ABSTRACT

JULIA F. STORM. Tentative Identification of Organic Compounds
in the Influent and Effluent of the High Point Westside
Wastewater Treatment Plant and Implications for Aquatic
Toxicity (Under the direction of DR. FRANCIS A. DIGIANO).

After identifying an acute toxicity problem, the North
Carolina Division of Environmental Management required the
High Point Westside Wastewater Treatment Plant (WWTP) to
institute periodic biomonitoring and reduce the toxicity.
Here, Westside WWTP samples are analyzed using the chemical-
specific approach to toxicity reduction in which potential
toxicants are identified.

WWTP samples determined as "toxic" or "nontoxic" by
Daphnia pulex bioassay, effluents from six categories of
industrial dischargers, and a domestic wastewater sample are
analyzed for organic chemicals using continuous solvent
extraction of wastewater samples and broad spectrum GC/MS
analysis. An extensive database is developed which includes
aquatic toxicity data and tentatively identified compounds in
WWTP samples and industrial effluents ranked according to
their potential for contribution to toxicity.

The study suggests that many compounds found in Westside
WWTP influent and effluent are of industrial origin since
they occur in both industrial samples and Westside WWTP

samples. Treatment does not remove some organic compounds exhibiting significant toxicity to aquatic organisms and shown to be present in "toxic" effluents and industrial samples.

Toxicity of Westside WWTP influent and effluent may be caused by a variety of industrial organic compounds in concentrations that alone would not be sufficient to produce a toxic effect but, because they may all produce toxicity by the same mechanism (narcosis) and thus may exhibit concentration addition, together produce a toxic effect. Recommendations for further analyses include confirmation of identifications using additional mass spectral techniques and determination of estimated or empirical aquatic toxicities.

TABLE OF CONTENTS

ACKNOWLEDGEMENTS

Thanks go to members of my committee, Dr. Charles M. Weiss and Dr. Russell F. Christman. I express special thanks to Dr. Francis A. DiGiano, my advisor, for his guidance and assistance.

For performing bioassays, providing information, and collecting samples, I wish to thank Glenda Botenheimer, Bill Frazier, Tom Gore, Frank Ward, and others on the staff of the Department of Water and Sewer of the City of High Point, North Carolina. Appreciation goes to Carol Haney of the North Carolina State University GC/MS Laboratory for performing GC/MS analyses. For her assistance in the use of the computer spreadsheet and other computer related matters, I thank Marty McClelland. And for the moral support, love, and encouragement that only a dear friend can give, thanks Marty.

1. INTRODUCTION

On February 5, 1987 the Water Quality Act of 1987 ammending the Clean Water Act of 1972 became law (Federal Register, 1987). This act requires states to develop by February 1989 water-quality based permit limitations for toxic pollutants to meet water quality standards beyond what can be accomplished by Clean Water Act technology-based requirements. Effluent biomonitoring is a cornerstone of this policy. EPA advocates its use as a problem identification tool and the use of toxicity as a control parameter in setting permit limits, where appropriate. EPA suggests that particular attention should be focused on POTWs having significant industrial input since studies have shown POTW's to be significant sources of toxic materials (Federal Register, 1984).

EPA's Complex EFfluent Toxicity Testing Program was carried out in support of the development and implementation of this policy ("Validity . . . ," 1986). The Technical Support Document for Water Quality-based Toxics Control (September, 1985) and a draft report, "Methods For Toxicity Reduction Evaluations," (January, 1987) were published to aid states and municipalities in implementing biomonitoring programs. There has been much discussion concerning the implementation of the policy of water-quality based

permitting (Roop and Hunsaker, 1985; Wall and Hanmer, 1987; Dunbar, 1987), some of it controversial (Carter, 1986; Grimes, 1987). For POTWs in particular, EPA's time frame for implementation is thought by some to be impractical, and its support documents have been attacked as inadequate (Grimes, 1987).

The state of North Carolina has been a leader in the implementation of a biomonitoring program for the control of toxics from industrial and municipal dischargers. During the last several years, 40% of over 400 toxicity tests performed by North Carolina's Division of Environmental Management (DEM) on industrial and municipal dischargers revealed effluent toxicity (Wall and Hanmer, 1987). Dischargers who have been identified as having toxic effluent are required to institute their own biomonitoring program and are responsible for reducing the toxicity.

Identifying toxicity problems has proved much easier than effecting toxicity reduction. This is especially true when dealing with the situation of a municipal wastewater treatment plant receiving a variety of industrial discharges.

The POTW that is the focus of this research, the Westside Wastewater Treatment Plant (WWTP) in High Point, North Carolina is an activated sludge treatment system having considerable industrial input. The Westside WWTP has had an intermittent problem with effluent toxicity over a period of several years. Although the NC DEM studied the situation and identified some sources of toxicity, toxic episodes have

continued, and a toxicity reduction strategy is needed.

There are two approaches to toxicity reduction: (1) the chemical-specific approach in which potential toxicants are identified and (2) the whole effluent toxicity approach in which treatment or control procedures are investigated without uncovering the specific chemical nature of the toxicants. The former approach is the one applied in this research.

The specific objectives of this research are:
(1) to create a database of organic chemicals identified frequently in Westside WWTP influent and effluent determined to be acutely toxic in aquatic bioassays and in Westside WWTP influent and effluent considered nontoxic,
(2) to analyze the implications regarding toxicity of the Westside WWTP influent and effluent by relating data from the toxicological literature to the findings of organic chemical analyses,
(3) to investigate possible sources of agents thought to be contributing to toxicity by analyzing industrial and domestic wastewater samples, and
(4) to make recommendations for further work in determining the source of toxicity at the Westside WWTP.

2. LITERATURE REVIEW

Approaches to the Study of Toxicants in Wastewater

Approaches to the study of toxicants in wastewater may be divided into three categories:

1) mutagenicity testing of selected fractions of wastewaters with various levels of chemical characterization of the wastewater,

2) identification of organic compounds in wastewater with evaluation of environmental significance using the toxicological literature, and

3) toxicity reduction evaluations of wastewater treatment plant effluent.

Neal, et al. (1980) evaluated the performance of selected advanced wastewater treatment plants for removing (or introducing) mutagenic chemicals and determined the distribution of detected mutagenic activity among various classes of chemical compounds. Salmonella, yeast, and mammalian cells were used to determine mutagenic activity. Sorption on polyurethane foam plugs, sorption on XAD resin, and solvent extraction techniques were used to recover organics from wastewater. Solvent extraction exhibited the best recovery of the three methods: %TOC recovered from secondary effluent equaled 24.6. Aromatic and oxygenated neutrals fractions of the solvent extraction of

pre-chlorination secondary effluent from an activated sludge treatment plant exhibited the greatest mutagenicity. The presence of many non-extracted polar mutagens was demonstrated.

Meier and Bishop (1985) evaluated conventional treatment processes for removal of mutagenic activity from municipal wastewaters. Their study investigated mutagen removal at various stages of treatment at several treatment plants: one receiving a heavily industrialized municipal waste, one receiving primarily domestic waste, and the EPA Test and Evaluation Facility in Cincinnati, Ohio, which receives an industrialized municipal waste. Mutagenicity tests were performed using Salmonella; wastewater was solvent extracted at low and high pH values. Meier and Bishop concluded that the mutagenic activity (both direct-acting and that requiring metabolic activation) was primarily industrial in origin because the domestic wastewater effluent exhibited a substantially lower mutagenicity. Removal of mutagenic activity by conventional treatment varied from none to two thirds of that initially present in the untreated wastewater, leading to the conclusion that "an appreciable portion of the responsible mutagens are relatively refractory to removal by conventional primary and activated sludge treatment." In contrast to findings of studies of drinking water, chlorination of secondary effluent did not substantially influence the mutagenicity of wastewater effluent. Mutagenic activity in the primary effluent was found in the

acid/neutral fraction. The base fraction of unchlorinated secondary effluent had the greatest specific mutagenic activity, although the acid fraction had the greatest overall mutagenic activity.It was recommended that identification of compounds responsible for mutagenic activity be undertaken to help determine the source and effective treatment methods for their removal.

Saxena and Schwartz (1979) investigated mutagens in wastewaters at various treatment stages of three advanced wastewater treatment plants representing three categories of advanced treatment processes: biological, physical-chemical, and land application. Influent to each of the three plants was secondary effluent from a conventional wastewater treatment plant. Mutagenicity assays on Salmonella were performed with and without mammalian metabolic activation. Both the biological and physical-chemical treatment processes failed to remove and in some cases introduced mutagenic substances.

Rappaport, et al. (1979) determined the mutagenicity (Ames bioassay) of five advanced wastewater treatment plants in urban areas. The sources of these wastewaters ranged from completely domestic to mixed domestic-industrial wastes. Wastewater samples of primary, secondary (pre-chlorination), and post-secondary (dechlorination employed at some plants) were collected. Organic compounds in the wastewater samples were concentrated by XAD resins. Mutagenic concentrates were separated into acid, base, and neutral fractions by solvent

extraction. Mutagenic samples were obtained only from plants having mixed domestic and industrial influent. Basic and neutral fractions appeared to contain most of the mutagenic activity. Nitrogenous bases, many of which are known to be mutagens, were probably among the compounds in the basic fractions. It was suggested that the activated sludge process may have converted inactive substances into mutagens since activity was observed in secondary and post-secondary effluents when none had been observed in primary effluent, even when tested at higher doses. They recommended compound identification in mutagenic fractions as a goal of future work.

Jungclaus, Lopez-Avila, and Hites (1978) analyzed the wastewater, receiving water, and receiving water sediments from a specialty chemicals manufacturing plant producing a wide range of compounds including pharmaceuticals, herbicides, antioxidants, thermal stabilizers, UV light absorbers, optical brighteners, and surfactants. The wastewater was treated by neutralization, biodegradation (in trickling filters), and clarification, achieving about 25% total BOD removal. Solvent extraction of water samples at low and high pH values and vapor stripping techniques were employed. Analysis was by GC/FID/ECD and GC/MS. Concentrations of the anthropogenic compounds ranged up to 15 ppm in the wastewater, 0.2 ppm in the river water, and several hundred ppm in the sediments. Mammalian toxicity data was quoted for several compounds. Aquatic toxicity

information involving Daphnia for s-triazine herbicides found in both the wastewater and river water were discussed. Jungclaus, Lopez-Avia, and Hites concluded that "a human health hazard is difficult to assess, but the long-term, low-level exposure to this wide variety of chemicals may have contributed to the lack of biota in the area."

Games and Hites (1977) identified organic compounds extracted from a dye manufacturing plant wastewater. Treatment of the wastewater involved neutralization, aeration lagoon biological degradation, and settling, resulting in 70% COD and 85% BOD removal. Some compounds were not removed at all by the treatment process; others were degraded or altered to produce compounds not present initially. Toxicity of compounds in both these categories were discussed in a limited manner. One compound found in the effluent is patented as a nematocide but was present as an impurity in a raw material used in dye manufacture. Games and Hites emphasized the benefit of broad spectrum analysis, as target compound analysis would not have discovered the potentially toxic nematocide. They recommended that a rapid screening test be developed to estimate the risk from chronic low level exposure to compounds such as those from the dye plant studied.

Brandes, Mount, and Wall (1986) used POTW effluent and ambient (Cuyahoga River) toxicity testing to determine if the POTW in question was causing an adverse impact on the quality of water in the Cuyahoga River. No observed effect levels of

the wastewater effluent ranged from 30 to 100 percent effluent, values Brandes, et al. considered characteristic of a moderately toxic effluent. To determine the cause of the toxicity, effluents were fractionated using solid phase extraction columns and fractions were tested for toxicity. Brandes, et al. concluded that toxicity was caused by different toxicants on different occasions. A moderately polar fraction containing 15 organic compounds, phenolic ones in particular, was responsible for causing toxicity.

Botts, et al. (1987) conducted a toxicity reduction evaluation of the Patapsco wastewater treatment plant in Baltimore, Maryland, an activated sludge biological treatment plant receiving approximately 60% domestic and 30% industrial influent. Periodic acute toxicity bioassays were conducted with _Ceriodaphnia dubia_ and _Mysidapsis bahia_ and chronic bioassays with _C. dubia_. They demonstrated that secondary treatment significantly reduces effluent toxicity. Toxicity tests of solid phase column fractions of the effluent indicated that non-polar compounds were responsible for the toxicity. Preliminary data from GC/MS analysis of non-polar organic fractions indicated that the complexity of chromatograms will make identification of specific compounds difficult. Botts, et al. found that the specific substrate utilization rate (at high COD levels) decreased for a "toxic" wastewater compared to a "typical" domestic wastewater, indicating that toxic compounds inhibit biodegradation at higher COD levels. Batch treatment tests of two industry

effluents indicated no pass-through toxicity. Further batch tests will determine the biodegradable component of industrial effluents. Toxicity treatability tests of other industrial effluents are planned.

Cary and Barrows (1981) conducted acute toxicity testing using fathead minnows and Daphnia magna of untreated and treated effluents from five pesticide manufacturers, one organic chemical manufacturer, and a bleached-kraft paper mill. Results indicated that the average toxicity reduction of the wastewater treatment plants was 98%, although significant mortality of test organisms still existed in treated effluents. No characterization of the treated or untreated effluents was made.

Horning, Robinson, and Petrasek (1984) used fathead minnow, Daphnia magna, and rainbow trout acute toxicity testing to evaluate the effectiveness of conventional wastewater treatment. Influent to the pilot-scale treatment system consisted of raw municipal wastewater mixed with a known concentration of 22 priority pollutants (nominally 50 ug/L of each). Concentrations of priority pollutants were reduced by 80% to greater than 99%. Toxicity reduction ranged from 65% to 83%; however significant toxicity was still present in the effluent. They concluded that removal efficiency is not necessarily a good indicator of the toxic properties of a conventionally treated wastewater effluent. They also submitted that "organism responses should be considered, in addition to physical and chemical

characterization, in determining the suitability of an effluent for discharge into the aquatic environment."

Aquatic Toxicological Studies

Research involving the toxicity of complex effluents to aquatic organisms has benefited from studies of quantitative structure-activity relationships (QSAR). In order to accomplish quick, effective hazard assessment of the tremendous number of industrial chemicals in use and being developed for use and to focus efforts on the more potentially hazardous chemicals, quantitative structure-activity relationships have been developed to predict toxicity.

Veith, et al. (1983) mention reviews showing narcosis to be a non-specific reversible physiological effect (central nervous system depression probably due to membrane perturbation, (Hermens, et al. 1984a)) caused by a wide variety of organic chemicals. Because this common mode of action of toxicity to aquatic organisms exists, structure-activity relationships may be determined. Conversely, chemicals for which QSARs exist are assumed to bring about acute toxicity by the same mode of action (Hermens 1984a). Veith, et al (1983) reported Konemann's findings obtaining a linear relationship between the n-octanol/water partition coefficient (log P) and acute toxicity to guppies of 50 anaesthetizing industrial pollutants. The relationship deviated from linearity for

chemicals with log P greater than 6 due to a deviation from linearity for bioaccumulation with such compounds. Veith et al. (1983) concluded that the 96 hour LC50 to fathead minnows of 50 industrial alcohols, ketones, ethers, alkyl halides, and substituted benzenes selected from the Toxic Substances Control Act industrial inventory can be estimated by a structure (n-octanol/water partition coefficient)-toxicity relationship.

Bobra, et al. (1983b) concluded from a study of 33 hydrocarbons and chlorinated hydrocarbons and their acute toxicities to D. magna in a closed system that different alkanes, cycloalkanes, monoaromatic, polynuclear aromatic, and chlorinated hydrocarbon solutions exhibit similar toxicity at similar fractions of their saturation concentration. She developed a formula from the relationship she observed for estimating the LC50s of compounds like those she studied:

0.2 x subcooled liquid solubility   x2 for linear compounds
                                    or x0.33 for small cyclics
                                    or x1 for large molecules.

The advantage of this model to those using logP values is that bioconcentration is taken into account, so that biotic concentration is being reflected in the ratio of the chemical's solubility in the organism to its subcooled liquid solubility. Bobra submitted that the limits of this predictive model for other compounds should be investigated. In another study (1983a), she showed that the model can be used to estimate toxicity of crude oils.

In an examination of QSAR models, Bobra, et al. (1985) suggested that when presenting QSAR data logarithmic plots of toxic concentration versus both solubility and o/w partition coefficient be prepared. In the case of the acute toxicity of chlorobenzenes to D. magna, the results showed that the nature of the toxic effect is nonspecific and that the toxic effect occurs when a critical concentration of toxicant is reached within the organism, i.e., the EC50 is controlled primarily by organism/water partitioning. Call, et al. (1985) developed a model based on partition coefficient for predicting subchronic toxicities to fathead minnows of ten narcotizing chemicals (ketones, benzenes, ethers, and alkyl halides). The model estimated maximum acceptable toxicant concentration (MATC).

Studies of the toxicity of mixtures of organic chemicals to D. magna using both experimental and QSAR-estimated toxicities utilize Konemann's mixture toxicity scale (Hermens, et al., 1984a) to describe the type of joint action exhibited by the mixture of chemicals, in which concentration addition is indicated by a mixture toxicity index of 1. Studies of chemical mixtures including industrial chemicals occurring in wastewater and of particular industrial wastewaters have been conducted (Broderius and Kahl, 1985; Hermens, et al., 1985; Hermens, et al., 1984a and 1984b; Bobra, et al., 1983a).

Various mixtures of up to 50 different chemicals from different classes thought to produce toxicity by the same

mode of action (narcosis) and tested in equal fractions of their LC50's were investigated by Broderius and Kahl (1985) and Hermens, et al. (1985). All the mixtures displayed a concentration additive acute joint action. The same conclusion was reached by both studies: even at no-effect levels of individual toxicants combinations of chemicals can produce a toxic effect. EPA's Technical Support Document for Water Quality-based Toxics Control presents data collected by Alabaster and Lloyd indicating that mixtures of toxicants found in sewage and industrial effluents exhibit acute toxicity additivity to aquatic organisms (p. 6). Alabaster and Lloyd's data deviating from additivity involved mixtures of pesticides which generally act according to a variety of specific mechanisms and not by narcosis.

Hermens, et al. (1984b) determined both the acute toxicity to and the inhibition of reproduction of D. magna of a mixture of 14 chemicals having varying chemical structures and probable modes of action. Results of the study showed that the potential for addition is reduced when more specific sublethal criteria, such as inhibition of reproduction in this study, are examined as opposed to mortality. However, even though chemicals were considered to have different modes of action, concentration addition was observed in the mortality study. It was concluded that this phenomenon of concentration addition of chemicals having different modes of toxic action is probably rare. Even though reduced joint toxicity was observed in the studies of inhibition of

reproduction (sublethal effect), the toxicity of the mixture was much higher than that of the individual chemicals and was near concentration addition. In a subsequent study, Hermens, et al. (1985) investigated the joint toxicity on inhibition of growth of _D. magna_ of a mixture of alcohols and chlorohydrocarbons. Concentration-additivity was observed, even at the no observable effect levels with sublethal toxicity criteria.

3. TOXICITY BACKGROUND AND DESCRIPTION OF SITE

Westside WWTP Description

The High Point Westside WWTP includes treatment by trickling filters and activated sludge in series. The effluent is filtered. A flow diagram of the plant is given in Figure 3.1. Prior to September of 1986, when operation of the expansion of the plant began, the plant operated with only one aeration basin.

Effluent from the plant is discharged into the Rich Fork of Abbotts Creek which empties into the Yadkin River at High Rock Lake (a source of drinking water for the town of Denton, NC). Rich Fork Creek has a 7Q10 (7 day, 10 year low flow) of 0.3 cubic feet per second; during periods of low flow the effluent comprises 95% of the creek's flow. (NC Division of Environmental Management, Jan. 23, 1984) Table 3.1 summarizes operational and influent characteristics of the plant. Effluent BOD5 and suspended solids are normally less than 20 mg/L. Values for suspended solids, BOD5, and COD removal efficiencies are given for March 1986 and March 1987 because sampling for this study was performed during these two months and because one month was prior to and the other following plant expansion and upgrading of treatment. It appears that improvement in these removal efficiencies has occurred since the upgrading of the plant. Infiltration occurs during
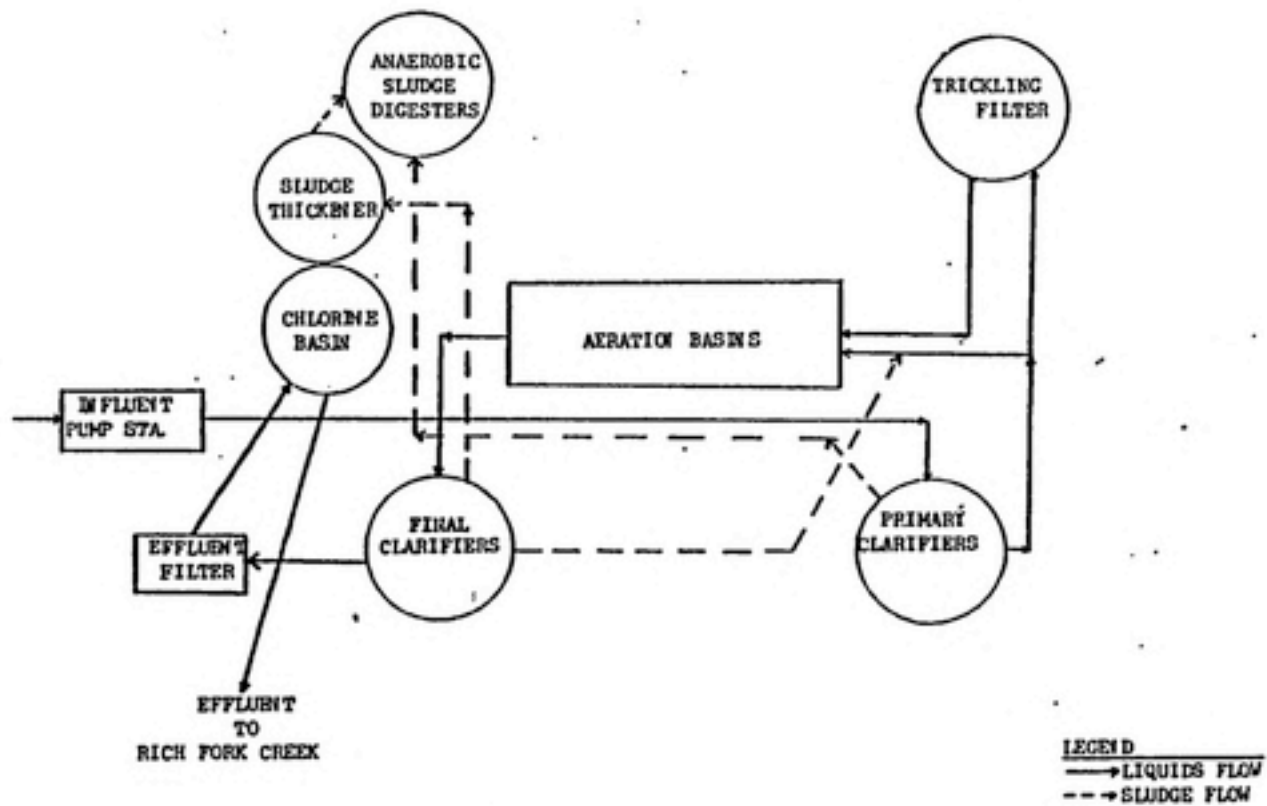
FIGURE 3.1 PROCESS FLOW DIAGRAM, HIGH POINT WESTSIDE PLANT

Table 3.1. OPERATIONAL AND INFLUENT CHARACTERISTICS

HIGH POINT WESTSIDE WASTEWATER TREATMENT PLANT

Characteristic	Value
Design flow	6.2 mgd
Average daily flow	3.5 mgd
Industrial flow	12% of total
Average daily influent BOD	178 mg/L
Industrial BOD contribution	78% of total
Typical influent TOC	150-300 mg/L
Weekday maximum TOC	1000 mg/L
Weekend minimum TOC	50 mg/L

	MARCH 1986	MARCH 1987
Average % total suspended solids removal	95	98
Average % BOD5 removal	92	96
Average % COD removal	80	90
Typical % TOC removal	82	

periods of heavy rain. While flows of 12-14 mgd may be
reached, these periods are of such short duration as not to
be reflected in the average daily flow.

Industrial contributions to the Westside plant are shown
in Table 3.2 to be a small percentage of the flow (12%) but a
large percentage of the BOD (78%). Industrial users of the
High Point Westside WWTP may be divided into the following
categories: organic chemical manufacturers, textile (dyeing
and finishing, milling), metal platers and formers, drum
cleaning, paints and coatings, and dairy operations. Table
3.2 lists each of these industrial categories and its
corresponding percentage of industrial flow to the wastewater
treatment plant. While dairy operations are responsible for
29% of the industrial flow, the effluent contributes mainly
BOD to the plant and makes no contribution to the toxicity of
the treatment plant influent. Disregarding the dairy
operations, the organic chemical manufacturers and metal
platers and formers are the largest contributors based on
flow.

Division of Environmental Management Assessment of Toxicity

The North Carolina Division of Environmental Management
(DEM) conducted a study in 1983 of the Westside WWTP and its
impact on Rich Fork Creek (NC DEM, 1984). Samples of effluent
collected prior to chlorination on three dates were submitted
to 48 hour static Daphnia pulex bioassays. These acute
toxicity tests resulted in LC50 values of less than 45%

Table 3.2. INDUSTRIAL USER PROFILE

HIGH POINT WESTSIDE WASTEWATER TREATMENT PLANT

Industry type	Contribution to flow
Organic Chemical Manufacturing	37%
Textile (dyeing, finishing, milling)	5%
Metal Platers and Formers	23%
Drum Cleaning	5%
Paints and Coatings	1%
Dairy	29%

effluent. In addition, a flow-through 96 hour LC50 using
fathead minnows was determined to be 64% effluent (prior to
chlorination). The study found that the numbers and diversity
of fish and benthic invertebrate populations were greatly
reduced downstream from the WWTP and concluded that the
effluent was greatly stressing downstream biota.

Results of chemical analyses of the effluent conducted at
the time of the benthic survey showed there to be high levels
of phenols and of formaldehyde, a tributyl tin compound at
ppb levels, and 10 unidentified peaks detected by GC/MS.
Vighi and Calamari (1985) found tributyltin chloride to have
a 24 hour LC50 of 0.013 mg/L (13 ppb) using Daphnia magna.
The DEM report concludes that while formaldehyde and tributyl
tin were components of the whole effluent toxicity,
additional toxic constituents probably exist. It also
suggests that if nonylphenol ethoxylates were a major
component of the phenols, that the municipality investigate
the possibility of having the textile industry substitute the
more biodegradable alcohol ethoxylates for them. The tributyl
tin compound used by the textile industry as a biocide was
substituted for with a less potently toxic compound.

High Point Toxicity Assessment Program

The Central Laboratory of the High Point Water and Sewer
Department has conducted acute Daphnia pulex toxicity tests
for several years on the recommendation of the state Division
of Environmental Management. Biomonitoring of wastewater

treatment plant effluent has sometimes been as frequent as two times per week. DEM defined acceptable levels of acute toxicity of the Westside WWTP effluent as and LC50 of greater than or equal to 95% effluent. From February 1986 to September 1986, prior to improvement in treatment facilities, the laboratory biomonitoring program found 8 of 13 influent and 13 of 43 effluent samples bioassayed as having LC50 values less than 90+%. Following upgrading of treatment processes, between September 1986 and April 1987, 5 of 5 influent and 9 of 41 effluent samples showed LC50 values of less than 90+%, showing some improvement in reduction of toxicity. Chronic toxicity of the treatment plant effluent has been documented also.

In the summer of 1987 the High Point Central Laboratory contracted with a private laboratory to conduct acute toxicity tests of industrial effluents discharged to the Westside plant and of an untreated domestic wastewater sample. Of the industrial effluents tested, 80% had LC50 values less than 10%. The LC50 values of the industrial effluents ranged from less than 0.1% to 71%. The industrial categories having at least one significant contributor (based on flow) having an LC50 of less than 1% are listed below:

textile	(minimum LC50 = 0.1%)
drum cleaning	(minimum LC50 = 0.1%)
metal plating	(minimum LC50 = 0.1%)
metal forming	
organic chemical manufacturing.	

The industrial effluent having the least toxicity (LC50=71%) was from an organic chemical manufacturer that pretreats by

an aerobic biological process. The least toxic untreated industrial effluent from an organic chemical manufacturer had an LC50 of 68%. An untreated domestic wastewater sample had an LC50 of 90%. These findings imply that the source of the toxicity of influent to the Westside plant is primarily industrial.

Attempts have been made by a private laboratory contracted by the High Point Central Laboratory to cultivate and maintain stock _Ceriodaphnia_ in Westside domestic wastewater treated in a batch reactor using activated sludge from the Westside plant. Although the daphnia live in this medium, they do not exhibit as high a reproductive rate as is required by EPA quality assurance guidelines for use in chronic bioassays. This suggests either that levels of toxic compounds present in the untreated domestic wastewater itself are high enough to depress reproductive rate or more probably that toxic compounds associated with the sludge are adversely affecting the reproductive rate. That sludge is a sink for heavy metals and polynuclear aromatic hydrocarbons has been well documented. Other compounds have been shown to be concentrated in sludge, as well. Giger, Brunner, and Schaffner (1984) reported that 4-nonylphenols, degradation products of nonylphenol polyethoxylates, are present in activated sludge (although anaerobically digested sludge has nearly 10 times the concentration of the activated sludge) and have toxicity to _Daphnia magna_ greater than that of cadmium.

4. MATERIALS AND METHODS

Sample Collection, Storage, and Handling

Samples of influent and effluent from the High Point Westside WWTP were collected on a weekly basis for a two month period in the spring of 1986 and as toxicity was discovered by periodic biomonitoring until April of 1987. An aeration basin grab sample was collected April 30, 1986 due to concern over a dramatic increase in the consumption of oxygen in the aeration basin. Table 4.1 lists the samples collected and corresponding results of acute toxicity tests. Wastewater samples exhibiting an LC50 of 90% or less in the 48 hour static Daphnia pulex bioassay are defined as "toxic." An LC50 of 90% means that in a solution composed of 90% by volume wastewater and 10% by volume pure dilution water mortality of 50% of the test organisms was observed. "Nontoxic" samples are defined as those having an LC50 of 90+%.

Wastewater samples were composited over 24 hours at a rate of one liter every six hours. Wastewater treatment plant effluent was collected prior to chlorination.

A 24 hour composite sample of domestic wastewater collected from a point in the sewer system having no industrial input was collected in the fall of 1987. In addition, samples of industrial wastewater from six

Table 4.1. HIGH POINT WESTSIDE WWTP SAMPLES
AND CORRESPONDING BIOMONITORING RESULTS

DATE	SAMPLE TYPE	COLLECTION METHOD	48 hour LC50 Daphnia pulex	TOXICITY DESIGNATION
2/3/86	EFF	COMPOSITE	56%	TOXIC
3/3/86	INF	COMPOSITE	AN	NONTOXIC
3/3/86	EFF	COMPOSITE	90+%	NONTOXIC
3/11/86	INF	COMPOSITE	15%	TOXIC
3/11/86	EFF	COMPOSITE	90+%	NONTOXIC
3/26/86	INF	COMPOSITE	AN	NONTOXIC
3/26/86	EFF	COMPOSITE	90+%	NONTOXIC
3/31/86	INF	COMPOSITE	AN	NONTOXIC
4/1/86	INF	COMPOSITE	33%	TOXIC
4/1/86	EFF	COMPOSITE	90+%	NONTOXIC
4/8/86	INF	COMPOSITE	AT	TOXIC
4/8/86	EFF	COMPOSITE	66%	TOXIC
4/30/86	AB	GRAB	49%	TOXIC
11/17/86	EFF	COMPOSITE	6%	TOXIC
11/18/86	EFF	COMPOSITE	6%	TOXIC
3/16/87	INF	COMPOSITE	AT	TOXIC
3/16/87	EFF	COMPOSITE	10%	TOXIC
3/17/87	EFF	COMPOSITE	6.1%	TOXIC

abbreviations: INF = influent; EFF = effluent;
                AB = aeration basin; AT = assumed toxic;
                AN = assumed nontoxic

categories: (1) organic chemical manufacturing, (2) textile, (3) metal finishing, (4) diecasting, (5) paints and coatings, and (6) drum cleaning were collected during this time period. Industrial wastewater samples in each category consisted of a mixture of 24 hour composites of two or more of the significant (based on flow) industrial contributors to the wastewater treatment plant.

Samples were stored in capped, two gallon acid-washed glass bottles with a minimum of headspace at 4 C, except during overnight shipping when samples were stored on ice in coolers. The majority of samples were extracted within one week of collection, except for some industrial composites which were stored for a maximum of one month prior to extraction.

General Characteristics of Westside Wastewater Samples

Table 4.2 provides characteristics of samples collected for this study. These data were obtained from the Central Laboratory of High Point's Department of Water and Sewer. Acute toxicity bioassay results (reported as percent effluent or influent causing mortality of 50% of Daphnia pulex test organisms), average daily flow, pH, BOD5, COD, and metals concentrations are given. In addition, monthly averages for each parameter except pH are provided. No value for any characteristic was also a maximum for the month a sample was collected. Most values for pH, BOD5, and COD are close to the monthly averages and appear normal.

Table 4.2. GENERAL CHARACTERISTICS OF WASTEWATER TREATMENT PLANT SAMPLES

METALS CONCENTRATIONS

48 hour LC50 Daphnia pulex	DATE	SAMPLE TYPE	FLOW RATE mgd	pH	BOD5 mg/L	COD mg/L	Cd mg/L	Cr mg/L	Cu mg/L	Fe mg/L	Pb mg/L	Ni mg/L	Zn mg/L	K mg/L	Na mg/L
AN	3/3/86	INF	3.02	6.7	240	620	.01	.06	.21	6.27	.01	.16	.28	10.5	53
15%	3/11/86	INF	2.97	6.5	140	320	.00	.01	.00	2.25	.0	.12	.06	4.7	29
AN	3/26/86	INF	2.49	6.5	96	150	.00	.09	.10	4.74	.00	.08	.16	4.4	26
AN	3/31/86	INF	2.06	6.0	340	650	NA	.10	.23	NA	NA	.10	.40	NA	NA
33%	4/1/86	INF	2.21	6.3	270	780	.00	.04	.15	3.3	.00	.27	.17	9.1	49
AT	4/8/86	INF	2.98	6.4	220	410	.00	.00	.07	2.86	.00	.07	.14	9.4	47
AT	3/16/87	INF	3.82	6.9	280	940	.00	.09	.22	9.4	.00	.39	.38	7.9	45
56%	2/3/86	EFF	2.89	6.8	8	100	.00	.00	.10	.83	.00	.09	.15	1.7	50
90+%	3/3/86	EFF	3.02	6.8	7	170	.01	.01	.08	.30	.0	.06	.05	7.1	40
90+%	3/11/86	EFF	2.97	6.7	24	90	.00	.01	.00	1.27	.0	.35	.11	10.5	58
90+%	3/26/86	EFF	2.49	6.7	21	130	NA	NA	NA	NA	NA	NA	NA	NA	NA
90+%	4/1/86	EFF	2.21	6.6	35	190	.00	.00	.09	1.03	.0	.00	.11	4.0	22
66%	4/8/86	EFF	2.98	6.5	18	140	.00	.00	.04	1.12	.0	.07	.08	13.6	52
6%	1/17/86	EFF	4.43	7.1	1	30	.00	.00	.04	.21	.0	.10	.10	8.4	60
6%	1/18/86	EFF	4.78	7.0	4	50	.00	.00	.03	.24	.0	.10	.11	9.3	65
10%	3/16/87	EFF	3.82	7.0	6	35	.00	.01	.05	.15	.0	.03	.04	6.8	39
6.1%	3/17/87	EFF	3.53	7.0	12	22	.00	.01	.03	.26	.0	.05	.07	7.4	48

MONTHLY AVERAGES

	DATE	SAMPLE TYPE	FLOW RATE mgd	pH	BOD5 mg/L	COD mg/L	Cd mg/L	Cr mg/L	Cu mg/L	Fe mg/L	Pb mg/L	Ni mg/L	Zn mg/L	K mg/L	Na mg/L
	3/86	INF	2.89		172	444	.00	.112	.149	4.5	.00	.20	.288	8.7	47
	4/86	INF	3.16		214	651	.01	.189	.13	4.5	.0	.16	.26	10.2	60
	3/87	INF	4.72		174	500	.00	.03	.10	4.25	.0	.20	.16	6.4	43
	2/86	EFF	2.77		13	107	.00	.00	.06	.47	.0	.07	.13	8.6	76
	3/86	EFF	2.89		14	90	.00	.01	.04	.54	.0	.17	.09	9.8	53
	4/86	EFF	3.16		22	160	.00	.01	.03	1.25	.0	.10	.06	12.7	56
	11/86	EFF	4.11		4	43	.00	.01	.02	.54	.0	.09	.10	9.9	67
	3/87	EFF	4.72		7	48	.00	.00	.04	.40	.0	.07	.09	5.9	40

Preparation and Analysis of Wastewater Samples

The preparation of samples for analysis is depicted in Figure 4.1. A procedural blank consisting of deionized distilled water was treated according to the same procedure as each set of three wastewater samples in order to detect any contamination entering the process from the extraction through the analysis stages. Wastewater samples (2 L) were continuously extracted for at least 16 hours with 250 mL of B and J residue analysis grade dichloromethane. Those collected before May 1986 were extracted at ambient pH, generally about pH 6.5. Wastewater samples collected after May 1986 were extracted first at a pH greater than 11 and then at a pH less than two in order to insure maximum recovery of organic bases and acids and to simplify chromatographic analyses. Sodium hydroxide (0.1 M) was used to adjust the wastewater samples to pH 11 or greater; adjustment to pH 2 or lower was accomplished by the addition of concentrated hydrochloric acid. Primary internal standards were added to wastewater samples prior to extraction as a means of determining the recovery of the extraction process. Wastewater samples extracted at ambient pH and acidified samples were spiked with 2,5-dimethylphenol; samples made basic were spiked with d8-anthracene. The continuous extraction apparatus was cleaned after each use with detergent and acid dichromate solution and rinsed thoroughly with deionized distilled water.

The dichloromethane extract was concentrated to a volume

24 HOUR CONTINUOUS EXTRACTION ——→ REDUCED PRESSURE ——→ FURTHER CONCENTRATION ————→ GC/MS ANALYSIS
                                  ROTARY EVAPORATION   BY MICRO-SNYDER
                                  OF EXCESS SOLVENT   EVAPORATION
                                  (from 250ml to 4ml)   (to .5ml, effluent only)
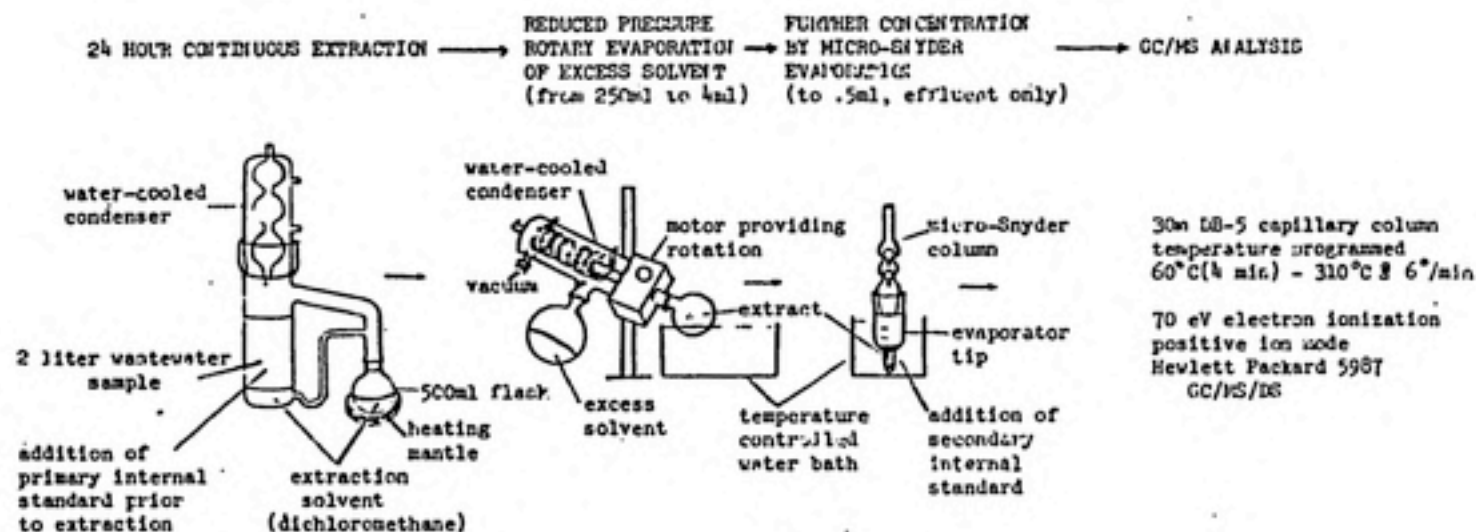
FIGURE 4.1. FLOW DIAGRAM OF ANALYTICAL METHOD

less than 5 mL using rotary evaporation at a temperature of approximately 32 C. Further concentration of the extract, if needed, was accomplished in micro-Snyder equipped concentrator tubes to which the extract had been quantitatively transferred. Extracts expected to be of greater TOC content, i.e. wastewater treatment plant influent and industrial effluents, were concentrated to approximately 5 mL. Wastewater treatment plant effluent and domestic wastewater extracts were concentrated to approximately 0.5 mL. Extracts were spiked with the secondary internal standard (1,4-dichlorobenzene or 1-chlorooctadecane) for the purposes of quantitation and transferred to 10 mL teflon-lined, screw-capped vials for storage in the freezer until analysis.

Extracts were analyzed by both GC/FID and GC/MS. The gas chromatographic column employed for the analysis of the samples collected prior to May 1986 was a J & W 30m, wide bore (0.32mm ID), thin film (0.25um) DB-5 fused-silica capillary column. To achieve maximum column life and performance, two separate, identical columns were used for the analysis of acid and base/neutral extracts (samples collected after May 1986). These columns were J & W 30m, narrow bore (0.25mm ID), thick film (1um) DB-5 fused silica capillary columns. Gas chromatographic conditions for GC/FID and GC/MS analyses are given in Table 4.3. GC/MS analyses were performed by Carol Haney of the North Carolina State University GC/MS laboratory. Performance of chromatographic columns used for base/neutral and acid extracts was monitored

Table 4.3. CONDITIONS FOR CHROMATOGRAPHIC ANALYSIS

	GC/FID	GC/MS/DS
instrument	Varian 3700	Hewlett-Packard 5987
temperature program	$60°(4')-280°a$ $6°/min$	$60°(4')-310°a$ $6°/min$
carrier gas	Helium	Helium
carrier flow rate	1 mL/min	1 mL/min
injector temperature	$280°C$	$300°C$
detector temperature	$300°C$	
ionization technique		EI, 70 eV
mode		positive ion
ion separation technique		quadropole mass filter
ion source temperature		$200°C$
transfer line temperature		$300°C$
mass spectral library		NBS-NIH
		(78,000 spectra)

by injection of the Grob mix prior to analysis of sample extracts by GC/FID. No significant degradation in column performance was observed.

Certainty Measures

Although primary internal standards were employed, no quantitative measure of recovery of the primary internal standard was determined. Because 1,4-dichlorobenzene was present in samples, it was a poor choice for an internal standard and could not be used as a basis for quantitation of recovery of the extraction process. The other secondary internal standard used, 1-chlorooctadecane, was either added to samples in too small a quantity to be detected or was not amenable to chromatography under the conditions used. In either case, because none was detected, quantitation of recovery of the primary internal standard could not be achieved. Despite these problems, 2,5-dimethylphenol was observed in a majority of samples. Thus, recovery of a compound spiked into the sample matrix prior to extraction was demonstrated. The fact that no compounds were identified in procedural blanks indicates that no contamination was introduced to samples by the analytical procedure itself.

Identification Process

The process of assigning identifications to compounds detected in samples included: 1) computer library search of the NBS-NIH mass spectral reference library, 2) manual

comparison of library identifications to reference spectra, and 3) inspection of spectra for reasonable fragmentation given the identification. Because spectra of standards were not generated on the mass spectrometer used for sample analysis for comparison with sample spectra, identifications may only be termed "tentative," as opposed to confirmed.

Acute Toxicity Tests

Bioassays of wastewater samples were performed by the Central Laboratory of the High Point Department of Sewer and Water. The bioassay method used was that developed by EPA (Peltier and Weber, 1985) and modified by the NC Division of Environmental Management to use Daphnia pulex, a waterflea which lives in soft water, as opposed to Daphnia magna, a hard water organism.

The method can be summarized as follows. Wastewater samples were diluted with well water to five concentrations ranging from 0 to 90% influent or effluent. Test organisms (10 Daphnia pulex individuals less than 24 hours old) were added to wastewater samples in 10 mL of dilution water; total volume of test medium was 100 mL. Mortality of the test organisms was recorded after 48 hours. Dissolved oxygen, temperature, and pH of the test medium were measured at the beginning and end of the test. Plots of log percent mortality versus wastewater concentration were constructed. The concentration at which 50% mortality occurred was obtained from this plot.

5. RESULTS

An Evaluation of Metals as Contributors to Toxicity

The focus of this research is on identification of organic compounds and their possible contribution to toxicity. However, it is first necessary to discuss the possible role of metals with the hope of eliminating them as a possible major contributor.

Table 5.1 provides information helpful in determining the contribution of Cu, Ni, and Zn to the toxicity of the Westside WWTP samples. Concentrations of metals expressed in terms of both mg/L and the percentage of their respective LC50 values from the literature (LC50 of Ni = 0.510 mg/L; LC50 of Zn = 0.66 mg/L; LC50 of Cu = 0.027 mg/L) as well as the combined values for Cu, Ni, and Zn are given (Nebeker, et al., 1985; Miller, et al., 1985; Ingersoll and Winner, 1982).

If the metals data for samples considered "toxic", i.e., LC50 < 90%, show concentrations that are less than their respective LC50s, it is possible to state that metals were not contributing to the toxicity of the samples. For all of the samples, Ni and Zn concentrations were less than their respective LC50 values. However, almost all of the samples, except one "toxic" influent and one "nontoxic' effluent, had Cu concentrations greater than 100% of the LC50 value for Daphnia, reaching a maximum of 852%. Five out of six

Table 5.1. DATA USEFUL IN DETERMINING CONTRIBUTION OF METALS TO THE TOXICITY OF WESTSIDE WASTEWATER SAMPLES

| 48 hour LC50 Daphnia pulex | DATE | SAMPLE TYPE | Individual Metal Concentration | | | | | | Combined Cu, Ni, Zn Values | |
			Cu mg/L	Cu % of LC50	Ni mg/L	Ni % of LC50	Zn mg/L	Zn % of LC50	mg/L	%ages of LC50s
AN	3/3/86	INF	.21	778	.16	31.4	.28	42.4	0.65	852.8
15%	3/11/86	INF	.00	0	.12	23.5	.06	9.1	0.18	32.6
AN	3/26/86	INF	.10	370	.08	15.7	.16	24.2	0.34	409.9
AN	3/31/86	INF	.23	852	.10	19.6	.40	60.6	0.73	932.2
33%	4/1/86	INF	.15	556	.27	52.9	.17	25.8	0.59	634.7
AT	4/8/86	INF	.07	259	.07	13.7	.14	21.2	0.28	293.9
AT·	3/16/87	INF	.22	815	.39	76.5	.38	57.6	0.99	949.1
56%	2/3/86 .	EFF	.10	370	.09	17.6	.15	22.7	0.34	410.3
90+%	3/3/86	EFF	.08	300	.06	11.8	.05	7.6	0.19	319.4
90+%	3/11/86	EFF	.00	0	.35	68.6	.11	16.7	0.46	85.2
90+%	3/26/86	EFF	NA	---	NA	---	NA	---	---	---
· 90+%	3/31/86	EFF	NA	---	NA	---	NA	---	---	---
90+%	4/1/86	EFF	.09	333	.00	0	.11	16.7	0.20	349.7
66%	4/8/86	EFF	.04	148	.07	13.7	.08	12.1	0.19	173.8
6%	11/17/86	EFF	.04	148	.10	19.6	.10	15.2	0.24	182.8
6%	11/18/86	EFF	.03	111	.10	19.6	.11	16.7	0.24	147.3
10%	3/16/87	EFF	.05	185	.03	5.9	.04	6.1	0.12	197
6.1%	3/17/87	EFF	.03	111	.05	9.8	.07	10.6	0.15	131.4

abbreviations: AN = assumed nontoxic; AT = assumed toxic; INF = influent; EFF = effluent; NA = not available

"nontoxic" samples (although 3 out 5 were assumed "nontoxic")
had Cu concentrations greater than the no observable effect
concentration (NOEC) of 0.020mg/L (Ingersoll and Winner,
1982), the highest being 0.09 mg/L. This apparent increase in
the concentration required to effect acute toxicity is
probably due to the phenomenon of complexation of metals by
high molecular weight organics or other compounds having
complexation capability (Winner, 1985; Flickinger, 1985).
Buckley (1983) showed wastewater treatment plant effluent to
have this kind of complexation capability. He found that
complexation of Cu by 40% sewage treatment plant effluent
diminishes the toxicity from total Cu to juvenile coho salmon
(LC50 = 0.286 mg/L as opposed to 0.022 mg/L). If the same
increase in the median lethan concentration of Cu (LC50) is
seen in wastewater with Daphnia, this would account for
samples having high concentrations of Cu exhibiting no
toxicity to Daphnia and would indicate that the toxicity of
"toxic" samples is due to something other than Cu.

Upon examination of Cu, Ni, and Zn concentration values,
the conclusion can be drawn that metals probably played no
role in the toxicity of the 3/11/86 influent sample having an
LC50 of 15%. However, because copper concentrations were
greater than 100% of the Cu LC50 for the other "toxic"
samples, other criteria for determining the toxic
contribution of metals was developed. Using the combined
concentrations of Cu, Ni, and Zn of the "nontoxic" effluent
sample as a basis for comparison (0.46 mg/L), and assuming

all other affects equal, "toxic" samples having a combined concentration of Cu, Ni, and Zn of less than 0.46 mg/L and whose toxicity thus appears not to be caused by metals are: 2/3/86 effluent, 4/8/86 influent and effluent, 11/17/86 effluent, 11/18/86 effluent, 3/16/87 effluent and 3/17/87 effluent.

Using the combined percentages of LC50 values for Cu, Ni, and Zn as given in Table 5.1, it appears that metals were not the major cause of toxicity in any of the "toxic" effluent samples, except perhaps the one collected 2/3/86. In all effluent samples except 2/3/86, the combined percentages of LC50s for the three metals were below 349.7%, the value reported for the 4/1/86 "nontoxic" effluent and used for comparison purposes. The 3/11/86 influent sample (LC50 = 15%) and the 4/8/86 influent sample (assumed "toxic") both had combined percentages of LC50s for Cu, Ni, and Zn below the 349.7% comparison value, indicating that toxicity in those influent samples thought to be toxic may not be due to metals.

Organic Compounds Found in Wastewater Samples

Organic compounds tentatively identified in seven High Point Westside WWTP influent samples and one aeration basin sample are listed in Table 5.2. Five out of the eight samples were defined as "toxic," three as "nontoxic." A "toxic" sample is one exhibiting an LC50 of 90% or less in the 48 hour static Daphnia pulex bioassay. A sample labelled

Table 5.2. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP INFLUENT

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: AN nontoxic 3/3/86	15% toxic 3/11/86	AN nontoxic 3/26/86	AN nontoxic 3/31/86	33% toxic 4/1/86	AT toxic 4/8/86	49% toxic 4/30/86	AT toxic 3/16/87 B/N(A)
1-(2-methoxypropoxy)-2-propanol	2	32	88		22	8	61	
benzoic acid, butyl ester		38						
1-(2-methoxy-1-methylethoxy)-2-propanol (early RT)		20	50		10	6	28	
1-(2-methoxy-1-methylethoxy)-2-propanol (late RT)		22	33		8	4	23	
1,2,4-trichlorobenzene	10.5	20	48		6	87	70	24(20)
1,1'-biphenyl	42	15.5	72	25	4	4	10	5(8)
undecane	7	11	20					
naphthalene	34.5	17	65		12	32	40	17
2-ethyl-1-hexanol	16	15	100	100	73	94	100	9
dimethylbenzene (early RT)	4	7.6	268		5	3		
2-butoxyethanol	31.5	7.6	80					
1- or 2-methylnaphthalene (early RT)		7.6			4	5	38	7(6)
1-(2-butoxyethoxy)ethanol		6						
1-chloro-2-, 3-, or 4-methylbenzene (early RT)	3	7	52			2	8	5
4,8,12-trimethyl-3,7,11-tridecatrienoic acid, methyl ester or tridecatrienenitrile	6	4						
1-heptacosanol	4	3.5						
1,2- or 1,3-dimethylnaphthalene	5.5	4					13	(3.5)
1-methylnaphthalene (late RT)	4	5.2			3	7	30	4(4)
caffeine	2	5	20			5		2
1,2,3- or 1,3,5-trichlorobenzene	3.5	5				19	20	4
2-methyl-2,4-pentanediol	3	2						
nonane		3						
5-(phenylmethyl)-2-thioxo-4-imidazolinone		2						
ethylbenzene		15	140		3			
octadecanoic acid, butyl ester (early RT)		2						

Table 5.2. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP INFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

LC50: / TOXICITY DESIGNATION: / SAMPLE DATE:

COMPOUND	AN nontoxic 3/3/86	15% toxic 3/11/86	AN nontoxic 3/26/86	AN nontoxic 3/31/86	33% toxic 4/1/86	RT toxic 4/8/86	49% toxic 4/30/86	RT toxic 3/16/87 B/N(A)
cis- or trans-α,α,4,5-tetramethyl-1-cyclopentene-1-methanol		3						
alkane at *RT 9.8		3						
2-ethyl-N,N-dimethyl-1-hexanamine		2						
octadecanoic acid, butyl ester (late RT)	4	2	30					
dodecane	4	3.5						
isothiocyanic acid, phenyl ester		3.5					22	
N,N-dimethylcyclohexanamine	8.4		368					6
3-methyl-1-butanol benzoate (isoamylbenzoate)		15.5	268			6	68	
toluene			118			17	17	360(27)
dimethylbenzene (late RT)	1.5		100			2	2	
α-terpineol	9	15	95	33	12	7	47	
benzenemethanol	30.5		80		9	17		34(7)
d-limonene			62					
1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester			35					(4)
alkane at *RT 36.21			25					
1-ethyl-2-, 3-, or 4-methylbenzene			16					
1,2,3-, 1,3,5-, or 1,2,4-trimethylbenzene			22					2
4-methylphenol	6.3		14	163	40	16	140	2
hexahydro-2H-azepin-2-one			13					4.5(4)
2-methylquinoline			16					
dodecanoic acid			18	68	8	9		(17)
tetradecanoic acid			20	80	6	4	40	(22)
hexadecanoic acid			22	75			96	(77)
1-hexadecene			15					
docosane			25					
alkane at *RT 33.42			15					

Table 5.2. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP INFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	AN nontoxic 3/3/86	15% toxic 3/11/86	AN nontoxic 3/26/86	AN nontoxic 3/31/86	33% toxic 4/1/86	AT toxic 4/8/86	49% toxic 4/30/86	AT toxic 3/16/87 B/N(A)
alkane at xRT 34.86				15					
alkane at xRT 40.04				12					
1,1-dicyclohexylheptane?				15					
1H-indole		13			80	10	12	116	5
phenol		4	2		73	7	7	70	2(22)
decanoic acid					60	6	5		(19)
molecular sulfur		2			20	4	7		
1,2-benzenedicarboxylic acid, butyl phenylmethyl ester							20	9	
1,2,4-trithiolane							5		
1,2,4,6-tetrathiepane							2		
nonylphenol isomer								7	
N,N,N',N'-tetraethyl-1,2-ethanediamine?								6	
1,2-benzenedicarboxylic acid, diisoctyl or dioctyl ester		12	14.5					29	
3-methyl-1H-indole								103	
dimethyltrisulfide		1.5						61	
1,1'-oxybisbenzene								47	
1,3-dihydro-2H-indol-2-one								39	
1,8-dimethylnaphthalene								22	(4)
2,6,10,15,19,23-hexamethyl-2,6,10,18,22-tetracosahexaene								20	
2-ethylhexanoic acid								16	
4-(2,2,3,3- or 1,1,3,3-tetramethylbutyl)phenol								12	
6-methyl-2-phenylindole? MW 207							2		
9,12-octadecedienoic acid		24	18						
14-methylcholestane		11	11.4						
unknown at xRT 46.2		7							
hexacosanol		5	5.2						

Table 5.2. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP INFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	AN nontoxic 3/3/86	15% toxic 3/11/86	AN nontoxic 3/26/86	AN nontoxic 3/31/86	33% toxic 4/1/86	AT toxic 4/8/86	49% toxic 4/30/86	AT toxic 3/16/87 B/N(A)
alkane at *RT 54.9, 54.6		6	3						
*RT 10.4, 1-methyl-2-, 3-, 4-(1-methylethyl), or 3-propyl-benzene or 1-ethyl-2,4- or 3,5-diaethylbenzene or 4-ethyl--1,2-diaethylbenzene or 2-ethyl-1,4-diaethylbenzene		6							
N-(4-hydroxyphenyl)acetamide or MW 169		5.3					5		
*RT 11.2, 1,2,4,5- or 1,2,3,5-tetramethylbenzene or methyl isopropylbenzene isomer		7							
*RT 11.4, isomer of *RT 11.2		7							
unknown at *RT 43.84				12				20	
9-octadecenoic acid								14	(33)
unknown at *RT 32.45, MW 2117					365				
unknown at RT 31.30, (*RT 24.0, 22.72), MW 203		3	11.2			18	16	6	42
unknown at RT 29.86, (*RT 23.4), MW 175		3	5						
2-isopropylidenedihydrobenzofuran-3-one or 4-methyl-5-phenyl 4-imidazolin-2-one or MW 189		2	6.2				6		
unknown at *RT 20.9, 20.8		2	2						
heptadecane		2							(10.5)
octadecane		2							(11)
unknown at *RT 26.8, MW 2017			2						
*RT 11.9, 2,3-dihydro-4- or 5-methylindene or (2-methyl-1-pr		4							
unknown at *RT 12.0, MW 147?		4.2							
*RT 12.1, isomer of *RT 11.9		4.2							
*RT 12.2, isomer of *RT 10.4		4.2							
ethyl-trimethylbenzene or diaethyl-isopropylbenzene isomer		4							
*RT 10.2, isomer of *RT 10.4		3.5							
*RT 10.9, isomer of *RT 11.2		1.5							

Table 5.2. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP INFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	AN nontoxic 3/3/86	15% toxic 3/11/86	AN nontoxic 3/26/86	AN nontoxic 3/31/86	33% toxic 4/1/86	AT toxic 4/8/86	49% toxic 4/30/86	AT toxic 3/16/87 B/N(A)
alkane at RT 13.9		2							
3-(1-methyl-2-pyrrolidinyl)pyridine (nicotine)		1.5							
1-(2-propenyloxy)-2-propanol		1.5							
azidocyclohexane?		1.5							
2-cyclohexen-1-ol		1.5							
2-cyclohexen-1-one		3.5							
decane		3							
1-methyl-2- or 4-propylbenzene or (1-methylpropyl)benzene		2							
RT 9.7, isomer of RT 11.2		3							
unknown at RT 31.8, 31.7		3		12					
nonadecanol?		2							
unknown at RT 33.6		4							
unknown at RT 34.1		6							
unknown at RT 50.0, MW 296		3							
unknown at RT 54.0, MW 296		3							
unknown at RT 31.72				4					
unknown at RT 21.86, MW 188?							4		
unknown at RT 32.3				4					
unknown at RT 36		4							
unknown at RT 31.18, MW 229?								88	
1,2 benzenedicarboxylic acid, diethyl ester			17						
hexanoic acid						13			(11)
tetrachloroethene									10
4-hydroxy-4-methyl-2-pentanone									12
2-(2-methoxyethoxy)ethanol									S(;1)
(chloromethyl)benzene									12

Table 5.2. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP INFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	AN nontoxic 3/3/86	15% toxic 3/11/86	AN nontoxic 3/26/86	AN nontoxic 3/31/86	33% toxic 4/1/86	AT toxic 4/8/86	49% toxic 4/30/86	AT toxic 3/16/87 B/N(A)
1-benzyl-2-methyl- or 3-methyl-1-(phenylmethyl)-azetidine									46(12)
unknown at RT 35.73, 36.01, MW 212									43
propanoic acid									(9)
2-methylpropanoic acid?									(3)
butanoic acid									(20.5)
unknown at RT 9.6, MW 104?									(9)
unknown at RT 10.15, MW 98?									(12)
pentanoic acid									(7.5)
unknown at RT 13.0, MW 139									(13)
unknown at RT 17.23, MW 116									(3)
benzoic acid									(64)
benzeneacetic acid									(6)
benzenepropanoic acid									(20)
pentadecane									(4.5)
hexadecane									(9)
2,6,10,14-tetramethylpentadecane									(4)
unknown at RT 31.42, MW 199									(6)
2,6,10,14-tetramethylhexadecane									(5)
nonadecane									(9)
alkane at RT 35.73									(7)
octadecanoic acid									(45)

abbreviations: AT=assumed toxic; ANT=assumed nontoxic; B/N=base/neutral extract; (A)=acid extract; RT=retention time; MW=molecular weight

"nontoxic" is one having an LC50 of 90+%. Identification of 146 different compounds at a detection limit of approximately 10 ppb was attempted in the influent/aeration basin samples. Tentative identification of 120 compounds was made. Insufficient information precluded the tentative identification of 24 detected compounds referred to as "unknown."

Table 5.3 contains a list of compounds identified in ten High Point Westside effluent samples, six of which were defined as "toxic" and four as "nontoxic." At a detection limit of approximately 1 ppb, the identification of 123 different compounds was attempted in these samples. Tentative identification of 82 compounds was made. Compounds referred to as "unknown" (41) were detected; however, information necessary to make tentative identification of these was lacking.

Although the approach employed in this work was that of broad spectrum analysis, some quantitative information can be extracted from the data. In addition to compound identification, Tables 5.2 and 5.3 present semi-quantitative data for each compound. This semi-quantitative data is expressed as the ratio of the height of a chromatographic peak in the total ion chromatogram (corresponding to a particular compound) to the noise level in the chromatogram. A value of 1.5 represents the detection limit of the mass spectrometer. Expressing the quantitative data in this way allows for comparisons of concentrations within a given

Table 5.3. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP EFFLUENT

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	56% toxic 2/3/86	90+% nontoxic 3/3/86	90+% nontoxic 3/11/86	90+% nontoxic 3/26/86	90+% nontoxic 4/1/86	66% toxic 4/8/86	6% toxic 11/17/86 B/N	6% toxic 11/18/86 B/N(A)	10% toxic 3/16/87 B/N(A)	6.1% toxic 3/17/87 B/N(A)
benzo[b]naphtho[2,1-d] or [1,2-d]thiophene							6				
N-(4-hydroxyphenyl)acetamide or MW 169?		81	50	2	8		5	2.5	36	3(4)	1.5
phosphoric acid, triethyl ester							92		36	2	
tetrachloroethene (tetrachloroethylene,perchloroethylene)							12		4(2)		2(3)
tetrahydro-2-furanmethanol							32				
1-(2-propenyloxy)-2-propanol							6				
4-hydroxy-4-methyl-2-pentanone (diacetone alcohol)							8			8(5)	(60)
toluene								1	3(3)	2(3)	
unknown at RT 9.54, ×(RT 4.3), MW 97			60						3.5(2)		
2-cyclohexen-1-ol			25						2(7)	2(8)	(10)
unknown at RT 11.21, 11.23, 11.35								2.5	2(16)		
2H-pyran-2-one or 2-cyclohexen-1-one			40						2(16)	1.5(3)	(5)
3,3,3-trichloro-1-propene									17		
unknown at RT 18.66, MW 168									7		
2-phenyl-1,3,2-dioxaborolane? MW 148							5				
1,3-isobenzofurandione									126		
2-isopropylidinedihydrobenzofuran-3-one or 4-methyl-5-phenyl -4-imidazolin-2-one or MW 189			40	3		22		4	10		
1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)			20					6	2(5)	(4)	(3)
unknown at RT 31.30, 31.50, ×(RT 24.02,22.73,22.68), MW 203			10	4.5		46		30	180(101)		
2-acetyl-2,8-dihydro-7-methyl-8-methylenepyrazolo- [5,1-c][1,2,4]triazine								4	10(21)		
unknown at RT 26.75, MW 207									5		
unknown at RT 40.14, ×(RT 32.7, 32.3, 32.4, 31.03), MW 204, (2,2,5,7-tetramethyl-1-tetralol?)		60	10	3		5			2(10)		
chloroform									220		
dibromochloromethane								1.5	5		
unknown at RT 16.22 (spectrum similar to RT 10.46)									2.5		
unknown at RT 17.37 (contains 2 chlorine?)									1.5		
unknown at RT 10.46									7		
2-isoxazolidinecarboxylic acid, ethyl ester? or MW 161?								2	3		
N,4-dimethylbenzenesulfonamide or (phenoxymethyl)benzene?									4		
4-methyl-3-penten-2-one or 2,5-dihydro-2,5-dimethylfuran										2	(18)
4-ethylpiperidine or 1-piperidinecarboxaldehyde		30	5						3	12(8)	40(32)

45

Table 5.3. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP EFFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	56% toxic 2/3/86	90+% nontoxic 3/3/86	90+% nontoxic 3/11/86	90+% nontoxic 3/26/86	90+% nontoxic 4/1/86	66% toxic 4/8/86	6% toxic 11/17/86 B/N	6% toxic 11/18/86 B/N(A)	10% toxic 3/16/87 B/N(A)	6.1% toxic 3/17/87 B/N(A)
N-acetyl-N-(2-methylpropyl)acetamide or 3-methyl-3-nonanamine			10			4	3	5	8	340(29)	19
cyclohexene or trans-2-methyl- or 4-methyl-1,3-pentadiene									560	210	80
7-oxabicyclo[4.1.0]heptane										3.5(39)	45(60)
MW 105 or dimethoxymethane (RT 10.03)										3.3	
unknown at RT 10.74, 10.99, MW 91?						6				6	2
benzenemethanol							2			2.0(5.5)	2(10)
2,3,6-trimethyl-4-octene or 1-butyl-2-ethyl-cyclopentane or (-)-Lavandulol										3.5	
unknown at RT 24.01, 24.31, MW 159										8.5(1.5)	1.5
1-benzyl-2- or 3-methyl-azetidine										8	12(6)
unknown at RT 26.64, 26.94, MW 203										10(2.5)	1.5(2)
unknown at RT 29.86, 30.21, MW 175 *(RT 23.65, 23.3, 23.42, 23.73, 22.12)		30	35	6.5	9	6				4	10
2-(1-methylheptyl)cyclopentanone		30	30	2						11.5(2.5)	90(63)
unknown at RT 34.05, 34.40, MW 232?										3	1.5
3,4-dihydro-5,7-dimethyl-1(2H)-naphthalenone or 7-methyl-4-Pteridinecarboxylic acid, ethyl ester										22	5
3,4-dihydro-6,7-dimethyl-1(2H)-naphthalenone										6	
1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) (bis(2-ethylhexyl)phthalate)										10(13.5)	1.5(10)
1,4-dioxane											2.5(5)
1,3-, 1,2-, or 1,4-dichlorobenzene											1.5
fluoromethylbenzene?											1.5
unknown at RT 14.7, MW 134										5.5	10
(3-chloropropyl)benzene?											7(2)
bromomethylbenzene? or (methylsulfonyl)methyl benzene?				3							2
5-methyl-2-hexanone										4	
unknown at RT 9.61, MW 184?										3	
3- or 1-chlorocyclohexene?										2.5	
benzaldehyde										2.5	7
3,7-dimethyl-1-octene?										3	
dichlorocyclohexane (MW 152) or 1-methyl-1H-pyrrole (MW 81)			16							4	5
unknown at RT 16.28, 16.25, MW 81 or 97 (brominated?)										4	5
1-nitrosopiperidine										7	13
unknown at RT 19.36, 19.32, MW 127, (similar to RT 16.28)										22	10

Table 5.3. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP EFFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	56% toxic 2/3/86	90+% nontoxic 3/3/86	90+% nontoxic 3/11/86	90+% nontoxic 3/26/86	90+% nontoxic 4/1/86	66% toxic 4/8/86	6% toxic 11/17/86 B/N	6% toxic 11/18/86 B/N(A)	10% toxic 3/16/87 B/N(A)	6.1% toxic 3/17/87 B/N(A)
unknown at RT 20.74, 20.30, MW 226 or 127 (similar to RT 16.28)									2	50	47
3-ethyl-4-methyl-1H-pyrrole-2,5-dione?										3	3
unknown at RT 20.95										6	6
unknown at RT 21.49, MW 246 or 244										3	12
3-bromocyclohexene										2	
a phthalate at RT 45.48										1.5	1.5
a phthalate at RT 47.18										3.5	
unknown at RT 5.82											13
dihydro-5,5-dimethyl-(3H)-furanone											5
unknown at RT 13.48, isomer of dihydro-dimethyl-furanone?											5
unknown at RT 15.89											3
3-nonyn-2-ol?											2
unknown at RT 19.97, MW 145, 1 chlorine											6.5
a phthalate at RT 36.32											1.5
α,α,4-trimethyl-3-cyclohexene-1-methanol (α-terpineol)					4						
dimethylbenzene (late RT) (xylene)					4	5					
hexahydro-2H-azepin-2-one				3	6						
N,N-dimethylbenzeneethanamine					4	3	10				
N,N-dimethylcyclohexanamine			400			144	3				
octadecanoic acid, butyl ester (late RT)					4						
phenyl carbamic acid, methyl ester or 1H-benzotriazole				3							
phthalate RT 45.2				2							
1,2-benzenedicarboxylic acid, diisooctyl or dioctyl ester (diisooctyl or dioctyl phthalate)		30	20	9	6	2					
1,2-benzenedicarboxylic acid, dimethyl ester (dimethylphthalate)				52.5							
1,2-benzenedicarboxylic aicd, dipentyl ester (dipentylphthalate)				3							
1-chloro-2-, 3-, or 4-methylbenzene (chlorotoluene) or (chloromethyl)benzene						2				2	
4-(1-methylethyl)benzoic acid, methyl ester				2							
caffeine				3		7	6				
1,2,3- or 1,3,5-trichlorobenzene (late RT)		350	80	4	5	3	65			4.5	7(47)
1,2,4-trichlorobenzene		770	300	15	18	8	232	6	2	4	16.5(11)
1,2-dichlorobenzene (IS)		60	60	12	6	22	52				
1-(methoxy-methylethoxy)-2-propanol (early RT)		30	5	6	54	25	36			2	10(16)
1-(methoxy-methylethoxy)-2-propanol (late RT)		25		4	36	19	20				4(8)

Table 5.3. COMPOUNDS TENTATIVELY IDENTIFIED IN HIGH POINT WESTSIDE WWTP EFFLUENT - continued

QUANTITATIVE DATA, SIGNAL TO NOISE RATIO

COMPOUND	LC50: TOXICITY DESIGNATION: SAMPLE DATE:	56% toxic 2/3/86	90+% nontoxic 3/3/86	90+% nontoxic 3/11/86	90+% nontoxic 3/26/86	90+% nontoxic 4/1/86	66% toxic 4/8/86	6% toxic 11/17/86 B/N	6% toxic 11/18/86 B/N(A)	10% toxic 3/16/87 B/N(A)	6.1% toxic 3/17/87 B/N(A)
1-(2-methoxypropoxy)-2-propanol (dipropylene glycol methyl ether)		30	10	13	78	47	72				5(6)
2,5-dimethylphenol (IS)		15	10	2	2	5			2		
2-ethyl-1-hexanol						26				1.5	
unknown at RT 12.05, MW 89?											2
hexanal?											
N,N,N',N'-tetraethyl-1,2-ethanediamine?						4	112				
unknown at RT 24.7, 24.43, MW 199		100		2							
unknown at RT 34.9, MW 251		20			2						
unknown at RT 36.7, 36.2, 36.33, 36.77, 35.03, MW 299?		70	35	22.5	10	3					
unknown at RT 35.4, 35.02, 33.6, MW 204 or 276 (isomer of RT 40.14?)		30		3		3					
unknown at RT 35.55, MW 279?		30									
unknown at RT 23.3, MW 227 or 269		20									
unknown at RT 27.97, MW 219 or 176		5									
1,4-bis(1-methylethenyl)benzene											
4-(1,1-dimethylpropyl)phenol			35	2							
1-ethyl-6-methyl-3-piperidinone			20								
unknown at RT 26.7, 26.8, 27.13, MW 201?			16	4	8						
unknown at RT 8.9			15								
unknown at RT 30.0, MW 134?			10	3							
1,2,4-, 1,3,5-, or 1,2,3-trimethylbenzene			10								
2-(1-methylethylidene)cyclohexanone?					18						
2-propyl-1,3-cyclohexanedione?					6						
unknown at RT 11.07, MW 157?					6						
unknown at RT 37.4					2						
unknown at RT 27.8					4						
unknown at RT 16.95, MW 141?					3						
1,2,3,4,6,7,12,12b-octahydroindolo 2,3-a quinolizine?					7.5						
unknown at RT 17.08							2				
unknown at RT 34.0, MW 226?					3						

abbreviations: B/N=base/neutral extract; (A)=acid extract; RT=retention time; MW=molecular weight

sample. However, because response factors were not determined and quantitative internal standards were not employed, strict comparisons within a given sample and comparisons from sample to sample cannot be made. Rigorous quantitation would have required deuterated analogs as internal standards and thus knowledge of what compounds were to be expected, and was not within the scope of this work.

Available Data Concerning Toxicological Significance of Organic Compounds Identified in Wastewater Samples

The toxicological literature was searched for studies dealing with toxicity of organic compounds individually or as mixtures to Daphnia pulex, Daphnia magna, Ceriodaphnia, and fathead minnows. Results of toxicity studies of these test organisms for particular compounds tentatively identified in this research and their sources are listed in Appendix I. Literature sources are referenced by a letter following the numeric test value listed in Appendix I; sources are listed on the last page of the table. Aquatic toxicological data for 60 individual compounds from 26 literature sources and for 5 complex mixtures from 5 literature sources were compiled.

Organic Compounds Found in Industrial Effluent and Domestic Wastewater Samples

A listing of the industrial effluents for which composites were collected and analyzed is given in Table 5.4. The table also includes the code letters used to identify these samples

Table 5.4. CATEGORIES OF INDUSTRIAL DISCHARGERS SAMPLED

INDUSTRIAL CATEGORY	CODE
Organic Chemical Manufacturing	OC
Textile	TX
Drum Cleaning	DC
Metal Finishing	MF
Diecasting	DI
Paints and Coatings	PC

in subsequent tables. The compounds tentatively identified in
each industrial effluent are listed in Appendices II - VII.
Although many compounds tentatively identified in industrial
effluents are also found on the list provided by the City of
High Point of process chemicals in use by industrial
dischargers, a significant number are not found on the list.
On the average, approximately 50 compounds were tentatively
identified in each categorical industrial effluent.
Subsequent tables will analyze further the influent and
effluent samples of the High Point Westside plant with the
aim of determining if specific compounds found in the
categorical listing of industrial effluents also appear in
the municipal plant.

In addition, a wastewater sample from a point in the
collection system where industrial effluents were not
discharged represents the category of domestic wastewater
(DW). The results of organic compound tentative
identification for this sample are given in Appendix VIII.
Analysis of the High Point Westside plant data appearing in
tables presented subsequently will also seek to identify
those compounds which may not be of industrial origin.

Organic Compounds in Toxic, Nontoxic, and Both Toxic and Nontoxic Wastewater Samples

Tables 5.5 - 5.7 subdivide the data provided in Table 5.2
and list compounds found only in toxic influent samples,
compounds found only in nontoxic influent samples, and

Table 5.5. COMPOUNDS TENTATIVELY IDENTIFIED ONLY IN TOXIC INFLUENT
AND THEIR SOURCES

COMPOUND	**FREQUENCY	SOURCE(S)	PROCESS CHEMICAL
1- or 2-methylnaphthalene (early RT)	5	OC	
isothiocyanic acid, phenyl ester	2		
1,2-benzenedicarboxylic acid, butyl phenyl-methyl ester (butyl benzyl phthalate)	2		Y
1,8-dimethylnaphthalene	2	OC	
9-octadecenoic acid	2	DW	Y
(chloromethyl)benzene (benzyl chloride)	1	OC	Y
alkane at *RT 9.8	1		
alkane at RT 35.73	1		
benzeneacetic acid	1	DW	
benzenepropanoic acid	1		
benzoic acid	1	OC,TX,DC,PC,DW	Y
benzoic acid, butyl ester	1	OC	Y
butanoic acid	1	DC,PC	
cis-/trans-α,α,4,5-tetramethyl-1-cyclopentene-1-methanol	1		
hexadecane	1	OC,TX,MF,DI	
N,N,N',N'-tetraethyl-1,2-ethanediamine?	1		
nonadecane	1	OC,TX,DC,MF,DI	
nonane	1		
nonylphenol isomer	1	MF,PC	
octadecanoic acid	1	TX,DC,DW	Y
octadecanoic acid, butyl ester (early RT)	1		Y
pentadecane	1	OC,TX,DC,MF	
pentanoic acid	1		
propanoic acid	1		Y
tetrachloroethene (perchloroethylene)	1	OC	Y
1,1'-oxybisbenzene	1		Y
1,2 benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate)	1	OC	Y
1,2,4,6-tetrathiepane	1	DW	
1,2,4-trithiolane	1	DW	
1,3-dihydro-2H-indol-2-one	1		
1-(2-butoxyethoxy)ethanol	1	MF,DW	
1-benzyl-2- or -3-methylazetidine	1	OC	
2,6,10,14-tetramethylpentadecane	1	TX,MF,DI	
2,6,10,14-tetramethylhexadecane	1	TX,MF,DI	
2,6,10,15,19,23-hexamethyl-2,6,10,18,22-tetra-cosahexaene	1		
2-(2-methoxyethoxy)ethanol	1		Y
2-ethyl-N,N-dimethyl-1-hexanamine	1		
2-ethylhexanoic acid	1	DC,PC	Y
2-methylpropanoic acid?	1	DC	
3-methyl-1H-indole	1		
4-(2,2,3,3- or 1,1,3,3-tetramethylbutyl)phenol	1	MF,PC	
4-hydroxy-4-methyl-2-pentanone	1	MF,PC	
5-(phenylmethyl)-2-thioxo-4-imidazolinone	1		
6-methyl-2-phenylindole? MW 207	1		
unknown at *RT 21.86, MW 188?	1		
unknown at *RT 26.8, MW 201?	1		
unknown at *RT 31.18, MW 229?	1		
unknown at *RT 31.72	1		
unknown at *RT 32.3	1		
unknown at RT 10.15, MW 98?	1		
unknown at RT 13.0, MW 139	1		
unknown at RT 17.23, MW 116	1		
unknown at RT 31.42, MW 199	1		
unknown at RT 35.73, 36.01, MW 212	1		
unknown at RT 9.6, MW 104?	1		

* Retention Time on column having 1 as opposed to .25 um film thickness
**out of 5 samples

Table 5.6. COMPOUNDS TENTATIVELY IDENTIFIED ONLY IN NONTOXIC
INFLUENT AND THEIR SOURCES

COMPOUND	**FREQUENCY	SOURCE(S)
alkane at *RT 13.9	1	
alkane at *RT 33.42	1	
alkane at *RT 34.86	1	
alkane at *RT 36.21	1	
alkane at *RT 40.04	1	
azidocyclohexane?	1	
d-limonene	1	DW
decane	1	DC,MF
docosane	1	MF,PC
ethyl-trimethylbenzene or dimethyl-isopropylbenzene isomer	1	
nonadecanol?	1	
1,1-dicyclohexylheptane?	1	
1-(2-propenyloxy)-2-propanol	1	
1-ethyl-2-, 3-, or 4-methylbenzene	1	
1-hexadecene	1	DW
1-methyl-2- or 4-propylbenzene or (1-methylpropyl)benzene	1	OC
2-cyclohexen-1-ol	1	
2-cyclohexen-1-one	1	DW
2-methylquinoline	1	
3-(1-methyl-2-pyrrolidinyl)pyridine (nicotine)	1	DW
*RT 10.2, isomer of *RT 10.4	1	OC
*RT 10.4, 1-methyl-2-, 3-, 4-(1-methylethyl), or 3-propyl-benzene or 1-ethyl-2,4- or 3,5-dimethylbenzene or 4-ethyl-1,2-dimethyl-benzene or 2-ethyl-1,4-dimethylbenzene	1	OC
*RT 10.9, isomer of *RT 11.2	1	
*RT 11.2, 1,2,4,5- or 1,2,3,5-tetramethyl-benzene or methyl-isopropylbenzene isomer	1	OC
*RT 11.4, isomer of *RT 11.2	1	OC,DI
*RT 11.9, 2,3-dihydro-4- or 5-methylindene or (2-methyl-1-propenyl)benzene	1	
*RT 12.1, isomer of *RT 11.9	1	OC
*RT 12.2, isomer of *RT 10.4	1	
*RT 9.7, isomer of *RT 11.2	1	OC
unknown at *RT 12.0, MW 147?	1	
unknown at *RT 31.8, 31.7	2	
unknown at *RT 32.45, MW 211?	1	
unknown at *RT 33.6	1	
unknown at *RT 34.1	1	
unknown at *RT 36	1	
unknown at *RT 46.2	1	
unknown at *RT 50.0, MW 296	1	
unknown at *RT 54.0, MW 296	1	

*Retention Time on column having 1 as opposed to .25 um film
  thickness
**out of 3 samples

Table 5.7. COMPOUNDS TENTATIVELY IDENTIFIED IN BOTH TOXIC AND NONTOXIC INFLUENT
AND THEIR SOURCES

COMPOUND	**FREQUENCY TOXIC	NONTOXIC	SOURCE(S)	PROCESS CHEMICAL
1-methylnaphthalene (late RT)	5	1	OC	
1,2,4-trichlorobenzene	5	2	OC	Y
naphthalene	5	2	OC,TX,DC	
phenol	5	2	DW	Y
1,1'-biphenyl	5	3	OC	Y
2-ethyl-1-hexanol	5	3	OC,TX,MF,PC	Y
1-(methoxy-methylethoxy)-2-propanol (early RT)	4	1		
1-(methoxy-methylethoxy)-2-propanol (late RT)	4	1		
1,2,3- or 1,3,5-trichlorobenzene	4	1	OC,DC	Y
1-(methoxy-methylethoxy)-2-propanol (early RT)	4	1		
1-(methoxy-methylethoxy)-2-propanol (late RT)	4	1		
1-(2-methoxypropoxy)-2-propanol	4	2		Y
1-chloro-2-, 3-, or 4-methylbenzene	4	2	OC,DC	Y
unknown at RT 31.30, (*RT 24.0, 22.72), MW 203	4	2	OC	
tetradecanoic acid	4	2	OC,TX,DC,DW	
1H-indole	4	2	DW	
4-methylphenol	4	3	PC,DW	
o-terpineol	4	3	DW	
1,2- or 1,3-dimethylnaphthalene	3	1	OC	
toluene (methylbenzne)	3	1	OC,DC	Y
decanoic acid	3	1	DC,OI	
3-methyl-1-butanol benzoate	3	1		
dimethylbenzene (early RT) (xylene)	3	2	OC,DC,PC	Y
dodecanoic acid	3	2	TX,DC,DI	Y
benzenemethanol	3	2	OC,DW	
caffeine	3	2	PC,DW	
ethylbenzene	2	1	OC,DC	Y
2-isopropylidenedihydrobenzofuran-3-one or 4-methyl-5-phenyl-4-imidazolin-2-one or MW189	2	1	OC	
1,2-benzenedicarboxylic acid, diisooctyl or di-octyl ester (diisooctyl or dioctyl phthalate)	2	1		
dimethylbenzene (late RT) (xylene)	2	2	OC,DC,PC	Y
2-butoxyethanol	2	2	OC,TX,DC,MF,DW	Y
hexadecanoic acid	2	2	OC,TX,DC,PC,DW	
molecular sulfur	2	2		

54

Table 5.7. COMPOUNDS TENTATIVELY IDENTIFIED IN BOTH TOXIC AND NONTOXIC INFLUENT
AND THEIR SOURCES - continued

COMPOUND	**FREQUENCY TOXIC-NONTOXIC		SOURCE(S)	PROCESS CHEMICAL
dodecane	1	1	DC,MF,DI	
hexahydro-2H-azepin-2-one	1	1	TX	
9,12-octadecedienoic acid	1	1	DC	
N-(4-hydroxyphenyl)acetamide or MW 169	1	1	TX,DC,PC	
unknown at RT 29.86, (*RT 23.4), MW 175	1	1	DC	
heptadecane	1	1	TX,DC,MF,DI	
octadecane	1	1	DC,TX,MF,DI	
hexanoic acid	1	1	DC	
1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) (2-ethylhexyl phthalate)	1	1	DC,MF,DW	
4,8,12-trimethyl-3,7,11-tridecatrienoic acid, methyl ester or tridecatrienenitrile	1	1		
1-heptacosanol	1	1		
2-methyl-2,4-pentanediol	1	1		
1,2,3-, 1,3,5-, or 1,2,4-trimethylbenzene	1	1		
dimethyltrisulfide	1	1		
14-methylcholestane	1	1		
hexacosanol	1	1		
alkane at *RT 54.9, 54.6	1	1		
unknown at *RT 43.84	1	1		
unknown at *RT 20.9, 20.8	1	1		
undecane	1	2	DC,DI	
octadecanoic acid, butyl ester (late RT)	1	2		Y
N,N-dimethylcyclohexanamine	1	2		

*Retention Time on column having 1 as opposed to .25 um film thickness
**out of 5 toxic and 3 nontoxic samples

compounds found in both toxic and nontoxic influent samples,
respectively. Tables 5.8 - 5.10 subdivide the data concerning
effluent samples provided in Table 5.2 in a similar fashion.
These tables also include: (1) frequency of occurrence of
each compound; (2) which, if any, industrial effluent
category (OC TX, DC, MF, DI, PC) and/or domestic wastewater
(DW) sample also contained the specific compound; and (3)
whether the compound appears (Y for yes) on the list provided
by the City of High Point of process chemicals in use by
industrial dischargers.

Organic Compounds Escaping Wastewater Treatment

A list of compounds escaping removal during the wastewater
treatment process was generated by comparing organic
compounds tentatively identified in Westside WWTP influent
and effluent samples collected on the same date. These
compounds are listed in Table 5.11. Although these compounds
were not completely removed by the treatment process, they
were attenuated by a factor of approximately one order of
magnitude. The majority of the compounds escaping treatment
are of industrial origin.

Table 5.8. COMPOUNDS TENTATIVELY IDENTIFIED ONLY IN TOXIC EFFLUENT
AND THEIR SOURCES

COMPOUND	**FREQUENCY	SOURCE(S)	PROCESS CHEMICAL
cyclohexene or 2- or 4-methyl-1,3-pentadiene	3	MF,DI,DW	
phosphoric acid, triethyl ester	3	OC	
tetrachloroethene (perchloroethylene)	3	OC	Y
toluene (methylbenzene)	3	OC,DC	
4-hydroxy-4-methyl-2-pentanone	3	MF	
a phthalate at RT 45.48	2		
benzaldehyde	2	MF	
dibromochloromethane	2		
1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester (2-ethylhexyl phthalate)	2	DC,MF,DW	
1-benzyl-2- or -3-methylazetidine	2	OC	
1-nitrosopiperidine	2		
2-acetyl-2,8-dihydro-7-methyl-8-methylene-pyrazolo[5,1-c][1,2,4]triazine	2	OC	
2-isoxazolidinecarboxylic acid, ethyl ester? or MW 161?	2	PC	
3,4-dihydro-5,7-dimethyl-1(2H)-naphthalenone or 7-methyl-4-Pteridinecarboxylic acid, ethyl ester	2		
3-ethyl-4-methyl-1H-pyrrole-2,5-dione?	2		
4-methyl-3-penten-2-one or 2,5-dihydro-2,5-dimethylfuran	2	PC	
7-oxabicyclo[4.1.0]heptane	2		
(3-chloropropyl)benzene?	1		
a phthalate at RT 36.32	1		
a phthalate at RT 47.18	1		
benzo[b]naphtho[2,1-d] or [1,2-d]thiophene	1		
chloroform	1		
dihydro-5,5-dimethyl-(3H)-furanone	1		
fluoromethylbenzene?	1		
MW 103 or dimethoxymethane (RT 10.03)	1		
N,4-dimethylbenzenesulfonamide or (phenoxymethyl)benzene?	1		
tetrahydro-2-furanmethanol	1		
1,3-, 1,2-, or 1,4-dichlorobenzene	1	DW	Y
1,3-isobenzofurandione	1	OC,DC,MF	
1,4-bis(1-methylethenyl)benzene	1		
1,4-dioxane	1		
1-(2-propenyloxy)-2-propanol	1		
2,3,6-trimethyl-4-octene or 1-butyl-2-ethyl-cyclopentane or (-)-Lavandulol	1		
2-phenyl-1,3,2-dioxaborolane? MW 148	1		
3,3,3-trichloro-1-propene	1		
3,4-dihydro-6,7-dimethyl-1(2H)-naphthalenone	1		
3,7-dimethyl-1-octene?	1		
3- or 1-chlorocyclohexene?	1		
3-bromocyclohexene	1		
3-nonyn-2-ol?	1		
5-methyl-2-hexanone	1		
unknown at *RT 12.05, MW 89?	1		
unknown at *RT 23.3, MW 227 or 269	1		
unknown at *RT 27.97, MW 219 or 176	1		
unknown at *RT 35.55, MW 279?	1		
unknown at RT 10.46	1		
unknown at RT 13.48, isomer of dihydro-dimethyl-furanone?	1		
unknown at RT 15.89	1		
unknown at RT 16.22 (RT 10.46 spectrum similar)	1		
unknown at RT 17.37 (contains 2 chlorine?)	1		
unknown at RT 18.66, MW 168	1		
unknown at RT 19.97, MW 145, 1 chlorine	1		
unknown at RT 26.75, MW 207	1		
unknown at RT 5.82	1		
unknown at RT 9.61, MW 104?	1		
unknown at RT 11.21, 11.23, 11.35	2		
unknown at RT 14.7, MW 134	2		
unknown at RT 16.28, 16.23, MW 81 or 97 (brominated?)	2		
unknown at RT 19.36, 19.32, MW 127 (RT 16.28 spectrum similar)	2		
unknown at RT 20.95	2		
unknown at RT 21.49, MW 246 or 244	2		
unknown at RT 24.01, 24.31, MW 159	2		
unknown at RT 26.64, 26.94, MW 203	2		
unknown at RT 34.05, 34.40, MW 232?	2		
unknown at RT 20.74, 20.30, MW 226 or 127 (spectrum similar to RT 16.28)	3		

*Retention Time on column having 1 as opposed to .25 um film thickness
**out of 6 samples

Table 5.9. COMPOUNDS TENTATIVELY IDENTIFIED ONLY IN NONTOXIC EFFLUENT
AND THEIR SOURCES

COMPOUND	**FREQUENCY	SOURCE(S)	PROCESS CHEMICAL
N,N-dimethylcyclohexanamine	3		
dimethylbenzene (late RT) (xylene)	2	OC,DC,PC	Y
hexahydro-2H-azepin-2-one	2	TX	
4-(1,1-dimethylpropyl)phenol	2		
o, ,4-trimethyl-3-cyclohexene-1-methanol (o-terpineol)	1	DW	
octadecanoic acid, butyl ester (late RT)	1		
phenyl carbamic acid, methyl ester or 1H-benzotriazole	1		Y
phthalate RT 45.2	1		
1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate)	1	OC	Y
1,2-benzenedicarboxylic aicd, dipentyl ester (dipentyl phthalate)	1		
4-(1-methylethyl)benzoic acid, methyl ester	1		
1-ethyl-6-methyl-3-piperidinone	1		
1,2,4-, 1,3,5-, or 1,2,3-trimethylbenzene	1		
2-(1-methylethylidene)cyclohexanone?	1		
2-propyl-1,3-cyclohexanedione?	1		
1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]-quinolizine?	1		
unknown at *RT 26.7, 26.8, 27.13, MW 201?	3		
unknown at *RT 30.0, MW 134?	2		
unknown at *RT 8.9	1		
unknown at *RT 11.07, MW 157?	1		
unknown at *RT 37.4	1		
unknown at *RT 27.8	1		
unknown at *RT 16.95, MW 141?	1		
unknown at *RT 17.08	1		
unknown at *RT 34.0, MW 226?	1		

*Retention Time on column having 1 as opposed to .25 um film thickness
**out of 4 samples

Table 5.10. COMPOUNDS TENTATIVELY IDENTIFIED IN BOTH TOXIC AND NONTOXIC EFFLUENT
AND THEIR SOURCES

COMPOUND	**FREQUENCY TOXIC-NONTOXIC		SOURCE(S)	PROCESS CHEMICAL
N-(4-hydroxphenyl)acetamide or MW 169?	6	3	TX,DC,PC	
1,2,4-trichlorobenzene	6	4	OC	Y
1,2-benzenedicarboxylic acid, diethyl ester (diethyl phthalate)	4	1	DW	
4-ethylpiperidine or 1-piperidinecarboxaldehyde	4	1		
N-acetyl-N-(2-methylpropyl)acetamide or 3-methyl-3-nonanamine	4	3		
1,2,3- or 1,3,5-trichlorobenzene (late RT)	4	4	OC,OC	Y
1-(methoxy-methylethoxy)-2-propanol (early RT)	4	4		
2-cyclohexen-1-ol	3	1		
2H-pyran-2-one or 2-cyclohexen-1-one	3	1	DW	
2-(1-methylheptyl)cyclopentanone	3	2		
1-(methoxy-methylethoxy)-2-propanol (late RT)	3	3		
unknown at RT 29.86, 30.21, MW 175 *(RT 23.65, 23.3, 23.42, 23.73, 22.12)	3	4	OC	
1-(2-ethoxpropoxy)-2-propanol (dipropylene glycol methyl ether)	3	4		Y
benzeneethanol	2	1	OC,OC,PC,DW	
dichlorocyclohexane or 1-methyl-1H-pyrrole	2	1		
2-isopropylidinedihydrobenzofuran-3-one or 4-methyl-5-phenyl-4-imidazolin-2-one or MW 189	2	3	OC	
unknown at RT 31,30, 31.50,*(Rt 24.02,22.73,22.68) MW 203	2	3	OC	
unknown at RT 40.14, *(RT 32.7, 32.3, 32.4, 31.03) MW 204 (2,2,5,7-tetramethyl-1-tetralol?)	2	3	OC	
1,2-dichlorobenzene (IS)	2	4		
2,5-diethylphenol (IS)	2	4		
bromomethylbenzene? or (methylsulfonyl)methyl benzene	1	1		
1-chloro-2-,3-, or 4-methylbenzene (chlorotoluene) or (chloromethyl)benzene (benzyl chloride)	1	1	OC	Y
2-ethyl-1-hexanol	1	1	OC,TX,OC,MF,PC	Y
N,N,N',N'-tetraethyl-1,2-ethanediamine?	1	1		
N,N-diethylbenzeneethanamine	1	2		
caffeine	1	2	PC,DW	
1,2-benzenedicarboxylic acid, diisooctyl or dioctyl ester (diisooctyl or dioctyl phthalate)	1	4		
unknown at *RT 35.4, 35.02, 33.6, MW 204 or 276 (isomer of RT 40.14?)	1	2		
unknown at *RT 36.7,36.2,36.33,36.77,35.03,MW 299?	1	4		
unknown at *RT 34.9, MW 251	1	1		
unknown at *RT 24.7, 24.43, MW 199	1	1		
unknown at RT 9.54, *(RT 4.3), MW 97	1	1		
unknown at RT 10.74, 10.95, MW 91?	2	1		

*Retention Time on column having 1 as opposed to .25 um film thickness
**out of 6 toxic samples and 4 nontoxic samples

Table 5.11. COMPOUNDS TENTATIVELY IDENTIFIED IN BOTH INFLUENT AND EFFLUENT SAMPLES ON THE SAME COLLECTION DATE,
THEREBY IMPLYING INCOMPLETE REMOVAL BY TREATMENT

	OCCURRENCE ON SAMPLE DATE					
toxicity status: influent effluent	3/3/86 ANT NT	3/11/86 TOX,15% NT	3/26/86 ANT NT	4/1/86 TOX,33% NT	4/8/86 AT TOX,66%	3/16,17/87 AT TOX,10%,6.1%
COMPOUND						
N-(4-hydroxyphenyl)acetamide or MW 169	x			x		
tetrachlorethene (perchloroethylene)						x
4-hydroxy-4-methyl-2-pentanone						x
toluene (methylbenzene)						x
2-cyclohexen-1-ol	x					
2-cyclohexen-1-one or 2H-pyran-2-one	x					
2-isopropylidenedihydrobenzofuran-3-one or 4-methyl-5-phenyl-4-imidazolin-2-one or MW189	x	x		x		
2-ethyl-1-hexanol				x		x
benzenemethanol				x		x
1-benzyl-2- or 3-methylazetidine						x
1,2-benznedicarboxylic acid, bis(2-ethylhexyl) ester (2-ethylhexyl phthalate)						x
dimethylbenzene (late RT) (xylene)			x	x		
hexahydro-2H-azepin-2-one			x			
N,N-dimethylcyclohexanamine	x		x			
octadeconaoic acid, butyl ester (late RT)			x			
1,2-benzenedicarboxylic acid, diisooctyl or dioctyl ester (diisooctyl or dioctyl phthalate)	x	x				
(chloromethyl)benzene (benzyl chloride)						x
1,2-benzenedicarboxylic acid, dimethyl ester (dimethyl phthalate)		x				
caffeine		x			x	
1,2,3- or 1,3,5-trichlorobenzene	x	x				x
1,2,4-trichlorobenzene	x	x	x	x	x	x
1-(2-methoxypropoxy)-2-propanol (dipropylene glycol methyl ether)	x	x	x	x	x	
1-(methoxy-methylethoxy)-2-propanol (early RT)		x	x	x	x	
1-(methoxy-methylethoxy)-2-propanol (late RT)		x	x	x	x	
unknown at RT 31.3, MW 203	x	x		x		
unknown at RT 29.86, MW 175	x	x				

abbreviations: ANT = assumed nontoxic; NT = nontoxic; TOX = toxic; AT = assumed toxic

6. DISCUSSION

Considerations for and Limitations to Data Interpretation

The relative nature of the term toxic cannot be emphasized too greatly in the discussion of results. A "toxic" sample is operationally defined in this study as exhibiting an LC50 of 90% or less in the 48 hour static Daphnia pulex bioassay. An LC50 of 90% means that in a solution composed of 90% by volume wastewater and 10% by volume pure dilution water 50% of the test organisms died. However, this also implies that samples labelled "nontoxic" (LC50 = 90+%) may very well be toxic to Daphnia pulex to some degree, as mortality of fewer than half the test organisms may have occurred.

The complexity of wastewater as a mixture of chemicals is one of the major limiting factors in the interpretation of the data. Although the Westside plant was selected for study because organic chemicals were considered by the Division of Environmental Management to be a major contributor to the toxicity of the effluent, it is still possible that metals played some role in producing the toxic effect. The possible role of metals was discussed in the Results section. Conclusions regarding the contribution of metals to toxicity of the wastewater samples were limited by the available information. It is also difficult, if not impossible, to

determine any synergistic or antagonistic effects of particular chemicals without further study. The authors of EPA's Technical Support Document for Water Quality-Based Toxics Control submit that antagonism among effluents of multiple sources has been ovserved, but that synergism is extremely rare and "may not be an important factor in the toxicological assessment of effluents."

The extraction and analytical methods used in this study, although fairly comprehensive, were not exhaustively so, and thus may be regarded as an additional limitation to data interpretation. Using similar techniques, Neal, et al (1980) recovered 25% of the TOC from secondary effluent of an activated sludge treatment plant. Volatile compounds and polar compounds could be better recovered using other methods.

For semi-volatile and non-volatile compounds, the method used in this research is successful. Using wastewater spiked with various industrial compounds, Bishop (1980) demonstrated recoveries of 76% ± 19% for acids and 68% ± 21% for base/neutrals. Due to a poor choice of internal standards, recoveries were not calculated for analyses performed in the study of High Point WWTP samples. However, 2,5-dimethylphenol, used as a primary internal standard for samples extracted at ambient pH and at acid pH, was observed in a majority of samples, demonstrating recovery of this compound.

It should be emphasized that identifications made in this research are tentative. Confirmation of these tentative identifications would require comparison of sample spectra to spectra of standard compounds generated on the same instrument used to analyze the WWTP samples. Additional mass spectral techniques such as chemical ionization and accurate mass determination would aid in lending more confidence to some identifications and in the identification of some as yet unidentified compounds. Fractionation of the extracts would result in less complex chromatograms and subsequently in improved compound identification.

Identification of sources of compounds is not complete. Not all compounds found in the Westside WWTP influent and effluent samples were found in industrial wastewater samples, in the domestic wastewater sample, or on the survey of process chemicals. Industrial samples were not collected on the same day as the treatment plant samples, and since industrial processes and thus chemicals used may change periodically, they are not necessarily representative of the entire range of chemicals entering the treatment plant. In addition, the survey of process chemicals may be incomplete: chemicals in use may not have been divulged and impurities and degradation products of these chemicals are not included.

Yet another limitation pertains to the toxicological literature. The database for toxicity of individual compounds to Daphnia pulex and particularly for aquatic toxicity of

complex chemical mixtures is sparse. The toxicological data
for non-aquatic organisms, although more extensive, is
difficult to relate to the situation being studied, although
attempts have been made to correlate aquatic and mammalian
toxicity data (Hodson, 1985).

Not all of the results of toxicological studies reported
in the literature are in agreement. Test conditions for
toxicity studies reported in this research sometimes vary.
The effect of test variables such as diet, chemistry of test
water, species, age of species, test duration, and organism
loading rates have been studied (Lewis, 1983) A study of
loading density, or the number of test organisms per volume
of test medium, showed that the "biological response
(mortality) did not vary more than three times in tests
conducted at density that ranged from 1 daphnid per 2 ml to 1
daphnid per 50 ml of test water" (Lewis, 1983) and that this
was acceptable variation. When volatile compounds are being
studied, the use of a closed or open test system influences
the accuracy of toxicity values particularly if nominal, as
opposed to measured, chemical concentrations are used. The
results of most of the toxicity test results reported in
Appendix I were obtained either using closed systems which
minimized losses due to volatilization or using analytically
measured test chemical concentrations. The exception to this
set of conditions is found in Le Blanc's study, whose values,
obtained in an open system and based on nominal test compound
concentrations, appear high in comparison to many other

researchers' findings. In general, however, when clearly
defined test protocols are employed, Daphnia magna effluent
toxicity data has been shown to be obtained with good
reproducibility both within and between laboratories (Grothe
and Kimerle, 1985).

Compounds identified in this research that are also on the
priorty pollutant list have been designated as such (Tables
6.1 - 6.4). It should be emphasized, however, that
non-inclusion on the list of priority pollutants does not
necessarily indicate that a compound has no toxic effect on
Daphnia.

Toxicity in this study also refers to the effect on a
particular organism: Daphnia pulex. The 48 hour static D.
pulex bioassay is among a battery of tests developed by EPA
to determine in-stream toxicity effects of effluents from
WWTP and industrial waste streams. EPA's Complex Effluent
Toxicity Testing Program established tht effluent toxicity is
directly correlated to impact in receiving waters (U.S. EPA,
1985, p. 2). As the Daphnia pulex is an invertebrate
indigenous to the eastern U.S. and a source of food for fish,
it does serve as both an indirect and direct indicator of
stream life quality. Thurston, et al (1985) concluded from a
study of comparative susceptibility of ten common aquatic
species to ten organic species causing lethality by four
modes of toxic action that "non-specific toxicants [which
constitute a majority of industrial chemicals] show little
variation in acutely lethal concentrations among aquatic

organisms." The possibility exists, however, that there are more or less sensitive organisms than the Daphnia pulex to the effluent from the Westside WWTP. Investigations of the comparative toxicity (both acute and subacute) of a variety of compounds to various species have shown Daphnia to frequently, but not always, be the most sensitive organism to a particular chemical (Slooff, et al, 1983; Slooff and Canton, 1983; and Blaylock, et al, 1985).

All these limitations make the determination of a cause/effect relationship impossible. The best use of the data from this study is therefore in pointing out directions for further study, which will be discussed in a later section. However, taking into account the limitations enumerated, some discussion regarding the implications of the results is warranted.

Framework for Data Interpretation

The presentation of the results reflects one approach for their interpretation. Figure 6.1 depicts in graphic form the approach employed and can be used as a key to the tables containing compound lists. Municipal wastewater samples were treated collectively as influent or effluent. Chemicals were divided into three categories: (1) chemicals found only in "toxic" samples, (2) chemicals found only in "nontoxic" samples, and (3) chemicals found in both "toxic" and "nontoxic" samples. These categories represent various degrees of suspicion for contribution to toxicity. Those

Figure 6.1.   Approach for Interpretation of Results

DOMESTIC WASTEWATER Appendix VIII

ORGANICS IN NON-TOXIC WWTP SAMPLES Tables 5.6, 5.9

ORGANICS IN TOXIC WWTP SAMPLES Tables 5.5, 5.8

Tables 5.7, 5.10

INDUSTRIAL WASTEWATER Appendices II-VII
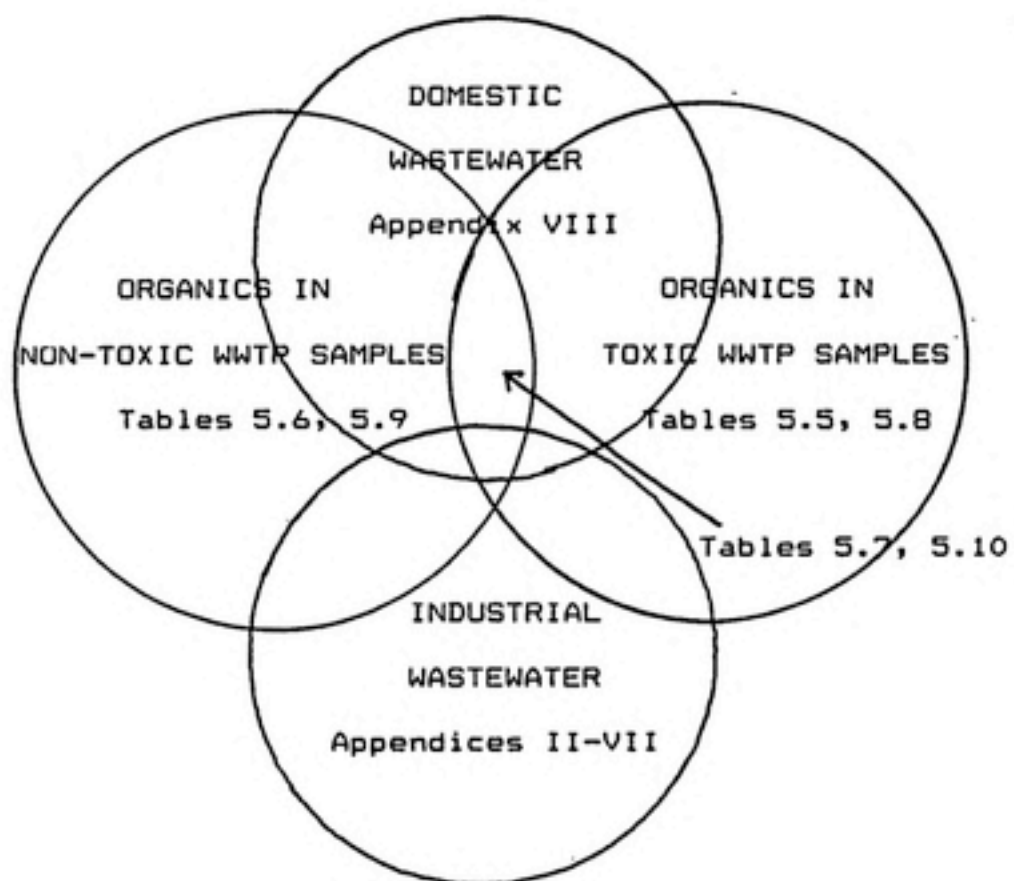
compounds found only in "toxic" samples are most suspect; those found only in "nontoxic" samples are least suspect. Compounds found in both "toxic" and "nontoxic" samples may be in combination with other compounds or in sufficient concentration to contribute to toxicity at some times and not at others. In addition, a greater frequency of occurrence of a compound in a particular category lends more credence to the implication for that compound regarding toxicity of that category.

The approach will indicate if the same compound or group of compounds is usually associated with toxicity. It will best elucidate the situation in which a particular chemical or group of chemicals is acting according to a specific mechanism of toxicity. If toxicity is resulting from a non-specific toxic mechanism, this approach will indicate what compounds occur most frequently, and in conjunction with toxicity, concentration, and treatability information, may be substituted for, disallowed from being discharged to the treatment plant, or treated in a more effective way.

The shaded area in Figure 6.2 depicts the compounds upon which discussion of results will focus, i.e., compounds tentatively identified in "toxic" WWTP samples and in industrial effluents but not in domestic wastewater. A close examination of chemicals of industrial orgin found in "toxic" samples at the Westside plant is warranted for two reasons. First, acute toxicity tests have shown most industrial effluents to be much more toxic than untreated domestic

Figure 6.2. Focus of Discussion of Results

organics in "toxic"
WWTP samples and
industrial but not
domestic
(Tables 6.1 - 6.4)
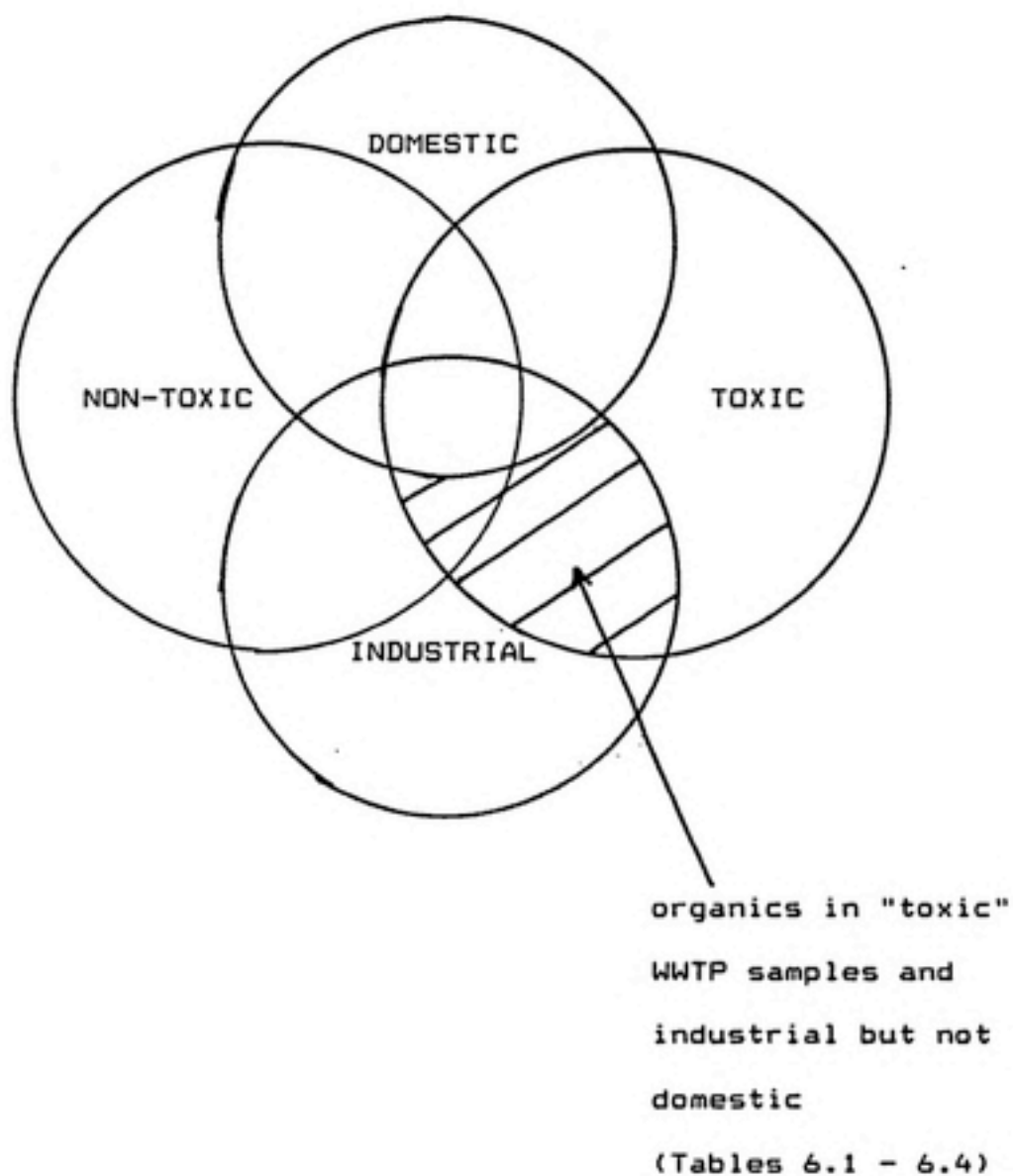
wastewater (LC50 of 80% of industrial effluents are less than 10% while LC50 of untreated domestic wastewater is 90%). Related research has shown mutagenicity of wastewater treatment plant effluent to be primarily of industrial origin (Meier and Bishop, 1985). Secondly, strategies for the control or treatment of compounds found in industrial effluents (in the event they are ultimately identified as toxic agents) can be more easily developed since their source has been identified. While this provides some justification, it in no way allows for drawing firm conclusions about a cause and effect relationship between specific industrial chemicals and toxicity to Daphnia pulex.

Possible Organic Compounds Contributing to Influent Toxicity

Of eight High Point Westside influent samples (including one aeration basin sample), five were "toxic," three "nontoxic." (See Table 4.1.) Table 6.1 lists those compounds that are most suspect of contributing to toxicity, according to the scheme described above.

The compound found with the greatest frequency in "toxic" influents is 1- or 2-methylnaphthalene. The isomers of methylnaphthalene have median lethal concentrations (48 hour LC50) to Daphnia magna of 1.42 mg/L and 1.85 mg/L for the 1- and 2-methyl isomers respectively.

Diphenylether (or 1,1'-oxybisbenzene) has a median lethal toxicity of 4.0 mg/L to fathead minnows over a 96 hour period under flow through test conditions. While not found in the

Table 6.1. COMPOUNDS TENTATIVELY IDENTIFIED ONLY IN TOXIC INFLUENT
AND THEIR INDUSTRIAL SOURCES

COMPOUND	×××FREQUENCY	INDUSTRIAL SOURCE(S)	PROCESS CHEMICAL
1- or 2-methylnaphthalene (early RT)	5	OC	
1,2-benzenedicarboxylic acid, butyl benzyl ester	2		Y
1,8-dimethylnaphthalene	2	OC	
(chloromethyl)benzene	1	OC	Y
benzoic acid, butyl ester	1	OC	Y
butanoic acid	1	DC,PC	
hexadecane	1	OC,TX,MF,DI	
nonadecane	1	OC,TX,DC,MF,DI	
nonylphenol isomer	1	MF,DI	
octadecanoic acid, butyl ester (early RT)	1		Y
pentadecane	1	OC,TX,DC,MF	
propanoic acid	1		Y
tetrachloroethene	1	OC	Y
1,1'-oxybisbenzene	1		Y
1,2 benzenedicarboxylic acid, dimethyl ester	1	OC	Y
1-benzyl-2- or -3-methylazetidine	1	OC	
2,6,10,14-tetramethylpentadecane	1	TX,MF,DI	
2,6,10,14-tetramethylhexadecane	1	TX,MF,DI	
2-(2-methoxyethoxy)ethanol	1		Y
2-ethylhexanoic acid	1	DC,PC	Y
2-methylpropanoic acid?	1	DC	
4-(2,2,3,3- or 1,1,3,3-tetramethylbutyl)phenol	1	MF,PC	
4-hydroxy-4-methyl-2-pentanone (diacetone alcohol)	1	MF,PC	

Aquatic toxicity data available
Aquatic toxicity (LC50) less than 4 mg/L
out of 5 samples

industrial effluents analyzed in this study, diphenylether is on the survey list of process chemicals used by High Point WWTP industrial users.

Toxicity data obtained in laboratory studies from several sources for tetrachloroethylene, a priority pollutant, shows it to have a median lethal toxicity to _Daphnia magna_ of 18 mg/L. In a field study carried out by Lay, et al. (1984), tetrachloroethylene in a pond was found to be toxic to all _Daphnia magna_ individuals in the compartment (about 100 daphnids) after 3 to 4 days of exposure to 0.44 mg/L of the chemical and after 3 hours to 2 days of exposure to 1.2 mg/L. This finding suggests that laboratory studies may have underestimated the toxicity of tetrachloroethylene in the environment.

Of the compounds on this list for which aquatic toxicity information is available (see Appendix I), nonylphenol, with an EC50 for _Daphnia magna_ of 0.18 mg/L and similar toxicities to shrimp and salmon, is the most toxic (McLeese, 1981). The compound p-tert-octylphenol is toxic (96hour LC50) to shrimp at 1.1 mg/L (McLeese, 1981).

Alkylphenols and alkylphenol polyethoxylates have been the subject of extensive study. Nonylphenol and octylphenol isomers are starting materials and metabolites of alkylphenol polyethoxylates, surfactants used primarily in the U.S. by industry and in Europe by both industry and households. Nonylphenol is also a major ingredient in a pesticide formulation. The presence of nonylphenols, nonylphenol

ethoxylates with one and two oxyethylene groups,

(nonylphenoxy)acetic acid, [(nonylphenoxy)ethoxy]acetic acid,

and octylphenol metabolites in sewage treatment plant

effluent, river water, and textile dyeing plant wastewater

has been reported in both Europe and the United States

(Stephanou and Giger, 1982; Ahel, Conrad, and Giger, 1987;

Ahel and Giger, 1985). Metabolites of nonylphenol

polyethoxylates, nonylphenol in particular, are much more

toxic (up to 5 orders of magnitude, depending on the number

of oxythylene groups) than the parent compounds (Stephanou

and Giger, 1982).

Giger, Brunner, and Schaffner (1984) and Ahel and Giger

(1985) reported nonylphenol concentrations (0.89 g/kg; 1.000

g/kg) of up to 2 orders of magnitude higher than usual

concentrations of heavy metals in anaerobically treated

sewage sludge. They found activated sludge to contain

4-nonylphenol concentrations of 0.09 to 0.15 g/kg dry matter

and mono- and diethoxylates in similar concentrations.

Concentrations of 467 ug/L of 4-nonylphenol were found in

effluent from the anaerobic sludge digester (Ahel and Giger,

1985). Digester effluent is normally returned to the

treatment plant (as it is in High Point) and contributes to

nonylphenol levels detected in treatment plant effluent and

in receiving waters.

Alkylphenol carboxylic acids and mono- and diethoxylates

were not identified in this study. However closer examination

of the mass spectra of compounds not identified as yet in

samples from the Westside WWTP and comparison to spectra in Stephanou and Giger (1982) and in Ahel, Conrad, and Giger (1987) is warranted. Nonyl and octylphenols were found in effluents of both the metal finishers and paints and coatings industries in High Point and in the Westside wastewater treatment plant influent. Dinonylphenol ethoxylate, octylphenoxypolyethoxy ethanol, octylphenoxypolyehtoxy ethyl benzyl ether, trioctylphenol ethoxylate, and nonylphenyl ethoxylate are all on the survey of process chemicals used by industries discharging waste to the High Point municipal wastewater treatment facilities. Thus the potential for the presence of alkylphenol and alkylphenol polyethoxylate metabolites in Westside WWTP influent and effluent exists.

An HPLC method developed by Ahel and Giger (1985) exhibits detection specificity of alkylphenols and alkyphenol polyethoxylate metabolites. Their method allows quantitative determination of these compounds in wastewater heavily loaded with other organic materials not possible by the method employed in the study of High Point samples without additional cleaning of extracts. This HPLC method might be employed in future analyses of High Point Westside WWTP samples in order to accurately characterize the presence of alkylphenols and alkylphenol polyethoxylate metabolites in WWTP samples.

It has been shown that biodegradation of alkylphenol polyethoxylates (APEO) is slower than for alcohol polyethoxylates (AEO) (Turner, et al., 1985). In influent

concentrations of up to 30 mg AEO/L, acute toxicity to fathead minnows was eliminated by secondary wastewater treatment. APEO concentration and acute toxicity to fish remained unchanged in laboratory die-away biodegradation tests reviewed by Truner, et al., while AEO acute toxicity disappeared more quickly than would be expected based on residual AEO concentrations. AEOs would thus be less toxic alternatives to APEOs.

Dimethyl and butyl benzyl phthalate, both priority pollutants, are the least toxic of the chemicals discussed thus far. Dimethyl phthalate, found in the organic chemical manufacturing effluent analyzed in this study, has a 48 hour LC50 to D. magna of 33 mg/L; the 48 hour LC50 of butyl benzyl phthalate to D. magna is 92 mg/L. Both chemicals are used in processes by industrial users of High Point's WWTPs. Except for information regarding 4-hydoxy-4-methyl-2-pentanone toxicity (24 hour LC50 greater than 5000 mg/L for goldfish), no aquatic toxicological data could be found for the remaining chemicals in Table 6.1.

In addition to compounds found only in "toxic" samples, compounds found in both "toxic" and "nontoxic" influent samples and in industrial effluents but not in domestic wastewater are suspect of contributing to toxicity. These compounds are listed in Table 6.2. Of particular interest are those compounds which occur more frequently in "toxic" than in "nontoxic" samples; these compounds are denoted by an asterisk.

Table 6.2. COMPOUNDS TENTATIVELY IDENTIFIED IN BOTH TOXIC AND NONTOXIC INFLUENT
AND THEIR INDUSTRIAL SOURCES

COMPOUND	***FREQUENCY TOXIC-NONTOXIC		INDUSTRIAL SOURCE(S)	PROCESS CHEMICAL
a** 1-methylnaphthalene (late RT)	5	1	OC	
a** 1,2,4-trichlorobenzene	5	2	OC	Y
a** naphthalene	5	2	OC,TX,DC	
** 1,1'-biphenyl	5	3	OC	Y
* 2-ethyl-1-hexanol	5	3	OC,TX,MF,PC	Y
a 1-(methoxy-methylethoxy)-2-propanol (early RT)	4	1	b	
a 1-(methoxy-methylethoxy)-2-propanol (late RT)	4	1	b	
a** 1,2,3- or 1,3,5-trichlorobenzene	4	1	OC,DC	Y
a 1-(2-methoxypropoxy)-2-propanol	4	2		Y
a** 1-chloro-2-, 3-, or 4-methylbenzene	4	2	OC,DC	Y
a unknown at RT 31.30, (*RT 24.0, 22.72), MW 203	4	2	OC	
a 1,2- or 1,3-dimethylnaphthalene	3	1	OC	
a* toluene	3	1	OC,DC	Y
a decanoic acid	3	1	DC,DI	
* dimethylbenzene (early RT)	3	2	OC,DC,PC	Y
dodecanoic acid	3	2	TX,DC,DI	Y
** ethylbenzene	2	1	OC,DC	Y
2-isopropylidenedihydrobenzofuran-3-one or 4-methyl-5-phenyl-4-imidazolin-2-one or MW189	2	1	OC	
** dimethylbenzene (late RT)	2	2	OC,DC,PC	Y
dodecane	1	1	DC,MF,DI	
hexahydro-2H-azepin-2-one	1	1	TX	
9,12-octadecedienoic acid	1	1	DC	
N-(4-hydroxyphenyl)acetamide or MW 169	1	1	TX,DC,PC	
unknown at RT 29.86, (*RT 23.4), MW 175	1	1	DC	
heptadecane	1	1	TX,DC,MF,DI	
octadecane	1	1	OC,TX,MF,DI	
hexanoic acid	1	1	DC	
undecane	1	2	DC,DI	
octadecanoic acid, butyl ester (late RT)	1	2		Y

a   Occur more frequently in toxic than nontoxic
*   Aquatic toxicity data available
** Aquatic toxicity (LC50) less than 4 mg/L
*** out of 5 toxic and 3 nontoxic
b   probable contaminants of 1-(2-methoxypropoxy)-2-propanol
*RT Retention Time on column having 1 as opposed to .25 um film thickness

Most of the toxicological data for compounds present in both "toxic" and "nontoxic" influents indicates that all of the compounds for which data is available have median lethal toxicities of 20 mg/L or less to _Daphnia_. Of the compounds that occur more frequently in "toxic" than in "nontoxic" influents, all have 48 hour median lethal toxicities to _Daphnia_ of less than 3 mg/L, except for naphthalene, 3- and 4-chlorotoluene, and toluene; (if LeBlanc's 1980 data which is consistently high when compared to all other sources is not included).

The compound occurring most frequently in "toxic" samples and most infrequently in "nontoxic" samples is 1-methylnaphthalene. Its toxicological data has already been discussed. (48 hour LC50, _D. magna_, = 1.42 mg/L) The trichlorobenzene isomers have median immobilization concentrations to _Daphnia_ of 1.29 - 2.66 mg/L and median lethal concentrations to _Daphnia_ of 1.8 - 2.7 mg/L for the 1,2,3- isomer and 2.1 mg/L for the 1,2,4- isomer. Only the 1,2,4- isomer is a priority pollutant. The 4- and 3-chlorotoluene isomers immobilize 50% of test _Daphnia_ population over a 48 hour time period in concentrations of 3.55 and 6.46 mg/L, respectively.

Toluene, another priority pollutant, has a 48 hour IC50 (immobilization) of 14.9 mg/L and a 48 hour LC50 of 11.5 mg/L for _D. magna_, while 48 hour _D. magna_ LC50 literature values for naphthalene, also a priority pollutant, range from 8.6 to 16.64 mg/L and the 96 hour LC50 for _D. pulex_ is 1 mg/L. The

large decrease in lethal concentrations of naphthalene from 48 to 96 hour exposure is probably due to the bioaccumulation of naphthalene by daphnids. Results of a study of the accumulation and elimination of naphthalene and other polynulcear aromatic hydrocarbons (PAH) by Daphnia pulex indicate that 24 hour accumulation factors in water, in algae, and in medium containing both naphthalene dosed water and algae are 677, 19844, and 2337 respectively (Trucco, et al., 1983). Naphthalene showed the greatest uptake of 5 PAH's evaluated. In addition, naphthalene had the lowest rate of clearance of the 5 PAH's: 17 - 30% cleared after 72 hours compared to 72 - 92% cleared by the other PAHs during the same time period.

No aquatic toxicological data are available for other compounds occurring more frequently in "toxic" than in "nontoxic" influents: dipropylene glycol methyl ether and its isomers; 1,2- or 1,3-dimethylnaphthalene; 3-methyl-butanol benzoate; and decanoic acid.

Compounds occurring equally as frequently or more frequently in "nontoxic" than "toxic" samples for which aquatic toxicity data were found, include 1,1'-biphenyl, ethylbenzene (a priority pollutant), two xylene isomers, and 2-ethyl-1-hexanol. Median immobilization concentrations (48 hour) for D. magna for the xylenes range form 8.6 to 14.3 mg/L. Median lethal concentrations (48 hour) for D. magna range from 3.18 mg/L (o-xylene) to 9.54 mg/1. The 48 hour LC50 of ethylbenzene for D. magna is 2.12 mg/L; that of

biphenyl is 3.08 - 4.7 mg/L. In a static 96 hour test 2-ethylhexanol was found to have a median lethal concentration to bluegill of 10 mg/L. Dimethylbenzene (late RT); hexahydro-2H-azepin-2-one; N,N-dimethylcyclohexanamine; terpineol; and trimethylbenzene were found only in "nontoxic" effluent samples.

Aquatic Toxicological Data for Compounds of Non-Industrial Origin Tentatively Identified in Influent Samples

Aquatic toxicological data are available for several compounds found in both "toxic" and "nontoxic" influents for which industrial sources were not identified or which were identified in domestic wastewater. (See Tables 5.7 and Appendix I.) Two of these compounds, 2-butoxyethanol and 2-methyl-2,4-pentanediol, have toxicities of greater than 1000 mg/L. The trimethylbenzenes have median lethal concentrations to $D.$ $magna$ of 3.6 to 6 mg/L. For phenol, 48 hour LC50s for $D.$ $magna$ range from 12.9 - 23 mg/L, while the no effect level concentration of diisooctyl or dioctylphthalate for $D.$ $magna$ reproduction is 0.32 mg/L.

Toxicological data for benzoic acid, found only in "toxic" influents and in domestic wastewater, is available. The Handbook of Environmental Data on Organic Chemicals gives a value of 255 mg/L for the 48 hour median tolerance limit of benzoic acid for the mosquito fish.

Many isomers of methyl and ethyl substituted benzene were found only in "nontoxic" influent. A toxicological study of

1,2,4,5-tetramethylbenzene found that the 48 hour LC50 for D. magna of this compound is 0.469 mg/L, indicating that appearance in a "nontoxic" sample does not necessarily show that a compound is not a potent toxicant. The 48 hour LC50 of decane to D. magna, also found only in a "non-toxic" sample, is 0.028 mg/L.

Possible Organic Compounds Contributing to Effluent Toxicity

Table 6.3 lists compounds most suspect of contributing to effluent toxicity. These are the compounds found only in "toxic" samples and also found in industrial effluents. Table 4.1 indicates that out of ten samples of effluent from the High Point Westside plant, six were "toxic" and four "nontoxic." Almost all of the compounds found in industrial effluents in Table 6.3 occur in more than one "toxic" sample.

Compounds found only in "toxic" effluents occur with greater frequency than do those found only in "toxic" influents, suggesting that the toxicity of effluents may be less variable than that of influents. However, fewer industrial sources of compounds found in effluent samples have been identified. This is probably because compounds undergo metabolism and degradation during the treatment process. Thus, the search for an industrial source of toxicity by effluent samples is made all the more difficult. Compounds that are in "toxic" effluent samples that appear to be related to ones identified in WWTP influent and industrial effluents include: 1-(2-propenyloxy)-2-propanol;

Table 6.3. COMPOUNDS TENTATIVELY IDENTIFIED ONLY IN TOXIC EFFLUENT
AND THEIR INDUSTRIAL SOURCES

	COMPOUND	**FREQUENCY	INDUSTRIAL SOURCE(S)	PROCESS CHEMICAL
	phosphoric acid, triethyl ester	3	OC	
*	tetrachloroethene	3	OC	Y
*	toluene	3	OC,DC	Y
*	4-hydroxy-4-methyl-2-pentanone	3	MF	
*	benzaldehyde	2	MF	
	1-benzyl-2- or -3-methylazetidine	2	OC	
	2-acetyl-2,8-dihydro-7-methyl-8-methylenepyrazolo[5,1-c]-[1,2,4]triazine	2	OC	
	2-isoxazolidinecarboxylic acid, ethyl ester? or MW 161?	2	PC	
	4-methyl-3-penten-2-one or 2,5-dihydro-2,5-dimethylfuran	2	PC	
	1,3-isobenzofurandione	1	OC,DC,MF	

* Aquatic toxicity data available
** out of 6 samples

3,4-dihydro-5,7- and 6,7-dimethyl-1(2H)-naphthalenone;
1,4-bis(1-methylethenyl)benzene; tetrahydro-2-furanmethanol;
dihydro-5,5-dimethyl-(3H)-furanone isomers; and
1-nitrosopiperidine.

Une of the compounds occurring frequently in "toxic"
effluent samples is triethylphospate, but no aquatic toxicity
data for it was found. However, a related compound,
tri-butylphosphate has a static 96 hour median letal
concentration to fathead minnows of greater than 10 mg/L.
Triethylphosphate is probably less toxic than
tributylphosphate, probably because of its less lipophilic
nature.

Tetrachloroethylene, toluene, and
4-hydroxy-4-methy-2-pentanone were all found in "toxic"
effluent samples with the same frequency as trietylphosphate
The toxicological data pertaining to these compounds have
been discussed. (See Appendix I.) Tetrachloroethylene and
toluene are much more toxic to Daphnia than
4-hydroxy-4-methy-2-pentanone.

Among compounds occurring somewhat less frequently is
benzaldehyde. The Handbook of Environmental Data on Organic
Compounds provides the only aquatic toxicological data found
concerning benzaldehyde: minnows stop eating when exposed to
17.1 mg/L of an 85% solution. The compound 1-benzyl-2- or
3-methylazetidine was also found only in "toxic" influent
samples, although no toxicological data exists for it.

Compounds found in both "toxic" and "nontoxic" Westside

effluents and also in industrial effluents but not in
domestic wastewater are also suspect of contributing to
effluent toxicity. Table 6.4 lists these compounds. Only N-
(4-hydroxyphenyl)acetamide occurred more frequently in
"toxic" than in "nontoxic" samples, however, no aquatic
toxicological data for this compound was found. The only
priority pollutant listed in Table 6.4 is
1,2,4-trichlorobezene. The toxicological literature indicates
that the two trichlorobenzene isomers, chlorotoluene, and
benzylchloride are all toxic to aquatic organisms in
concentrations of 10 mg/L or less.

Even though samples to be bioassayed were collected prior
to chlorination, normal procedure is to dechlorinate the
wastewater sample with sodium thiosulfate prior to initiation
of the toxicity test. Effluent samples collected 3/16/87 and
3/17/87 were not dechlorinated prior to being bioassayed and
contained compounds not present in any other samples and
possibly arising from chlorination reactions. Compounds of
this type include two unknowns suspected of containing
chlorine and bromine, 3-bromocyclohexene, chlorocyclohexene,
(3-chloropropyl)benzene, and fluoromethylbenzene. (See Table
5.8.)

Although not identified in industrial effluents,
3,3,3-trichloropropene; chloroform; dibromochloromethane;
1,4-dioxane; dichlorobenzene; and 5-methyl-2-hexanone were
all present only in "toxic" WWTP effluent samples (see Table
5.8) and are possibly of industrial origin, present as

Table 6.4. COMPOUNDS TENTATIVELY IDENTIFIED IN BOTH TOXIC AND NONTOXIC EFFLUENT
AND THEIR INDUSTRIAL SOURCES

	COMPOUND	xxxFREQUENCY TOXIC-NONTOXIC		INDUSTRIAL SOURCE(S)	PROCESS CHEMICAL
a	N-(4-hydroxyphenyl)acetamide or MW 169?	6	3	TX,DC,PC	
xx	1,2,4-trichlorobenzene	6	4	OC	Y
xx	1,2,3- or 1,3,5-trichlorobenzene (late RT)	4	4	OC,DC	Y
	1-(2-methoxy-1-methylethoxy)-2-propanol (early RT)	4	4		
	1-(2-methoxy-1-methylethoxy)-2-propanol (late RT)	3	3		
	unknown at RT 29.86, 30.21, MW 175 x(RT 23.65, 23.3, 23.42, 23.73, 22.12)	3	4	DC	
	1-(2-methoxypropoxy)-2-propanol	3	4		Y
	2-isopropylidinedihydrobenzofuran-3-one or 4-methyl-5-phenyl-4-imidazolin-2-one or MW 189	2	3	OC	
	unknown at RT 31,30, 31.50,x(Rt 24.02,22.73,22.68) MW 203	2	3	OC	
	unknown at RT 40.14, x(RT 32.7, 32.3, 32.4, 31.03) MW 204 (2,2,5,7-tetrmethyl-1-tetralol?)	2	3	OC	
xx x	1-chloro-2-, 3-, or 4-methylbenzene or (chloromethyl)benzene	1	1	OC	Y
	2-ethyl-1-hexanol	1	1	OC,TX,DC,MF,PC	Y

x   Aquatic toxicity data available
xx   Aquatic toxicity (LC50) less than 4 mg/L
a   Occurs more frequently in toxic than nontoxic
xxx out of 6 toxic and 4 nontoxic samples

contaminants in the drinking water supply, or arise (in some cases) from chlorination reactions. Toxicity data for all these compounds may be found in Appendix I.

Aquatic toxicological studies of benzo[b]naphtho[2,1-d] or [1,2-d]thiophene (BNT), found only in a "toxic" effluent sample, indicate that the 2,1-d isomer is non-toxic, while the 1,2-d isomer has a 48 hour LC50 for D. magna of 0.220mg/L. The structurally similar PAH chrysene is not acutely toxic to Daphnia. In addition, Eastmond, et al. predicted a maximum bioconcentration factor of 8000 for BNT, greater than that of chrysene (5200), and an elimination half life of 23 hours compared to 18 hours for chrysene. Results indicated that daphnids metabolize BNT.

Compounds Escaping Removal

Compounds escaping removal (regardless of whether samples were "toxic" or "nontoxic") at the Westside WWTP have been presented in Table 5.11 and the available aquatic toxicological data for each in Appendix I. Many of these chemicals were also found in the industrial samples from High Point. The fact that some of these compounds, most notably tetrachloroethene, toluene, 2-ethyl-1-hexanol, dimethylbenzene, and the trichlorobenzenes, exhibit considerable toxicity to aquatic organisms is impetus for improving treatment or seeking substitute compounds of lower toxicity and better removal efficiency.

Incomplete removal of some of the compounds listed in

Table 5.11 has been reported in the literature. In a pilot plant study, removal efficiencies of bis(2-ethylhexyl)phthalate and di-n-octylphthalate were found to be 79% and 83%, respectively (Petrasek, et al, 1983). The primary removal mechanism for both these compounds was found to be association with sludge. Incomplete removal of 1,2,4-trichlorobenzene was observed in laboratory studies of activated sludge treatment systems (Weber and Jones, 1986). Losses of the nonbiodegradable compound were attributed to volatilization.

Weber and Jones (1986) found toluene and o-xylene to be biodegraded in the activated sludge process. Because only semi-quantitative results were obtained in the study of High Point Westside samples, it is difficult to determine the effectiveness of treatment of these two compounds.

Toxicity of Complex Mixtures

The implication from the literature involving mixture toxicity studies is that combinations of potent toxicants acting similarly (usually by narcosis) to produce toxicity can produce a toxic effect even at concentrations near or below their no effect levels. In addition combinations of a great number of toxicants that may not be considered potent toxicants may be sufficient to produce acute toxicity to aquatic organisms.

Table 6.5 was prepared assuming that the additive effect of sub-lethal concentration in a mixture could apply to the

Table 6.5. EXAMPLE OF CONCENTRATIONS NECESSARY TO PRODUCE TOXIC
INFLUENT GIVEN CONCENTRATION ADDITION

COMPOUND	LC50 mg/L	FRACTION OF LC50 (1/14) mg/L
1-methylnaphthalene	1.42	.1
nonylphenol	.18	.013
octylphenol	1.1	.08
tetrachloroethene	18	1.28
1,1'-oxybisbenzne	4	.28
biphenyl	3.08	.22
2-ethylhexanol	10	.71
1,3,5-trichlorobenzene	1.43	.1
4-chlorotoluene (chloro-methylbenzene)	3.5	.25
1,2,4-trichlorobenzene	2.1	.15
naphthalene	16.64	1.19
toluene	11.5	.82
ethylbenzene	2.12	.15
2-butoxyethanol	1051	75

chemicals found at the Westdie WWTP. The 14 chemicals in Table 6.5 were chosen because they were all present in at least one influent sample bioassayed as "toxic" and acute toxicity data were available. According to the principle of concentration addition, each chemical present at 1/14 of it LC50 value should produce acute toxicity in the mixture. The resulting concentrations given in Table 6.5 are in the range of those found in Westside WWTP influent samples: 100 ppb to 1 ppm.

Based on the available aquatic toxicological data, p-nonylphenol was the only compound found which may act according to a specific mode of action as pesticides, for instance, usually do. However, because the toxicological database is so small in comparison to the number of chemicals identified in this study, the possibility of the presence of other specifically acting chemicals exists.

7. CONCLUSIONS AND RECOMMENDATIONS

The approach taken in this research was to attempt to relate identification of chemical compounds to toxicity of Westside WWTP samples. At the outset, the definition of toxicity given by the North Carolina regulatory authority depends on the minimal dilution capability of the receiving stream. That is, at the High Point Westside WWTP a sample is "toxic" if it exhibits an LC50 of less than 95% to Daphnia pulex because Rich Fork Creek has a 7Q10 of only 0.3 cfs. This is a very rigid definition of toxicity because 50% of the test organisms must survive with very little dilution (5%) of the wastewater. Given this definition a number of samples (Table 4.1) were classified as being toxic (including both influent and effluent samples).

An extensive database of extractable organic constituents tentatively identified in both "toxic" and "nontoxic" Westside WWTP influent and effluent, industrial wastewater, and domestic wastewater and of available aquatic toxicity data was compiled. Many compounds found in Westside WWTP influent and effluent are of industrial origin as demonstrated by their occurrence in both industrial samples and Westside WWTP samples. Treatment does not remove some organic compounds exhibiting significant toxicity to aquatic organisms and shown to be present in "toxic" effluents and

industrial samples. With the possible exception of nonylphenol isomers, no compound known to act according to a specific mechanism of acute toxicity (such as pesticides normally do) was identified, although because of the sparsity of the aquatic database this conclusion should be regarded with caution. Many compounds known to or thought to act according to the general toxic mechanism of narcosis were tentatively identified. Toxicity of Westside WWTP influent and effluent may be caused by a variety of industrial organic compounds in concentrations that alone would not be sufficient to produce a toxic effect but, because they may all produce toxicity by the same mechanism (narcosis) and thus may exhibit concentration addition, together produce a toxic effect. Metals appear to have had only a minor contribution, if any, to toxicity of most "toxic" effluent samples and some influent samples, while the extent of the contribution to toxicity of other of the influent samples is unknown without further investigation.

The success of the toxicity reduction evaluation program based on identification of specific toxic organic chemicals at the High Point Westside WWTP remains open to question. EPA has developed alternative procedures that rely on broader and simpler screening of causes of toxicity, but eventually may lead to removal of specific chemicals by industrial contributors (U.S. EPA, 1985; Anderson-Carnahan and Mount, 1987). That is not, however, to say the approach used in this research is of no value.

Because the compounds contributing to the toxicity of the Westside WWTP effluent may be different from toxic episode to toxic episode, a system of prioritization could be established based on toxicity to aquatic organisms, persistence in the environment, bioaccumulation, mutagenicity, effectiveness of available treatment or pretreatment methods, and concentration and frequency of occurrence in "toxic" samples. An example of a hazard rating system incorporating some of these parameters is discussed by Calamari, et al. (1983). Using a system of this type, compounds tentatively identified thus far as the most suspect of contributing to toxicity could be targeted for the appropriate treatment or pretreatment action. For example, if the highly toxic nonyl and octylphenol isomers tentatively identified in "toxic" influent and in industrial samples are present as a result of the use of alkyphenol polyethoxylate surfactants as seems to be the case, the more biodegradable and less toxic alcohol polyethoxylate surfactants should be substituted for the isomers currently used by industries discharging waste to the Westside WWTP.

Because the database still has large gaps, a more accurate target list could be generated once the missing information has been gathered. Priority in obtaining additional information should be given to those compounds shown to be escaping removal by the treatment process. (See Table 5.11.) Recommendations for filling in these data gaps include:

1) confirmation of identification of tentative

identifications made in this research by obtaining a spectrum on the mass spectrometer used in this research of a standard for each compound tentatively identified and subsequent comparison of these reference spectra to the spectra of compounds tentatively identified in samples;

2) continued monitoring of compounds identified thus far as being suspect of contributing to toxicity;

3) determination of estimated aquatic toxicities by use of quantitative structure-activity relationships such as those determined by Veith, Hermens, Broderius, Bobra, Schultz, or Calamari; this approach is limited by availability and accuracy of structural descriptors (e.g., octanol/ water partition coefficients or subcooled liquid solubility) used by the models;

4) empirical determination of aquatic toxicities;

5) fractionation of existing sample extracts and subsequent toxicity tests of fractions and identification of compounds in the most toxic fractions;

6) quantitation of target compounds in existing extracts;

7) application of further mass spectral identification techniques (using existing extracts) such as exact mass determination (allowing assignment of possible molecular formula) and chemical ionization techniques (allowing greater chance of molecular ion identification and thus molecular weight determination); and

8) measurement of acute toxicity of wastewater at various points in the treatment process (e.g. primary clarifier

effluent, trickling filter effluent, sludge digester aqueous effluent) to determine the processes responsible for reduction or introduction of toxicants.

REFERENCES

Ahel, M. and W. Giger, "Determination of Alkylphenold and Alkylphenol Mono- and Diethoxylates in Environmental Samples by High-Performance Liquid Chromatography," _Analytical Chemistry_, Vol. 57, No. 8, pp. 1577-1583, July 1985.

Ahel, M., I. Conrad, and W. Giger, "Persistent Organic Chemicals in Sewage Effluents. 3. Determinations of Nonylphenol Carboxylic Acids by High-Resolution Gas Chromatography/Mass Spectrometry and High-Performance Liquid Chromatography," _Environmental Science and Technology_, Vol. 21, No. 7, pp. 697-703, 1987.

Anderson-Carnahan, L. and D. I. Mount, "Methods for Toxicity Reduction Evaluations," U.S. Environmental Protection Agency, draft report, Water Division, Water Quality Branch, Chicago, IL, Jan. 1987.

Bishop, D. F., "GC/MS Methodology for Measuring Priority Organics in Municipal Wastewater Treatment," U.S. Environmental Protection Agency, Municipal Environmental Research Laboratory, Cincinnati, Ohio, EPA-600/S2-80-196, Dec. 1980.

Blackburn, J. W., W. L. Troxler, K. N. Truong, R. P. Zink, S. C. Meckstroth, J. R. Florance, A. Groen, G. S. Sayler, R. W. Beck, R. A. Minear, S. Breen, and O. Yagi, "Project Summary: Organic Chemical Fate Prediction in Activated Sludge Treatment Processes," U.S. Environmental Protection Agency, Water Engineering Research Laboratory, Cincinnati, Ohio, EPA/600/S2-85/102, Nov. 1985.

Blaylock, B. G., M. L. Frank, and J. F. McCarthy, "Comparative Toxicity of Copper and Acridine to Fish, _Daphnia_ and Algae," _Environmental Toxicology and Chemistry_, Vol. 4, pp. 63-71, 1985.

Bobra, A. M., W. Y. Shiu, and D. Mackay, "Acute Toxicity of Fresh and Weathered Crude Oils to _Daphnia magna_," _Chemoshpere_, Vol. 12, No. 9/10, pp. 1137-1149, 1983a.

Bobra, A. M., W. Y. Shiu, and D. Mackay, "A Predictive Correlation for the Acute Toxicity of Hydrocarbons and Chlorinated Hydrocarbons to the Water Flea (_Daphnia magna_)," _Chemosphere_, Vol. 12, No. 9/10, pp. 1121-1129, 1983b.

Bobra, A. M., W. Y. Shiu, and D. Mackay, "Quantitative Structure-Activity Relationships for the Acute Toxicity of Chlorobenzenes to _Daphnia magna_," _Environmental Toxicology and Chemistry_, Vol. 4, pp. 297-305, 1985.

Botts, J. A., E. C. Sullivan, J. W. Braswell, W. L. Goodfellow, Jr., W. L. McCulloch, A. G. McDearmon, D. F. Bishop, "Toxicity Reduction Evaluation at a Municipal Wastewater Treatment Plant," working paper Engineering-Science, Inc., Fairfax, VA., 1987.

Brandes, R., D. Mount, T. Wail, "Effluent Toxicity Assessment and Control for a Publicly Owned Treatment Works Causing Toxic Water Quality Impact," Abstracts of the 59th Annual Conference of the Water Pollution Control Federation, Oct. 1986.

Broderius, S. and M. Kahl, "Acute Toxicity of Organic Chemical Mixtures to the Fathead Minnow," Aquatic Toxicology, Vol. 6, pp. 307-322, 1985.

Brown, D., and R. S. Thompson, "Phthalates and the Aquatic Environment : Part I** The Effect of Di-2-Ethylhexyl Phthalate (DEHP) and Di-Isodecyl Phthalate (DIDP) on the Reproduction of Daphnia magna and Observations on their Bioconcentration." Chemoshpere, Vol. 11, No. 4, pp. 417-426, 1982.

Buckley, J. A., "Complexation of Copper in the Effluent of a Sewage Treatment Plant and an Estimate of its Influence on Toxicity to Coho Salmon," Water Research, Vol. 17, No. 12, pp. 1929-1934, 1983.

Buckley, J. A., G. A. Yoshida, N. R. Wells, and R. T. Aquino, "Toxicities of Total and Chelex-Labile Cadmium to Salmon in Solutions of Natural Water and Diluted Sewage with Potentially Different Cadmium Complexing Capacities," Water Research, Vol. 19, No. 12, pp. 1549-1554, 1985.

Calamari, D., R. Da Gasso, S. Galassi, A. Provini, and M. Vighi, "Biodegradation and Toxicity of Selected Amines on Aquatic Organisms," Chemosphere, Vol. 9, pp. 753-762, 1980.

Calamari, D., R. Da Gasso, F. Setti, and M. Vighi, "Toxicity of Selected Chlorobenzenes on Aquatic Organisms," Chemosphere, Vol. 12, pp. 253-262, 1983.

Call, D. J., L. T. Brooke, M. L. Knuth, S. H. Poirier, and M. D. Hoglund, "Fish Subchronic Toxicity Prediction Model for Industrial Organic Chemicals That Produce Narcosis," Environmental Toxicology and Chemistry, Vol. 4, pp. 335-341, 1985.

Carter, K. B., "Controlling Toxicity: An Integrated Strategy," Journal of the Water Pollution Control Federation, Vol. 58, No. 1, pp. 6-11, Jan. 1986.

Cary, G. A. and M. E. Barrows, "Reduction of Toxicity to Aquatic Organisms by Industrial Wastewater Treatment," U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth, MN, EPA-600/S3-81-043, Aug. 1981.

Cowgill, U. M., I. T. Takahashi, and S. L. Applegath, "A Comparison of the Effect of Four Benchmark Chemicals on Daphnia magna and Ceriodaphnia Dubia-Affinis Tested at Two Different Temperatures," Environmental Toxicology and Chemistry, Vol. 4, pp. 415-422, 1985.

DeGraeve, G. M., D. L. Geiger, J. S. Meyer, and H. L. Bergman, "Acute and Embryo-larval Toxicity of Phenolic Compounds to Aquatic Biota," Archives of Environmental Contamination and Toxicology, Vol. 9, pp. 557-568, 1980.

Dunbar, L. E., "Implementation of a Water Quality-Based Strategy for Protection of Aquatic Life," Journal of the Water Pollution Control Federation, Vol. 59, No. 8, pp. 761-766, August 1987.

Eastmond, D. A., G. M. Booth, and M. L. Lee, "Toxicity, Accumulation, and Elimination of Polycyclic Aromatic Sulfur Heterocycles in Daphnia magna," Archives of Environmental Contamination and Toxicology, Vol. 13, pp. 105-111, 1984.

Flickinger, A. L, "Chronic Toxicity of Mixtures of Copper, Cadmium and Zinc to Daphnia pulex," DA8425424, Dissertation Abstracts International B, Vol. 45, pp. 2466, 1985.

Games, G. M. and R. A. Hites, "Decomposition, Treatment Efficiency, and Environmental Significance of Dye Manufacturing Plant Effluents," Analytical Chemistry, Vol. 49, No. 9, pp. 1433-1440, Aug. 1977.

Giger, W., P. H. Brunner, and C. Schaffner, "4-Nonylphenol in Sewage Sludge: Accumulation of Toxic Metabolites form Nonionic Surfactants," Science, Vol. 225, pp. 623-625, Aug. 1984.

Glaze, W. H., G. R. Peyton, C. F. Young, and C. Lin, "Fate of Naphthalene in a Rotating disc Biological contactor," Journal of the Water Pollution Control Federation, Vol. 58, No. 7, pp. 792-798, July 1986.

Grimes, M. M., "The Impact of EPA's Biomonitoring Policy on POTWs," Journal of the Water Pollution Control Federation, Vol. 59, No. 8, pp. 755-760, August 1987.

Grothe, D. R., and R. A. Kimerle, "Inter- and Intralaboratory Variability in Daphnia magna Effluent Toxicity Test Results," Environmental Toxicology and Chemistry, Vol. 4, pp. 189-192, 1985.

Hermens, J. , E. Broekhuyzen, H. Canton, and R. Wegman, "Quantitative Structure Activity Relationships and Mixture Toxicity Studies of Alcohols and Chlorohydrocarbons: Effects on Growth of Daphnia magna," Aquatic Toxicology, Vol. 6, pp. 209-217, 1985.

Hermens, J., H. Canton, P. Janssen, and R. De Jong, "Quantitative Structure-Activity Relationships and Toxicity Studies of Mixtures of Chemicals with Anaesthetic Potency: Acute Lethal and Sublethal Toxicity to Daphnia Magna," Aquatic Toxicology, Vol. 5, pp. 143-154, 1984a.

Hermens, J., H. Canton, N. Steyger, and R. Wegman, "Joint Effects of a Mixture of 14 Chemical on Mortality and Inhibition of Reproduction of Daphnia magna," Aquatic Toxicology, Vol. 5, pp. 315-322, 1984b.

Hodson, P. V., "A Comparision of the Acute Toxicity of Chemicals to Fish, Rats, and Mice," Journal of Applied Toxicology, Vol. 5, No. 4, pp. 220-226, 1985.

Horning II, W. B., E. L. Robinson, and A. C. Petrasek, Jr., "Reduction in Toxicity of Organic Priority Pollutants by Pilot-Scale Conventional Wastewater Treatment Process," Archives of Environmental Contamination and Toxicology, Vol. 13, pp. 191-196, 1984.

Ingersoll, C. G. and R. W. Winner, "Effect on Daphnia Pulex (De Geer) of Daily Pulse Exposures to Copper or Cadmium," Environmental Toxicology and Chemistry, Vol. I, pp. 321-327, 1982.

Jungclaus, G. A., V. Lopez-Avilla, and R. A. Hites, "Organic Compounds in an Industrial Wastewater: A Case Study of Their Environmental Impact," Environmental Science and Technology, Vol. 12, No. 1, Jan. 1978.

Lay, J. P., W. Schauerte, W. Klein, and F. Korte, "Influence of Tetrachloroethylene on the Biota of Aquatic Systems: Toxicity to Phyto- and Zooplankton Species in Compartments of a Natural Pond," Archives of Environmental Contamination and Toxicology, Vol. 13, pp. 135-142, 1984.

LeBlanc, G. A., "Acute Toxicity of Priority Pollutants to Water Flea (Daphnia magna)," Bulletin of Environmental Contamination and Toxicology, Vol. 24, pp. 684-691, 1980.

Lewis, M. A., "Effects of Loading Density of the Acute Toxicities of Surfactants, Copper, and Phenol to Daphnia magna Straus," Archives of Environmental Contamination and Toxicology, Vol. 12, pp. 51-55, 1983.

Manual of Acute Toxicity: Interpretations and Database for 410 Chemicals and 66 Species of Freshwater Animals, Resource Publication #160, U.S. Department of the Interior, 1986.

McCarthy, J. F., and D. K. Whitmore, "Chronic Toxicity of Di-N-Butyl and Di-N- Octyl Phthalate to Daphnia magna and the Fathead Minnow," Environmental Toxicology and Chemistry, Vol. 4, pp. 167-179, 1985.

McLeese, D. W., V. Zitko, D. B. Sergeant, L. Burridge, and C. D. Metcalfe, "Lethality and Accumulation of Alkylphenols in Aquatic Fauna," Chemosphere, Vol. 10, No. 7, pp. 723-730, 1981.

Meier, J. R. and D. F. Bishop, "Evaluation of Conventional Treatment Processes for Removal of Mutagenic Activity form Municipal Wastewaters," Journal of the Water Pollution Control Federation, Vol. 57, No. 10, pp. 999-1005, Oct. 1985.

Miller, W. E., S. A. Peterson, J. C. Greene, and C. A. Callahan, "Comparative Toxicology of Laboratory Organisms for Assessing Hazardous Waste Sites," Journal of Environmental Quality, Vol. 14, No. 4, pp. 569-574, 1985.

N.C. Division of Environmental Management, "Toxicological Examination of High Point Westside Waste Water Treatment Facility NPDES #NC0024228," Technical Services Unit, Aquatic Toxicology Group, Jan. 1984.

Neal, M. W., L. Mason, D. J. Schwartz, and J. Saxena, "Assessment of Mutagenic Potential of Mixtures of Organic Substances in renovated Water," U.S. Environmental Protection Agency, Washington, D.C., EPA-600/1-81-016, Feb. 1980.

Nebeker, A. L., Carol Savonen, and D. G. Stevens, "Sensitivity of Rainbow Trout Early Life Stages to Nickel Chloride," Environmental Toxicology and Chemistry, Vol. 4, pp. 223-239, 1985.

Peltier, W., and C. I. Weber, "Methods for Measuring the Acute Toxicity of Effluents to Freshwater and Marine Organisms," 3rd. edition, Environmental Monitoring and Support Laboratory, U.S. Environmental Protection Agency, Cincinnati, Ohio, EPA 600/4-85/013, March 1985.

Petrasek, A. C., I. J. Kugelman, B. M. Austern, T. A. Pressley, L. A. Winslow, and R. H. Wise, "Fate of Toxic Organic Compounds in Wastewater Treatment Plants," Journal of the Water Pollution Control Federation, Vol. 55, No. 10, pp. 1286-1296, Oct. 1983.

Rapport, S. M, M. G. Richard, M. C. Hollstein, and R. E. Talcott, "Mutagenic Activity in Organic Wastewater Concentrates," Environmental Science and Technology, Vol. 13, No. 8, pp. 957-961, Aug. 1979.

Richter, J. E., S. F. Peterson, and C. F. Kleiner, "Acute and Chronic Toxicity of Some Chlorinated Benzenes, Chlorinated Ethanes, and Tetrachloroethylene to Daphnia magna," Archives of Environmental Contamination and Toxicology, Vol. 12, pp. 679-684, 1983.

Roop, R. D., and C. T. Hunsaker, "Biomonitoring for Toxics Control in NPDES Permitting," Journal of the Water Pollution Control Federation, Vol. 57, No. 4, pp. 271-277, April 1985.

Saxena, J. and D. J. Schwartz, "Mutagens in Wastewaters Renovated by Advanced Wastewater Treatment," Bulletin of Environmental Contamination and Toxicology, Vol. 22, pp. 319-326, 1979.

Schultz, T. W., and B. A. Moulton, "Structure-Activity Relationships for Nitrogen-Containing Aromatic Molecules," Environmental Toxicology and Chemistry, Vol. 4, pp. 353-359, 1985.

Slooff, W., J. H. Canton, and J. L. M. Hermens, "Comparison of the Susceptibility of 22 Freshwater Species to 15 Chemical Compounds. I. (Sub)acute Toxicity Tests," Aquatic Toxicology, Vol. 4, pp. 113-128, 1983.

Slooff, W., and J. H. Canton, "Comparison of the Susceptibility of 11 Freshwater Species to 8 Chemical Compounds. II. (Semi)chronic Toxicity Tests," Aquatic Toxicology, Vol. 4, pp. 271-282, 1983.

Stephanou, E. and W. Giger, "Persistent Organic Chemicals in Sewage Effluents. 2. Quantitative Determinations of Nonylphenols and Nonylphenol Ethoxylates by Glass Capillary Gas Chromatography," Environmental Science and Technology, Vol. 16, No. 11, pp. 800-805, 1982.

Thurston, R. V, T. A. Gilfoil, E. L. Meyn, T. K. Zajdel, T. I. Aoki, and G. D. Veith, "Comparative Toxicity of Ten Organic Chemicals to Ten Common Aquatic Species," Water Research, Vol. 19, No. 9, pp. 1145-1155, 1985.

Trucco, R. G., F. R. Engelhardt, and B. Stacey, "Toxicity, Accumulation and Clearance of Aromatic Hydrocarbons in Daphnia pulex," Environmental Pollution, Vol. 31, pp. 191-202, 1983.

Turner, A. H., F. S. Abram, V. M. Brown, and H. A. Painter, "The Biodegradability of Two Primary Alcohol Ethoxylate Nonionic Surfactants under Practical Conditions, and the Toxicity of the Biodegradation Products to Rainbow Trout," Water Research, Vol. 19, No. 1, pp. 45-51, 1985.

U.S. Environmental Protection Agency, "Development of Water Quality-Based Permit Limitation for Toxic Pollutants: National Policy," Federal Register, Vol. 49, 1984.

U.S. Environmental Protection Agency, "Technical Support Document for Water Quality-Based Toxics Control," Office of Water, Washington, D.C., EPA-440/4-85-032, Sept. 1985.

U.S. Environmental Protection Agency, "Report to Congress on the Discharge of Harzardous Wastes to Publicly Owned Treatment Works," Office of Water Regulations and Standard, Washington, D.C., EPA/530-SW-86-004, Feb. 1986.

U.S. Environmental Protection Agency, "Water Quality Act of 1987 Implementation; Draft Guidance Availability," Federal Register, Vol. 52, No. 172, September 4, 1987.

Validity of Effluent and Ambient Toxicity Tests for Predicting Biological Impact, Kanawha River, Charleston, WV, edited by D. I. Mount and T. Norberg-King, EPA/600/3-86/006, US EPA, July 1986.

Veith, G. D., D. J. Call, and L. T. Brooke, "Structure-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals," Canadian Journal of Fisheries and Aquatic Science, Vol. 40, pp 743-748, 1983.

Vighi, M. and D. Calamari, "QSARs fo Organotim Compounds on Daphnia magna," Chemosphere, Vol. 14, No. 11/12, pp. 1925-1932, 1985.

Wall, T. M., and R. W. Hanmer, "Biological Testing to Control Toxic Water Pollutants," Journal of the Water Pollution Control Federation, Vol. 59, No. 1, pp. 7-12, Jan. 1987.

Weber, W. J. and B. E. Jones, "Project Summary: Toxic Substance Removal in Activated Sludge and PAC Treatment Systems," U.S. Environmental Protection Agency, Water Engineering Research Laboratory, Cincinnati, Ohio, EPA/600/S2-86/045, June 1986.

Westlake, G. F., J. B. Sprague, and D. W. Rowe, "Sublethal Effects of Treated Liquid Effluent from a Petroleum Refinery. V. Reproduction of Daphnia pulex and Overall Evaluation," Aquatic Toxicology, Vol. 4, pp. 327-339, 1983.

Winner, R. W., "Bioaccumulation and Toxicity of Copper as
Affected by Interactions Between Humic Acid and Water
Hardness," Water Research, Vol. 19, No. 4, pp. 449-455, 1985.

APPENDIX I

AQUATIC TOXICOLOGICAL DATA FOR SELECTED CHEMICALS

2-methyl-1-propanol

flowthrough 96 hour LC50 fathead minnow mg/L	NOEC growth Daphnia magna log umol/L	48 hour LC50 Daphnia magna -log mol/L
1430 a 1430 b	3.77 c	1.824 j

cyclohexanol

flowthrough
96 hour LC50
fathead minnow
mg/L

704 a

2-methoxyethanol

48 hour IC50
immobility
Daphnia magna
log umol/L

5.39 e

2-methyl-2,4-pentanediol

flowthrough 96 hour LC50 fathead minnow mg/L	48 hour LC50 Daphnia magna -log mol/L
10700 a	1.224 j

2-butoxyethanol

48 hour IC50
immobility
Daphnia magna
log umol/L

3.95 e

5-methyl-2-hexanone

flowthrough
96 hour LC50
fathead minnow
mg/L

159 a

4-methyl-2-pentanone

flowthrough 96 hour LC50 fathead minnow mg/L	estimated MATC fathead minnow mg/L
505 a 537 b	77.4 m

2-(2-ethoxyethoxy)ethanol

flowthrough
96 hour LC50
fathead minnow
mg/L

27400 a

p-xylene

48 hour IC50 immobility Daphnia magna umol/L	48 hour LC50 Daphnia magna mmol/m3
1.91 e	80 r

diphenyl ether   (1,1'-oxybisbenzene)

flowthrough 96 hour LC50 fathead minnow mg/L	24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L	NOEC mortality mg/L
4.0 a	1.4 w	0.67 w	0.41 w

o-xylene

48 hour IC50 immobility Daphnia magna log umol/L	48 hour LC50 Daphnia magna mmol/m3
1.91 e	30 r

tetrahydrofuran

flowthrough
96 hour LC50
fathead minnow
mg/L

2160 a

1,2-dichlorobenzene

NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day EC50 reproduction Daphnia magna log umol/L	16 day LC50 Daphnia magna log umol/L
0.60 c	1.41 e	0.51 e	1.01 e

48 hour LC50 Daphnia magna	24 hour IC50 immobility Daphnia magna mg/L	14 day EC50 reproduction Daphnia magna mg/L	14 day EC16 reproduction Daphnia magna mg/L
16 mmol/m3 n <44 mmol/m3 r 2.4 mg/L w	0.78 q	0.55 q	0.37 q

24 hour LC50 Daphnia magna mg/L	NOEC mortality mg/L
2.4 w	0.36 w

105

1,3-dichlorobenzene

flowthrough 96 hour LC50 fathead minnow mg/L	48 hour LC50 Daphnia magna mg/L	EC50 reproduction Daphnia magna mg/L	48 hour IC50 immobility Daphnia magna
7.8 a 9.12 b	1.7 - 5.6 d 7.4 v 28 w	1.4 - 1.8 d	1.51 umol/L e 4.2 mg/L v

MATC fathead minnow log mol/L	28 day LOEC reproduction or growth Daphnia magna mg/L		24 hour LC50 Daphnia magna mg/L
-4.99 l	1.5 v		48 w

NOEC
mortality
Daphnia magna
mg/L

6.0 w

1,2,3-trichlorobenzene

48 hour IC50 immobility Daphnia magna log umol/L	48 hour LC50 Daphnia magna mmol/m3	24 hour IC50 immobility Daphnia magna mg/L	14 day EC50 reproduction Daphnia magna mg/L
0.90 e	10 n 15 r	0.35 q	0.20 q

14 day EC16
reproduction
Daphnia magna
mg/L

0.08 q

1,4-dichlorobenzene

flowthrough 96 hour LC50 fathead minnow mg/L	NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna log umol/L
4.0 a	0.60 c	1.51 e	1.01 e

16 day EC50 reproduction Daphnia magna log umol/L	MATC fathead minnow log mol/L	24 hour IC50 immobility Daphnia magna mg/L	14 day EC50 reproduction Daphnia magna mg/L
0.51 e	-5.29 l	1.6 q	0.93 q

14 day EC16 reproduction Daphnia magna mg/L	24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
0.64 q	42 w	11 w	0.68 w

1,3,5-trichlorobenzene

NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna log umol/L	16 day EC50 reproduction Daphnia magna log umol/L
-0.04 c	0.90 e	0.58 e	0.03 e

1,2,4-trichlorobenzene

flowthrough 96 hour LC50 fathead minnow mg/L	NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna
2.9 a 2.76 b	0.00 c	1.17 e	0.49 log umol/L e 0.56 mg/L e

16 day EC50 reproduction Daphnia magna	16 day NOEC reproduction mg/L	16 day NOEC mortality mg/L	MATC fathead minnow log mol/L
0.17 log umol/L e 0.27 mg/L e	0.10 e	0.32 e	-5.41 l

24 hour IC50 immobility Daphnia magna mg/L	14 day EC50 reproduction Daphnia magna mg/L	14 day EC16 reproduction Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L
1.2 q	0.45 q	0.32 q	2.1 v 50 w

28 day LOEC reproduction or growth Daphnia magna mg/L	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L	
0.69 v	110 w	<2.4 w	

m-xylene

NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna log umol/L	16 day EC50 reproduction Daphnia magna log umol/L
1.02 c	2.13 e	1.29 e	0.83 e

48 hour LC50 Daphnia magna			
90 mmol/m3 r			

tetrachloroethylene

flowthrough 96 hour LC50 fathead minnow mg/L	48 hour IC50 immobility Daphnia magna	16 day LC50 Daphnia magna log umol/L	16 day EC50 reproduction Daphnia magna log umol/L
23.8 b	2.04 log umol/L e 8.5 mg/L v	1.38 e	0.93 e

48 hour LC50 Daphnia magna mg/L	28 day LOEC reproduction or growth Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L	LTO Daphnia magna field study in pond days
18 v 18 w	1.1 v	10 w	1/8 – 2 ∂1.2 mg/L x 3 –4 ∂ 0.44 mg/L x

toluene

NOEC growth Daphnia magna lug umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna log umol/L	16 day EC50 reproduction Daphnia magna log umol/L
1.49 c	2.21 e	1.61 e	1.19 e

static 96 hour LC50 bluegill mg/L	48 hour LC50 Daphnia magna	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
74 – 840 h	125 mmol/m3 r 310 mg/L w	310 w	28 w

phenol

48 hour LC50 Daphnia magna mg/L	EC50 reproduction Daphnia magna mg/L	48 hour LC50 Ceriodaphnia dubia/affinis mg/L	48 hour LC50 Daphnia pulicaria mg/L
23 d 12.9 ∂ 20 dg.C k 12.8 ∂ 24 dg.C k 31.9 mmol/m3 r 12 w	10 d	12.1 ∂ 20 dg.C k (4.3) ∂ 24 dg.C k	>109.0 t

96 hour LC50 fathead minnow mg/L	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L	
67.5 ∂ 14 dg.C t 24.9 ∂ 25 dg.C t	29 w	2.2 w	

3-chlorotoluene

48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna log umol/L	16 day EC50 reproduction Daphnia magna log umol/L	
1.71 e	1.15 e	0.67 e	

4-chlorotoluene

NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	16 day LC50 Daphnia magna	16 day EC50 reproduction Daphnia magna
0.40 c	1.45 e	1.10 log umol/L e 1.6 mg/L e	0.66 log umol/L e 0.58 mg/L e

16 day NOEC reproduction Daphnia magna mg/L	16 day NOEC mortality Daphnia magna mg/L		
0.32 e	1.0 e		

chloroform

NOEC growth Daphnia magna log umol/L	48 hour IC50 immobility Daphnia magna log umol/L	24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L
2.10 c	2.88 e	29 w	29 w

NOEC
mortality
Daphnia magna
mg/L

<7.8 w

o-cresol

48 hour LC50 Daphnia pulicaria mg/L	96 hour LC50 fathead minnow mg/L	48 hour NOLC Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L
>94.0 t	18.2 t	2.9 g	9.5 g

48 hour NOLC Daphnia pulex mg/L	48 hour LC50 Daphnia pulex mg/L
5.2 g	9.6 g

m-cresol

48 hour LC50 Daphnia pulicaria mg/L	96 hour LC50 fathead minnow mg/L
>99.5 t	55.9 t

p-cresol

48 hour LC50 Daphnia pulicaria mg/L	96 hour LC50 fathead minnow mg/L
22.7 t	28.6 t

tri-n-butylphosphate

static
24 hour LC50
fathead minnow
mg/L

>10 h

2-ethylhexanol

static
96 hour LC50
bluegill
mg/L

10 h

ethylbenzene

static 96 hour LC50 bluegill mg/L @ various pH and T	48 hour LC50 Daphnia magna	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
56 - 285 h	20 mmol/m3 r 75 mg/L w	77 w	6.8 w

bis-2-ethylhexyl phthalate

static 96 hour LC50 bluegill mg/L	flowthrough 96 hour LC50 fathead minnow mg/L	48 hour EC50 immobility Daphnia magna mg/L	21 day NOEC reproduction Daphnia magna mg/L
>100 h	>10 h	0.169 - 0.304 p	>0.100 p

24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
>68 w	11 w	1.1 w

2,3,5-trimethylnaphthalene

static
96 hour LC50
fathead minnow
mg/L

6.4 h

2,3,6-trimethylnaphthalene

static
96 hour LC50
fathead minnow
mg/L

>6.7 h

trans-1,2-dichlorocyclohexane

estimated MATC
fathead minnow
mg/L

0.77 l

diethyl phthalate

24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
52 w	52 w	10 w

di-n-butyl phthalate

estimated 48 hour LC50 Daphnia magna mg/L	NOEC reproduction Daphnia magna mg/L	NOEC hatching success fathead minnow mg/L	LC50 fathead minnow mg/L
5.2 m	0.56 m	0.56 m	2.02 m

butyl benzyl phthalate

24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L	NOEC mortality mg/L
>460 w	92 w	<36 w

di-n-octyl phthalate

NOEC reproduction Daphnia magna mg/L	NOEC hatching success fathead minnow mg/L
0.32 m	3.2 m

dimethyl phthalate

24 hour LC50 Daphnia magna mg/L	48 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
150 w	33 w	<1.7 w

morpholine

24 hour IC50 immobility Daphnia magna mg/L
119 o

cyclohexylamine

24 hour IC50
immobility
Daphnia magna
mg/L

58 o

octane

48 hour LC50
Daphnia magna
mmol/m3

3.3 r

decane

48 hour LC50 Daphnia magna	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
0.2 mmol/m3 r 18 mg/L w	23 w	1.3 w

cyclohexane

48 hour LC50
Daphnia magna
mmol/m3

45 r

1,2,4-trimethylbenzene

48 hour LC50
Daphnia magna
mmol/m3

30 r

1,3,5-trimethylbenzene

48 hour LC50
Daphnia magna
mmol/m3

50 r

cumene

48 hour LC50
Daphnia magna
mmol/m3

5 r

1,2,4,5-tetramethylbenzene

48 hour LC50
Daphnia magna
mmol/m3

3.5 r

naphthalene

48 hour LC50 Daphnia magna	96 hour LC50 Daphnia pulex mg/L	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
130 mmol/m3 r 22.6 mg/L u 8.6 mg/L w	1.000 s	17 w	0.60 w

1-methylnaphthalene

48 hour LC50
Daphnia magna
mmol/m3

10 r

2-methylnaphthalene

48 hour LC50
Daphnia magna
mmol/m3

13 r

biphenyl

48hour LC50 Daphnia magna	24 hour LC50 Daphnia magna mg/L	NOEC mortality Daphnia magna mg/L
20 mmol/m3 r 4.7 mg/L w	27 w	<2.2 w

<u>benzo[b]naphtho[2,1-d]thiophene</u>

Daphnia magna

nontoxic u

<u>benzo[b]naphtho[1.2-d]thiophene</u>

48 hour LC50
Daphnia magna
mg/L

0.220 u

<u>phenanthrene</u>

48 hour LC50 Daphnia magna	96 hour LC50 Daphnia pulex mg/L
6.5 mmol/m3 r 0.843 mg/L u	0.100 s

<u>nonylphenol polyethoxylates</u>
(by average # of oxyethylene groups)

	NDEC mortality Daphnia mg/L
30 oxyethylene	>10,000 y
20 "	1000 y
10 "	10 y
7 "	10 y
6 "	5 y
4 "	5 y

<u>nonylphenol</u>

EC50 Daphnia magna mg/L	96 hour LC50 fingerling brook trout mg/L	96 hour LC50 fingerling rainbow trout mg/L
0.18 z	0.145 aa	0.230 aa

p-nonylphenol

96 hour LC50 shrimp mg/L	96 hour LC50 salmon mg/L
0.30 aa (Eastman and Rohm and Haas)	0.19, 0.16 (flowthrough) aa (Eastman) 0.13 (flowthrough) aa (Rohm and Haas)

p-tert-octylphenol

96 hour LC50
shrimp
mg/L

1.1 aa

SOURCES OF AQUATIC TOXICOLOGICAL DATA

n Bobra, Shiu, and Mackay, 1985.
r Bobra, Shiu, and Mackay, 1983b.
b Broderius and Kahl, 1985.
p Brown and Thompson, 1982.
q Calamari, Da Gasso, Setti, and Vighi, 1983.
o Calamari, Da Gasso, Galassi, Provini and Vighi, 1980.
l Call, Brooke, Knuth, Poirier, and Hoglund, 1985.
k Cowgill, Takahashi, and Applegath, 1985.
t DeGraeve, Geiger, Meyer, and Bergman, 1980.
u Eastmond, Booth, and Lee, 1984.
z Giger, Brunner, and Schaffner, 1984.
d Hermens, Canton, Steyger, and Wegman, 1984.
c Hermens, Broekhuyzen, Canton, and Wegman, 1985.
e Hermens, Canton, Janssen, and De Jong, 1984.
x Lay, Schauerte, Klein, and Korte, 1984.
w LeBlanc, 1980.
m McCarthy and Whitmore, 1985.
aa McLeese, Zitko, Sergeant, Burridge, and Metcalfe, 1981.
v Richter, Peterson, and Kleiner, 1983.
g Slooff, Canton, and Hermens, 1983.
y Stephanou and Giger, 1982.
j Thurston, Gilfoil, Meyn, Zujdel, Aoki, and Veith, 1985.
s Trucco, Engelhardt, and Stacey, 1983.
h U.S. Department of the Interior, 1986.
a Veith, Call, and Brooke, 1983.
f Westlake, Sprague, and Rowe, 1983.

APPENDIX II

RT	COMPOUND, PAINTS AND COATINGS, ACID EXTRACT	AMOUNT (SIGNAL/NOISE)
5.15	butanoic acid	8
6.13	unknown	4
6.54	unknown	4
7.28	unknown	2.5
10.8	unknown	4
10.9	2-ethyl-1-hexanol	12
13.8	2-ethylhexanoic acid?	6
15.3	benzoic acid	7
15.4	1- or 2-dodecene	21
20.4	2-isoxazolidinecarboxylic acid, ethyl ester? MW 145?	3
21	N-(4-hydroxyphenyl)acetamide (MW 151) or MW 169?	30
23.8	alkane MW?	4
25.3	octylphenol isomer	30
26.4	nonylphenol isomer?	2
27.1	MW 199? or MW 177? (nonylphenol isomer?)	5
27.3	MW 220? nonylphenol isomer?	13
27.4	nonylphenol isomer	15
27.6	nonylphenol isomer	12
27.6	nonylphenol isomer	5
27.8	nonylphenol isomer	4
28.0	nonylphenol isomer?	4
28.2	nonylphenol isomer	12
28.4	2-methyl-4-(1,1,3,3-tetramethylbutyl)phenol	3
30.2	signal too weak	3
31.8	hexadecanoic acid	15
32.0	similar to RT 30.22, MW 179?	5
32.1	MW 264? similar to RT 30.22	7
32.8	unknown similar to RT 30.22	4
33.0	MW 242?	5
34.0	alkane?	5
35.1	MW 284?	5

	COMPOUND, PAINTS AND COATINGS, BASE/NEUTRAL EXTRACT	
4.11	4-methyl-3-penten-2-one	4
4.84	N-methylacetamide?	4
5.3	4-hydroxy-4-methyl-2-pentanone	28
6.07	xylene (early RT)	4
6.4	1,1'-oxybisbutane	4
6.81	2- or 3-pentanone? and xylene (late RT)	2
7.72	unknown	4
9.49	unknown	2
10.2	signal too weak	2
10.9	2-ethyl-1-hexanol	118
11.1	benzenemethanol	2
11.7	2-methylphenol	2
12.9	methylphenol and MW 124	8
13.4	2-methoxy-N-(2-methoxyethyl)acetamide (MW 147)	102
15.5	MW 128? and MW 116?	13

16.5	unknown	24
16.6	1,3,5,7-tetraazatricyclo[3.3.1.13,7]decane (MW 140)	3
18.2	tridecane and unknown	2
19.6	(S)-3-(1-methyl-2-pyrrolidinyl)pyridine (MW 162)	18
20.6	unknown at RT 24.71, 24.69, MW 161	155
21.2	N-(4-hydroxyphenyl)acetamide? or MW 169?	165
21.3	unknown MW 158 or 9?	28
24.1	unknown MW 161? similar to RT 20.55	12
25.3	octylphenol isomer	48
26.7	unknown MW 167?	9
27.1	nonylphenol isomer	3
27.3	octyl or nonylphenol isomer	16
27.4	nonylphenol isomer	16
27.5	nonylphenol isomer	10
27.6	nonyl or octylphenol isomer	10
27.7	nonylphenol isomer	8
27.8	nonylphenol isomer	6
28.0	nonylphenol isomer and unknown	6
28.2	octylphenol isomer (4-(1,1,3,3-tetramethylbutyl)phenol)	11
28.4	a phthalate?	4
30.2	caffeine?	3
31.7	signal weak	3
32.1	signal weak	6
32.6	MW 221?	3
34.0	heneicosane or 10-methyleicosane	4
35.6	docosane? MW 310?	4
38.9	unknown	4

APPENDIX III

RT	COMPOUND, DIECASTING, ACID EXTRACT	AMOUNT (SIGNAL/NOISE)
4.58	2-methyl-1-propanol or 2-butanol	4
8.10	butanoic acid	9
12.71	MW 99?	8
15.42	2-methyldecane	5
15.63	3-methyldecane?	5
16.22	6-decen-5-one, MW 154	3
16.50	undecane	52
16.73	MW 154? (signal weak)	3
16.99	3,6-dimethyldecane?	3
17.27	decahydro-2-methylnaphthalene (2-methyldecalin)	6
17.29	alkane	2
17.45	1,2,4,5- or 1,2,3,4-tetramethylbenzene or diethylbenzene	2
17.47	MW 149?	2
17.78	MW 152, pulegone?	6
18.25	6-dodecene, MW 168	6
18.68	5-methyl-5-undecene?	12
18.89	3-methyl-3-undecene? or 3-methyl-4-undecene?, MW 168	10
19.17	1-, 5-, or 4-dodecene	104
19.29	1-dodecene or cyclodocecane, MW 168	108
19.35	dodecane, MW 170	80
19.53	5-, 2-, or 4-dodecene	156
19.78	2-, 4-, or 1-dodecene	76
20.69	benzothiazole	10
24.02	decanoic acid	102
25.25	two compounds: MW 156 and MW 185	6
25.88	2,4-, 2,5-, or 2,6-bis(1,1-dimethylethyl)phenol	23
28.23	trimethylnaphthalene or methyl-ethylnaphthalene, MW 170	22
28.38	dodecanoic acid	44
28.92	hexadecane	11
29.71	MW 213?	8
31.01	heptadecane	13
31.12	2,6,10,14-tetramethylpentadecane	10
32.97	octadecane, MW 254	13
33.19	2,6,10,14-tetramethylhexadecane, MW 282	24
34.85	nonadecane, MW 268	18

RT	COMPOUND, DIECASTING, BASE/NEUTRAL EXTRACT
4.10	2- or 3- or 4-methyl-1,3-pentadiene
5.68	2-methyl-2-butenal
6.78	dihydro-2,5-furandione?
7.38	morpholine
9.35	MW 103
10.18	MW 115
10.46	2-(diethylamino)ethanol
10.78	2,4-hexadienal or 3,4-heptadiene
11.19	1-(1,1-dimethylethyl)-3-azetidinol?
12.68	MW 99
13.65	MW 143, spectrum similar to RT 11.19, N,N-dipropyl-1-propanamine?

```
13.86    MW 142
14.47    2- or 5-ethyl-5- or 2-methylpyridine
14.90    MW 137, 2-ethyl-4-pentenal?
16.30    5-methyldecane or 2,6-dimethylnonane
16.33    4-methyl-2-thiazolamine
17.15    4-(1-butenyl)-morpholine? or 2-methyl-4-(1-methylethyl)thiazole?
17.53    1-(1-methylethyl)-3-azetidinol?
17.89    MW 145
17.92    MW 155
18.10    MW 171?
18.40    MW 171, isomer of RT 18.10
18.89    cyclododecane
18.99    MW 168, 1-dodecene?
19.08    MW 170, alkane?
19.24    MW 168, similar spectrum to RT 18.89
19.70    4-(1,3-butadienyl)morpholine
20.28    3,4-dihydro-3,5,8-trimethyl-1(2H)-maphthalenone
20.11    MW 147
20.46    benzothiazole or 1,2-benzisothiazole
23.11    3-(3,3-dimethylbutyl)cyclohexanone?, MW 182
23.39    MW 165?
23.85    MW 201?
24.91    N-methyl-phenyl-urethane or 2-methyl-N,N-dimethylthiobenzamide or
         ethyl-N-methyl-N-phenylcarbamate?
25.52    2,6-bis(1,1dimethylethyl)phenol   (2,6-di-tert-butylphenol)
26.23    MW 207
26.67    MW 207
26.95    MW 206
27.36    signal too weak
27.84    MW 191, isomer of RT 29.31?
28.11    MW 205
29.31    MW 191, 1-hydroxy-2,2-dimethyl-5-phenylpyrrolidine
30.04    unknown
32.70    4-ethyltetradecane?
33.41    MW 215
34.36    nonadecane
34.72    3- or 4-methyldibenzothiophene
36.10    eicosane
36.20    poor spectrum
36.76    MW 212, 4,9-dimethylnaphtho[2,3-b]thiophene
36.93    isomer of RT 36.76
37.39    isomer of RT 36.76
37.56    MW 220, 2-(4-morpholinyl)benzothiazole
37.93    2,3- or 2,5-dimethylphenanthrene
```

APPENDIX IV

RT	COMPOUND, METAL FINISHING, ACID EXTRACT	AMOUNT (SIGNAL/NOISE)
8.57	4-hydroxy-4-methyl-2-pentanone	10
11.74	carbonic acid, dimethyl ester	13
12.83	1,2-dioxepane?	9
13.47	decane	28
13.88	2-(2-ethoxyethyoxy)ethanol	12
14.55	2-ethyl-1-hexanol	21
14.72	3,4-dihydro-2H-pyran?	20
15.67	signal weak	9
16.54	2-methyldecane	52
17.01	3,6-dimethyldecane	7
17.76	MW 154, pentylcyclohexane?	11
17.80	signal weak	
18.34	2,5-dimethylphenol (primary internal standard)	26
19.35	dodecane	60
20.09	siganl weak	38
20.75	benzothiazole	22
22.00	tridecane	68
23.28	1,3-isobenzofurandione, MW 148	68
24.49	tetradecane	74
25.94	4,6-dimethyldodecane?	32
26.83	pentadecane	104
29.03	hexadecane	108
30.02	2,6,10-trimethylpentadecane	34
31.12	heptadecane	118
31.22	2,6,10,14-tetramethylpentadecane	64
33.09	octadecane	66
33.27	2,6,10,14-tetramethylhexadecane	40
34.93	nonadecane	70
36.69	eicosane	44
38.36	2,6,10,15-tetramethylheptadecane or heneicosane	25
39.96	docosane	14
47.48	bis(2-ethylhexyl)phthalate?	12

RT	COMPOUND, METAL FINISHING, BASE/NEUTRAL EXTRACT
4.12	2- or 4-methyl-1,3-pentadiene
7.24	3-hexen-2-one or 2,5-dihydro-2,5-dimethylfuran
8.63	4-hydroxy-4-methyl-2-pentanone
10.47	1,4-dioxan-2-ol?
10.63	2-butoxyethanol
11.61	benzaoldehyde
13.70	2-(2-ethoxyethoxy)ethanol
14.28	N,N-dimethylmethanethioamide?, MW 89
14.39	2-ethyl-1-hexanol
14.55	3,4-dihydro-2H-pyran?
14.83	1,1'-[methylenebis(oxy)]bis-ethane? or isomer of RT 14.95
14.95	bis(1-methyl-2-hydroxyethyl)ether
19.10	1- or 2-(2-butoxyethoxy)ethanol

```
19.90   1,2,3-trimethoxypropane
21.59   unknown
26.06   2-butoxypentane?
26.75   2-[2-(2-methoxyethoxy)ethoxy]ethanol
26.96   unknown
28.11   unknown
28.64   2,5-dimethyltetradecane
31.13   nonylphenol isomer
31.33   octylphenol isomer
31.46   nonylphenol isomer
31.61   4-nonlyphenol or other isomer
31.74   nonylphenol isomer
31.92   nonylphenol isomer
32.15   nonylphenol isomer
32.25   octylphenol isomer, possibly 4-(1,1,3,3-tetramethylbutyl)phenol
32.35   nonylphenol isomer
32.83   signal too weak
46.73   bis(2-ethylhexyl)phthalate
```

APPENDIX V

RT	COMPOUND, DRUM CLEANING, ACID EXTRACT	AMOUNT
4.70	MW 72	7.5
6.17	toluene	6
7.14	hexanal	10
9.05	2-methylpropanoic acid	54
9.33	butanoic acid	31
9.40	2-methyl-2-propanoic acid	18
10.25	nonane	7
11.38	2,6-dimethyloctane?	2
12.28	4-methylnonane, MW 142	5
12.36	alkane, MW 140	4
12.57	3-methylnone, MW 142	5
13.36	2-pentylfuran, MW 138	5
13.49	decane, MW 142	28
14.20	2,6-dimethylnonane	12
14.31	hexanoic acid?, MW 116	18
14.56	2,5,6-trimethyloctane	6
14.70	MW 140, (1-methylpropyl)- or butylcyclohexane and MW 156	7
15.24	5-methyldecane?, MW 156	6
15.34	4-methyldecane	5
15.46	2-methyldecane?	12
15.65	3-methyldecane	12
16.24	6-decen-5-one, MW 154	6
16.52	undecane, MW 156	58
17.31	4-methylundecane, MW 170	9
17.79	signal too weak	6
17.95	2-nitrophenol, MW 139	8
18.06	methylundecane?, MW 170?	8
18.34	2-,3-,or 5-methylundecane, MW 170	12
18.43	2-ethylhexanoic acid, MW 144	24
19.34	dodecane	38
20.25	octanoic acid, MW 144	40
21.00	benzoic acid	128
21.72	MW 158?	14
22.00	nonanoic acid	23
23.13	1,3-isobenzofurandione	148
24.07	decanoic acid	26
24.45	tetradecane, MW 198	7
26.76	pentadecane, MW 212	8
27.76	signal weak	6
28.42	dodecanoic acid, MW 200	138
29.01	MW 168?	42
30.79	MW 210?	10
30.93	MW 152?	18
31.00	heptadecane, MW 240	8
32.45	tetradecanoic acid, MW 228	84
32.97	7,9-dimethylhexadecane?, MW 254	9
34.83	nonadecane, MW 268	6
36.18	hexadecanoic acid, MW 256	152
36.89	1,1',1''-ethylidynetrisbenzne, MW 258	6
39.41	9,12-octadecadienoic acid and 9,17-octadecadienal	220

```
39.76   octadecanoic acid, MW 284                                    115
43.53   1,2,3,4,4a,9.10,10a-octah-(1. , 4 . , 10 . )1-phenantrene-
        carboxylic acid                                               10
47.40   1,2-benzendicarboxylic acid, bis(2-ethylhexyl) ester          10
```

```
RT      COMPOUND, DRUM CLEANING, BASE/NEUTRAL EXTRACT
---------------------------------------------------------------------------
 3.84   1-butanol
 4.07   1-methoxy-2-propanol
 4.93   2-ethoxyethanol
 5.58   4-methyl-2-pentanone
 6.36   methylbenzene  (toluene)
 7.46   cis-1,3- or 1,4-dimethylcyclohexane or 2,2-dimethyl-3-hexene,
        MW 112 and MW 86
 9.27   ethylbenzene
 9.52   xylene  (dimethylbenzene isomer)
10.30   xylene  (dimethylbenzene isomer)
10.12   2-heptanone
10.86   2-butoxyethanol
11.45   propylcyclohexane
12.24   1-chloro-2-methylbenzene
12.60   1-heptanol
13.43   decane
13.86   2-(2-ethoxyethoxy)ethanol
14.14   4-methyldecane
14.63   butylcyclohexane and MW 154
14.79   benzenemethanol
15.25   4- or 5-methyldecane
15.36   4- or 2-methyldecane and MW 154
15.56   3-methyldecane
16.05   unknown
16.27   4-methyl-2-decene?
16.41   3,7-dimethylnonane
17.18   MW 152
17.35   MW 134
17.40   MW 164
17.46   unknown
18.49   1-decanol
19.20   1-(2-methoxyethoxy)butane? and MW 170
19.38   naphthalene
19.69   2- or 3-(1,1-dimethylethyl)thiophene
20.15   1,2,3- or 1,3,5-trichlorobenzene
21.82   MW 150, an alcohol?
21.95   4-(1,1-dimethylethyl)phenol  (p-tertbutylphenol)
22.28   MW 130?
22.38   MW 130? isomer of 22.28?
24.73   N-(4-hydroxyphenyl)acetamide or MW 169?
28.12   dodecanoic acid
29.93   MW 175
31.32   unknown
31.72   MW 175, isomer of RT 29.93?
31.86   1,6-dimethyl-4-(1-methylethyl)naphthalene
32.08   tetradecanoic acid
33.47   isomer of RT 31.86
```

35.76 hexadecanoic acid
39.07 9,12-octadecadienoic acid
43.03 1,2,3,4,4a,9,10,10a-octah-(1 ,4 ,10)-1-phenanthrenecarboxylic
       acid
46.76 bis(2-ethylhexyl) ester of 1,2-benzenedicarboxylic acid

APPENDIX VI

```
RT      COMPOUND, TEXTILE, ACID EXTRACT
--------------------------------------------------------------------------
11.67   2-hydroxypropanoic acid, methyl ester or 1,2-propanediol?
13.91   MW 89
14.93   2-ethyl-4-pentenal
19.61   octanoic acid?
19.89   benzoic acid
22.13   hexahydro-sH-azepin-2-one
27.16   pentadecane
29.35   hexadecane
30.37   6- or 7-propyltridecane
31.43   heptadecane
31.54   2,6,10,14-tetramethylpentadecane
32.68   tetradecanoic acid
33.38   octadecane
33.58   signal too weak
35.25   nonadecane
36.53   hexadecanoic acid
39.71   cyclopentaneundecanoic acid?
39.98   octadecanoic acid


RT      COMPOUND, TEXTILE, BASE/NEUTRAL EXTRACT
--------------------------------------------------------------------------
 7.17   methylguanidine or N,N-dimethylformamide
10.94   2-butoxyethanol
14.80   2-ethyl-1-hexanol
19.78   naphthalene
22.11   hexahydro-2H-azepine-2-one
25.27   N-(4-hydroxyphenyl)acetamide
25.63   1,3dihydro-1,3,3-trimethyl-2H-indol-2-one or 1,3,3-
        trimethoxyindole or 3-methoxy-2,3-dimethyl-3H-indole
26.55   1-dodecanol
26.99   pentadecane
27.16   N,N-dimethyl-1-dodecanamine, MW 213
28.49   dodecanoic acid?
29.18   hexadecane
30.20   2,6,10-trimethyltetradecane?, MW 240
30.66   signal too weak
30.89   1-octadecanol
31.26   heptadecane, MW 240
31.37   2,6,10,14-tetramethylpentadecane
31.54   signal too weak
31.79             "
32.10             "
32.63   tetradecanoic acid
33.21   octadecane
33.42   2,6,10,14-tetramethylhexadecane
35.08   nonadecane
36.37   hexadecanoic acid
36.85   signal too weak
39.61             "
40.74             "
```

APPENDIX VII

RT	ORGANIC CHEMICAL MANUFACTURING, ACID EXTRACT
12.67	1-chloro-2-, 3-, or 4-methylbenzene (chlorotoluene)
14.90	2-ethyl-4-pentenal
16.82	1- or 2- or 4-ethyl-1,2-, 1,3- 1,4-, or 2,4-dimethylbenzene or 1-methyl-2-, 3-, or 4-(1-methylethyl)benzene
17.76	MW 134 or 1,2,4,5-tetramethylbenzene or 1-ethyl-3,5-dimethyl-benzene and MW 116
17.91	1,2,4,5- or 1,2,3,5-tetramethylbenzene or 1-methyl-4-(1-methyl-ethyl)benzene or 1-ethyl-3,5-dimethylbenzene or 2-ethyl-1,4-dimethylbenzene
18.89	2,3-dihydro-4-methyl-1H-indene or (2-methyl-2- or 1-propenyl)-benzene and isomers as in RT 17.91
19.73	benzoic acid and 1,2,4-trichlorobenzene
20.01	naphthalene
20.78	1,2,3- or 1,3,5-trichlorobenzene
22.98	1- or 2-methylnaphthalene
23.46	1- or 2-methylnaphthalene
24.13	1,3-isobenzofurandione
24.84	3-methyltridecane
25.05	1,1'-biphenyl
25.44	1- or 2-ethylnaphthalene
25.72	1,7-, 2,7-, 1,5-, 2,6-, 1,8-, 1,3- 2,3- 1,6-dimethynaphthalene
26.10	1,8, 1,3-, 1,4-, 1,7-, 2,3-, 12,-, 1,5-, 2,7-, or 2,6-dimethyl-naphthalene
26.20	dimethylnaphthalene isomer
26.59	dimethylnaphthalene isomer
26.71	dimethylnaphthalene isomer
27.15	2,6,11-trimethyldodecane
29.03	MW 189?, 2-isopropylidenedihydrobenzofuran-3-one or 4-methyl-5-phenyl-4-imidazolinone
29.34	hexadecane
31.74	MW 203
32.14	benzoic acid, phenyl ester?, MW 198
33.38	octadecane
33.57	signal too weak
35.24	nonadecane
36.46	hexadecanoic acid
37.34	2-acetyl-2,8-dihydro-7-methyl-8methylenepyrazolo[5,1-c][1,2,4]triazine?
39.89	poor spectrum
40.20	"
43.99	"

RT	ORGANIC CHEMICAL MANUFACTURING, BASE/NEUTRAL EXTRACT
5.87	cycloyexane
6.00	pyridine
6.43	toluene
7.75	tetrachloroethene
8.51	MW 112 or 84?
8.95	MW 75?

```
 9.44   ethylbenzene
 9.71   xylene
10.51   xylene
10.76   3-methyl-2-cyclohexen-1-one?
11.28   2-butoxyethanol
11.63   N-butylidene-1-butanamine (MW 127)
12.51   1-chloro-2-, 3-, ro 4-methylbenzene
13.41   unknown
13.61   2,2,5,5-tetramethyl-3-hexene?
14.48   1-chloro-2-, 3-, or 4-methylbenzene or (choromethyl)benzene
15.09   2-ethyl-1-hexanol
15.32   benzenemethanol
15.60   1-methy-2- or 4-propylbenzene or (1-methylpropyl)benzene
15.80   1-ethyl-2,3-, 2,4-, or 3,5-dimethylbenzene or 1-methyl-3- or 4-
        (1-methylethyl)benzene or 4-ethyl-1,2-dimethylbenzene
16.39   isomer as in RT 15.80 or 3-ethenyl-1,2-dimethyl-1,4-cyclohexadiene
16.45   isomers as in Rt 15.80
16.63            "
17.57   1,2,3,5- or 1,2,4,5-tetramethylbenzene or isomers as in RT 15.80
17.70   1,2,3,5- or 1,2,4,5-tetramethylbenzene? or isomers as in RT 16.39
17.95   phosphoric triethyl ester, MW 182
18.67   1-ethenyl-3-ethyl or 1-ethenyl-4-ethylbenznene or (1-methyl-1-
        propenyl)benzene or 2,3-dihydro-2-methyl-aH-indene
19.52   1,2,4-trichlorobenzene
19.80   naphthalene
20.54   trchlorobenzene
22.76   2- or 1-methynaphthalene
23.07   MW 160? and MW 127, hexahydro-4-methyl-2H-azepin-2-one?
23.22   2- or 1-methylnaphthalene
24.83   1,1'-biphenyl, MW 154
25.22   1- or 2-ethylnaphthalene
25.49   1,7-, 1,5-, 2,6-, or 1,6-dimethylnaphthalene
25.80   N-(2-(1-methylethenyl)phenyl)acetamide?
25.98   1-benzyl-2- or 3-methylazetidine
26.41   1,2-benzenedicarboxylic acid, dimethyl ester
26.49   1-dodecanol
26.79   1,2-,1,4-, or 1,8-dimethylnaphthalene
26.95   pentadecane
27.28   3- or 4-methyl-1,1'-biphenyl or 1,1'-methylenebisbenzene?
27.45   MW 207?
27.78   MW 189 or 2-isopropylidenedihydrobenzofurna-3-one or 4-methyl-
        5-phenyl-4-imidazolin-2-one
28.09   [1,1'-biphenyl]-2-ol
28.42   1,4,6-, 1,4,5-, or 2,3,6-trimethylnaphthalene
29.14   hexadecane
30.08   unknown
30.18   N-butylbenzamide
30.87   1-tetradecanol
31.27   MW 203
31.88   bezoic acid, 2-methyl-propyl ester ?, MW 178
32.54   tetradecanoic acid
36.32   hexadecanoic acid
```

37.38   2-acetyl-2,8-dihydro-7-methyl-8-methylenepyrazole[5,1-c][1,2,4]-
        triazine? MW 190
40.29   MW 204?, similar spectrum to RT 37.38

APPENDIX VIII

RT	COMPOUND, DOMESTIC WASTEWATER, ACID EXTRACT	AMOUNT
9.28	acetic acid?	2.5
9.64	signal too weak	
13.1	phenol	2
16.0	4-methylphenol	2
16.6	methyl-2-2propenyldisulfide? MW 120?	2
16.9	1,2,4-trithiolane	3.3
18.2	2,5-dimethylphenol (primary internal standard)	2
18.8	benzoic acid	3
21.2	benzeneacetic acid	12
30.9	1,2,3,5,6-pentathiepane MW 188	3
32.3	tetradecanoic acid	8
34.6	1-hexadecene	19
36.1	hexadecanoic acid	68
37.2	signal too weak	
38.2	3- or 5-octadecene	32
39.2	9-octadecenoic acid MW 282	12
39.5	octadecanoic acid	53
47.4	1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester	4

COMPOUND, DOMESTIC WASTEWATER, BASE/NEUTRAL EXTRACT

RT	
4.09	4-methyl-1,3-pentadiene or cyclohexene?
5.71	dimethyldisulfide
7.46	1,2-ethanedithiol
9.2	unknown
10.2	unknown, MW 115
10.6	2-butoxyethanol
11.0	sulfonylbismethane
11.6	2-cyclohexen-1-one
12.0	MW 109? 2 chlorine present
13.0	phenol
13.7	2-(2-ethoxyethoxy)ehanol
14.1	isocineole MW 154 and dichlorobenzene MW 146
14.4	N,N-dimethylmethanethioamide
14.5	limonene (p-mentha-1,8-diene)
14.7	MW 154? and benzenemethanol
15.9	4-methylphenol
16.8	1,2,4-trithiolane
17.2	benzeneethanol
17.7	m-mentha-1,8-diene
18.0	1-methyl-4-(1-methylethenyl)cyclohexanol
18.6	1,7,7-trimethyl-exo_bicyclo[2.2.1]heptan-2-ol (isoborneol)
18.8	5-methyl-2-(1-methylethyl)cyclohexanol (menthol)
19	1-4-terpineol or p-menth-1-en-4-ol
19.1	1- or 2-(2-butoxyethoxy)ethanol
19.4	o-terpineol
19.5	(-)-cis-caran-trans-3-ol
22.2	1H-indole

23.6	3-(1-methyl-2-pyrrolidinyl)pyridine (nicotine)
26.0	1-dodecanol?
26.5	2,3-dihydro-4-methyl-1H-indole
27.6	[1,1'-biphenyl]-2-ol
28.0	1,2,4,6-tetrathiepane
28.9	1,2-benzenedicarboxylic acid, diethyl ester
30.3	signal too weak
30.6	unknown, MW 188
31.2	signal too weak
32.0	tetradecanoic acid
32.8	signal too weak
33.2	siganl too weak
33.3	signal too weak
33.6	1-(1-cyclohexen-1-yl)-4-methoxybenzene?
34.2	cyclohexadecane
34.4	caffeine
35.7	hexadecanoic acid
37.8	hydrocarbon or long chain alcohol?
38.1	N,N-dimethyl-1-octadecanamine