release from *Pentace triptera* rather than at high pH the color seem to be easily appearing in solution when the adsorbent get into the solution. Based on the color appearance, it is also give some affect on pH different on the adsorption. pH of samples after adsorption are recorded to shown the pH different before and after adsorption takes place.

Referring to the bar chart provided shown a different pH before and after adsorption. For benzene and toluene sample, the result had shown that pH of sample move towards to neutral sample. For benzene sample with pH 2.67 before adsorption, the pH of the sample increase to 4.69 after adsorption and toluene pH sample after adsorption increase to 4.02 from 2.66 before adsorption. Alkaline sample of benzene and toluene also reduce to 7.31 and 7.23 respectively after adsorption. Based on pH study, the neutral sample which is at pH 7 or pure water normally contain: $[H^+] = [OH^-] = 1 \times 10^{-7}$ Adsorption process is attempted to neutralize the sample. From an acidic sample solution of pH 2 before adsorption, after adsorption sample seem to be neutralize which less $[H^+]$ ion contain in sample rather than before adsorption. Same principle also for alkaline sample solution which the pH sample before adsorption is 12 and after adsorption pH of sample reduce to neutral meaning that less $[OH^-]$ ion contain in sample rather than before adsorption. Basically, we can say that adsorption process seem to neutralize the sample pH which contain nearly same $[H^+]$ ion and $[OH^-]$ ion in sample.

Concentration of organic compound before and after adsorption:

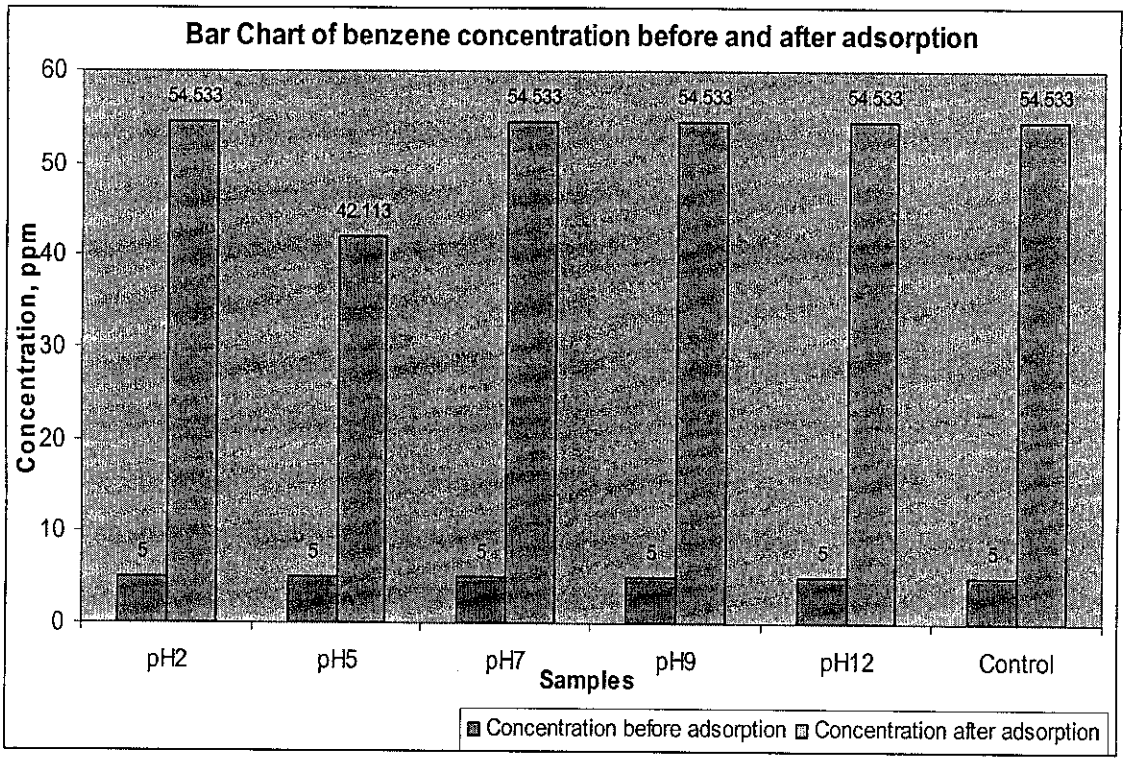

Figure 4.7: Bar Chart of concentration before and after adsorption of benzene

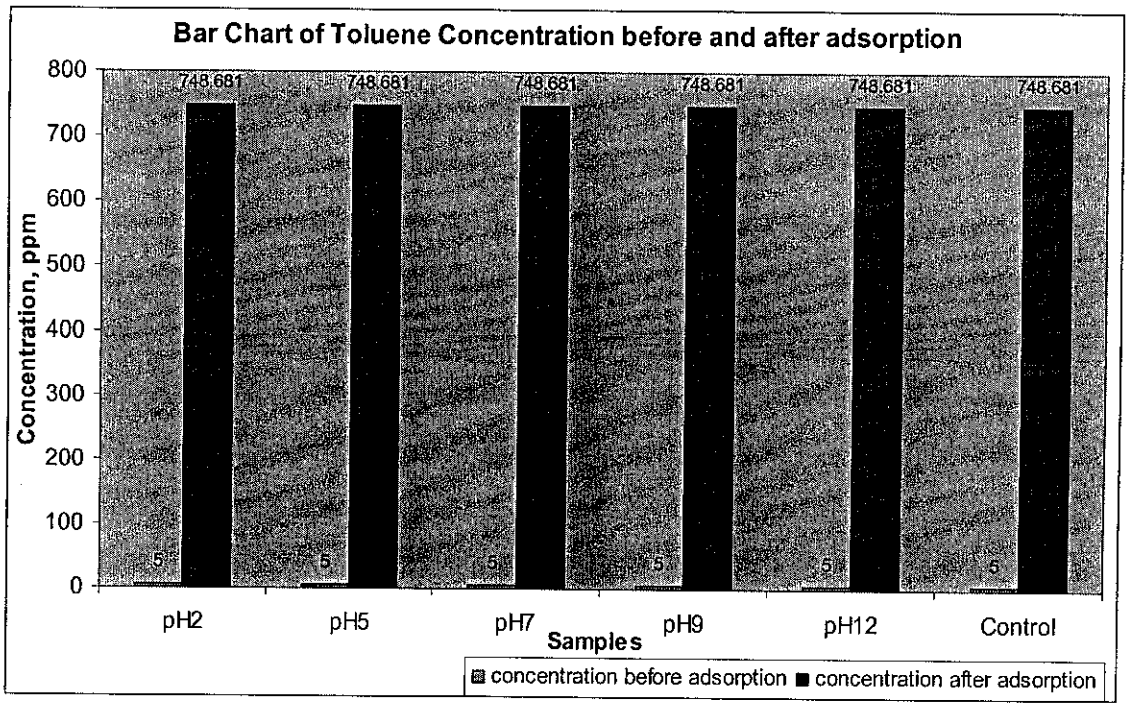

Figure 4.8: Bar Chart of concentration before and after adsorption of toluene

Result above shown a different concentration of organic compound (benzene and toluene) before and after adsorption for varies of pH sample solution. Before concentration determined by UV-vis instrumentation, calibration curve should be prepared so that the concentration will be qualitatively measured by UV-Vis. UV-Vis is a type of analytical instrument that used qualitative method to test or measure the sample. Calibration curve was created using three standard solutions which is at 1 ppm, 3 ppm and 5 ppm. In this project, concentration of benzene and toluene is fixed at 5 ppm while pH of the solution varies. From theoretical study for adsorption process, *Pentrace triptera* leaves will adsorb benzene and toluene contains in the sample and the sample concentration should be lower than the concentration of benzene and toluene before adsorption.

Figure 4.7 shown a comparison different of benzene concentration varies in pH before and after adsorption. Six samples at different pH (pH 2, 5, 7, 9, 12 and control) were tested. Comparison show concentration of benzene after adsorption are higher than before adsorption where at pH 2, 5, 7, 9 and 12 gives same benzene concentration of 54.5 ppm while at pH 5 benzene concentration is 42.1 ppm. Due to UV-vis result, first hypothesis applied was desorption of benzene to solution. In figure 4.8, show comparison toluene concentration before and after adsorption. Toluene concentrations after adsorption are higher than before adsorption where all sample at varies of pH gives same toluene concentration of 748.6 ppm. First hypothesis applied where toluene are desorp rather than adsorb by *Pentace triptera.*

4.3 GAS CHROMATOGRAPGY MASS SPECTROMETER (GCMS) RESULTS

Due to UV-Vis Spectrophotometer unpredicted result, the project continue by using another analytical equipment in order verify and analyze the sample. Gas chromatography mass spectroscopy (GCMS) has been used in determining the concentration of sample based on the retention time of benzene and toluene. Under GCMS instrumentation, component analysis contain in sample solution have been analyze based on peak appearance on chromatogram.

Results for GCMS are shown in appendices (*Refer Appendix C*). Due to time constraint, sample tested under GCMS instrument are benzene and toluene at pH 2, 7, 12 and control sample where all sample are at fix concentration of 5 ppm. Standard for Benzene and Toluene are prepared at 5ppm of concentration. Standard sample analyze with gas chromatography which for benzene, the retention time is 3.787 and for toluene, the retention time is 3.8.

Qualitative analysis has been done for the tested sample (sample after adsorption). Each samples required about one-half hour to complete the testing. In qualitative method analysis by GCMS, sample was analyzed based on retention time of component to be tested. Appendices C1.1 showed a qualitative analysis of benzene sample at four different pH. The sample was analyzed at the reference retention time of benzene (3.787) based on standard benzene concentration of 5 ppm. No peak appears show for the all sample. Peak area of for targeted benzene is equal to zero for all sample. In GCMS, concentration of component contain in mixture depend on the peak area. Zero peak area detected for benzene on chromatogram show that the concentration of benzene in sample is 0 ppm. In Appendices C1.2 showed a qualitative analysis of toluene sample at four different pH. Same result also shown for toluene sample where toluene are not detected in the sample meaning the peak area equal to zero and concentration of toluene is 0 ppm for all sample.

GCMS result shown different result from UV-vis instrument. In UV-vis, concentration of benzene determined was 54.533 ppm and concentration of toluene is 748.611 ppm while for GCMS benzene and toluene are not detected. There are opposite measurement show between UV-vis and GCMS. In first hypothesis using UV-vis, desorption of benzene and toluene are not relevant because GCMS does not give same result.

In gas chromatography, component mixture was analyzed and separated based vapor pressure of the component and their retention time detected by mass spectrometer detector. All sample have being analyze to check the component exist in the sample. Based on the peak value and shape on the chromatogram display, GCMS scans the possible component (compound name) from three sources of GCMS library named, 1. Wiley229.lib; 2. Nist21.lib; 3. Nist107.lib.

Chromatogram of component mixture separation show in Appendices C2.1: Benzene at pH 2, C2.2: Benzene at pH 7, C2.3: Benzene at pH 12, C2.1: Benzene at control sample. For pH 2 (acidic sample), chromatogram shown 9 components exist in sample. First peak at retention time 3.250 show higher peak area meaning that higher concentration of the component in the sample. The possibilities component for peak 1 is carbon dioxide (CO_2) and carbamic acid (CH_3NO_2). Other components exist in the sample in lower concentration are amine group, carboxylic acid group, aldehydes group, alcohol group and ester group. The entire components are organic compound that contain Carbon, Nitrogen, Hydrogen and Oxygen. For pH 7 (neutral sample), chromatogram show 3 peak appearance meaning that only 3 component exist at pH 7 sample. Nearly neutral sample result in lower component exists in sample. Component of higher concentration contain in samples are benzenesulfonamide ($C_{25}H_{31}NO_4S$). Other components are amino, alcohol and carboxylic acid group. For pH 12 (Alkaline sample) shown the higher component exist in sample which is 11 component. Highest concentration of component contain in this sample is carbamic acid where it is appear in large peak area 2 and 6. Other component contain in the sample are acetic acid, gaseous

compound (CO_2 and NO_2), ketone group, amine group and carboxylic group. For control sample of benzene chromatogram show 11 component exist in sample. Main component exist is also carbamic acid. From result, at high pH and low pH, extraction and digestion of compound seem to be actively occurring and produce high component contain in sample.

In appendices C3 show a chromatogram for toluene analyzing sample. The appendices are C3.1: Toluene at pH 2, C3.2: Toluene at pH 7, C3.3: Toluene at pH 12 and C3.4: Toluene at control sample. For pH 2 (acidic sample), high component extracted and exist in sample. 8 components contain in sample. Higher peak area is peak 4 and 6 where the component is carbamic acid. Other components exist in sample including the carboxylic acid and amine group. For pH 7 (neutral sample), Only 7 component contain in sample where highest peak area is at peak 2. The component exist is carbamic acid. Other lowest amount of component contain in sample are ketone group and aldehydes group. For pH 12 (alkaline sample), about 13 component extracted from leaves and highest amount of component contain in sample are ethanedoic acid ($C_2H_2O_4$) at peak 2 and carbamic acid (peak 1, 3, 4, 5 and 6). Other component contain in sample are ketone group, amine group, aldehydes group and alcohol group. For control sample, 8 component extracted which high amount of component contain in sample are carbamic acid and 2-propanone (C_3H_6O).

Hypothesis from GCMS result were the carcinogenic compound shown by benzene and toluene. From qualitative measurement, concentration of benzene and toluene is zero after adsorption. Different between GCMS and UV-vis explaining the qualitative measurement by Uv-Vis may contribute to error in measurement of benzene and toluene concentration. After adsorption process, sample tested using GCMS as shown by chromatogram result in many component exists in the solution. Second hypothesis is benzene and toluene were adsorbed by *Pentace triptera* and at the same time benzene and toluene extract and digest *Pentace triptera* leaves. Leaves normally contain chlorophyll and many other organic compounds such as amine group. Carbamic acid is the component that identifies to be mostly extracted from *Pentace triptera* leaves where

toluene gives more formation of carbamic acid in sample. Number and amount of component exist also depend on the pH of sample where at high pH and low pH, extraction and digestion of compound seem to be actively occurring and produce high component contain in sample.

4.4 QUALITATIVE METHOD OF UV-Vis Spectrophotometer

As we understand, UV-VIS is one type of quantitative instrumental analysis. Qualitative instrumental analysis mostly involve sophisticated electronic instrument that generates electrical signal that are related to some property of analyte and proportional to the analyte's concentration in a solution. In other word, the standards and sample are provided to the instrument, the instrument measures the property, the electrical signal is generated, and the signal, or often the numerical value of the property itself, is displayed on readout and subsequently related to concentration.

Spectroscopic methods involve the use of light and measure the amount of either light absorbed (absorbance) or light emitted by solutions of the analyte under certain conditions. Along with the determination of the weight or volume of the prepared sample, one or several standard solutions must be prepared. Such solutions needed to calibrate the instrument. In general term, calibration is a procedure by which any instrument need to be tested with the standard in order to determine its response for an analyte in a sample for which the true response is already known or needs to be established.

The problem in using the qualitative instrumental may lead to the error in measuring the sample which is concentration of the solute by using UV-Vis spectrophotometer. In this case, the true response may need to be established; this is done by measuring the response of the standard (the known quantities). Usually, series of standard used to create of calibration curve which in this project we use 1ppm, 20ppm, 60ppm and 100ppm for varies of concentration.

A calibration curve is plotted which the instrument response, Abs vs. the concentration, or of known quantities, of the standard. This shown the qualitative instrumental analysis in measuring the concentration of tested sample.

Interferences are quite common in quantitative and quantitative analysis by UV-VIS spectrophotometer, interference is a contaminating substance that gives and absorbance signal at the same wavelength or wavelength range selected range selected for analyte. For qualitative analysis this would show up as an incorrect absorption spectrum, thus possibly leading to erroneous conclusions if the contaminant was not known to be present. For quantitative analysis, this would result in a higher absorbance than one would measure otherwise. Absorbance are additive. This means that the total absorbance measured at a particular wavelength is the sum of absorbance of all absorbing species present.

Thus if an interference present, if an interference is present, the correct absorbance can be determined by subtracting the absorbance of the interference at the wavelength used, if it is known. In order to encounter these problems is to utilize separation such as liquids-liquids extraction or liquid chromatography to separate the interfering substance from the analyte prior to the spectrophotometer measurement.

Deviations from Beer's law are in evidence when the Beer's law plot is not linear. This probably most often observed at higher concentration of analyte, as indicated in the standard solution for calibration curve. Instrument deviations occur because it is possible for an instrument to be accurate at extremely high or low transmittance values that are approaching either 0 or 100%T. The normal working range is between 15 and 80%, corresponding to absorbance between 0.1 and 0.82. It is recommended that standards be prepared to measure in this range and that unknown samples be diluted if necessary.

Deviations due to chemical interference occur when a high or low concentration of analyte cause chemical equilibrium shifts in the solution that directly or indirectly affect its absorbance. It may be necessary in these instances to work in a narrower concentration range than expected. This means that unknown samples may also need to be further diluted, as in the instrument deviation case. Basically, Instrument operators may also want to conduct periodic wavelength calibrations. It is important to know that the wavelength displayed or dialed in really is the wavelength passing through the sample compartment. One way to check for proper wavelength calibration is to prepare a solution of an analyte for which the wavelength, it may be that the wavelength. Control is out of calibration.

Contamination, as indicated, manifested itself in the absorption spectrum. If a sample contaminated with a chemical that has its own absorption spectrum in a range studied, the absorption pattern which the spectrum of the analyte will not match the expected pattern. If a contaminant is suspected, it may originate from any of the chemicals used in the procedure including the solvent, the analyte used to prepare standards, or any the chemical added to the solutions tested. In that case, repeating the solution preparation using chemicals from fresh, unopened containers may help solve the problem.

Basically, from the sample as shown in appendices which turn into high brownish color which may contaminate the sample. From the basis understanding of spectrochemical which is wavelength can vary in distance from as little fraction of atomic diameters to as long as several miles. This suggests the existence of an extremely broad of wavelength. In the point of view, what is the nature of the interaction between light and matter that causes certain wavelength of light to be absorbed? The answer lies in the structure of the atoms and molecules of which matter is composed. First consider atoms. The modern theory of the atoms states that electrons exist in energy levels around the nucleus. Electrons can be moved from one energy level to a higher one if conditions are right. For example, the outermost electron of a sodium atom (which has electron $1s^2s^2p^63s^1$) can be moved from 3s level to the vacant 3p level if conditions are right.

These conditions consist of:

1) The addition of a specific amount of energy to the electron which the energy difference between 3s and 3p level.
2) A vacant for electron with this greater energy in a certain higher energy level which in this case 3p level.

So in other words, if an electron absorbs energy required for it to be promoted to a higher vacant energy level, then it is promoted (or elevated) to that level. When the light of certain wavelength of this energy strikes an atoms and cause an electron to be promoted to a higher energy level, the energy of light becomes part of the electron energy and therefore disappears. It is absorbed. The light coming in must be exactly the same energy as the energy difference between the two electronic levels, otherwise it is not absorb. (Kenkel, 2002)

Other research study, benzene and toluene are very carcinogenic compound and at high concentration, benzene and toluene can effect and attack the cell and chlorophyll of leaves (Cossich, 2002). Although in this experiment we are using low concentration of benzene and toluene, but the leaves has been dried and its structure strength has been disturbed and benzene and toluene easily attack the leaves structure. The effect from this matter, chlorophyll of leaves comes out from the leaves and introduces a color to the sample. The interference might occur since the residue contain in sample and also the color of solution that turn out the result to be at same concentration which mean at same Absorbance value. The residue contain in sample could be at the same wavelength of benzene and toluene which also have same value of energy difference of electron of sample. Other analysis also conducted for other for different benzene and toluene concentration after adsorption. The contaminant the contribute to error in measurement of the sample is carbamic acid which exist in sample based on GCMS result due to physical color of carbamic acid is a prism from toluene and benzene.

4.5 COMPARISON STUDY FROM PREVIOUS RESEARCH PROJECT

In the previous study by Othman (2001), optimum uptake capacity and optimum concentration for metals adsorption on *Pentace triptera* was determined. The project was done by Aida Othman. Concentration of metal ion (Cu^{2+}, Ni^{2+} and Pb^{2+}) plays an important role for the adsorption and ion exchange study. It will show the capacity of the adsorbent and ion exchange for the metal uptake system. There are two types of biomass used in this experiment, which were the naturally dried leaves (sun dried) and the fresh leaves (dried in the oven at 60°C for 24 hours). In the experiment, 0.5 g of biomass was mixed with 50-ml metal ion solutions (Pb^{2+}, Cu^{2+}) at different concentrations; 1 ppm, 5 ppm, 10 ppm, 15 ppm and 20 ppm. The mixture was shook in the rotary shaker for 6 hours at the speed of 150 rpm and room temperature. It was the separated using the laboratory sieve and the metal ion solutions were analyzed using the AAS. After the experiment is conducted, the results shows that the best adsorption occur by dry biomass is when the initial concentration at 15.6 ppm for Pb^{2+} solution which is the metal uptake is 1.06g metal/ g biomass, and at 11.7 ppm for Cu^{2+} solutions which is the metal uptake is 0.5g metal/ g biomass. As for fresh biomass, the optimum adsorption can occur for 0.5 g biomass in 50 mL metal solution is when the initial concentration at 10.5 ppm Pb^{2+} which is the metal uptake is 0.66g metal/ g biomass solution and 12.8 ppm Cu^{2+} solution which is the metal uptake is 0.28g metal/ g biomass. In binary and ternary solutions, the results exhibit that lead is the most metal uptake compared to copper and nickel. Followed by copper, the second metal uptake and lastly nickel. (Othman, 2001)

From the research, it is shown that *Pentace triptera* work efficiently with metal adsorption. This can be seemed from the metal uptake by adsorbent (*Pentace triptera*). Comparing between the two research projects is the adsorbate use for adsorption which in previous project, metal ion (Pb, Cu, Ni) while in these project organic compound are used. Based on UV-VIS result, benzene and toluene concentration after adsorption are higher than before adsorption which totally different expectation result in early stage

project objective. This result shown *Pentace triptera* is not a best adsorbent for organic compound. Basically, the finding between two research studies, *Pentace triptera* is only available for metal adsorption rather than organic compound which we can say that ion-exchange between metals ion and *Pentace triptera* leaves and metal are not a solvent compound that can dissolve the material such as *Pentace triptera*. Other comparison could be the contact time for adsorption between the two researches which for metal biosorption, the contact time is 6hr and for organic material adsorption is 24hr. The effect could be the contact time different that introduce extent of reaction between leaves with organic material and production of microbes due to long time adsorption and open-close the Erlenmeyer flask cover.

4.6 CHLOROPHYLL

From research conducted, which from journal study on effect of various indifferent organic solvents on the leaf pigments. Laminum leaf has been subjected in this research to study effect of organic solvent. The softness of the Laminum leaves and the approximate neutrality of their tissue juice marked them as especially suitable objects. Alcohols (methyl, ethyl, and amyl), acetone, acetaldehyde, ether, chloroform, benzene and toluene are solvent used. These solvents, acting on fresh (ground) or dry leaves, dissolve all the pigments equally and abundantly. The carotin can be completely extracted in this way. Dried leaves (dried at low temperature!) likewise give their carotin to the solvent, and in somewhat purer condition. Tissues cooked or warmed at higher temperatures, however, when ground with the solvent give a green extract, a fact which will be explained later. Benzene, xylene, toluene, carbon disulfide also give an action on leaf pigments intermediate between the solvents of the first groups.

Basically, hypothesis in this project were extraction of chlorophyll and digestion occur toward the leaf by organic compound. From the sample appearance, color formation after adsorption contact. For vary of concentration, it is shown the same color appearance for benzene and toluene. For vary of pH where at low pH shows light green-yellow color appearance and the sample color become darken as the pH increase.

At low pH which is in acidic solution sample, the acidic solution could prevent the extraction of chlorophyll from the leaf. At high pH value which is in alkaline solution sample, in experimentation work, after adding up the biomass to alkaline sample for both benzene and toluene, the color of sample change instantaneously, so from this observation, alkali act as a catalyst in extraction of chlorophyll. (Tswett, 1872-1919)

4.7 CARBAMIC ACID

Hypothesis from GCMS result, Carbamic acid is the component that identifies to be mostly extracted from Pentace triptera leaves where toluene gives more formation of carbamic acid in sample. $C_3H_7NO_2$ is a weaker acid. Apparent color of acid carbamic is colorless, columnar crystals or white, granular powder, prisms from benzene and toluene. [11]. Referring to its apparent color which is prism from toluene and benzene, this parameter shown acid carbamic will have the same wavelength for benzene and toluene. So as a result from UV-VIS analysis, the concentration contain in the sample should be acid carbamic. As pH test conducted also, pH of sample after adsorption shown a result near neutral sample which mean that these pH shown acid carbamic. An alkaline sample at pH 9 and 12 seem to be neutralized by reducing it pH value after adsorption. While at an acidic sample which pH 2 and 4, as acid carbamic form in the sample, sample tend to contain more weaker acid so that pH of sample increase. From previous discussion, toluene and benzene attack by extracted and digested the leaves structure as see that color introduce to the sample and toluene and benzene extract carbamic acid from *Pentace triptera* leaves.

This is a new finding of the carcinogenic of toluene and benzene compound toward biomass adsorbent and formation of carbamic acid from the toluene and benzene from adsorption with *Pentace triptera*. Research founded that carbamic acid have a lot of usage and mainly for agriculture side and textile industries. The major use of ethyl carbamate is as an intermediate in the synthesis of a variety of products and as a solubilizer and cosolvent for pesticides and fumigants (Johnson, 2004).

Other research conducted that carbamates is an ester of carbamic acid. Adding of carbon and benzene ring to carbamic acid could produce carbamates. This carbamate compound is an active compound.

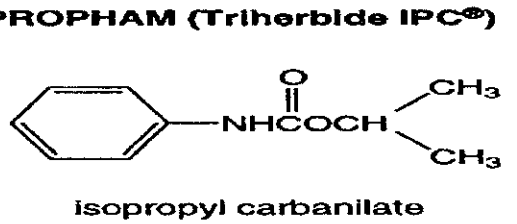

Figure 4.9 Chemical Structure of Carbamates compound

Carbamates were discovered in 1945, the carbamates are used primarily as selective pre-emergence herbicides, but some are also effective in post-emergence use. The first product was propham (Triherbide IPC®) (Fig. 6), also known as IPC. Others are chlorpropham (Furloe®, CIPC) and asulam (Asulox®). They kill plants by stopping cell division and plant tissue growth. Two effects are noted: cessation of protein production and shortening of chromosomes undergoing mitosis (duplication). Carbamates are readily translocated and inhibit meristematic development. Basically, Herbicides, or chemical weed killers, have largely replaced mechanical methods of weed control in countries where intensive and highly mechanized agriculture is practiced. Herbicides provide a more effective and economical means of weed control than cultivation, hoeing, and hand pulling. Together with fertilizers, other pesticides, and improved plant varieties, they have made an important contribution to the increased yields we now have and serve to combat rising costs and shortages of agricultural labor. The heavy use of herbicides is confined to North America, Western Europe, Japan, and Australia. Without the use of herbicides, it would have been impossible to mechanize fully the production of cotton, soybeans, sugar beets, all grains, potatoes, and corn, (Ware, 2000). This shown a new finding of this project that *Pentace triptera* could produce carbamic acid by react it with benzene and toluene.

CHAPTER 5
CONCLUSION AND RECOMMENDATION

5.1 CONCLUSION

The main objective this research project is to study the effect of solution pH and initial solute concentration of organic compound on adsorption by *Pentace triptera*. Benzene and toluene is the organic compound which are effluent of petroleum refinery to waste water. *Pentace tripetra* used as and adsorbent to adsorb the organic compound. Furthermore, the project expected that optimum Solution pH and initial concentration will be finding for best adsorption to occur.

After the experiment is conducted, the result from UV-VIS Spectrophotometer shown that the concentration of benzene and toluene after adsorption higher than before adsorption. For varies of initial solute concentration (1, 5 10, 20, 40, 60, 80 and 100ppm), all sample gives benzene solution concentration after adsorption for nearly same concentration of 212.9 while for toluene concentration it gives also nearly same concentration at 2814.9. For varies of pH sample (pH 2, 5, 7, 9 12) fix concentration of 5ppm, result gives that after adsorption, for benzene, the concentration is 54.5ppm while for toluene, result gives the sample concentration after adsorption is 748.6ppm.

Based on the result, we could conclude that the equipment used for testing which is UV-Vis Spectrophotometer which work on qualitative method analysis. The error would occur in qualitative analysis which is interference by material with same wavelength of desired testing material. Contamination of sample and deviation of Beer's law also contribute to inaccurate result of UV-VIS equipment.

In order to verify and identify the component of mixture in sample after adsorption, Gas Chromatography Mass Spectroscopy has been selected in this project. Sample only conducted for sample at pH 2, 7, 12 and controlled sample at 5ppm for both benzene and toluene. Based on result, benzene and toluene concentration shown zero value meaning no benzene and toluene detected in the sample. While in sample component mixture analysis, it shown many peak in sample exist and mostly the possibilities of the formation of carbamic acid in the sample.

As a conclusion, *Pentace triptera* is not suitable adsorbent for adsorption of organic compound but applicable for biosorption of metal ion. From GCMS result (peaks chromatogram) and color of sample, Chlorophyll of dried biomass (*Pentace triptera leaf*) was extracted and leaf was digested by organic compound. A new finding from this project is the carcinogenic of Benzene and Toluene on Biomass and the formation of carbamic acid in the sample from extraction and digested of leaf by organic compound. .

5.2 RECOMMENDATION

Based on result determine by UV-VIS Spectrophotometer and Gas Chromatography Mass Spectrophotometer, in order to make sure and identify the component in sample mixture, High Performance Liquid Chromatography should be used in this project. HPLC is an instrumental chromatography in which the mobile phase is a liquid. Advantage of HPLC is that HPLC is a modern column technology and gradient solvent elution system for extremely complex system and can be analyze in short of time.

Pentace triptera is not suitable adsorbent for adsorption of organic compound due to carcinogenic of benzene and toluene from this research project. It is recommend that to change with other biomass prospect like chatosan and micro degraded of organic compound by microorganism.

Seems from the sample analysis by GCMS found the formation of carbamic acid from *Pentace triptera* in contact with benzene and toluene, further analysis could be study so that we could find a new way of producing carbamic acid which carbamic acid are widely use as an intermediate in the synthesis of a variety of products and as a solubilizer and co solvent for pesticides and fumigants. Carmates of carbamic acid also one type of natural herbicide. Herbicides, or chemical weed killers, have largely replaced mechanical methods of weed control in countries where intensive and highly mechanized agriculture is practiced.

Extraction of chlorophyll and other compound from *Pentace triptera* leaf by organic compound also one new finding from this research project and further study should also be study. Referring to journal by Sung, Y. Y. (1997) found that flavonoid is extracts from the leaves of *Ginkgo biloba* L. have been therapeutically used in Asian countries for centuries. Organic solvents are generally employed to extract metabolites from whole plants or plant materials and further purification of the metabolites is necessary. (Sung, 1997)

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APPENDIX A: Picture

A1: Adsorbent

A1.1 Pentace Triptera Leaves

A1.2 Grinding Pentace Triptera (size: 0.5- 1mm)

A2: Tools and Equipment

A2.1 Mortar Grinder

A2.2 Sieving Machine

A2.3 Toluene

A2.4 Benzene

A2.5 HCl

A2.6 NaCl

A2.7 Different Concentration Preparation

A2.8 pH meter

A2.9 Weighing Balance

A2.10 Sample before shaking

A2.11Rotary Shaker

A2.12 UV-VIS Spectrophotometer

A3: Sample

A3.1 Vary of Concentration

A3.1.1 Benzene

A3.1.2 Toluene

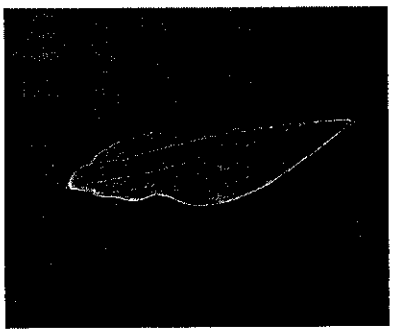
A3.2 Vary of pH

A3.2.1 Benzene

A3.2.2 Toluene

APPENDIX A: PICTURE

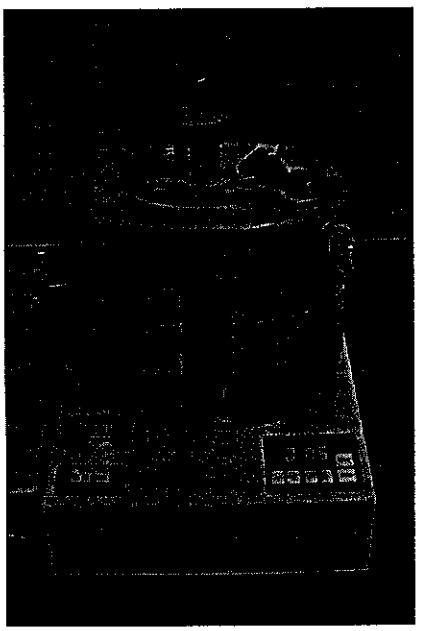
A1. Adsorbent:



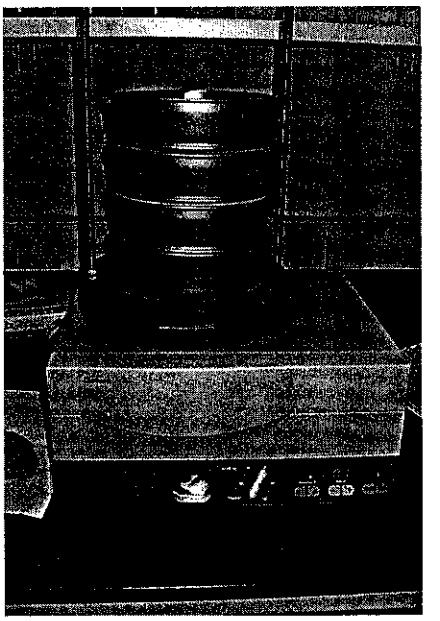
A1.1 *Pentace Triptera Leaves*

A1.2 *Grinding Pentace Triptera (size: 0.5- 1mm)*

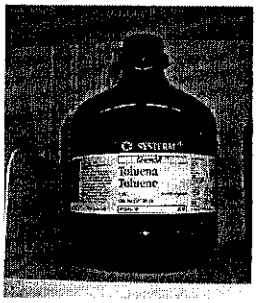
A2. Tools and Equipments:



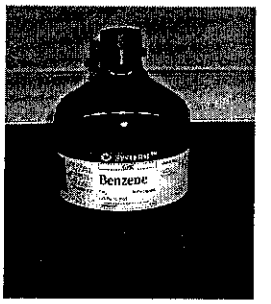
A2.1 *Mortar grinder*



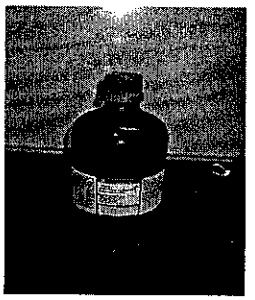
A2.2 *Sieving Machine*



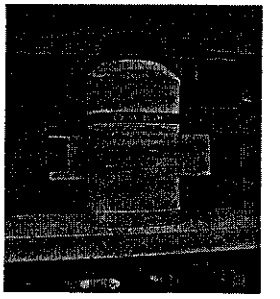
A2.3 Toluene



A2.4 Benzene

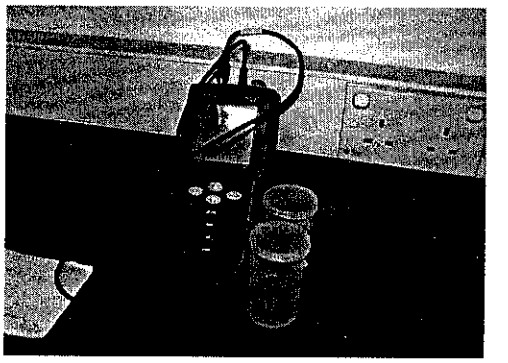


A2.5 HCl

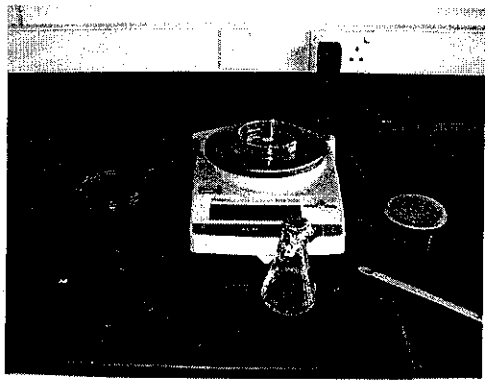


A2.6 NaCl

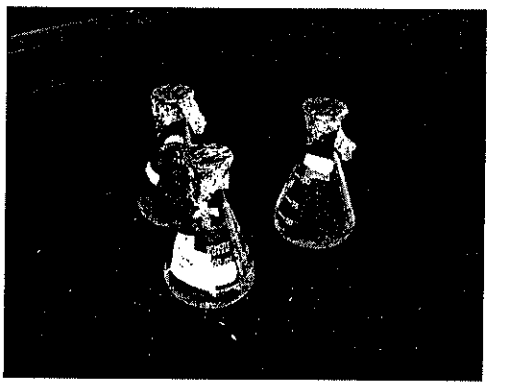
A2.7 Different Concentration preparation



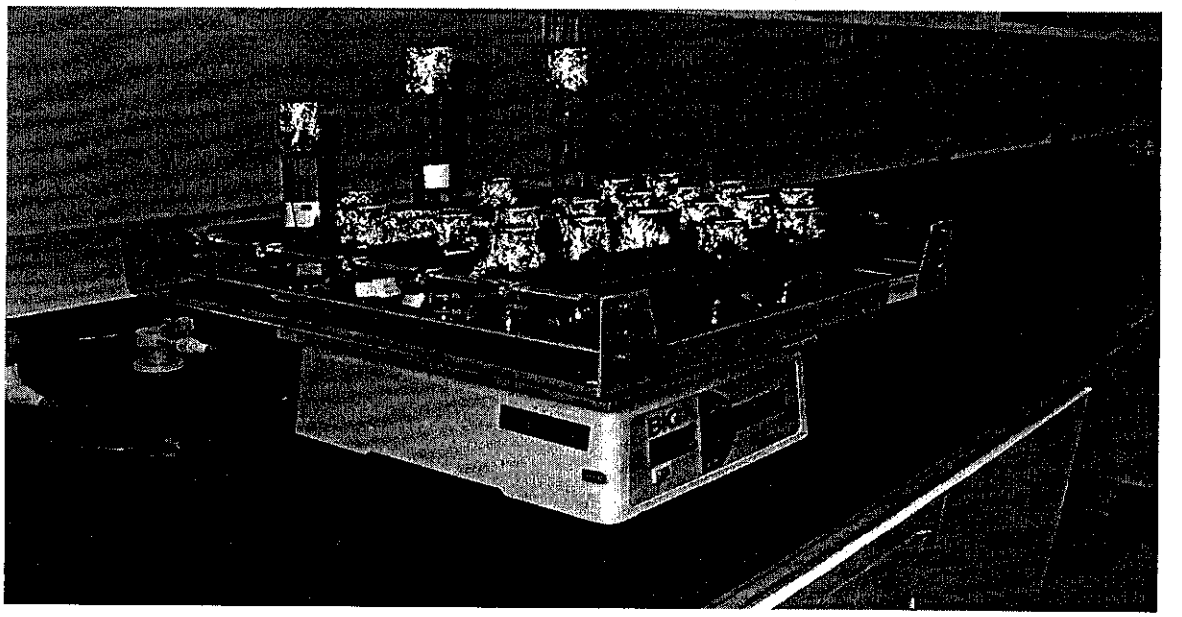
A2.8 pH meter: Measure pH sample



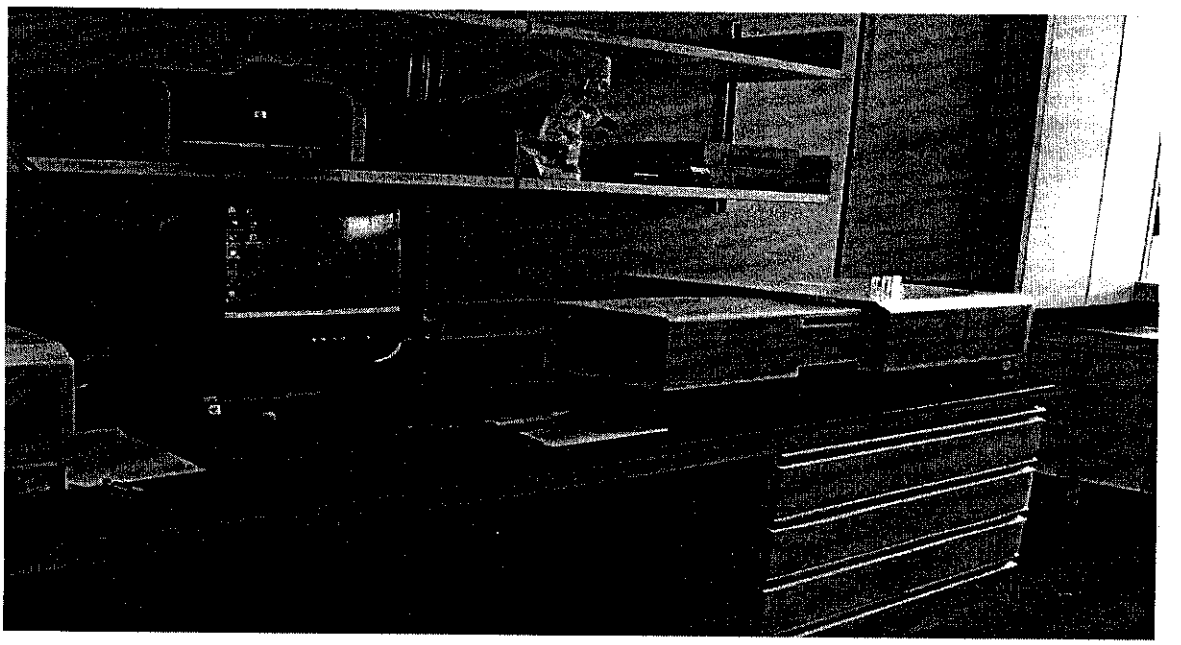
A2.9: Weighing Balance: Weight Sample



A2.10 Sample before Shaking



A2.11 *Rotary Shaker: Adsorption Process*



A2.12 *UV-VIS Spectrophotometer Unit: Testing Sample*

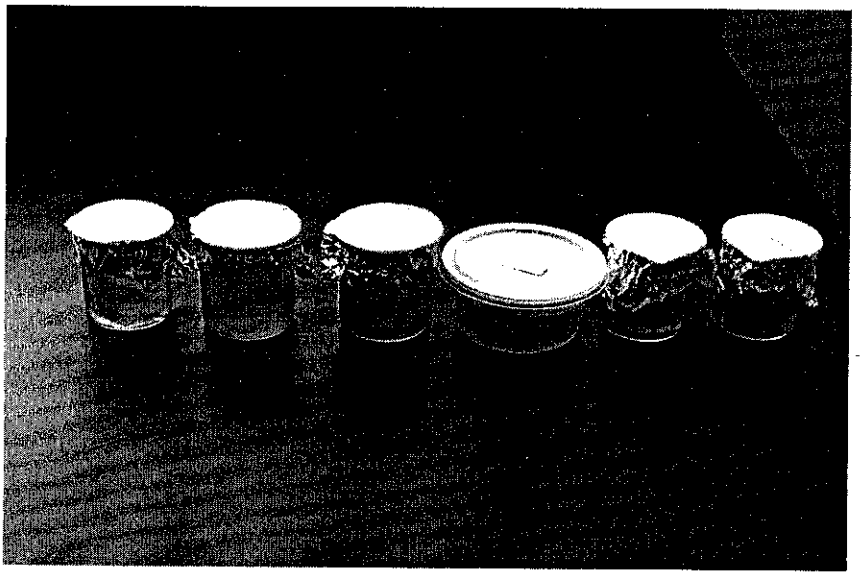
A3. Sample:

A3.1 Vary of Concentration:

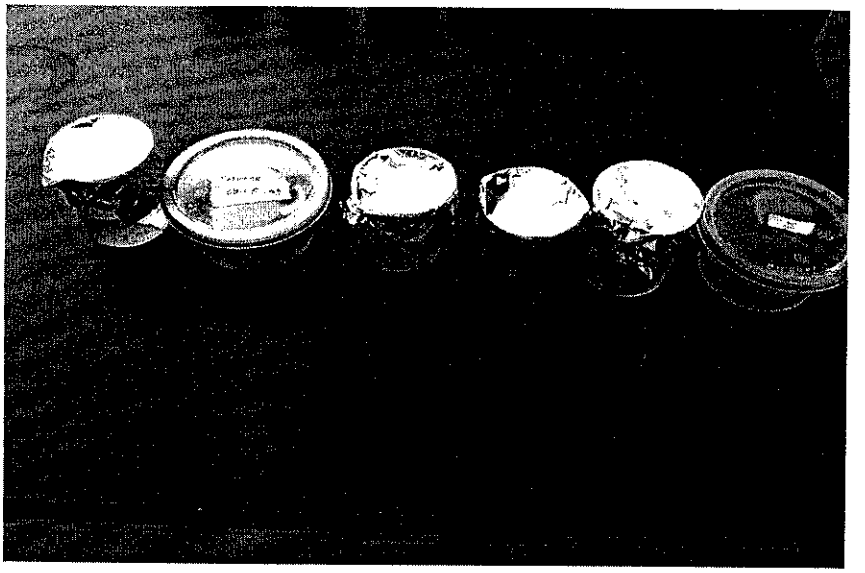
A3.1.1 *Benzene*

A3.1.2 *Toluene*

A3.2 Vary of pH



A3.2.1 *Benzene*



A3.2.2 *Toluene*

APPENDIX B: UV-VIS RESULT

B1: Standard Calibration Curve

B1.1 Standard Benzene Vary Concentration Calibration Curve

B1.2 Standard Toluene Vary Concentration Calibration Curve

B1.3 Standard Benzene Vary pH Calibration Curve

B1.3 Standard Toluene Vary pH Calibration Curve

B2: Sample Tested

B2.1 Vary Benzene Concentration Tested Sample

B2.2 Vary Toluene Concentration Tested Sample

B2.3 Vary Benzene pH Tested Sample

B2.4 Vary Toluene pH Tested Sample

B3: Spectrum Analysis

B3.1 50ppm Benzene Standard Sample Spectrum Analysis.

B3.2 5ppm Toluene Standard Sample Spectrum Analysis.

B3.3 60ppm Benzene Tested Sample Spectrum Analysis.

B3.4 60ppm Toluene Tested Sample Spectrum Analysis.

B3.5 pH 2 Benzene Tested Sample Spectrum Analysis

B3.6 pH 2 Toluene Tested Sample Spectrum Analysis

B3.7 pH 12 Benzene Tested Sample Spectrum Analysis

B3.8 pH 12 TolueQne Tested Sample Spectrum Analysis

APPENDIX C: GCMS RESULT

C1: Qualitative Analysis

C1.1 Qualitative Analysis of Benzene Samples

C1.2 Qualitative Analysis of Toluene Samples

C2: Chromatogram Separation of Benzene Sample

C2.1 Benzene of pH 2

C2.2 Benzene of pH 7

C2.3 Benzene of pH 12

C2.4 Benzene Control Sample

C3: Chromatogram Separation of Toluene Sample

C3.1 Toluene of pH 2

C3.2 Toluene of pH 7

C3.3 Toluene of pH 12

C3.4 Toluene Control Sample

.1 : Standard Benzene Vary Concentration Calibration curve

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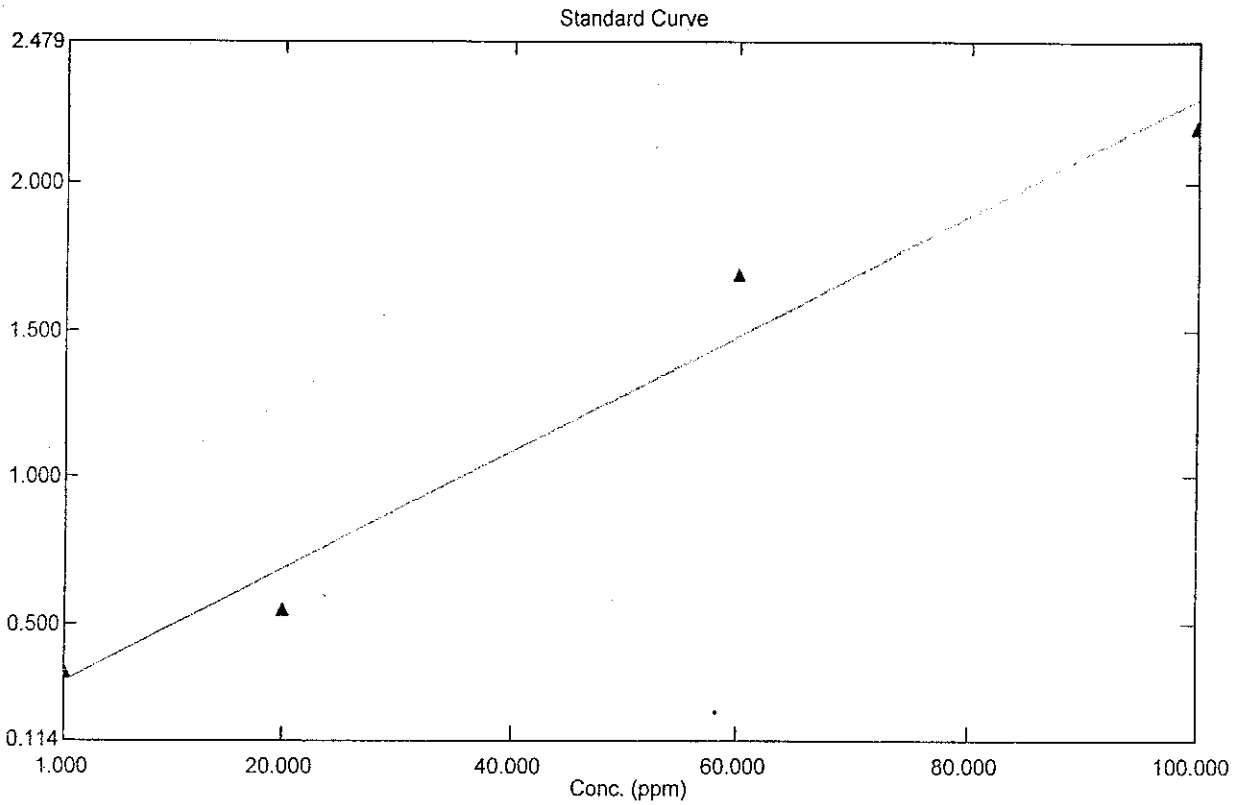

ard Table

	Sample ID	Type	Ex	Conc	WL204.1	Wgt.Factor	Comments
	Std1	Standard		1.000	0.345	1.000	
	Std2	Standard		20.000	0.547	1.000	
	Std3	Standard		60.000	1.689	1.000	
	Std4	Standard		100.000	2.191	1.000	

B1. 2 : Standard Toluene Vary Concentration Calibration Curve

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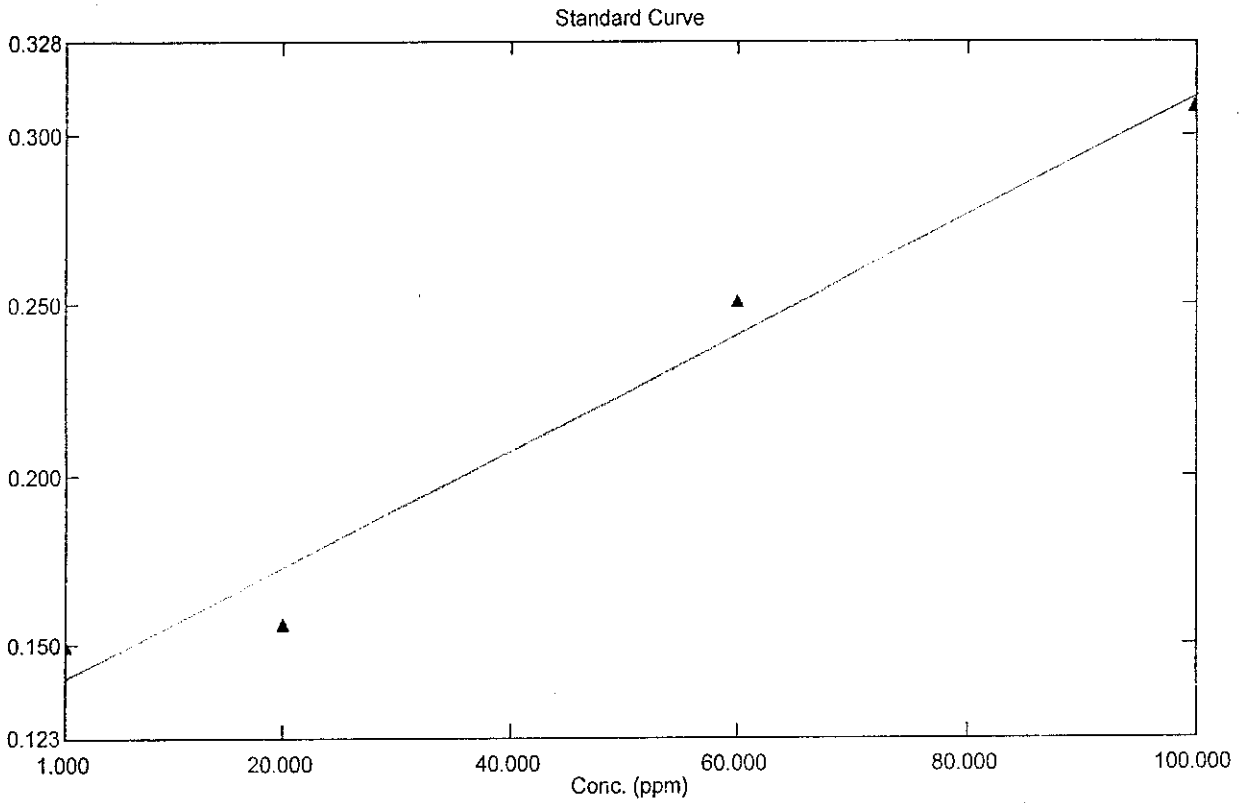
03/29/2004 11:31:33 AM

e Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\Std_Toluene.pho



idard Table

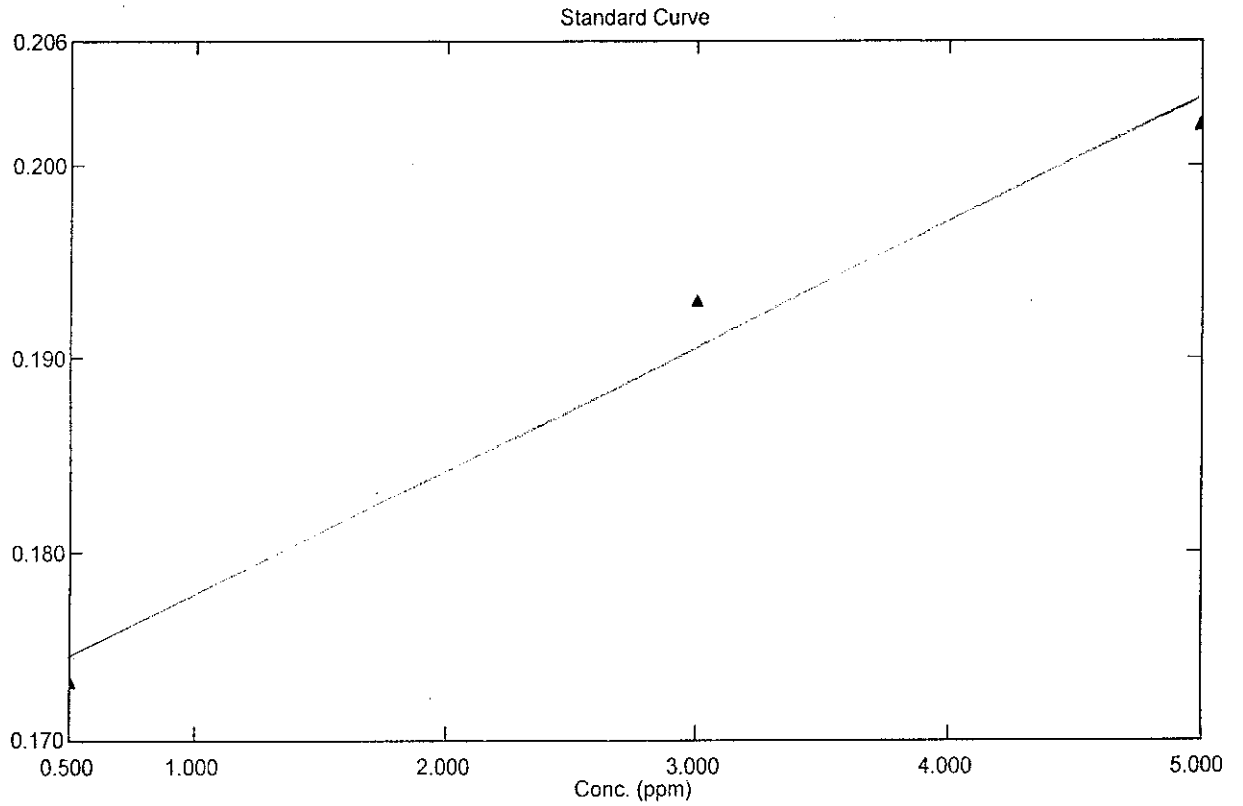
	Sample ID	Type	Ex	Conc	WL260.9	Wgt.Factor	Comments
	Std1	Standard		1.000	0.149	1.000	
	Std2	Standard		20.000	0.156	1.000	
	Std3	Standard		60.000	0.251	1.000	
	Std4	Standard		100.000	0.308	1.000	

51.3 : Standard Benzene vary pH Calibration Curve

:andard Table Report

04/08/2004 11:04:26 AM

Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH study\stdPpHtoluene.pho



ard Table

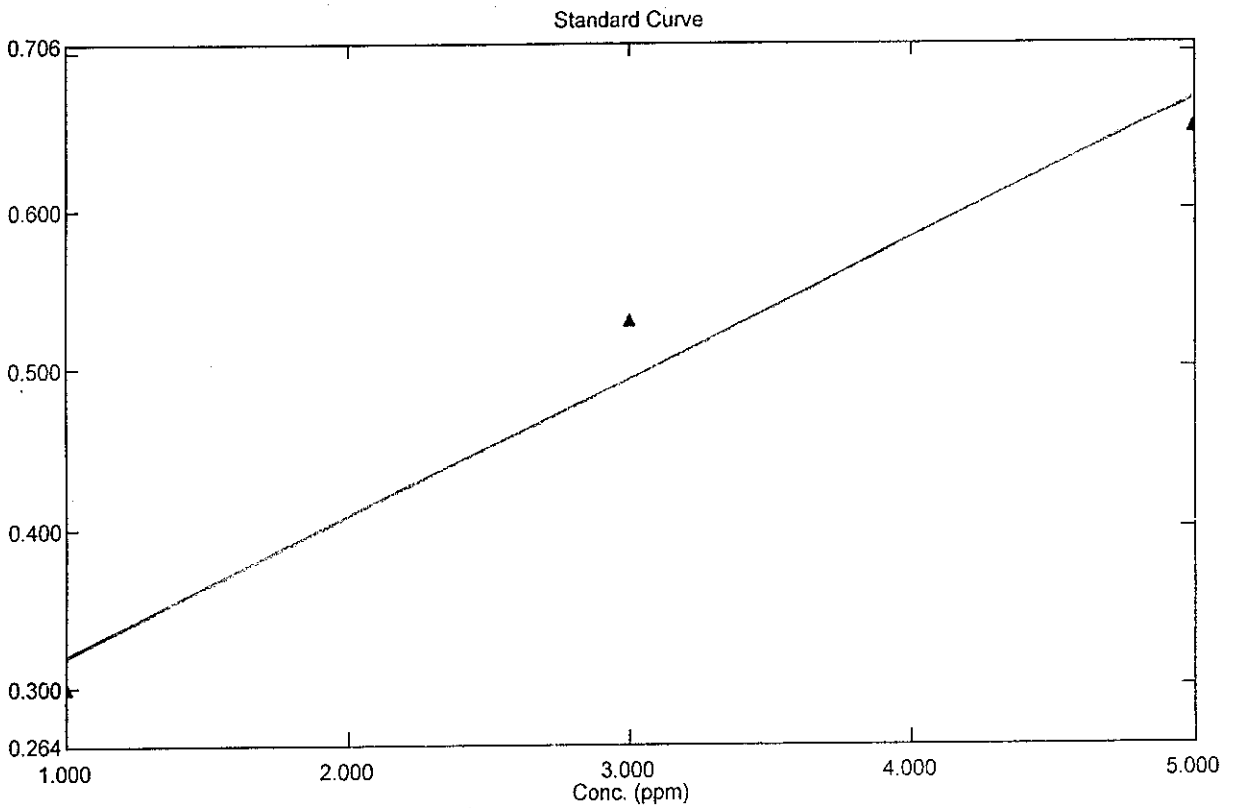
	Sample ID	Type	Ex	Conc	WL260.9	Wgt.Factor	Comments
	Std_pHT	Standard		5.000	0.202	1.000	
	Std_pHT2	Standard		3.000	0.193	1.000	
	Std_pHT3	Standard		0.500	0.173	1.000	

B1.4 : Standard Toluene Vary pH Calibration Curve

tandard Table Report

04/08/2004 11:04:02 AM

e Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH study\std_pHbenzene2.pho



ıdard Table

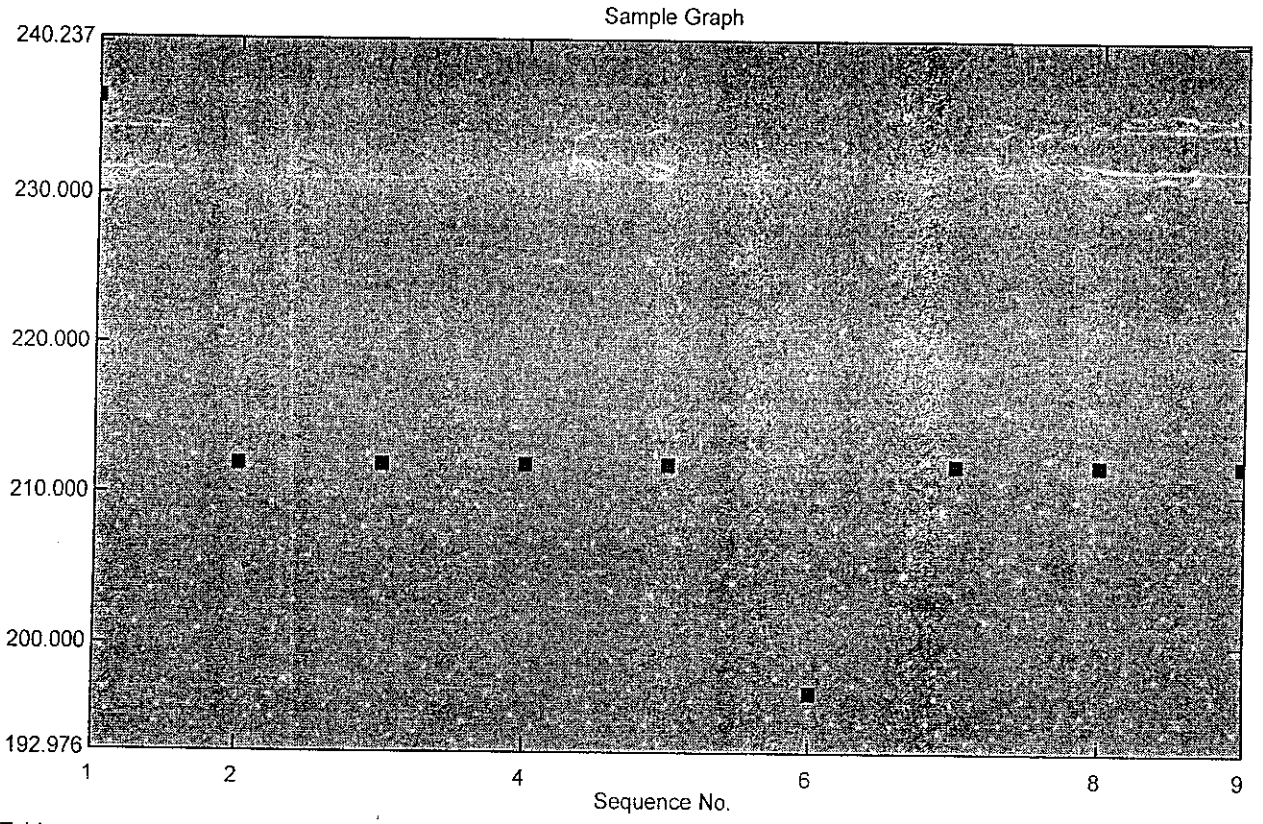
	Sample ID	Type	Ex	Conc	WL204.1	Wgt.Factor	Comments
	Std_pB1	Standard		1.000	0.301	1.000	
	Std_pB2	Standard		3.000	0.531	1.000	
	Std_pB3	Standard		5.000	0.651	1.000	

B.L.1 : Vary Benzene Concentration Tested Sample

ample Table Report

03/29/2004 11:32:17 AM

e Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\Std_Benzenetry2.pho



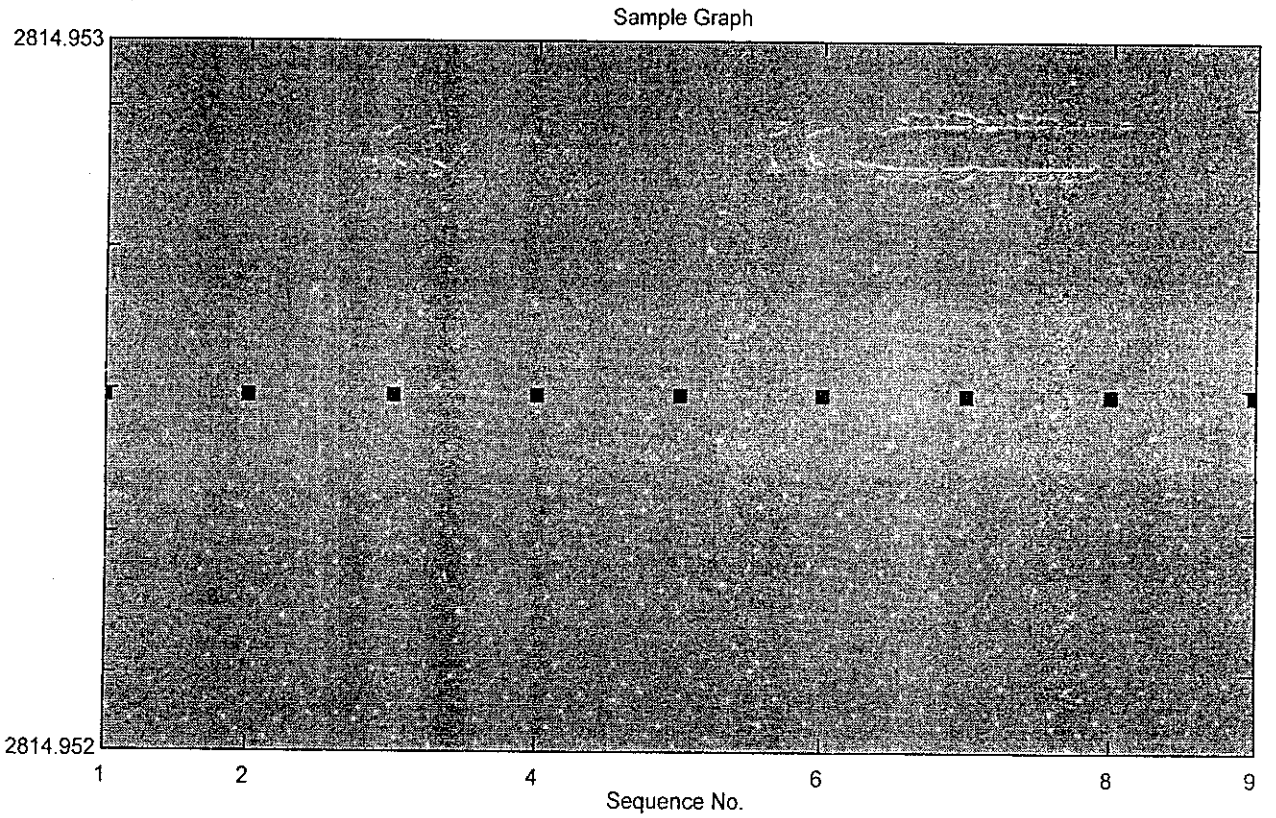
e Table

	Sample ID	Type	Ex	Conc	WL204.1	Comments
	C8	Unknown		236.299	5.000	
	C9	Unknown		212.024	4.516	
	C1	Unknown		212.024	4.516	
	C5	Unknown		212.024	4.516	
	C6	Unknown		212.024	4.516	
	C7	Unknown		196.914	4.215	
	C2	Unknown		212.024	4.516	
	C3	Unknown		212.024	4.516	
	C4	Unknown		212.024	4.516	

;ample Table Report

03/29/2004 12:19:28 PM

le Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\Std_TolueneC1.pho



ole Table

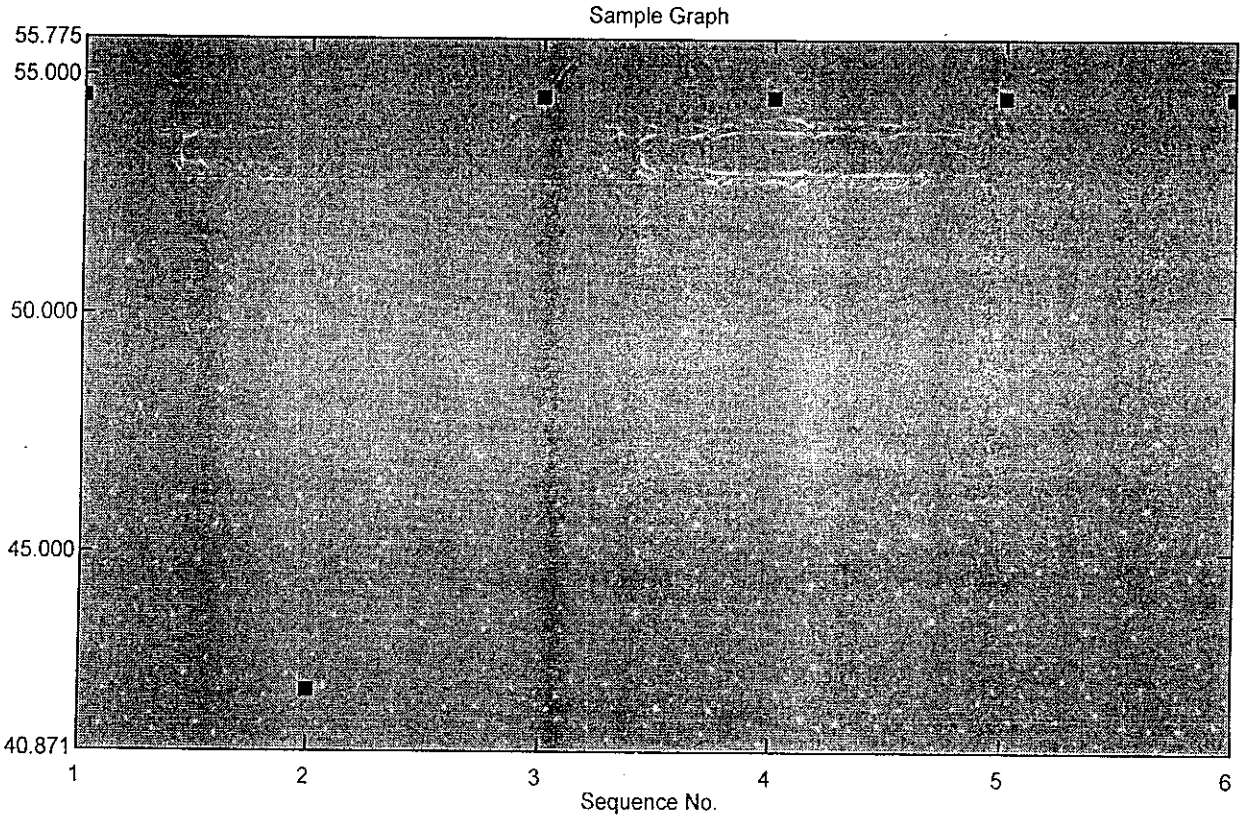
	Sample ID	Type	Ex	Conc	WL260.9	Comments
	CT1	Unknown		2814.952	5.000	
	CT2	Unknown		2814.952	5.000	
	CT3	Unknown		2814.952	5.000	
	CT4	Unknown		2814.952	5.000	
	CT5	Unknown		2814.952	5.000	
	CT6	Unknown		2814.952	5.000	
	CT7	Unknown		2814.952	5.000	
	CT8	Unknown		2814.952	5.000	
	CT9	Unknown		2814.952	5.000	

B2 · 3 : Vary. Benzene pH tested Sample

ample Table Report

03/29/2004 01:00:21 PM

e Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH study\test1.pho



le Table

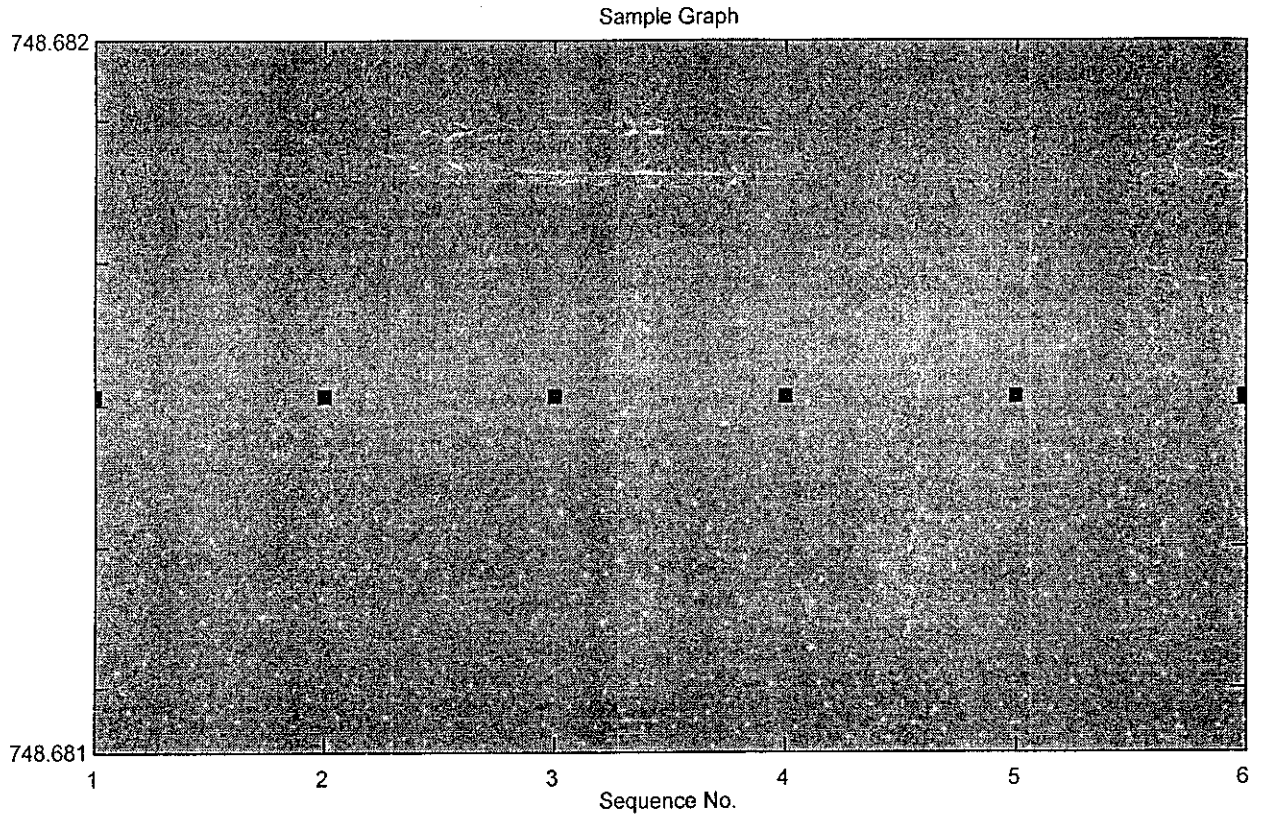
	Sample ID	Type	Ex	Conc	WL204.1	Comments
	pH2	Unknown		54.533	5.000	
	pH5	Unknown		42.113	3.914	
	pH7	Unknown		54.533	5.000	
	pH9	Unknown		54.533	5.000	
	pH12	Unknown		54.533	5.000	
	Control	Unknown		54.533	5.000	

B2.A : Vary toluene pH tested sample

ample Table Report

04/08/2004 11:05:58 AM

e Name: C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH study\test2.pho



ple Table

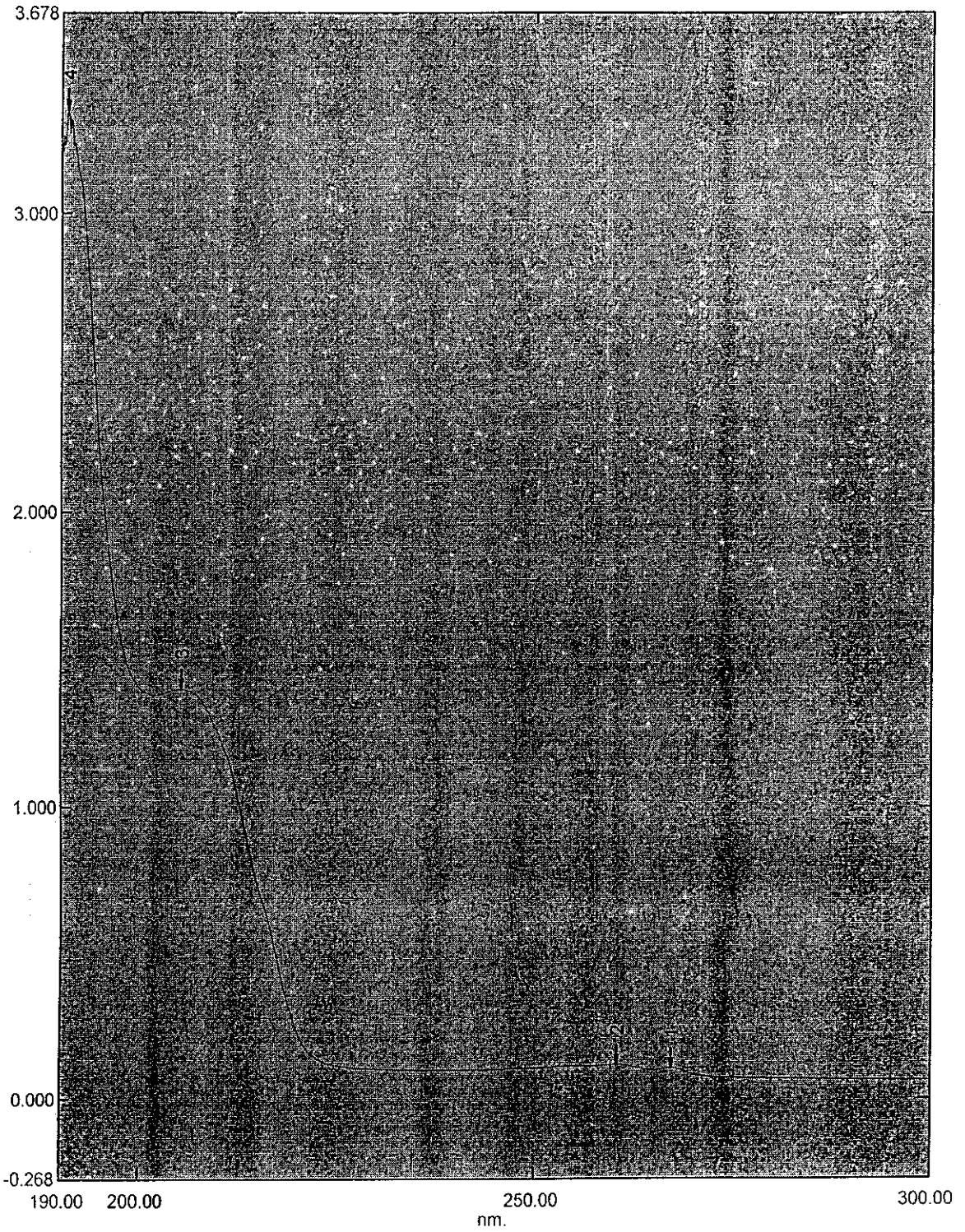
	Sample ID	Type	Ex	Conc	WL260.9	Comments
	pH2	Unknown		748.681	5.000	
	pH5	Unknown		748.681	5.000	
	pH7	Unknown		748.681	5.000	
	pH9	Unknown		748.681	5.000	
	pH12	Unknown		748.681	5.000	
	Control	Unknown		748.681	5.000	

B3.1 : 50 ppm Benzene Std Spectrum Analysis

/erlay Spectrum Graph Report

03/26/2004 05:52:21 PM

Storage 174728 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\yh\50ppmbenzene.spc

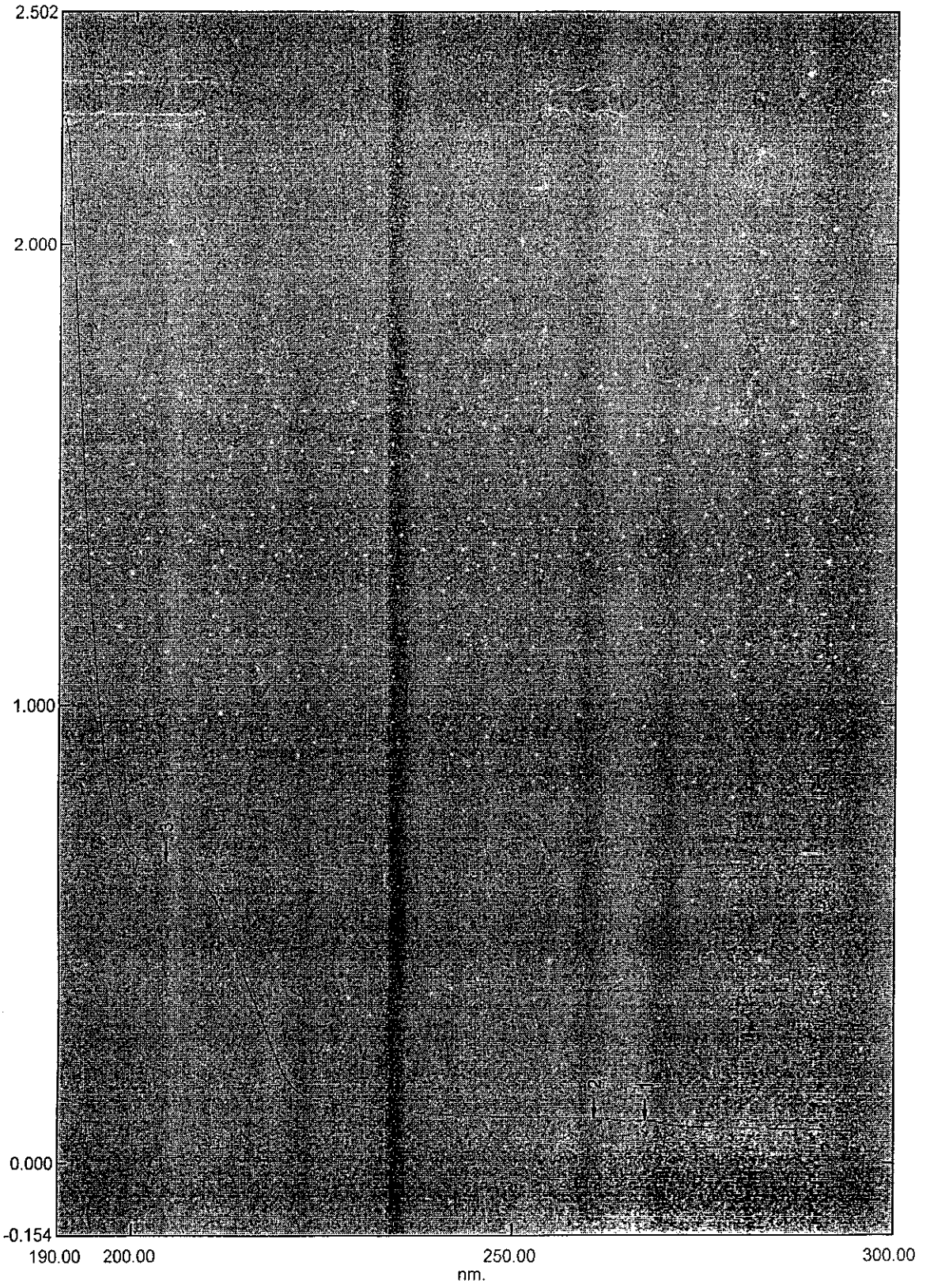


B5-2. . 5 ppm

Active Spectrum Graph Report

03/29/2004 12:43:31 PM

Data Set: Storage 124154 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\5ppmtry.spc

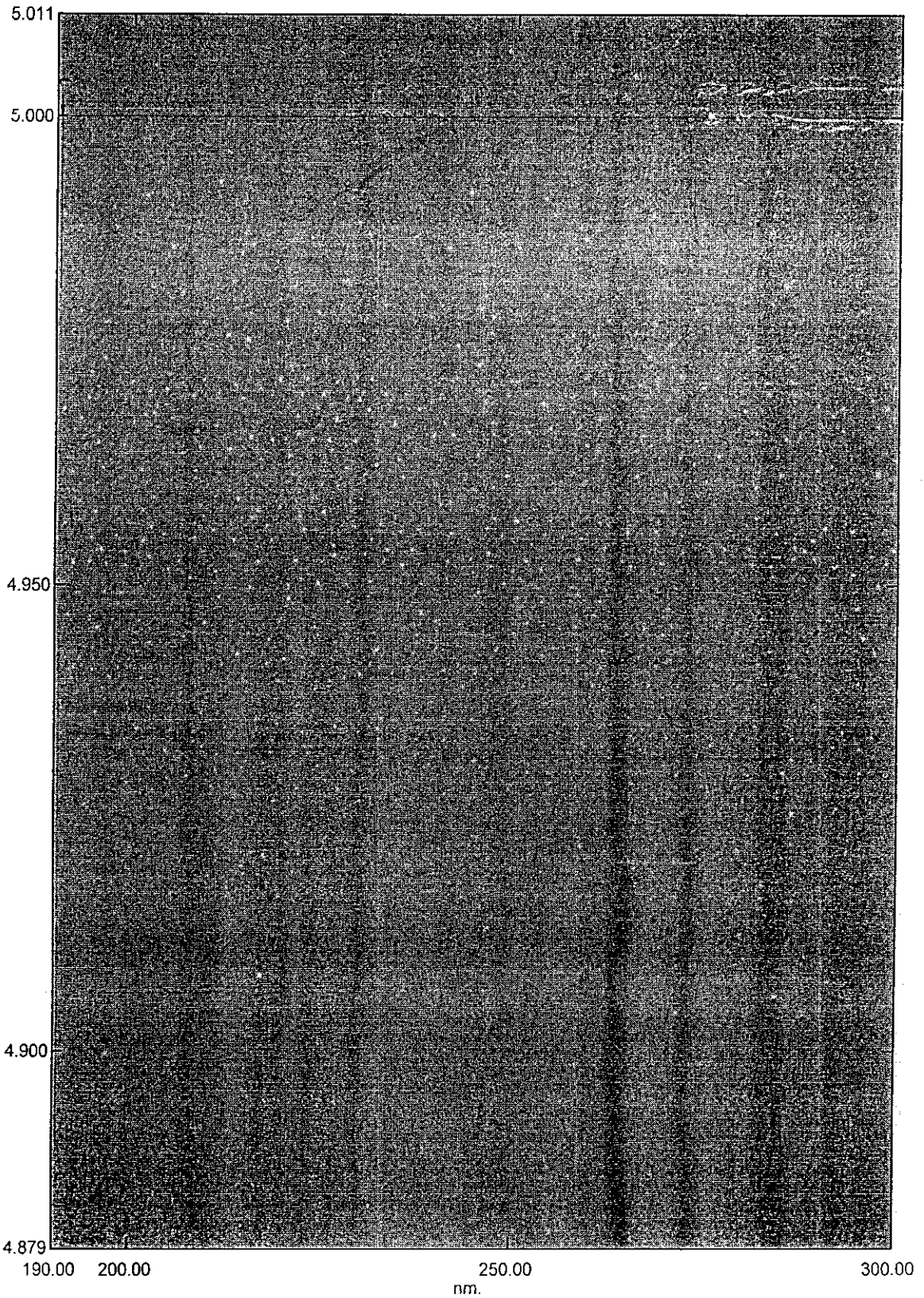


B3. 4 : 60 ppm Benzene Tested Sample Spectrum Analys

ctive Spectrum Graph Report

04/05/2004 02:45:16 PM

ta Set: Storage 144354 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\Abenzene60ppm.spc

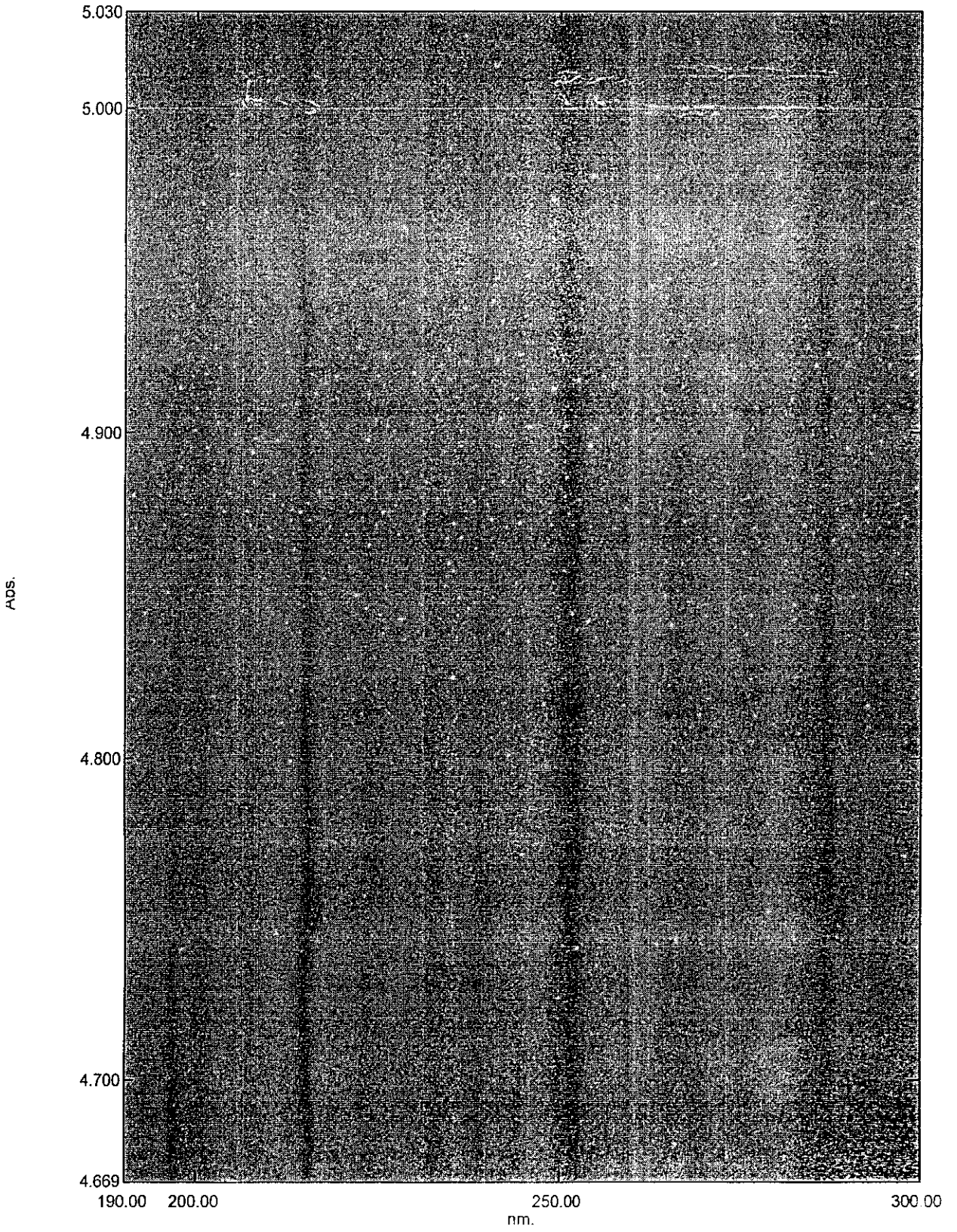


B3-4 : 60ppm Toluene tested sample spectrum Analysis.

Active Spectrum Graph Report

04/08/2004 11:32:32 AM

Data Set: Storage 113143 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\60ppmT.spc

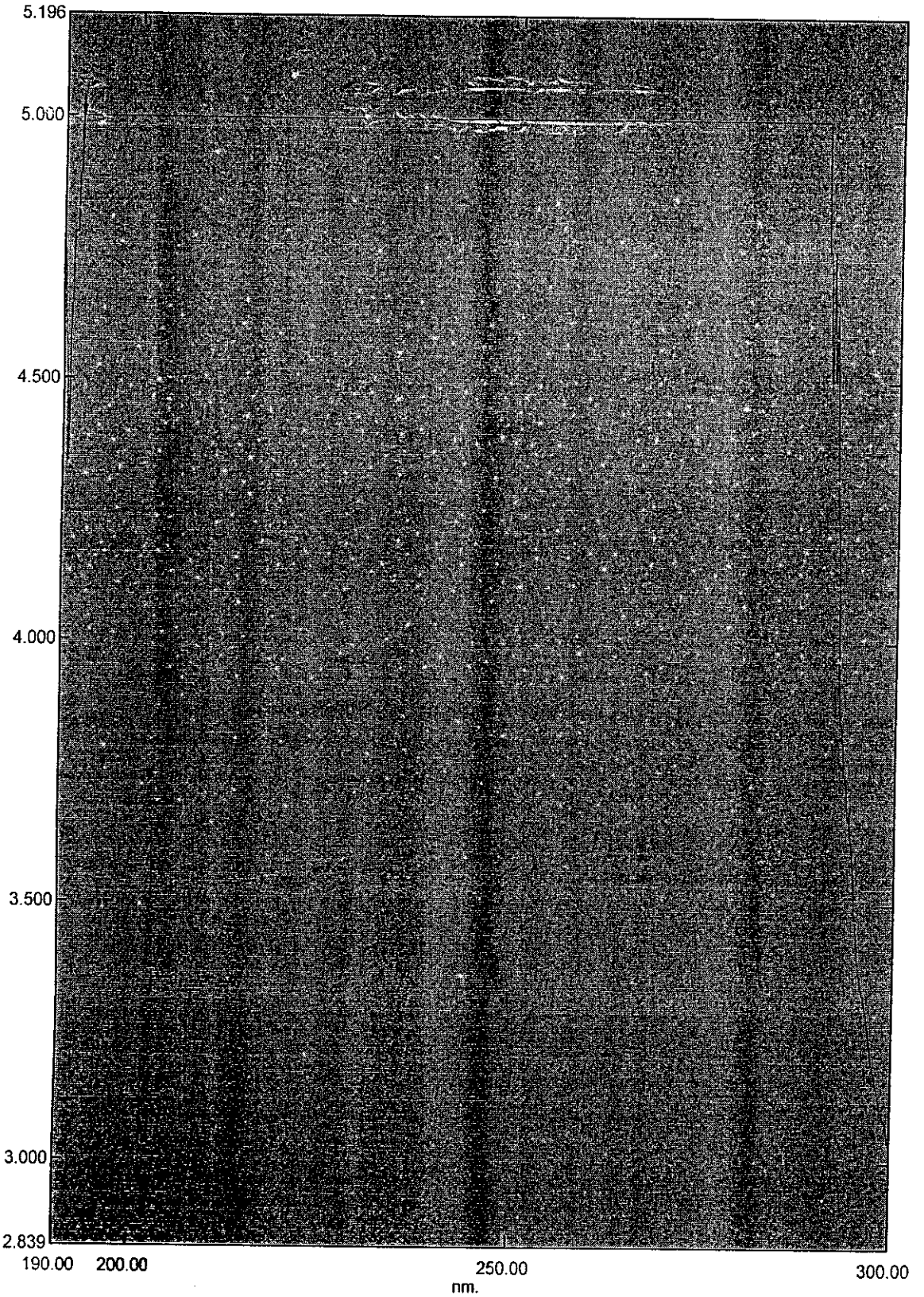


3.5 : pH2 Benzene Tested Sample Spectrum Analysis

ctive Spectrum Graph Report

04/08/2004 11:13:59 AM

ta Set: Storage 111336 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH2ben.spc

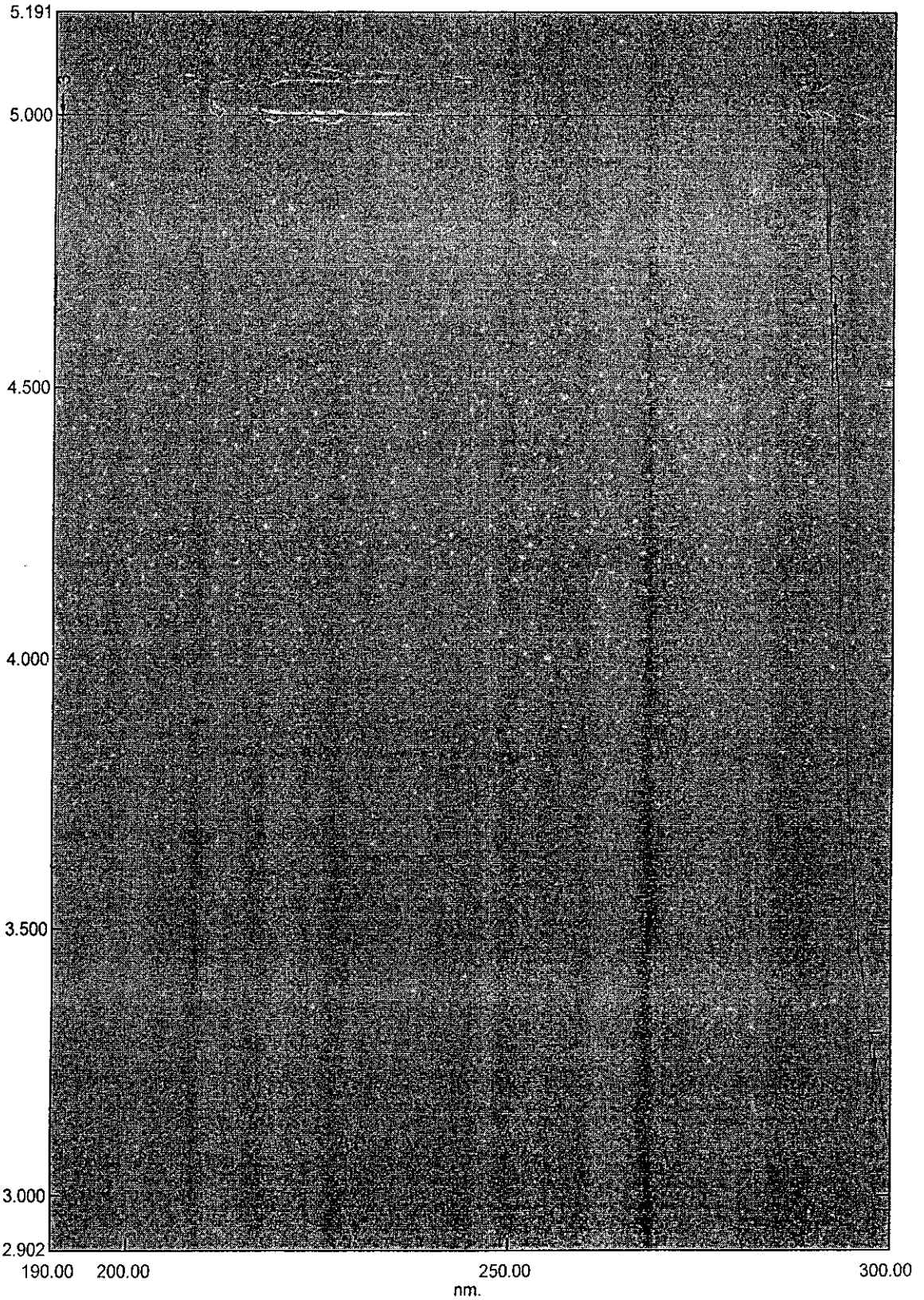


B 3.6 : pH 2 Toluna Tested Sample Spectrum Analysis

ıctive Spectrum Graph Report

04/08/2004 11:15:54 AM

ata Set: Storage 111534 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH2Tou.spc

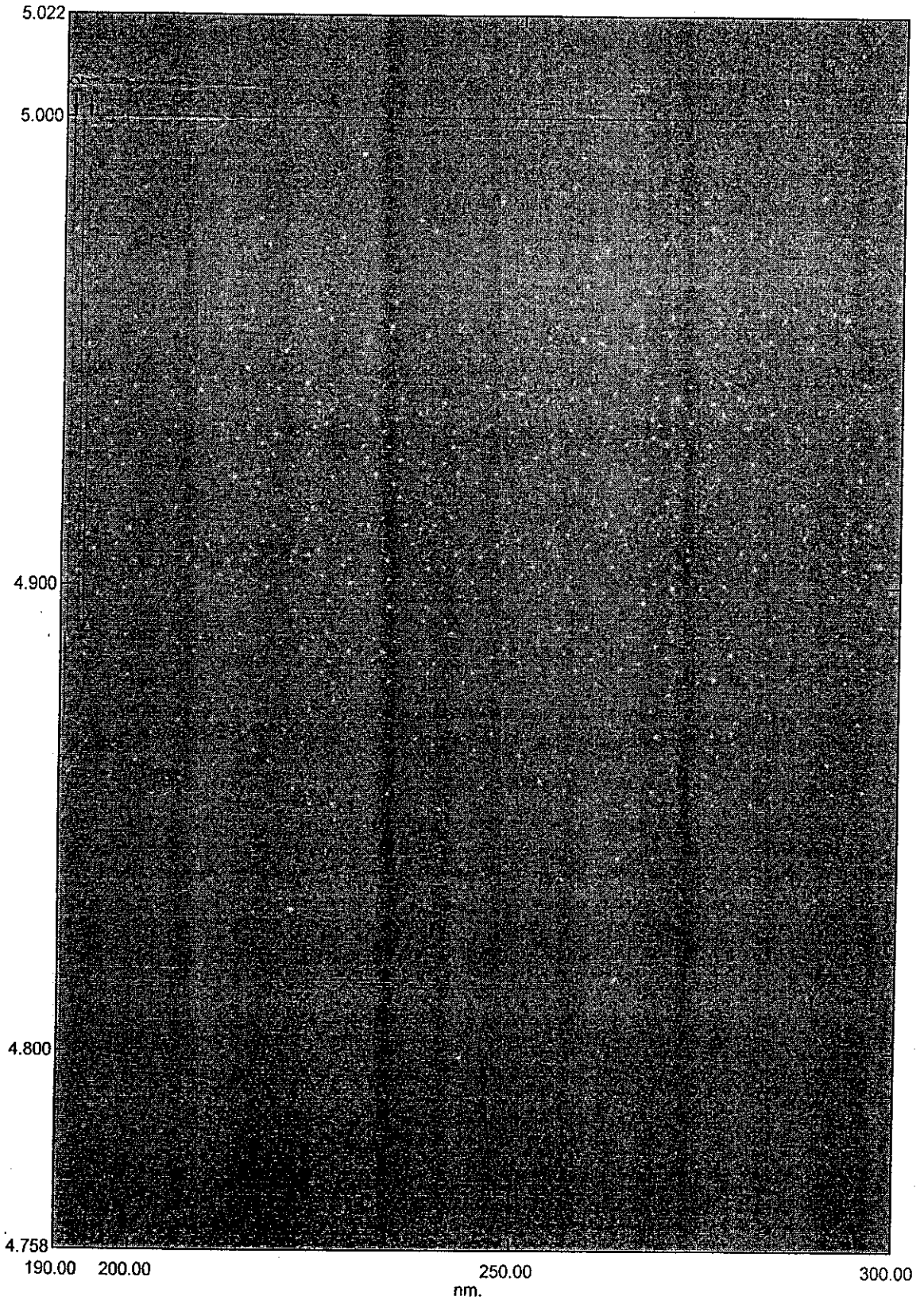


B3.7 : pH 12 Benzene Tested Sample Spectrum Analysis.

ctive Spectrum Graph Report

04/08/2004 11:18:54 AM

a Set: Storage 111835 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH12ben.spc

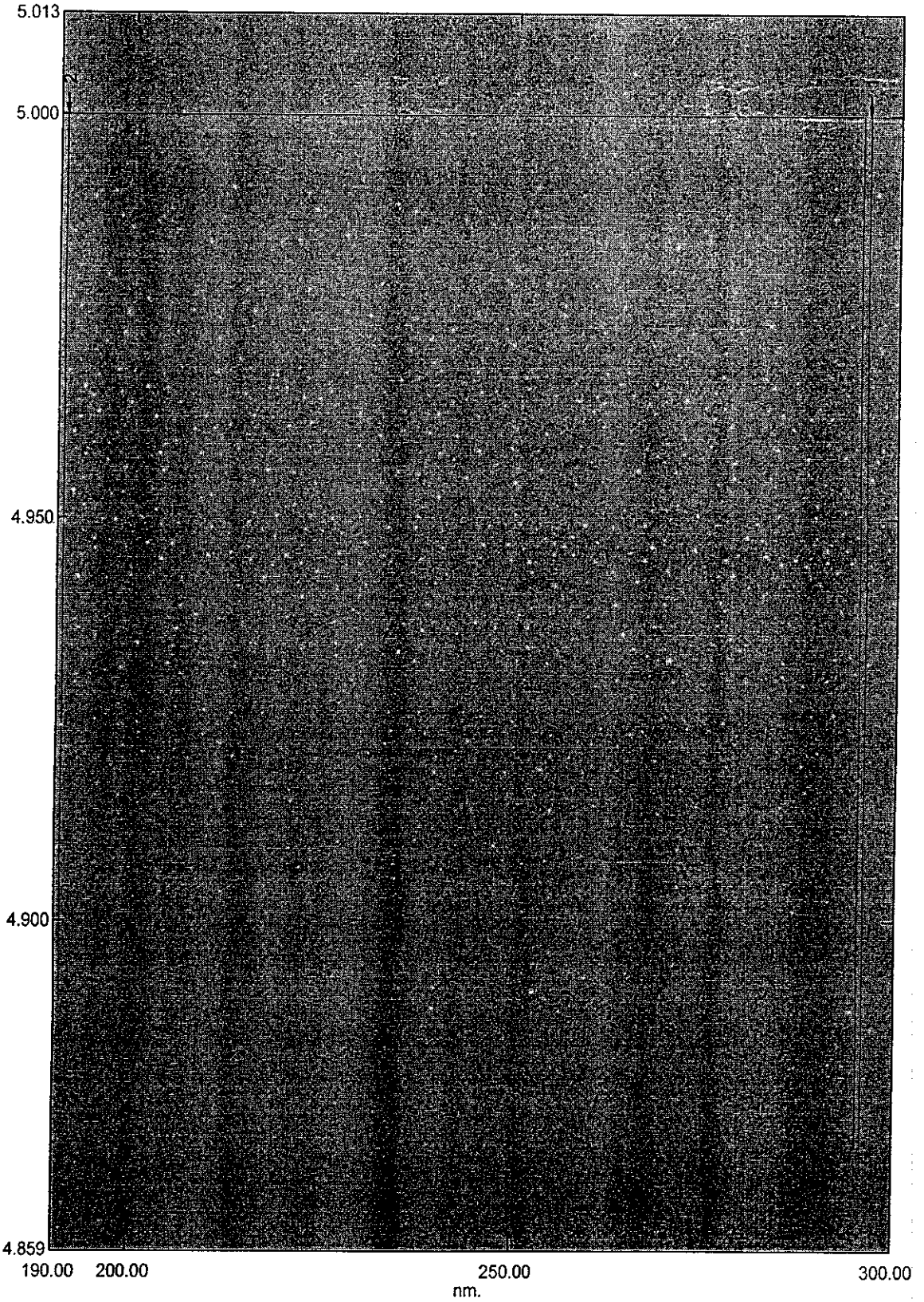


B3.8 : pH 12. 10 nm. tested sample Spectrum Analysis

Active Spectrum Graph Report

04/08/2004 11:21:04 AM

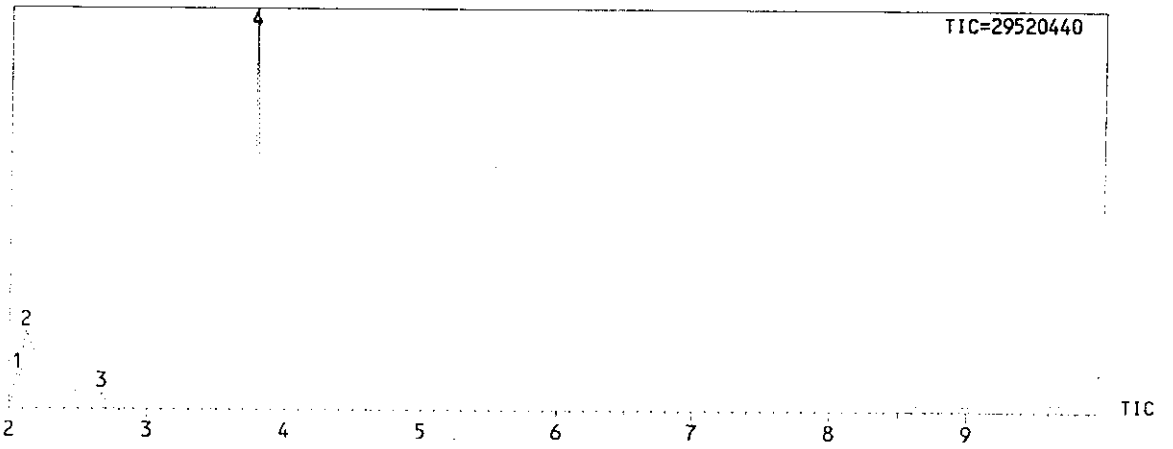
Data Set: Storage 112044 - RawData - C:\Program Files\Shimadzu\UVProbe\Data\fyp_2004\malik\pH12tou.spc



*** CLASS-5000 *** Report No. = 21 Data : HO-BEN.D02 04/04/22 11:54:45

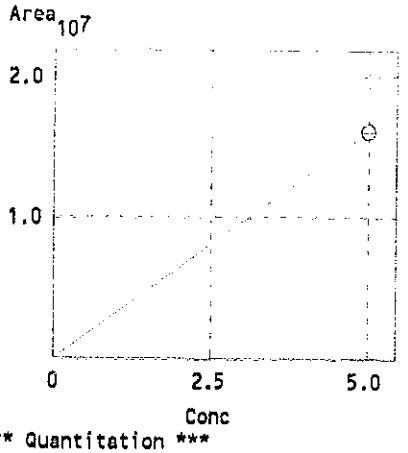
Sample : std ben
ID :
Type : Standard
Method File Name : HO-BEN.MET

*** Chromatogram ***



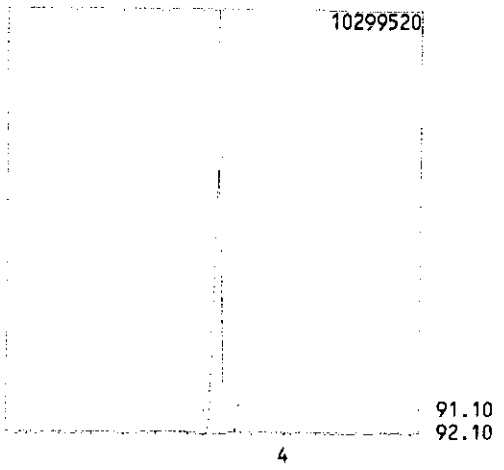
*** Calibration Curve ***

ID # 1 M/Z : 91.10 Name : benzene
Area = 3.21868e+006 * (Conc.) r2 = 1.000000



	Conc.(ppm)	Area
1	5.000	16093376

*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : benzene

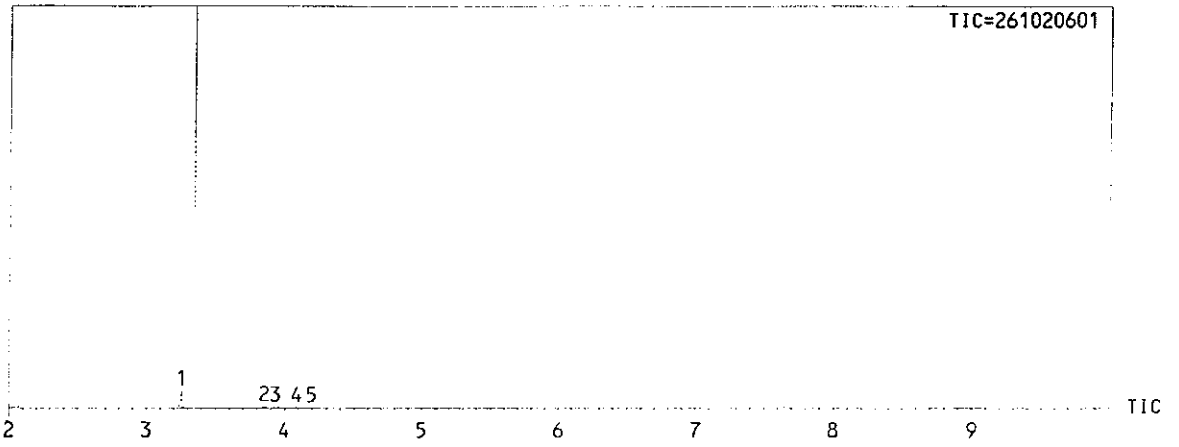
Time : 3.787
Area : 16093376

	M/Z	Area	%Rel.Int.to Target
1	92.10	10200428	63

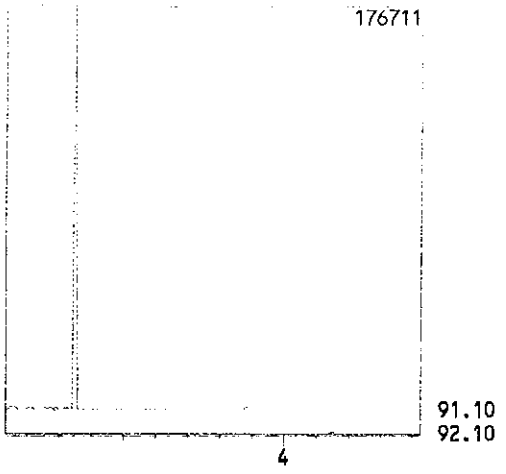
*** CLASS-5000 *** Report No. = 22 Data : MALIK.D01 04/04/27 10:45:18

Sample : BenzenepH2
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : benzene

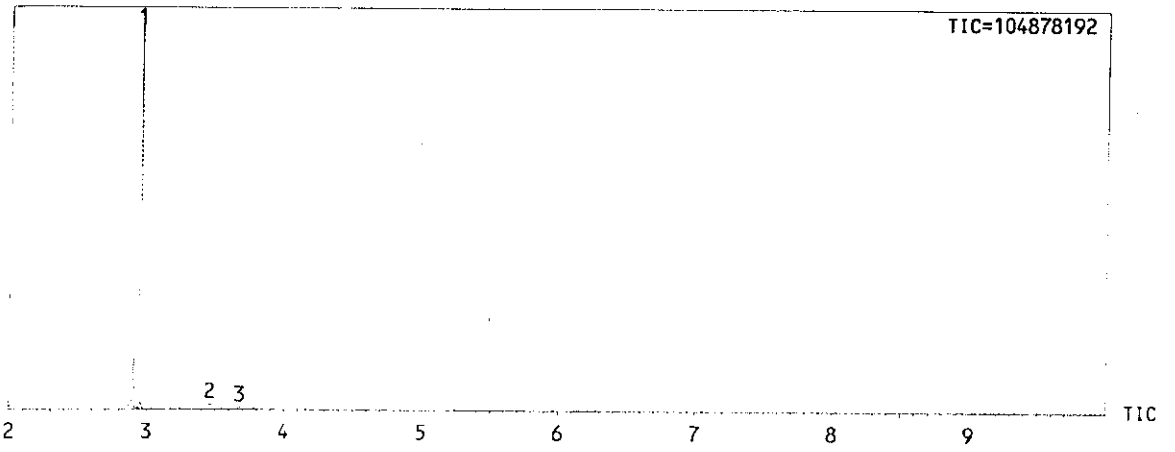
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

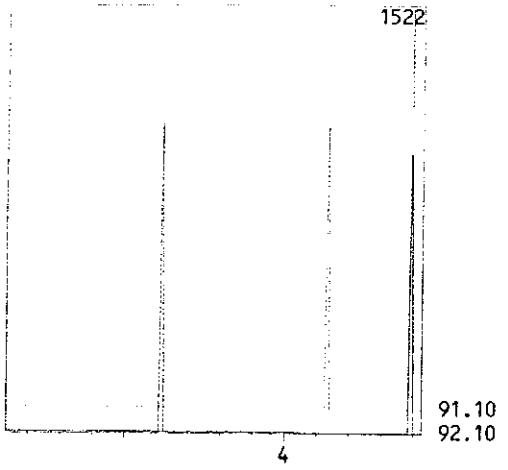
*** CLASS-5000 *** Report No. = 23 Data : MALIK.D02 04/04/27 11:18:44

Sample : BenzenepH7
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : benzene

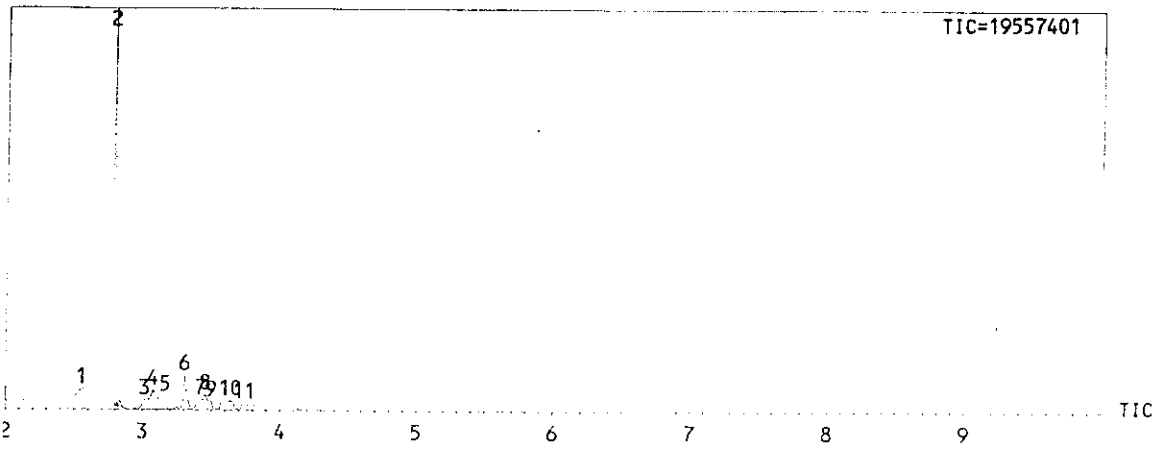
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

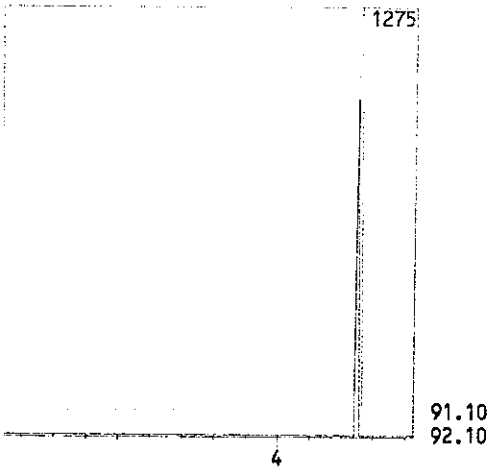
*** CLASS-5000 *** Report No. = 24 Data : MALIK.D03 04/04/27 11:54:52

Sample : BenzenepH12
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : benzene

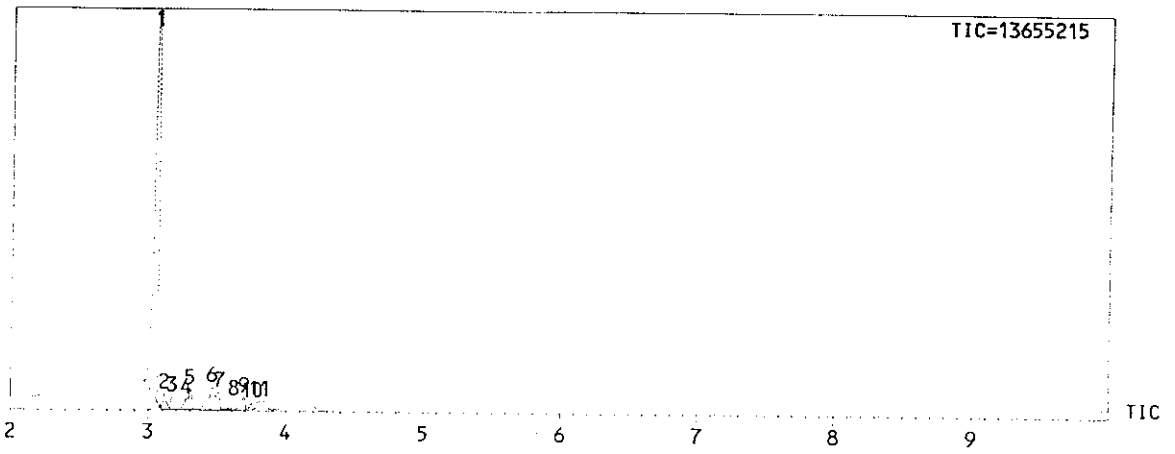
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

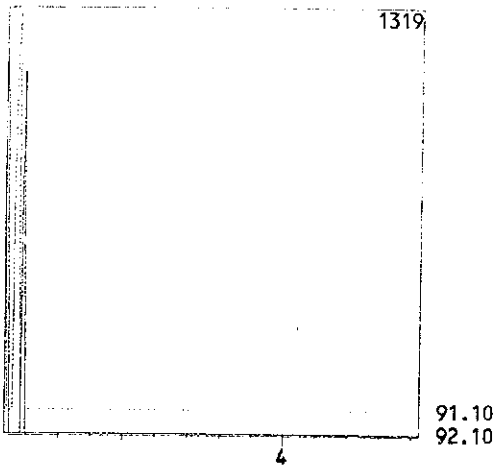
*** CLASS-5000 *** Report No. = 25 Data : MALIK.D04 04/04/27 12:42:02

Sample : BenzeneControl
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : benzene

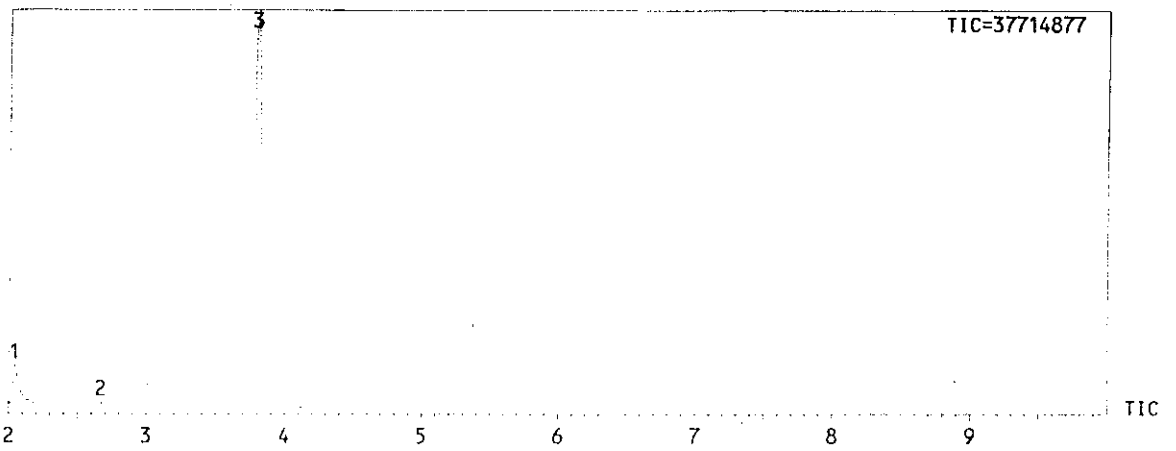
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

*** CLASS-5000 *** Report No. = 26 Data : HO-BEN.D10 04/04/22 16:46:30

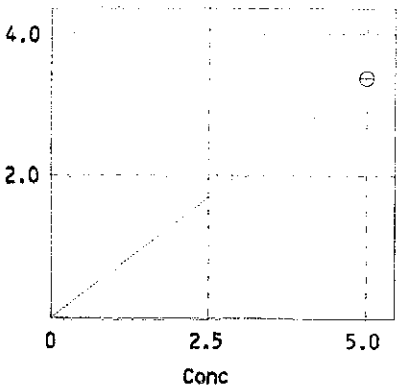
Sample : std tol
ID :
Type : Standard
Method File Name : HO-BEN.MET

*** Chromatogram ***



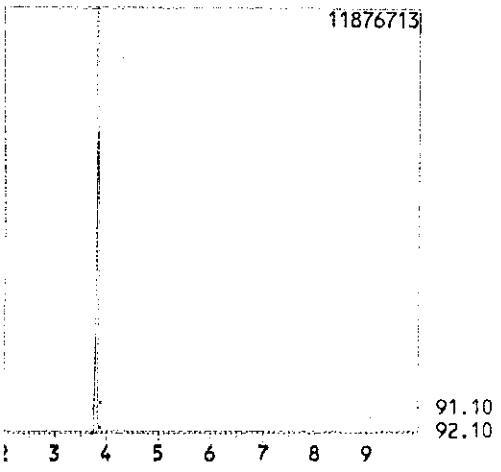
*** Calibration Curve ***

ID # 1 M/Z : 91.10 Name : toluene
Area = 6.74797e+006 * (Conc.) r2 = 1.000000



	Conc.(ppm)	Area
1	5.000	33739837

*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : toluene

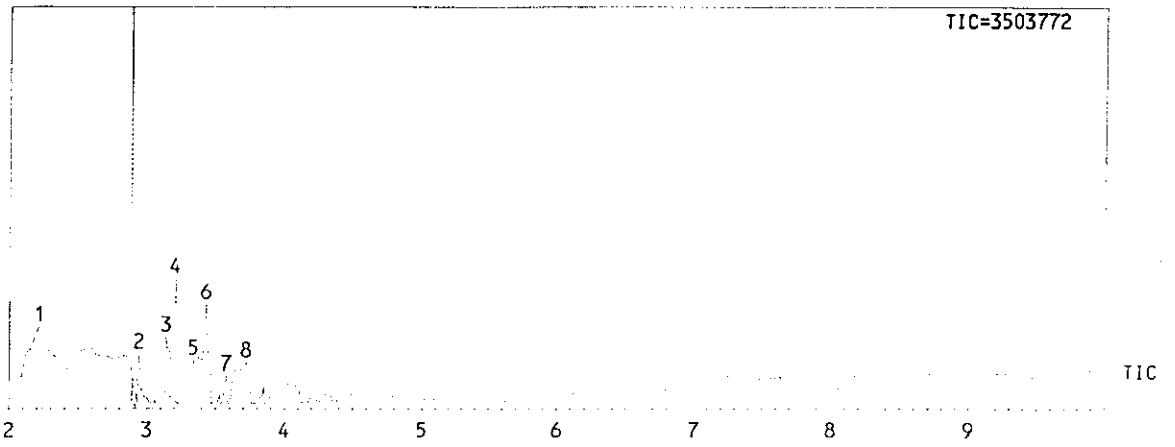
Time : 3.800
Area : 33739837

	M/Z	Area	%Rel.Int.to Target
1	92.10	23538131	70

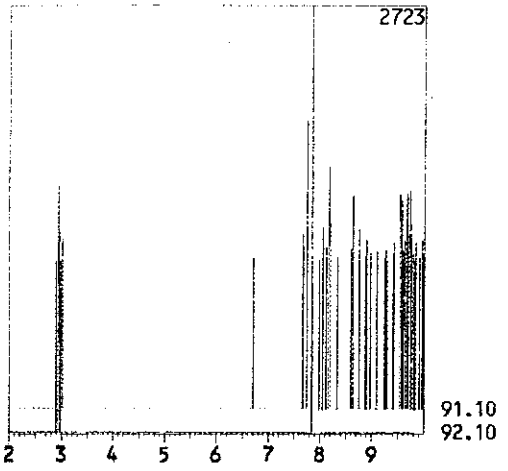
*** CLASS-5000 *** Report No. = 27 Data : MALIK.D05 04/04/27 13:12:45

Sample : ToulenepH2
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : toluene

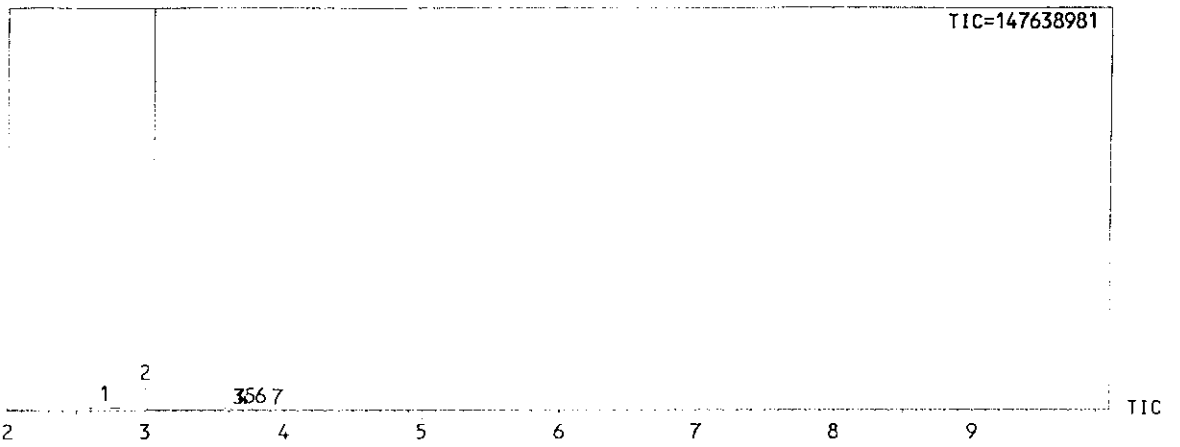
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

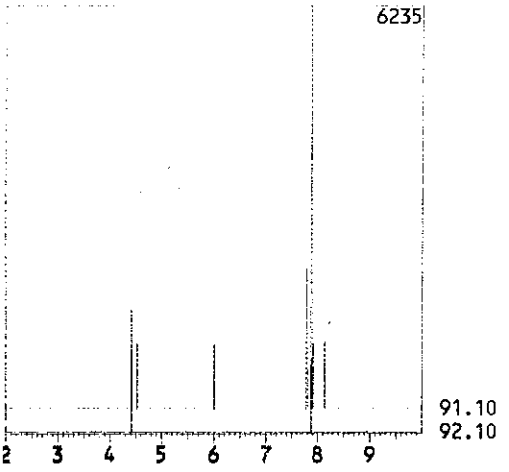
*** CLASS-5000 *** Report No. = 28 Data : MALIK.D06 04/04/27 13:42:56

Sample : ToulenepH7
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : toluene

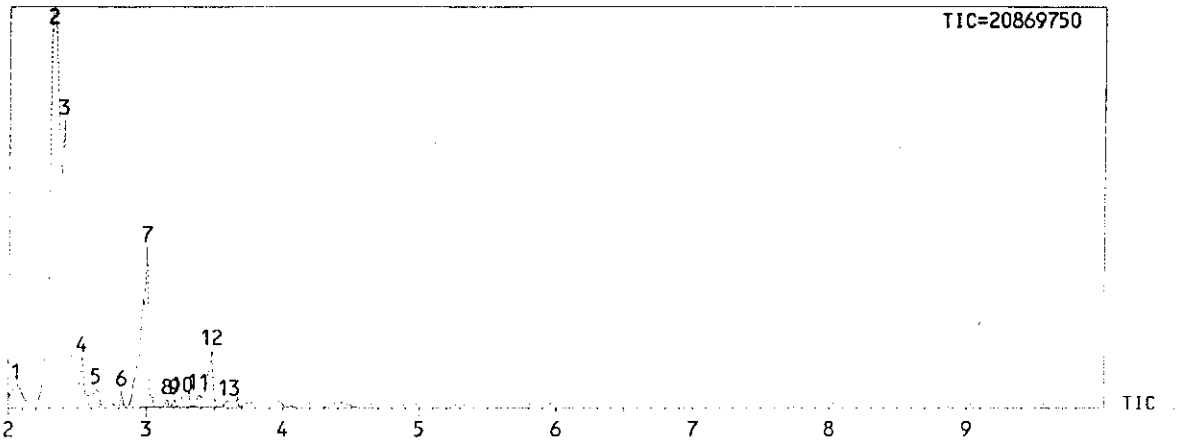
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

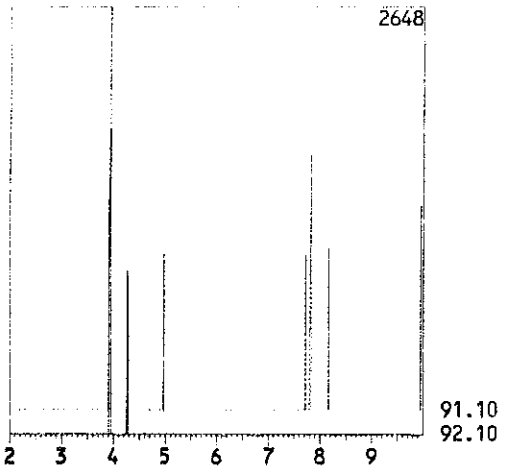
*** CLASS-5000 *** Report No. = 29 Data : MALIK.D07 04/04/27 14:13:04

Sample : TolunepH12
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***



ID : 1 M/Z : 91.10
Type : Target
Name : toluene

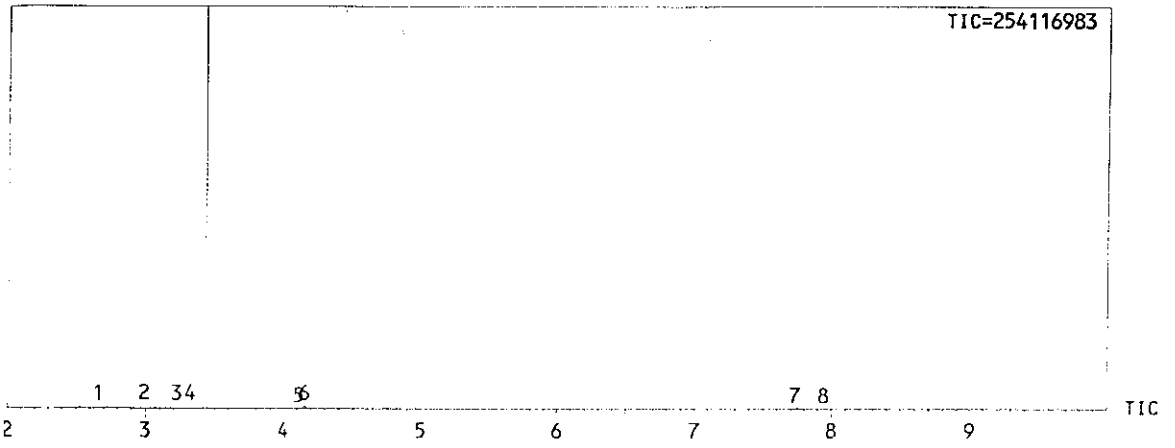
Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

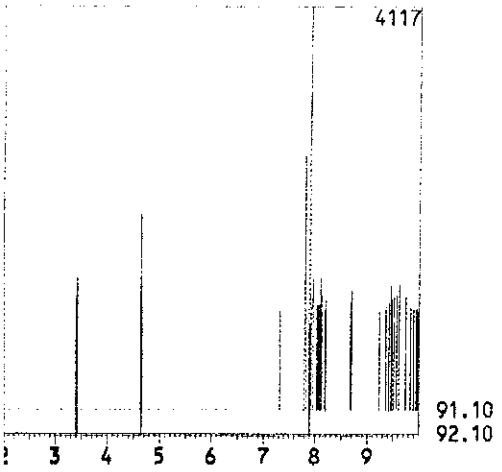
*** CLASS-5000 *** Report No. = 30 Data : MALIK.D08 04/04/27 14:43:07

Sample : Controltoluene
ID :
Type : Unknown
Method File Name : HO-BEN.MET

*** Chromatogram ***



*** Quantitation ***

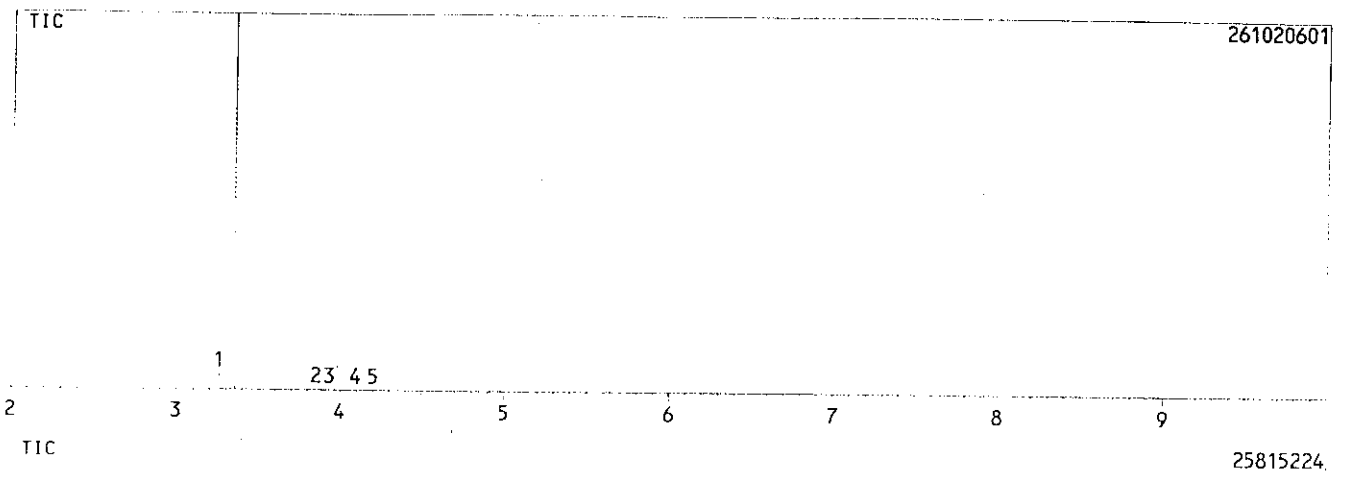


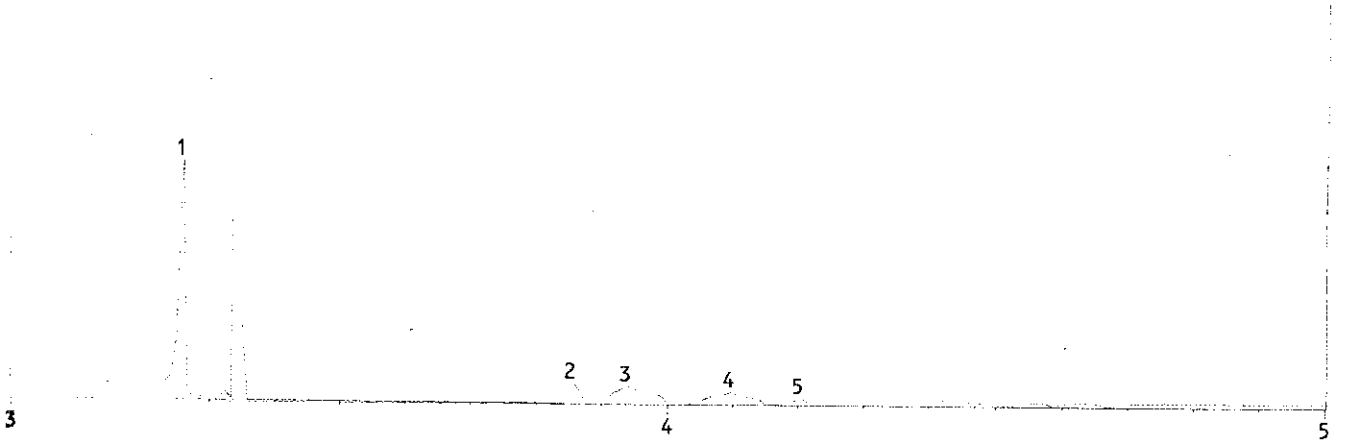
ID : 1 M/Z : 91.10
Type : Target
Name : toluene

Time : ?
Area : 0
Conc. : 0.000(N.D.)

	M/Z	Area	%Rel.Int.to Target
1	92.10	Can not find Reference Peak !	

Data : MALIK.D01 04/04/27 10:45:18
Sample : BenzenepH2
ID :
Method File Name : HO-BEN.MET





<Unknown Spectrum>
PKNO : 1 Ret .Time : 3.250
Scan # : 152 B.G. Scan # :155
Base Peak : 44.00(8544466)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	96	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
3	96	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 3.850
Scan # : 224 B.G. Scan # :227
Base Peak : 44.00(347276)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
2	87	45	$C_2 H_7 N$	1
			Methanamine, N-methyl- (CAS) Dimethylamine $$ N,N--dimethylamine $$ N,N-Dimethylamine $$	
3	87	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

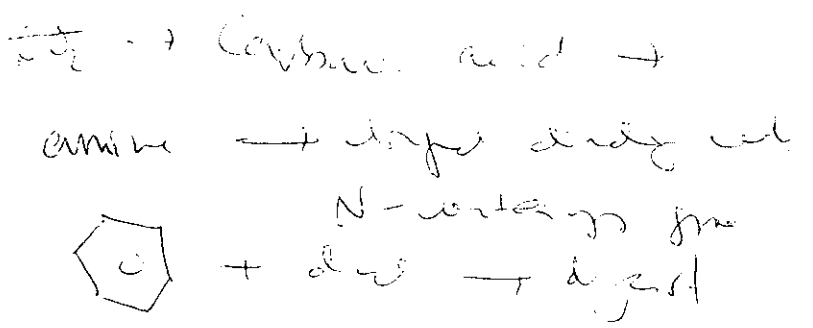
<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.940
Scan # : 234 B.G. Scan # :242
Base Peak : 44.00(411385)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	91	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
2	91	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	
3	90	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 4.100
Scan # : 253 B.G. Scan # :260
Base Peak : 44.00(96045)



<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound
1	79	100	$C_6 H_{12} O$
			4-Penten-1-ol, 3-me
2	79	100	$C_6H_{12}O$
			4-Penten-1-ol, 3-me
3	78	100	$C_6 H_{12} O$
			Hexanal (CAS) n-He
			$$ Caproic aldehyde
			naldehyde $$

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NI

<Unknown Spectrum>

PKNO : 5 Ret .Time : 4.200
Scan # : 265 B.G. Scan # :269
Base Peak : 44.00(50268)

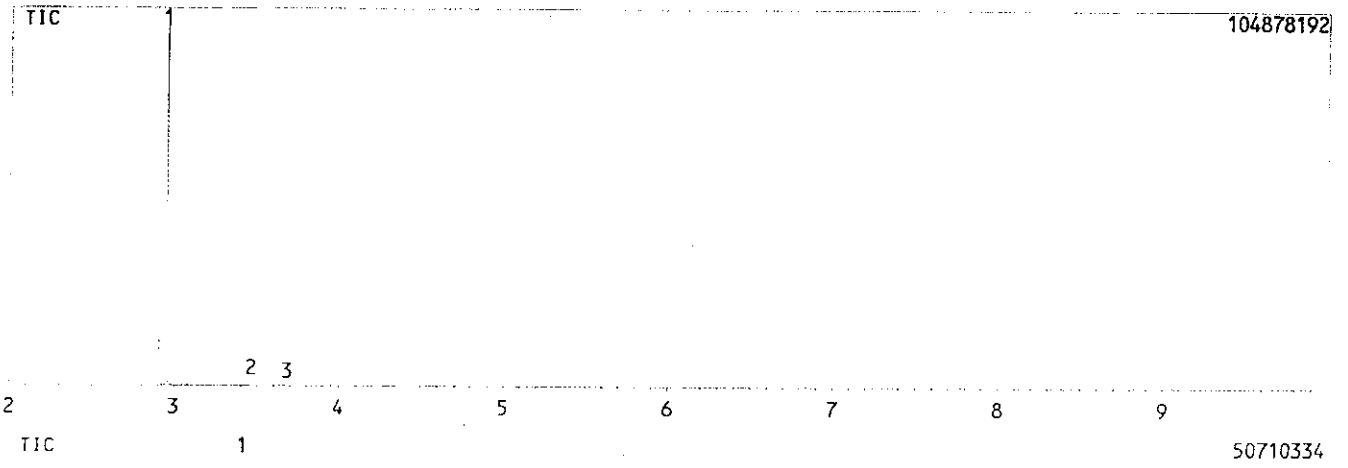
<Hit List>

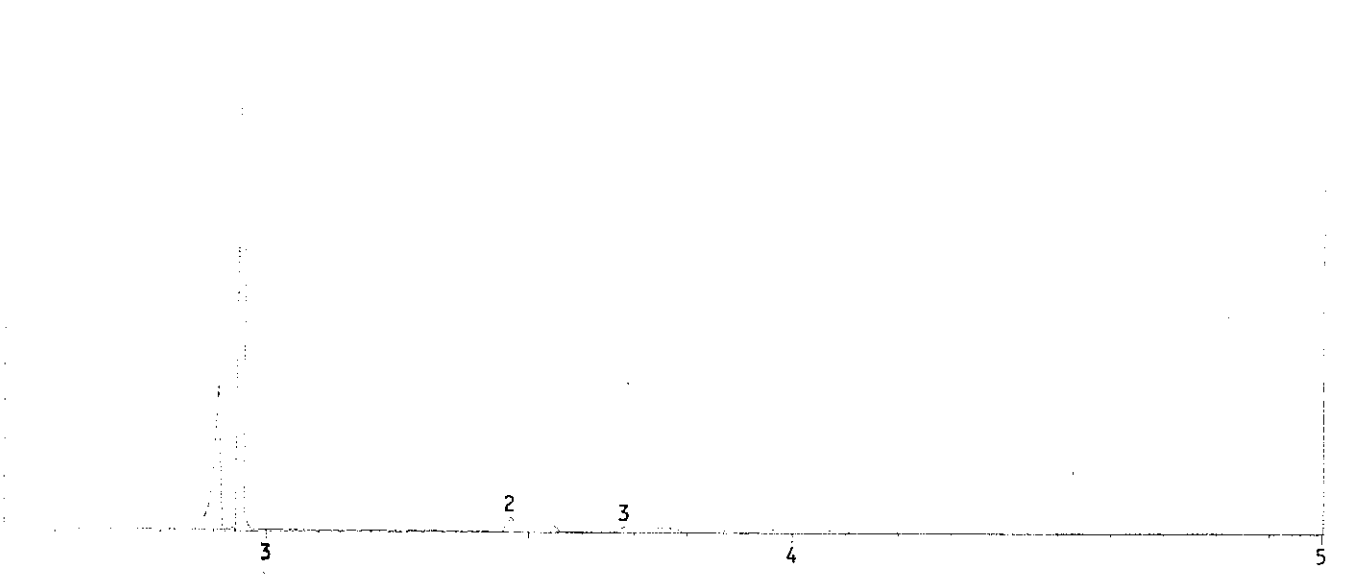
No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	85	72	$C_3H_4O_2$	1
			Formic acid, ethenyl ester (CAS) Vinyl formate $$ Formic acid, vinyl ester $$	
2	85	72	$C_3H_4O_2$	2
			Formic acid, ethenyl ester	
3	84	74	$C_3H_6O_2$	1
			Oxiranemethanol (CAS) Glycidol $$ Glycide $$ Glycidyl alcohol $$ Epihydrin alcohol $$ Allyl alcohol oxide $$ 2,3-Epoxy-1-propanol $$ 1-Propanol, 2,3-epoxy- $$ 2-(Hydroxymethyl)oxirane $$ 3-Hydroxypropylene oxide $$ 1,2-Epoxy-3-hydroxypropane $$ 1-Hydroxy-2,3-epoxypropane $$ 3-Hydroxy-1,2-epoxypropane $$ 2-hydroxymethyl-oxirane $$ Oxiranylmethanol $$ Epiol OH $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

Lab 2 Benzene at pH 7

Data : MALIK.D02 04/04/27 11:18:44
Sample : BenzenepH7
ID :
Method File Name : HO-BEN.MET





<Unknown Spectrum>
PKNO : 1 Ret .Time : 2.950
Scan # : 115 B.G. Scan # :118
Base Peak : 377.00(44057944)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	63	441	$C_{25}H_{31}NO_4S$	1
			Benzenesulfonamide, N,4-dimethyl-N-(6a,7,10,10a-tetrahydro-1-methoxy-6,6,9-trimethyl-6H-diben zo[b,d]pyran-3-yl)-, (6aR-trans)- (CAS) (-)-1-METHOXY-3-(METHYLTOSYL-AMINO)-6,6,9-TRIMETHYL-6 A,10A-TRANS-6A,7,10,10A-TETRAHYDRO-6H-DIBENZO(B,D)PYRAN $$	
2	61	475	$C_{32}H_{29}NO_3$	3
			Diphenylacetic acid, 4-((pyrrolidinocarbonyl)diphenylmethyl)- $$	
3	60	484	$C_{14}H_{18}BR_2O_7SI$	1
			1,7-dibromo-11,12-bis(methoxycarbonyl)-4,4-dimethyl-3,5,9-trioxa-4-silatricyclo[5.3.2.0(2,8)] dodec-11-ene $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 3.460
Scan # : 177 B.G. Scan # :190
Base Peak : 44.00(555259)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	75	C_3H_9NO	1
			1-Propanol, 2-amino- (CAS) 2-Amino-1-propanol $$ Alaninol $$ 2-Aminopropanol $$ .beta.-Propan olamine $$ 2-Amino-2-methylethanol $$ 1-Hydroxy-2-aminopropane $$ 1-Methyl-2-hydroxyethylamin e $$	
2	87	89	$C_3H_7NO_2$	1
			DL-.ALPHA.-ALANINE $$	
3	85	230	$C_5H_{10}O_{10}$	1
			Cyclopentanedecol (CAS) DECAHYDROXYCYCLOPENTANE $$ Cyclopentanepentone, pentahydrate $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

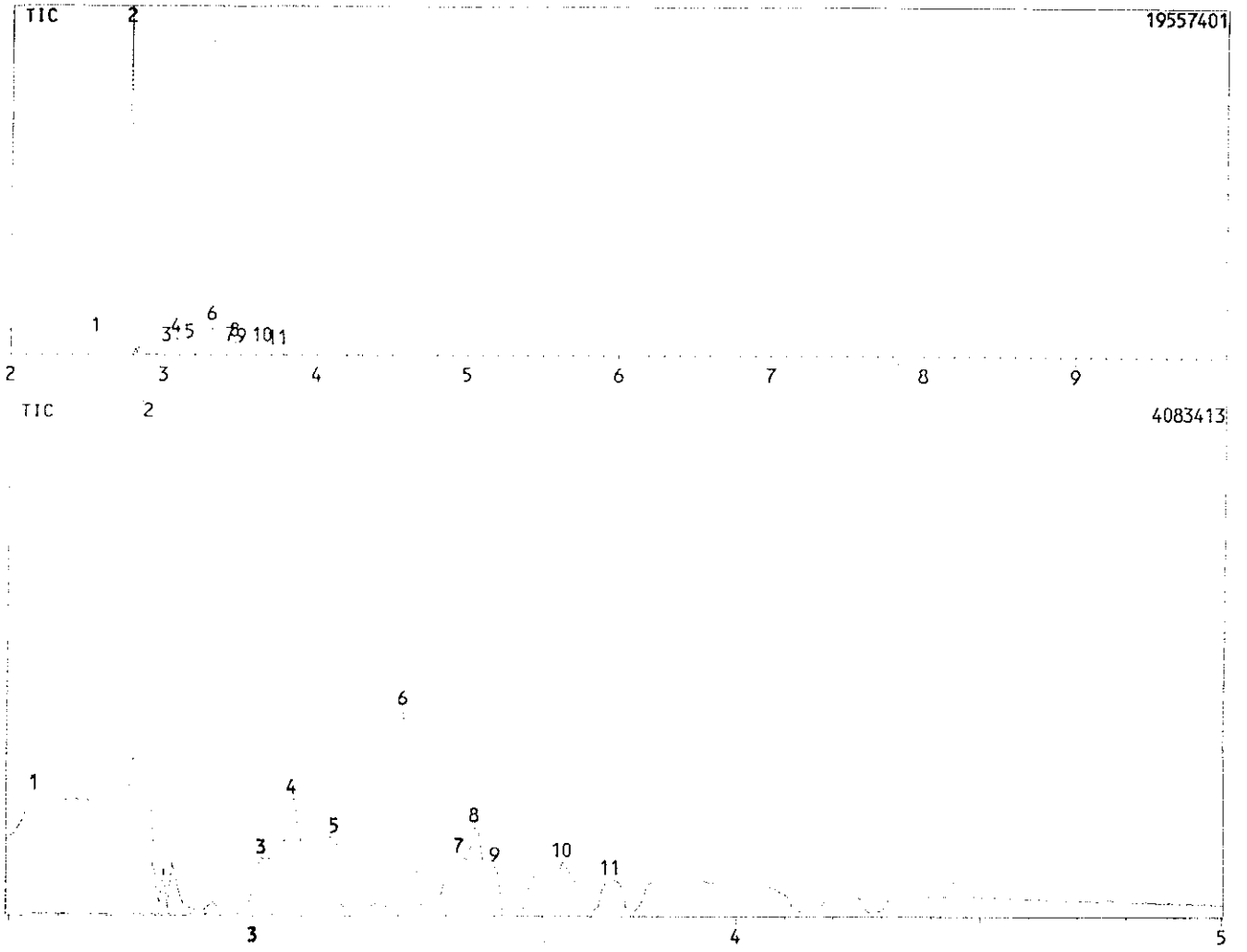
<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.680
Scan # : 203 B.G. Scan # :216
Base Peak : 44.00(326496)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	89	89	$C_3H_7NO_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alani ne $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic ac id $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic aci d $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	
2	88	75	C_3H_9NO	3
			(R)-(-)-2-Amino-1-propanol $$	
3	88	89	$C_3H_7NO_2$	3
			d-Alanine $$ D-.alpha.-Alanine $$ dl-Alanine $$ (R)-Alanine $$ Alanine, D- $$ Ba 2776 $$ D(-) -.alpha.-Alanine $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

Data : MALIK.D03 04/04/27 11:54:52
Sample : BenzenepH12
ID :
Method File Name : HO-BEN.MET



<Unknown Spectrum>
PKNO : 1 Ret .Time : 2.550
Scan # : 67 B.G. Scan # :89
Base Peak : 44.00(37239)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	95	44	N_2O	1
			Nitrogen oxide (N2O) (CAS) Nitrous oxide $$ Laughing gas $$ Dinitrogen oxide $$ Dinitrogen monoxide $$ Nitrus oxide $$	
2	92	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
3	92	44	CO_2	3
			Carbon dioxide $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$ Carbonic anhydride $$ Dry ice $$ CO2 $$ Anhydride carbonique $$ Carbonice $$ Kohlendioxyd $$ Kohlensaure $$ UN 1013 $$ UN 1845 $$ UN 2187 $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 2.780
Scan # : 95 B.G. Scan # :106
Base Peak : 44.00(14292073)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	96	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	95	61	CH_3NO_2	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
3	95	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.010
Scan # : 123 B.G. Scan # :127
Base Peak : 60.00(8527)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	83	60	$C_2H_4O_2$	1
			Acetic acid (CAS) Ethylic acid $$ Vinegar acid $$ Ethanoic acid $$ Glacial acetic acid $$ Methanecarboxylic acid $$ Ethanoic acid monomer $$ Aci-Jel $$	
2	83	60	$C_2H_4O_2$	1
			Acetic acid (CAS) Ethylic acid $$ Vinegar acid $$ Ethanoic acid $$ Glacial acetic acid $$ Methanecarboxylic acid $$ Ethanoic acid monomer $$ Aci-Jel $$	
3	81	60	$C_2H_4O_2$	3
			Acetic acid $$ Ethanoic acid $$ Ethylic acid $$ Glacial acetic acid $$ Methanecarboxylic acid $$ Vinegar acid $$ CH3COOH $$ component of Aci-Jel $$ Acetasol $$ Acide acetique $$ Acido acetico $$ Azijnzuur $$ Essigsaeure $$ Octowy kwas $$ Acetic acid, glacial $$ Kyselina octova $$ UN 2789 $$ UN 2790 $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 3.080
Scan # : 131 B.G. Scan # :135
Base Peak : 43.00(132970)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	77	86	$C_5H_{10}O$	2
			2-Butanone, 3-methyl-	
2	77	86	$C_5H_{10}O$	1
			2-Butanone, 3-methyl- (CAS) 3-Methyl-2-butanone $$ Methyl isopropyl ketone $$ Methyl butanone-2 $$ Methylbutanone $$ Isopropyl methyl ketone $$ Ketone, isopropyl methyl $$ 3-Methylbutan-2-one $$ 2-Acetylpropane $$ 2-Methylbutan-3-one $$	
3	77	102	$C_5H_{10}O_2$	3
			CH3CH(OH)CH2C(O)CH3 $$ 2-Pentanone, 4-hydroxy- $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 5 Ret .Time : 3.160

Scan # : 141 B.G. Scan # :145
Base Peak : 44.00(279067)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	90	89	$C_3 H_7 N O_2$ DL-.ALPHA.-ALANINE $$	1
2	89	124	$C_7 H_8 O_2$ 4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	1
3	89	89	$C_3 H_7 N O_2$ L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	1

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 6 Ret .Time : 3.300
Scan # : 158 B.G. Scan # :163
Base Peak : 44.00(1282550)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	61	$C H_3 N O_2$ Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	1
2	97	44	$C O_2$ Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	1
3	97	78	$CH_6N_2O_2$ Carbamic acid, monoammonium salt	2

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 7 Ret .Time : 3.420
Scan # : 172 B.G. Scan # :174
Base Peak : 31.00(7124)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	82	76	$C_2 H_4 O_3$ Acetic acid, hydroxy- (CAS) Glycolic acid $$ Hydroxyacetic acid $$ Glycollic acid $$ Hydroxyethanoic acid $$ .alpha.-Hydroxyacetic acid $$ 2-Hydroxyacetic acid $$	1
2	81	32	CH_4O Methyl Alcohol	2
3	81	130	$C_4H_5ClN_3$ 2-Amino-5-chloropyrimidine $$ 2-Pyrimidinamine, 5-chloro- $$ Pyrimidine, 2-amino-5-chloro- $$	3

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 8 Ret .Time : 3.450
Scan # : 176 B.G. Scan # :179
Base Peak : 43.00(189315)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	58	$C_3 H_6 O$ 2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	1
2	97	58	C_3H_6O Acetone	2
3	96	58	$C_3 H_6 O$ 2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	1

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 9 Ret .Time : 3.500
Scan # : 181 B.G. Scan # :184
Base Peak : 44.00(154251)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#

1	86	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-D imethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
2	86	230	$C_5 H_{10} O_{10}$	1
			Cyclopentanedecol (CAS) DECAHYDROXYCYCLOPENTANE $$ Cyclopentanepentone, pentahydrate $$	
3	85	45	$C_2 H_7 N$	1
			Methanamine, N-methyl- (CAS) Dimethylamine $$ N,N--dimethylamine $$ N,N-Dimethylamine $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 10 Ret .Time : 3.640
Scan # : 198 B.G. Scan # :202
Base Peak : 44.00(230985)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	90	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-D imethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
2	88	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alani ne $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic ac id $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic aci d $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	
3	88	75	C_3H_9NO	3
			(R)-(-)-2-Amino-1-propanol $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

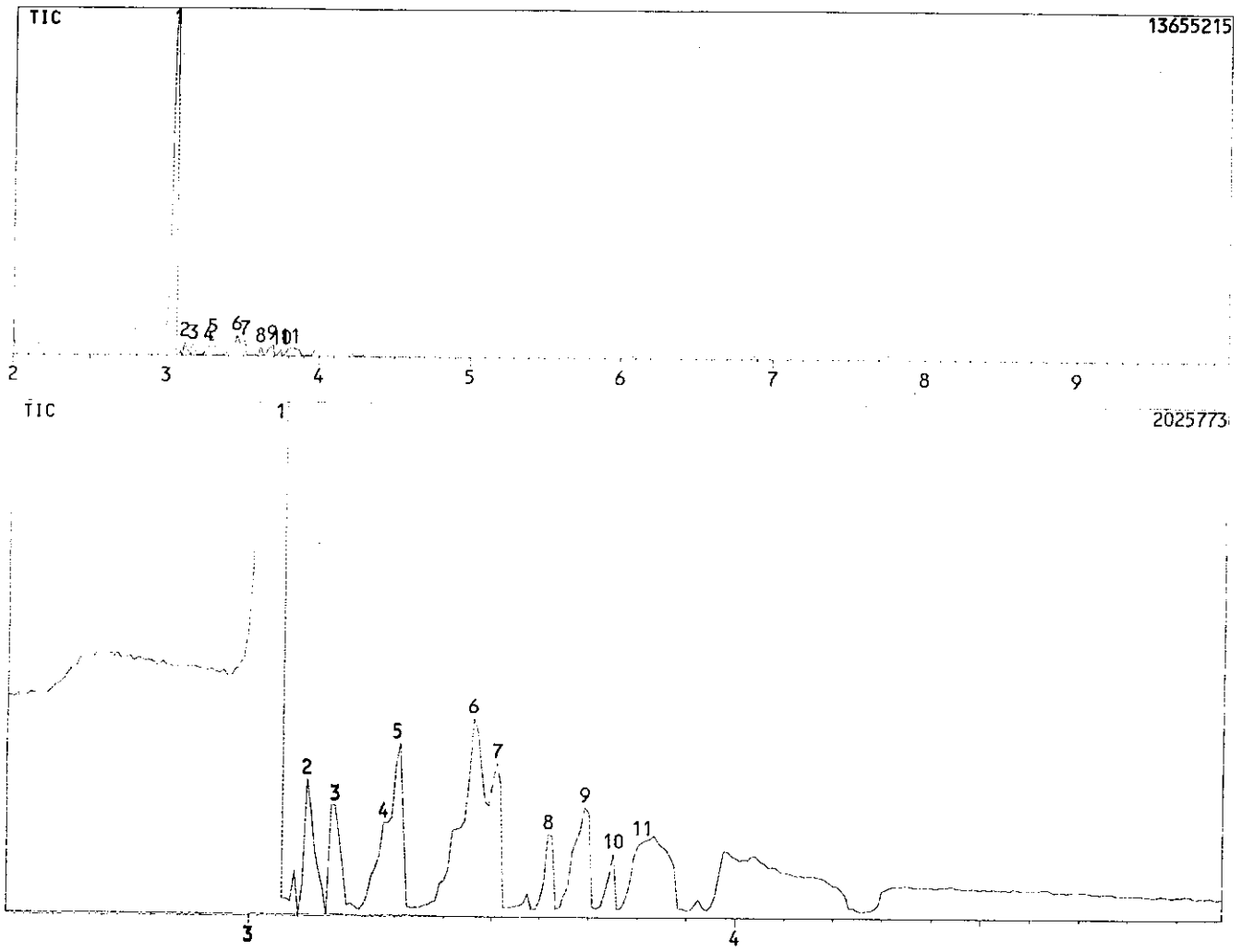
<Unknown Spectrum>
PKNO : 11 Ret .Time : 3.740
Scan # : 210 B.G. Scan # :215
Base Peak : 44.00(97584)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	86	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
2	85	45	$C_2 H_7 N$	1
			Methanamine, N-methyl- (CAS) Dimethylamine $$ N,N--dimethylamine $$ N,N-Dimethylamine $$	
3	85	75	$C_3 H_9 N O$	1
			1-Propanol, 2-amino- (CAS) 2-Amino-1-propanol $$ Alaninol $$ 2-Aminopropanol $$ .beta.-Propan olamine $$ 2-Amino-2-methylethanol $$ 1-Hydroxy-2-aminopropane $$ 1-Methyl-2-hydroxyethylamin e $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

Data : MALIK.D04 04/04/27 12:42:02
Sample : BenzeneControl
ID :
Method File Name : HO-BEN.MET



<Unknown Spectrum>
PKNO : 1 Ret .Time : 3.050
Scan # : 127 B.G. Scan # :133
Base Peak : 44.00(11128474)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	98	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	98	61	CH_3NO_2	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
3	98	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 3.110
Scan # : 135 B.G. Scan # :140
Base Peak : 422.00(2691)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	37	154	$C_4H_{10}O_4S$	1
			Sulfuric acid, diethyl ester (CAS) DES $$ Diethyl sulphate $$ Ethyl sulfate $$	
2	36	142	$C_6H_{11}BO_3$	1
			ERYTHRIT, 1,4-ANHYDRO-2,3-O-(ETHYLBORANDIYL)- $$	
3	36	184	$C_9H_{17}BO_3$	1
			1,3,2-Dioxaborolane, 2-ethyl-4-(3-oxiranylpropyl)- (CAS) 6-EPOXYHEPTANE, 1,2-O-(ETHYLBORANDIYL)- $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.170
Scan # : 142 B.G. Scan # :145
Base Peak : 80.00(2867)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	32	212	$C_8H_8N_2O_5$	3
			Benzene, 2-methoxy-1-methyl-3,5-dinitro- $$	
2	31	174	$C_{11}H_{14}N_2$	3
			1,2,5,6-Tetrahydropyridine, 1-methyl-6-[2-pyridyl]- $$	
3	30	195	$C_8H_5NO_5$	3
			6-Nitropiperonal $$ 3,4-(Methylenedioxy)-6-nitrobenzaldehyde $$ 4,5-Methylenedioxy-2-nitrobenzaldehyde $$ 1,3-Benzodioxole-5-carboxaldehyde, 6-nitro- $$ Piperonal, 6-nitro- $$ 1,3-Benzodioxole, 5-formyl-6-nitro- $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 3.270
Scan # : 154 B.G. Scan # :156
Base Peak : 29.00(5284)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	65	85	C_4H_7NO	1
			2-methyl-3-oxazoline $$	
2	64	166	$C_6H_{15}O_3P$	1
			Phosphonic acid, ethyl-, diethyl ester (CAS) Diethyl ethylphosphonate $$ Diethyl ethanephosphonate $$ Diethoxyethylphosphine oxide $$	
3	64	146	$C_6H_{10}O_4$	1
			Ethanedioic acid, diethyl ester (CAS) Diethyl oxalate $$ Ethyl oxalate $$ Diethyl ethanedioate $$ Oxalic acid, diethyl ester $$ Diethyl ester of oxalic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 5 Ret .Time : 3.300
Scan # : 158 B.G. Scan # :161
Base Peak : 44.00(479798)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	94	61	CH_3NO_2	1

```
                    Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$
                    Monoammonium salt of carbamic acid $$
 2      94      78  CH6N2O2                                    2
                    Carbamic acid, monoammonium salt
 3      94      44  C O2                                       1
                    Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon ox
                    ide (CO2) $$ Carbonic acid, gas $$

Library Name
 (1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 6    Ret .Time : 3.450
Scan #      : 176    B.G. Scan # :180
Base Peak   :    44.00(    219436)

<Hit List>
No      SI Mol.Wgt. Mol.Form./Compound Name                LIB#
 1      89     124  C7 H8 O2                                   1
                    4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-D
                    imethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$
 2      89      61  C H3 N O2                                  1
                    Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$
                    Monoammonium salt of carbamic acid $$
 3      89      90  C2 H2 O4                                   1
                    Ethanedioic acid (CAS) Oxalic acid $$ Aquisal $$ Aktisal $$ Oxiric acid $$ Iron potassium oxa
                    late $$

Library Name
 (1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 7    Ret .Time : 3.500
Scan #      : 182    B.G. Scan # :185
Base Peak   :    44.00(    400879)

<Hit List>
No      SI Mol.Wgt. Mol.Form./Compound Name                LIB#
 1      93      61  C H3 N O2                                  1
                    Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$
                    Monoammonium salt of carbamic acid $$
 2      92      44  C O2                                       1
                    Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon ox
                    ide (CO2) $$ Carbonic acid, gas $$
 3      92      78  CH6N2O2                                    2
                    Carbamic acid, monoammonium salt

Library Name
 (1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 8    Ret .Time : 3.610
Scan #      : 195    B.G. Scan # :200
Base Peak   :    44.00(     64574)

<Hit List>
No      SI Mol.Wgt. Mol.Form./Compound Name                LIB#
 1      85      72  C3 H4 O2                                   1
                    Formic acid, ethenyl ester (CAS) Vinyl formate $$ Formic acid, vinyl ester $$
 2      85      72  C3H4O2                                     2
                    Formic acid, ethenyl ester
 3      85      72  C4H8O                                      3
                    Cyclobutanol $$ Cyclobutyl hydroxide $$

Library Name
 (1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 9    Ret .Time : 3.690
Scan #      : 204    B.G. Scan # :208
Base Peak   :    44.00(    241153)

<Hit List>
No      SI Mol.Wgt. Mol.Form./Compound Name                LIB#
 1      92     124  C7 H8 O2                                   1
                    4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-D
                    imethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$
 2      89      61  C H3 N O2                                  1
                    Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$
                    Monoammonium salt of carbamic acid $$
 3      88      75  C3 H9 N O                                  1
                    Ethanol, 2-(methylamino)- $$ .beta.-(Methylamino)ethanol $$ Methylethanolamine $$ (Hydroxyeth
                    yl)methylamine $$ (2-Hydroxyethyl)methylamine $$ Methyl(.beta.-hydroxyethyl)amine $$ Methyl(h
```

ydroxyethyl)amine $$ Methyl(2-hydroxyethyl)amine $$ Methylaminoethanol $$ Methylethylolamine $$ Monomethylaminoethanol $$ Monomethylethanolamine $$ Monomethylmonoethanolamine $$ N-(2-Hydroxyethyl)methylamine $$ N-Methyl-N-(.beta.-hydroxyethyl)amine $$ N-Methyl-N-(2-hydroxyethyl)amine $$ N-Methyl-N-hydroxyethylamine $$ N-Met

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 10 Ret .Time : 3.750
Scan # : 211 B.G. Scan # :214
Base Peak : 44.00(119590)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	91	61	CH_3NO_2	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
2	90	89	$C_3H_7NO_2$	3
			Alanine $$ L-Alanine $$ Alanine, L- $$ .alpha.-Alanine $$ .alpha.-Aminopropionic acid $$ (S)-Alanine $$ L-.alpha.-Alanine $$ L-.alpha.-Aminopropionic acid $$ L-(+)-Alanine $$ L-2-Aminopropanoic acid $$ L-2-Aminopropionic acid $$ Propanoic acid, 2-amino- $$ Propanoic acid, 2-amino-, (S)- $$ L-CH3CH(NH2)COOH $$ (S)-2-Aminopropanoic acid $$	
3	90	89	$C_3H_7NO_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 11 Ret .Time : 3.800
Scan # : 218 B.G. Scan # :236
Base Peak : 44.00(115325)

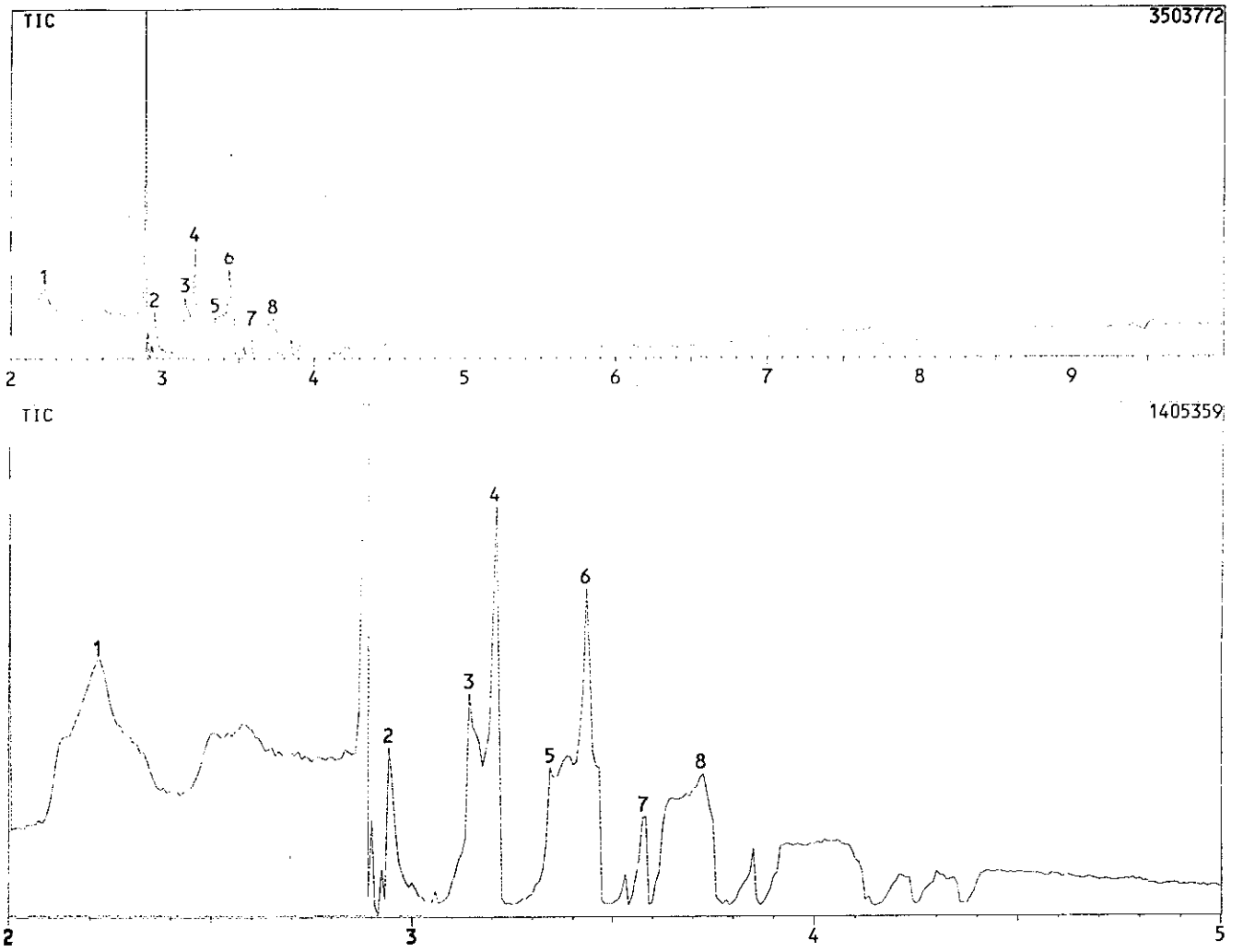
<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	93	124	$C_7H_8O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
2	89	89	$C_3H_7NO_2$	1
			DL-.ALPHA.-ALANINE $$	
3	89	89	$C_3H_7NO_2$	2
			dl-Alanine	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

L3.1 : Toluene at pH 2.

Data : MALIK.D05 04/04/27 13:12:45
Sample : ToulenepH2
ID :
Method File Name : HO-BEN.MET



<Unknown Spectrum>
PKNO : 1 Ret .Time : 2.220
Scan # : 28 B.G. Scan # :36
Base Peak : 28.00(89059)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	82	296	$C_8H_{10}BR_2O_2$ cis-(1S,3R)-Deltamethrinic acid $$ Cyclopropanecarboxylic acid, 3-(2,2-dibromoethenyl)-2,2-dimethyl-, (1S-cis)- $$	1
2	82	32	O_2 Air $$	1
3	82	124	$C_7H_8O_2$ 4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	1

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 2.940
Scan # : 114 B.G. Scan # :120
Base Peak : 264.00(2493)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	30	382	$C_{23}H_{42}O_4$ Tetrahydropyran, 5-hydroxy-6-hydroxymethyl-2-[4-(4-pentylcyclohexyl)cyclohexyloxy]- $$	3
2	29	263	$C_{12}H_{10}ClN_3O_2$ Benzoylamide, 2-amino-5-hydroxy-N-[2-chloro-3-pyridyl]- $$	3
3	27	390	$C_{22}H_{35}BO_5$ Pregnan-20-one, 3,11-dihydroxy-17,21-[(methylborylene)bis(oxy)]-, (3.alpha.,5.beta.,11.beta.)- (CAS) 3.ALPHA.,11.BETA.,17.ALPHA.,21-TETRAHYDROXY-5.BETA.-PREGNAN-20-ONE METHYL BORONATE $$ 5.beta.-Pregnan-20-one, 3.alpha.,11.beta.,17,21-tetrahydroxy-, cyclic 17,21-methaneboronate $$	1

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.140
Scan # : 138 B.G. Scan # :142
Base Peak : 44.00(57727)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	83	46	CH_6Si Silane, methyl- $$ Methylsilane $$ Silaethane $$ CH3SiH3 $$	3
2	83	88	$C_4H_8O_2$ Ethanol, 2-(ethenyloxy)- (CAS) Vinyloxyethanol $$ 2-(Vinyloxy)ethanol $$ Ethanol, 2-(vinyloxy)- $$ 2-Hydroxyethyl vinyl ether $$ Ethylene glycol vinyl ether $$ Ethyleneglycol monovinyl ester $$ Ethylene glycol monovinyl ether $$	1
3	83	88	$C_4H_8O_2$ Ethanol, 2-(ethenyloxy)- $$ Ethanol, 2-(vinyloxy)- $$ Ethylene glycol monovinyl ether $$ Ethylene glycol vinyl ether $$ Ethyleneglycol monovinyl ester $$ Vinyloxyethanol $$ 2-(Vinyloxy)ethanol $$ 2-Hydroxyethyl vinyl ether $$ Ethylenglycol monovinyl ester $$ Mveeg $$	3

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 3.200
Scan # : 146 B.G. Scan # :149
Base Peak : 44.00(749002)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	91	61	CH_3NO_2 Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	1
2	91	90	$C_2H_2O_4$ Ethanedioic acid (CAS) Oxalic acid $$ Aquisal $$ Aktisal $$ Oxiric acid $$ Iron potassium oxalate $$	1
3	90	44	CO_2 Carbon dioxide $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$ Carbonic anhydride $$ Dry ice $$ CO2 $$ Anhydride carbonique $$ Carbonice $$ Kohlendioxyd $$ Kohlensaure $$ UN 1013 $$ UN 1845 $$ UN 2187 $$	3

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 5 Ret .Time : 3.340

Scan # : 162 B.G. Scan # :170
Base Peak : 43.00(18199)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	89	60	$C_2 H_4 O_2$	1
			Acetic acid (CAS) Ethylic acid $$ Vinegar acid $$ Ethanoic acid $$ Glacial acetic acid $$ Methanecarboxylic acid $$ Ethanoic acid monomer $$ Aci-Jel $$	
2	88	60	$C_2 H_4 O_2$	1
			Acetic acid (CAS) Ethylic acid $$ Vinegar acid $$ Ethanoic acid $$ Glacial acetic acid $$ Methanecarboxylic acid $$ Ethanoic acid monomer $$ Aci-Jel $$	
3	88	60	$C_2H_4O_2$	3
			Acetic acid $$ Ethanoic acid $$ Ethylic acid $$ Glacial acetic acid $$ Methanecarboxylic acid $$ Vinegar acid $$ CH3COOH $$ component of Aci-Jel $$ Acetasol $$ Acide acetique $$ Acido acetico $$ Azijnzuur $$ Essigsaeure $$ Octowy kwas $$ Acetic acid, glacial $$ Kyselina octova $$ UN 2789 $$ UN 2790 $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 6 Ret .Time : 3.430
Scan # : 173 B.G. Scan # :179
Base Peak : 44.00(571743)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	91	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
2	90	90	$C_2 H_2 O_4$	1
			Ethanedioic acid (CAS) Oxalic acid $$ Aquisal $$ Aktisal $$ Oxiric acid $$ Iron potassium oxalate $$	
3	90	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 7 Ret .Time : 3.570
Scan # : 190 B.G. Scan # :195
Base Peak : 44.00(61998)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	75	$C_3 H_9 N O$	1
			1-Propanol, 2-amino- (CAS) 2-Amino-1-propanol $$ Alaninol $$ 2-Aminopropanol $$ .beta.-Propanolamine $$ 2-Amino-2-methylethanol $$ 1-Hydroxy-2-aminopropane $$ 1-Methyl-2-hydroxyethylamine $$	
2	87	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
3	87	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 8 Ret .Time : 3.720
Scan # : 208 B.G. Scan # :213
Base Peak : 44.00(161836)

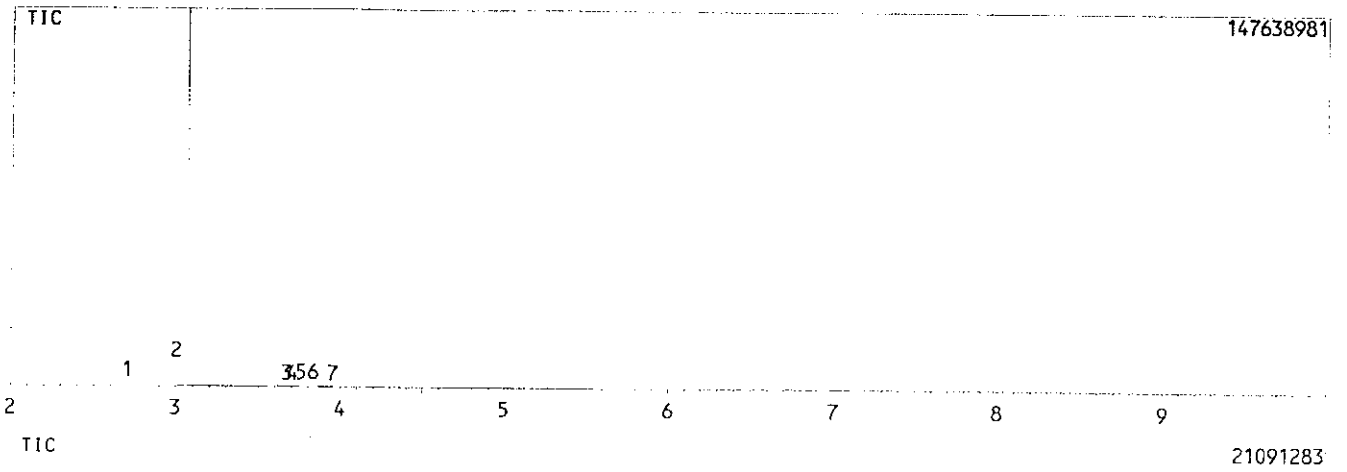
<Hit List>

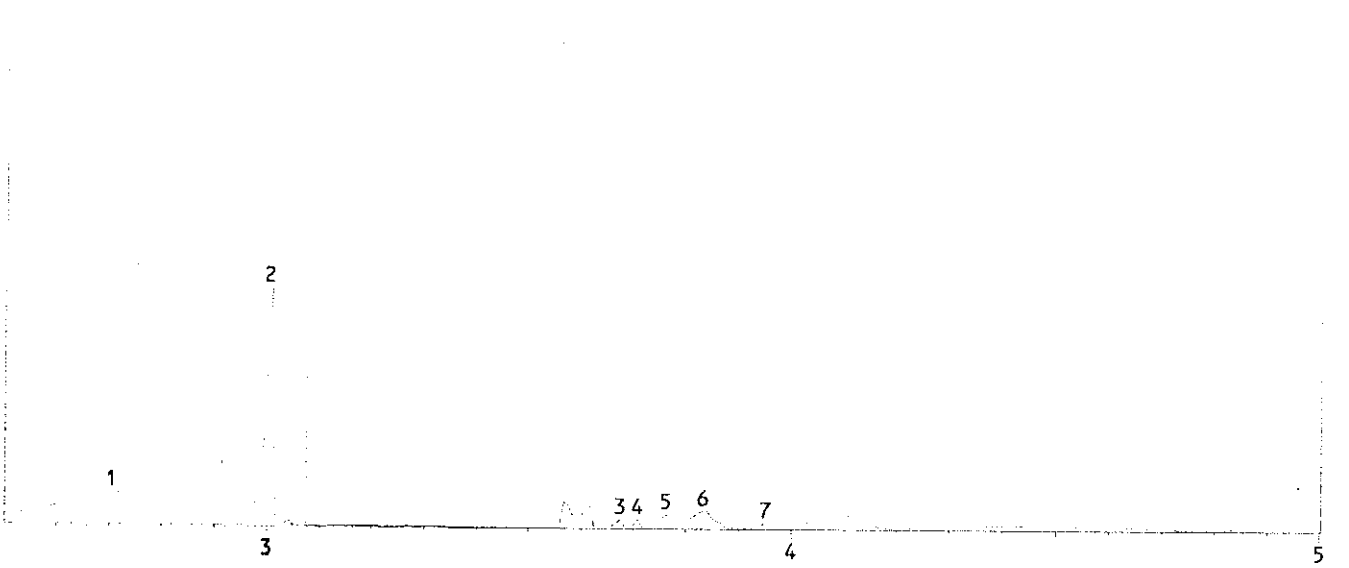
No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
2	87	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	
3	87	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

C5. 2 · Toluene at pH 7

Data : MALIK.D06 04/04/27 13:42:56
Sample : ToulenepH7
ID :
Method File Name : HO-BEN.MET





<Unknown Spectrum>
PKNO : 1 Ret .Time : 2.700
Scan # : 86 B.G. Scan # :101
Base Peak : 43.00(292673)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	97	58	C_3H_6O	2
			Acetone	
3	97	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 3.000
Scan # : 122 B.G. Scan # :130
Base Peak : 44.00(7306332)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	98	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	98	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
3	97	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.670
Scan # : 202 B.G. Scan # :204
Base Peak : 44.00(153583)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	91	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
2	89	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
3	89	89	$C_3 H_7 N O_2$	1
			L-Alanine (CAS) Alanine, L- $$ L-(+)-.ALPHA.-ALANINE $$ (S)-Alanine $$ Alanine $$ L-(+)-Alanine $$ .alpha.-Alanine $$ L-.alpha.-Alanine $$ L-2-Aminopropionicacid $$ L-2-Aminopropanoic acid $$ Propanoic acid, 2-amino- $$ .alpha.-Aminopropionic acid $$ L-.alpha.-Aminopropionic acid $$ Propanoic acid, 2-amino-, (S)- $$ (S)-2-Aminopropanoic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 3.700
Scan # : 206 B.G. Scan # :210
Base Peak : 44.00(204148)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	96	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
2	96	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
3	96	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 5 Ret .Time : 3.760
Scan # : 213 B.G. Scan # :217
Base Peak : 44.00(170610)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	99	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	99	44	CO_2	2
			Carbon dioxide	
3	99	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 6 Ret .Time : 3.840
Scan # : 222 B.G. Scan # :228
Base Peak : 43.00(213550)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	87	58	C_3H_6O	2
			Acetone	
3	86	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 7 Ret .Time : 3.950
Scan # : 235 B.G. Scan # :252
Base Peak : 250.00(2044)

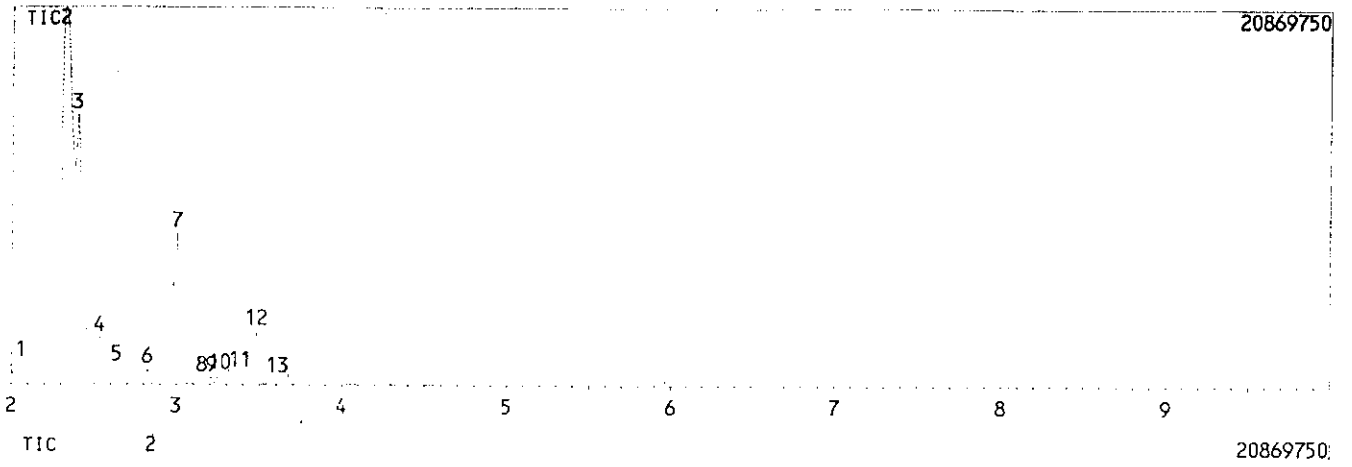
<Hit List>

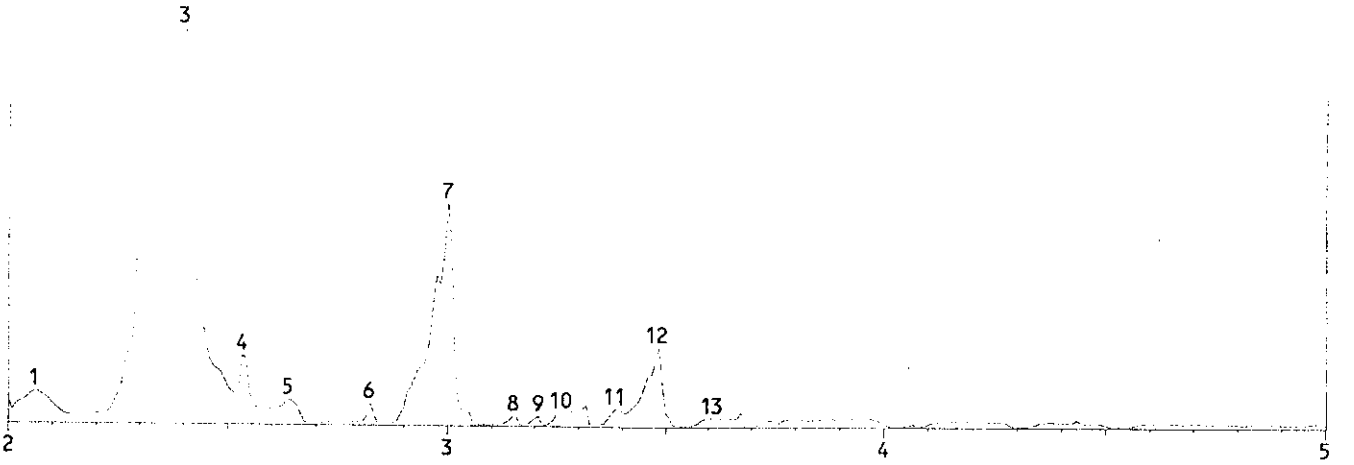
No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	57	250	$C_{16}H_{26}O_2$	3
			3,5-Di-t-butyl-4-methoxy-1,4-dihydrobenzaldehyde $$	
2	53	250	$C_{15}H_{22}O_3$	3
			Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy- $$ Benzoic acid, 3,5-di-tert-butyl-4-hydroxy- $$ 3,5-Di-tert-butyl-4-hydroxybenzoic acid $$ 3,5-di-t-Butyl-4-hydroxy benzoic acid $$	
3	49	250	$C_{16}H_{26}O_2$	3
			Phenol, 2,6-bis(1,1-dimethylethyl)-4-(methoxymethyl)- $$ p-Cresol, 2,6-di-tert-butyl-.alpha.-methoxy- $$ Ethyl Antioxidant 762 $$ Ionol 4 $$ 2,6-di-tert-Butyl-.alpha.-methoxy-para-cresol $$ DTB $$ Methyl ether of 3,5-di-tert-butyl-4-hydroxybenzene $$ Phenol, 2,6-di-tert-butyl-4-methoxymethyl- $$ 2,6-Di-tert-butyl-4-methoxymethylphenol $$ 2,6-Di-tert-butyl-.alpha.-methoxy-p-cresol $$ 3,5-Di-tert-butyl-4-hydroxybenzyl methyl ether $$ 4-Methoxymethyl-2,6-di-tert-butylphenol $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

C 5 . 3 . Toluene at pH 12.

Data : MALIK.D07 04/04/27 14:13:04
Sample : ToulenepH12
ID :
Method File Name : HO-BEN.MET





<Unknown Spectrum>
PKNO : 1 Ret .Time : 2.050
Scan # : 8 B.G. Scan # :18
Base Peak : 44.00(566874)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	92	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
2	90	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
3	90	90	$C_2 H_2 O_4$	1
			Ethanedioic acid (CAS) Oxalic acid $$ Aquisal $$ Aktisal $$ Oxiric acid $$ Iron potassium oxalate $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 2.320
Scan # : 40 B.G. Scan # :47
Base Peak : 44.00(4400477)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	92	90	$C_2 H_2 O_4$	1
			Ethanedioic acid (CAS) Oxalic acid $$ Aquisal $$ Aktisal $$ Oxiric acid $$ Iron potassium oxalate $$	
2	87	230	$C_5 H_{10} O_{10}$	1
			Cyclopentanedecol (CAS) DECAHYDROXYCYCLOPENTANE $$ Cyclopentanepentone, pentahydrate $$	
3	86	90	$C_2 H_2 O_4$	1
			Ethanedioic acid (CAS) Oxalic acid $$ Aquisal $$ Aktisal $$ Oxiric acid $$ Iron potassium oxalate $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 3 Ret .Time : 2.400
Scan # : 49 B.G. Scan # :63
Base Peak : 44.00(11516049)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	99	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	98	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
3	98	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 2.530
Scan # : 65 B.G. Scan # :71
Base Peak : 44.00(1773998)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	99	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
2	99	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
3	99	44	CO_2	3
			Carbon dioxide $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$ Carbonic anhydride $$ Dry ice $$ CO2 $$ Anhydride carbonique $$ Carbonice $$ Kohlendioxyd $$ Kohlensaure $$ UN 1013 $$ UN 1845 $$ UN 2187 $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 5 Ret .Time : 2.640
Scan # : 78 B.G. Scan # :84
Base Peak : 44.00(197011)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	74	74	$C_3H_6O_2$	3
			Glycidol $$ Oxiranemethanol $$ 1-Propanol, 2,3-epoxy- $$ Allyl alcohol oxide $$ Epihydrin alcohol $$ Glycide $$ Glycidyl alcohol $$ 1-Hydroxy-2,3-epoxypropane $$ 1,2-Epoxy-3-hydroxypropane $$ 2-(Hydroxymethyl)oxirane $$ 2,3-Epoxy-1-propanol $$ 3-Hydroxy-1,2-epoxypropane $$ 3-Hydroxypropylene oxide $$ Hydroxymethyloxirane $$ 2,3-Epoxypropanol-1 $$ Methanol, oxiranyl- $$ Monoepoxide glycidol $$ NCI-C55549 $$ Oxiranylmethanol $$ 2,3-Epoxypropanol $$ Hydroxymethyl ethylene oxide $$ Epoxypropyl alcohol $$	
2	74	74	$C_3 H_6 O_2$	1
			Oxiranemethanol (CAS) Glycidol $$ Glycide $$ Glycidyl alcohol $$ Epihydrin alcohol $$ Allyl alcohol oxide $$ 2,3-Epoxy-1-propanol $$ 1-Propanol, 2,3-epoxy- $$ 2-(Hydroxymethyl)oxirane $$ 3-Hydroxypropylene oxide $$ 1,2-Epoxy-3-hydroxypropane $$ 1-Hydroxy-2,3-epoxypropane $$ 3-Hydroxy-1,2-epoxypropane $$ 2-hydroxymethyl-oxirane $$ Oxiranylmethanol $$ Epiol OH $$	
3	73	75	$C_2 H_5 N O_2$	1
			Carbamic acid, methyl ester (CAS) Methyl carbamate $$ Urethylane $$ Methylurethane $$ Carbamic acid methyl ester $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 6 Ret .Time : 2.820
Scan # : 100 B.G. Scan # :103
Base Peak : 44.00(625320)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	44	$C O_2$	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	97	61	$C H_3 N O_2$	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
3	97	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 7 Ret .Time : 3.000
Scan # : 121 B.G. Scan # :130
Base Peak : 43.00(4185431)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	97	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
3	97	58	C_3H_6O	2
			Acetone	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 8 Ret .Time : 3.150
Scan # : 139 B.G. Scan # :143
Base Peak : 44.00(118591)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	45	$C_2 H_7 N$	1
			Methanamine, N-methyl- (CAS) Dimethylamine $$ N,N--dimethylamine $$ N,N-Dimethylamine $$	
2	86	75	$C_3 H_9 N O$	1
			1-Propanol, 2-amino- (CAS) 2-Amino-1-propanol $$ Alaninol $$ 2-Aminopropanol $$ .beta.-Propanolamine $$ 2-Amino-2-methylethanol $$ 1-Hydroxy-2-aminopropane $$ 1-Methyl-2-hydroxyethylamine $$	
3	86	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 9 Ret .Time : 3.200
Scan # : 146 B.G. Scan # :148
Base Peak : 44.00(123935)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	87	75	$C_3 H_9 N O$	1
			1-Propanol, 2-amino- (CAS) 2-Amino-1-propanol $$ Alaninol $$ 2-Aminopropanol $$ .beta.-Propanolamine $$ 2-Amino-2-methylethanol $$ 1-Hydroxy-2-aminopropane $$ 1-Methyl-2-hydroxyethylamine $$	
2	85	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
3	85	45	$C_2 H_7 N$	1
			Methanamine, N-methyl- (CAS) Dimethylamine $$ N,N--dimethylamine $$ N,N-Dimethylamine $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 10 Ret .Time : 3.250
Scan # : 152 B.G. Scan # :163
Base Peak : 44.00(129485)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	86	72	$C_3 H_4 O_2$	1
			Formic acid, ethenyl ester (CAS) Vinyl formate $$ Formic acid, vinyl ester $$	
2	86	72	$C_3H_4O_2$	2
			Formic acid, ethenyl ester	
3	85	132	$C_3 H_4 N_2 O_4$	1
			Acetic acid, [(aminocarbonyl)amino]oxo- (CAS) Oxaluric acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 11 Ret .Time : 3.380
Scan # : 167 B.G. Scan # :170
Base Peak : 43.00(92101)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	95	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	95	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
3	95	58	C_3H_6O	2
			Acetone	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 12 Ret .Time : 3.480
Scan # : 179 B.G. Scan # :184
Base Peak : 43.00(1384692)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	95	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	95	58	C_3H_6O	2
			Acetone	
3	95	58	$C_3 H_6 O$	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 13 Ret .Time : 3.600
Scan # : 194 B.G. Scan # :207
Base Peak : 44.00(110552)

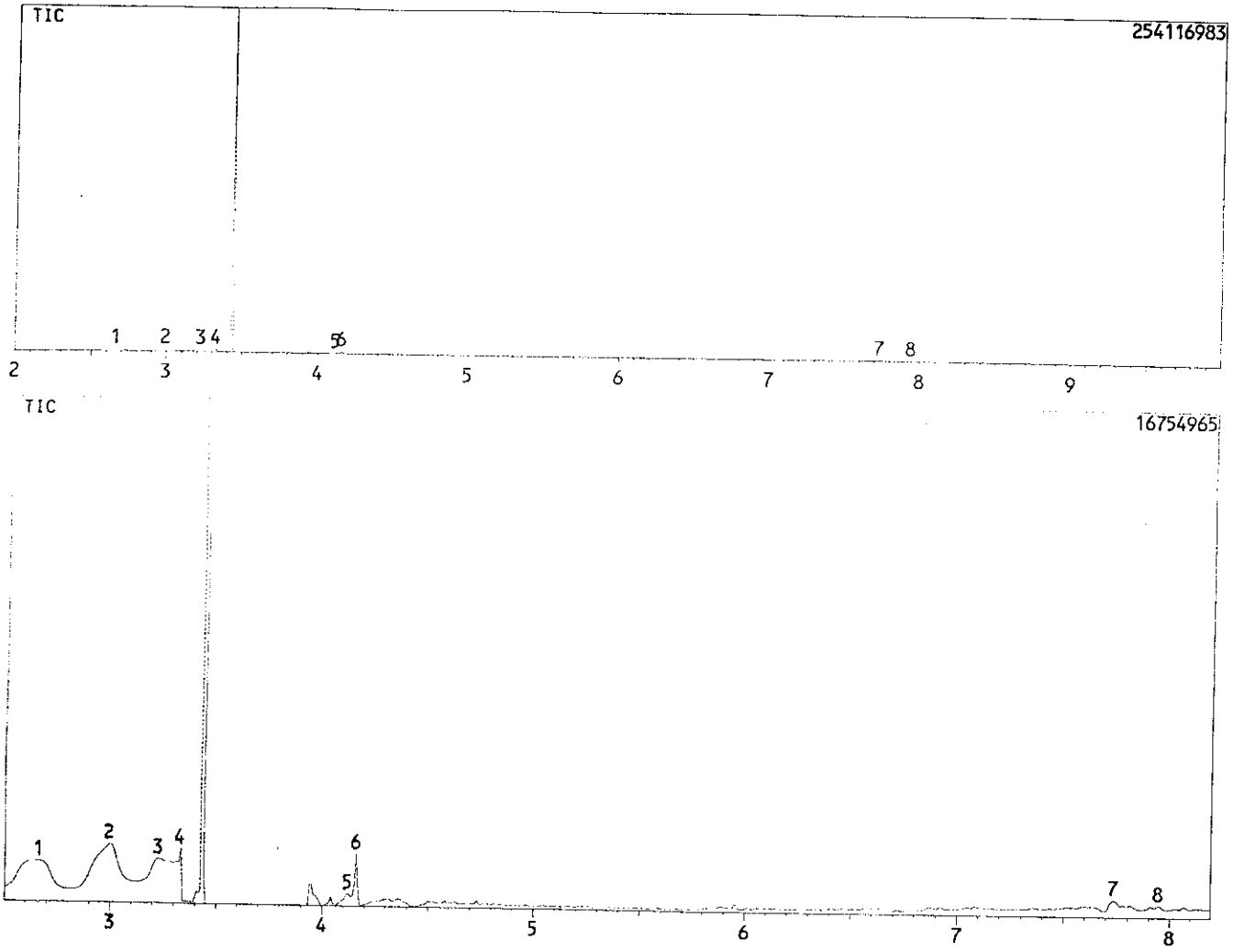
<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	84	230	$C_5 H_{10} O_{10}$	1
			Cyclopentanedecol (CAS) DECAHYDROXYCYCLOPENTANE $$ Cyclopentanepentone, pentahydrate $$	
2	83	89	$C_3 H_7 N O_2$	1
			DL-.ALPHA.-ALANINE $$	
3	83	124	$C_7 H_8 O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-D	

imethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

Data : MALIK.D08 04/04/27 14:43:07
Sample : Controltoluene
ID :
Method File Name : HO-BEN.MET



<Unknown Spectrum>
PKNO : 1 Ret .Time : 2.660
Scan # : 81 B.G. Scan # :95
Base Peak : 44.00(643447)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	94	61	CH_3NO_2	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	
2	93	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
3	92	44	N_2O	1
			Nitrogen oxide (N2O) (CAS) Nitrous oxide $$ Laughing gas $$ Dinitrogen oxide $$ Dinitrogen monoxide $$ Nitrus oxide $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 2 Ret .Time : 2.990
Scan # : 120 B.G. Scan # :134
Base Peak : 43.00(691113)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	98	58	C_3H_6O	2
			Acetone	
2	98	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
3	98	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 3 Ret .Time : 3.220
Scan # : 148 B.G. Scan # :159
Base Peak : 43.00(221734)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	58	C_3H_6O	2
			Acetone	
2	97	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
3	96	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 4 Ret .Time : 3.330
Scan # : 161 B.G. Scan # :163
Base Peak : 44.00(1076183)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	95	124	$C_7H_8O_2$	1
			4H-Pyran-4-one, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-pyrone $$ 2,6-DIMETHYL-1,4-PYRONE $$ 2,6-Dimethyl-4H-pyran-4-one $$ 2,6-Dimethyl-4-pyranone $$ 2,6-Dimethyl-.gamma.-pyrone $$	
2	91	75	C_3H_9NO	1
			Ethanol, 2-(methylamino)- $$ .beta.-(Methylamino)ethanol $$ Methylethanolamine $$ (Hydroxyethyl)methylamine $$ (2-Hydroxyethyl)methylamine $$ Methyl(.beta.-hydroxyethyl)amine $$ Methyl(hydroxyethyl)amine $$ Methyl(2-hydroxyethyl)amine $$ Methylaminoethanol $$ Methylethylolamine $$ Monomethylaminoethanol $$ Monomethylethanolamine $$ Monomethylmonoethanolamine $$ N-(2-Hydroxyethyl)methylamine $$ N-Methyl-N-(.beta.-hydroxyethyl)amine $$ N-Methyl-N-(2-hydroxyethyl)amine $$ N-Methyl-N-hydroxyethylamine $$ N-Met	
3	89	61	CH_3NO_2	1
			Carbamic acid, monoammonium salt (CAS) Ammonium carbamate $$ Carbamic acid, ammonium salt $$ Monoammonium salt of carbamic acid $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>

PKNO : 5 Ret .Time : 4.110
Scan # : 255 B.G. Scan # :258
Base Peak : 44.00(117510)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	
2	97	78	$CH_6N_2O_2$	2
			Carbamic acid, monoammonium salt	
3	97	44	CO_2	1
			Carbon dioxide (CAS) Dry ice $$ R 744 $$ Carbonic acid gas $$ Carbonic anhydride $$ Carbon oxide (CO2) $$ Carbonic acid, gas $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 6 Ret .Time : 4.150
Scan # : 260 B.G. Scan # :263
Base Peak : 43.00(862492)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	97	58	C_3H_6O	2
			Acetone	
3	97	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 7 Ret .Time : 7.730
Scan # : 689 B.G. Scan # :693
Base Peak : 43.00(117946)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	97	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	97	58	C_3H_6O	2
			Acetone	
3	96	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB

<Unknown Spectrum>
PKNO : 8 Ret .Time : 7.950
Scan # : 715 B.G. Scan # :719
Base Peak : 43.00(64964)

<Hit List>

No	SI	Mol.Wgt.	Mol.Form./Compound Name	LIB#
1	93	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	
2	93	58	C_3H_6O	2
			Acetone	
3	91	58	C_3H_6O	1
			2-Propanone (CAS) Acetone $$ propan-2-one $$ Propanone $$ Methyl ketone $$ Dimethyl ketone $$ Pyroacetic ether $$ .beta.-Ketopropane $$ Dimethylformaldehyde $$ ACETONE (2-PROPANONE) $$	

Library Name
(1) WILEY229.LIB (2) NIST21.LIB (3) NIST107.LIB