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OAK RIDGE Y-12 PLANT

LOCKHEED MARTIN

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OZONE/UV TREATMENT TO ENHANCE BIODEGRADATION OF SURFACTANTS IN INDUSTRIAL WASTEWATER

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ABSTRACT

The new owners of a surfactant manufacturing plant wanted to triple production but were limited by the plant's wastewater treatment capacity. Mass balance calculations indicated that little aerobic biodegradation was occurring in the plant's wastewater treatment system. Literature reviews and laboratory tests confirmed that as much as 60% of the plant's products might resist aerobic biodegradation. Overall chemical losses, both solid and aqueous, were estimated at ~3.8% of theoretical. Organic loadings to the wastewater treatment system were ~170 kg/d of which ~50 kg/d reached the biological treatment system. Pollution prevention measures have allowed a >20% increase in production levels with a >30% decrease in effluent volume and no increase in discharge of chemical oxygen demand (COD). A new dissolved air floatation (DAF) system removes ~70% of the organic loading. Sludge volumes are lower by an order of magnitude than with the clarifier/drum-filter process it replaced.

Key factors impacting performance of the wastewater treatment system are solubility and biodegradability. Polyethyloxylates manufactured by the plant are intended specifically to enhance water solubility. The DAF system efficiently removes suspended solids and marginally soluble compounds which are adsorbed on bentonite clay used with the DAF. Water-soluble compounds pass through the DAF and clarifier. If these soluble compounds are to be removed at all, it must be either by biodegradation or by physical/chemical methods of which ozonation and ultrafiltration are two examples.

A 1000 MWCL membrane further reduced the COD by ~30% but was less effective than anticipated in rejecting dissolved surfactants.

Pilot-scale tests showed that ozone/UV treatment significantly increased the bioavailability of five of the six compounds tested. In every case, COD was consumed more rapidly than total organic carbon (TOC) indicating that oxidation of organic substrates took place at faster rates than mineralization to carbon dioxide and water. About 0.5 mg O_3/mg COD was sufficient to increase biological oxygen demand (BOD) to the highest levels achieved. The highest *ratios* of BOD to COD required 1 to 2 g O_3/g COD. Ozone consumption ranged from ~1 g up to ~9 g O_3/g COD and from ~4 g up to ~33 g O_3/g of TOC. Clearly, ozone/UV treatment would benefit waste treatment both by enhancing biodegradability and by direct destruction of COD. A nominal load of 20,000 L/d at 6,000 mg/L as COD (DAF effluent) and an ozone demand of 0.5 mg O_3/mg COD would require ~60 kg/d (132 lb/d) of ozone.

Many of the plant's products are both water soluble and well known to resist biodegradation.These include alkyl phenol ethoxylates (APEs) and derivatives of polypropylene oxide. Biological treatment is highly unlikely to degrade these compounds. The only options are further source reduction or an effective physical/chemical treatment.

Alkyl ethoxylates are entirely different. Alkyl ethoxylates are widely regarded as readily biodegradable. Failure of the plant's treatment system to degrade alkyl ethoxylates is the likely result of three factors acting in concert. First and foremost, required nutrients, mainly nitrogen and phosphorous but also trace elements (iron, zinc, manganese etc) are likely to be absent in the treatment system. Second, microbes capable of degrading alkyl ethoxylates either have been killed by biotoxins or have failed to acclimate. Failure to acclimate often indicates that fluctuations in composition or concentration are too extreme. Third, and less likely, surfactant concentrations may be so high as to damage the microbes.

OBJECTIVES

The intended product of this Department of Energy Defense Programs Small Business Initiative Cooperative Research and Development Agreement (CRADA) was a practical demonstration of advanced oxidation processes (AOPs) which promote aerobic digestion of aqueous wastes containing concentrated surfactants produced for the textile, food, and personal care industries. Surfactants inherently are emulsifiers and difficult to remove from water by physical chemical treatments; some are resistant to microbial digestion; some are biocides. Advanced oxidation alone was not intended or expected completely to destroy the surfactant wastes; rather, the goal was to promote inexpensive aerobic digestion.

ACCOMPLISHMENTS

The host for this technology demonstration was Specialty Industrial Products, Inc. (Spartanburg, SC). Sun River Innovations, Ltd. (Lexington, KY) provided advanced oxidation equipment and technical expertise. Lockheed Martin Energy Systems, Inc.,[1] (Oak Ridge, TN) provided project coordination and technical support. Dr. Craig Adams[2] (Clemson University, Clemson, SC) provided specialized expertise on the effects of advanced oxidation on the biodegradation of organic compounds. Points of contact are listed in Appendix 1.

Pilot-scale tests clearly showed that ozone/UV treatment would benefit waste treatment both by enhancing biodegradability and by direct destruction of COD. Ozone/UV treatment significantly increased the bioavailability of five of six compounds tested. In all cases, COD was consumed more rapidly than TOC, indicating that oxidation proceeded more rapidly than mineralization to carbon dioxide and water. About 0.5 mg O_3/mg COD was sufficient to increase BOD to the highest levels achieved. The highest *ratios* of BOD to COD required 1 to 2 g O_3/g COD. Ozone demand to consume COD and TOC ranged from ~1g up to ~9 g O_3/g COD and from ~4 g up to ~33 g O_3/g of TOC.

These results were reported at the 89th Conference of the Air and Waste Management Association, Nashville, TN, June 23-28, 1996.

BENEFITS TO DOE DEFENSE PROGRAMS

The advanced oxidation technologies demonstrated through this CRADA are directly applicable to the highly varied wastes generated at production facilities and laboratories owned by the United States Department of Energy and the United States Department of Defense. These technologies also are applicable to environmental restoration and waste management efforts to decommission a host of federally owned facilities contaminated by defense wastes. Specifically, these technologies are applicable at the Oak Ridge Y-12 Plant. In concept, advanced oxidation will destroy all organic constituents of mixed, radioactive, and RCRA wastes while raising inorganic constituents to their highest oxidation states so that they can be removed predictably and repeatably by conventional treatment processes.

BENEFITS TO NON-FEDERAL PARTICIPANTS

Implementation of the Clean Water Act of 1990 places surfactant producers and industrial users at significant economic and legal risk.. Wastewater discharge standards will be difficult and expensive to achieve with conventional treatment technologies. The United States annually consumes ~7.5 billion pounds[3,4] of surfactants valued at over $2 billion. Global surfactant consumption is projected to exceed 22 billion pounds/year by 2000. Anionic surfactants, typified by the linear alkyl sulfonates, comprise ~65% of the domestic market. Non-ionic surfactants, typified by the linear alcohol ethoxylates, are ~25% of the market. An estimated 45% of all surfactants are consumed directly in industrial processes while ~55% go into consumer products. The domestic textile industry alone consumes ~1.5 billion pounds of surfactants each year.

Specialty Industrial Products manufactures and formulates surfactant products for the textile, food, and personal care products industries. Major product lines include fatty acid esters derived from sorbitol and linear alkyl alcohol and alkylphenol derivatives of polyoxyethylene (EO) and polyoxypropylene (PO). The Spartanburg plant ships ~36 million lb/year of product of which ~16 million lb/year are synthesized on-site.

Surfactant-bearing wastes are generated both in surfactant manufacture and in industrial and domestic use. Implementation of improved waste treatment technologies would allow Specialty Industrial Products to expand production while meeting discharge standards at reduced cost and liabilities relative to current treatment methods. Availability of effective treatment technologies would allow surfactant users to continue to purchase surfactant products from Specialty Industrial Products.

The CRADA demonstrated expertise and equipment offered for sale by Sun River Innovations in a significant new application. Sun River Innovations will be able to share CRADA results with prospective clients.

Academic participants may use their own results in technical publications, presentations, theses/dissertations, and the classroom and have access to all non-proprietary information resulting from the CRADA.

BACKGROUND

Specialty Industrial Products, as the new owners and managers of a surfactant manufacturing plant in Spartanburg, SC, wanted to triple production but were limited by the plant's wastewater treatment capacity. This project was conceived as a practical evaluation of advanced oxidation processes (AOPs) for enhancing aerobic digestion of concentrated aqueous wastes containing surfactants that normally resist aerobic digestion. AOPs were neither expected or intended to destroy the surfactants completely; rather, partial oxidation was expected to substantially enhance the availability of these compounds for inexpensive aerobic digestion.[5]

AOPs include the use of ozone, hydrogen peroxide, ultraviolet (UV) light, and catalysts - alone or in combination - to oxidize organic materials. Ozone[6,7] is an extraordinarily powerful oxidant that has been used in Europe since about 1905 to treat drinking water and wastewater; ozonation has gained acceptance in the United States only in arid regions and in applications where chlorination is unacceptable. Home swimming pools, large aquaria, and a limited number of water utilities use ozone to supplement or replace chlorination.

Ozone is generated by a corona discharge through dry air or oxygen. Its chemistry in water is strongly influenced by pH.[8] Highly energetic free radical reactions are favored in basic solution whereas somewhat slower and more selective molecular reactions are favored in acidic media.

Like ozone, hydrogen peroxide is a clean, powerful oxidant. Like molecular oxygen, hydrogen peroxide often requires a catalyst or UV light to promote reaction. In principle, ultraviolet light breaks the HO-OH peroxide bond creating two highly reactive hydroxyl radicals. While the liquid form of hydrogen peroxide and its relative stability are functional advantages, performance is limited by the penetrating power of ultraviolet light and the susceptibility of peroxides to disproportionation.

In concept, AOPs can destroy the organic components of waste mixtures while raising inorganic constituents to their highest oxidation states for easy and predictable removal by conventional treatment processes. Complete oxidation is seldom cost effective; rather, the goal was integration of AOPs with pollution prevention and conventional treatment options. Specifically, the goal was to partially oxidize biorecalcitrant surfactant molecules to intermediates that could be more easily treated by traditional aerobic digestion.

This project was the result of a technical assistance request initiated through the Southeast Manufacturing Technology Center (SMTC), Greenville, SC, on behalf of Specialty Industrial Products. The SMTC is a not-for-profit corporation serving South Carolina and other southeastern states. One of the three original Centers sponsored by the National Institute of Standards and Technology (NIST), the SMTC is funded by a combination of federal, state, and private funds through an agreement with the University of South Carolina. Enterprise Development, Inc., of South Carolina, a private not-for-profit firm, is responsible for management of the SMTC.

METHODS AND RESULTS

Characterization of the Wastewater Treatment System

The wastewater treatment system, shown schematically in Figure 1, is based on aerobic digestion. Discharge permits are based on the mass loading of organic wastes measured as COD. Table 1 shows typical wastewater analyses. The DAF system was installed in April, 1995, to remove suspended solids and emulsified organics. The DAF process removes ~70% of the organic loading. Sludge volumes are lower by an order of magnitude than with the clarifier/drum-filter process it replaced. Net organic loadings to the wastewater treatment system are ~170 kg/d of which ~50 kg/d pass through the DAF process to reach the biotreatment system:

Volume = 15,000 L/d
COD (DAF-IN) = 23 g/L
Conversion factor = ~0.5 g compound/g COD
Net organic loading = ~15,000 * 23 * 0.5/1000 = ~172 kg/d
Organic loading to biotreatment system = 0.3 * 172 = ~52 kg/d

Biodegradability Assessments

Mass balance calculations showed that little biodegradation occurred anywhere in the system. Each raw material and product was categorized as to its expected biodegradability. Compounds known or suspected to resist aerobic digestion were ranked according to their probable wastewater loading. Selected compounds were tested for biodegrability at Clemson University.[9] Literature sources and specific laboratory assessments showed that as much as

60% by weight of the plant's probable wastes might resist aerobic biodegradation. Raw material and product lists are shown in Appendices 2 and 3 along with assessments of their aerobic biodegradability.

Pollution Prevention Assessments

Pollution prevention assessments were conducted during site visits in November, 1994. In decreasing order of estimated importance, aqueous wastes were generated by tank/reactor cleaning; hose, pump, and filter cleaning; spills during flaking and drum loading; drum cleaning; and miscellaneous spills.

While procedures adequately assured product quality, available records were not sufficiently detailed to confidently estimate product yields.

Many raw materials inherently are mixtures of variable composition. Coconut oil fatty acids are typically ~50% C12, 15-20% C14, and 5-10% each of C8, C10, C16, and C18. Tallow fatty acids are typically ~66% C18 and 33% C16 with a few percent of C14. EO- and PO-derived polymers typically are complex mixtures of compounds varying in the length of the polymer chain.

Chemical additions were routinely monitored using load cells; however, batch sheets almost always showed the amounts called for by procedure rather than those actually measured. Several load cells were out of service. Reactor volumes were well calibrated to fill-height, but fill-heights were not monitored or recorded. Water removal during esterifications was monitored to assure complete reaction, but amounts were not recorded for the production record. Product yields were not easily tied back to specific batches.

That said, shop-floor logs and observations during site visits allowed product yields for routine esterifications to be estimated at ~97% of theoretical. Based on net shipments of 2,655,546 kg (5.8 million pounds) for January-June, 1994, routine material losses were ~450 kg/day:

Actual Yield = 0.97* Theoretical Yield = 2,655,546 kg product
Theoretical Yield = 2,737,676 kg product
Losses = 82,130 kg = 451 kg/d (based on 182 days for period)

Several known or suspect biotoxins were identified. Giv Gard DXN (6-acetoxy-2,4-dimethyl-m-dioxane or 1,3-dioxan-4-ol 2,6-dimethyl acetate) is a bacteriostat/fungistat added to several formulations. Softener 44 is a quaternary ammonium compound which may be a biotoxin. Several of the Sipamines and Sipophoses may be toxic to microbes.

One major additional waste stream was identified. Esterification of fatty acids with sorbitol typically produces two phases the denser of which is "decanted" away from the desired product and dumped directly to the wastewater treatment system. Net yields for sorbitol esterifications were estimated at 93% of theoretical. If routine yields are 97%, decant losses are about 4%. Based on reported shipments of 572,332 kg of sorbitol-derived ("Sorbac") esters for January - June, 1994, estimated losses as decant were 24,616 kg or ~135 kg/d.

While decant is certainly the largest single source of water-borne waste, much of this material is likely to be removed as suspended solids early in the wastewater treatment process. While some of the Sorbitol esters *per se* were judged to be biorecalcitrant, the decants were not characterized nor was the solubility of any decant determined.

To summarize, routine chemical losses were estimated at 3% of theoretical or ~450 kg/d; losses as decant from sorbitol esterifications were ~4% of theoretical equivalent to ~135 kg/d; overall chemical losses were ~585 kg/d (less than three 55-gallon drums/d) equivalent to ~3.8% of theoretical.

Source Term Reductions

Specialty Industrial Products has worked to quantify and reduce material losses. Batch sheets were revised to collect better mass balance information. Mass flow controllers were installed to improve stoichiometric accuracy. A new warehouse and tank yard reduced spills and improved production efficiency. Several processes were modified to reduce or eliminate wastes; buy-versus-make strategies for several product lines were reassessed. Where consistent with quality requirements, washdown from aqueous blends now is added to product, eliminating washdown as a waste. Discharge of biotoxins has been significantly curtailed. Although production rates still are limited by waste treatment capacity, source reduction measures have allowed a >20% increase in production levels with no net increase in organic loading and a >30% reduction in discharge volume.

Pilot-Scale Ozone/UV Studies.

Pilot-scale ozone/UV studies were conducted in Spartanburg in May and June, 1995. Table 2 shows the experimental matrix. Results are compiled in Table 3.

The tests used an SR-2000 system provided and operated by Sun River Innovations. The ozone generator was fed with pure oxygen bled from a liquid oxygen storage container. Water to be treated was pumped into the SR-2000 at ~50 gpm. An eductor injected ozone along with unreacted oxygen. The mixture was divided and passed in turbulent flow through two sets of 2-in.-diameter stainless steel pipe, each ~70 ft long and convoluted through 24 full 180° turns. The mixture then passed through the UV chamber, where it was exposed to UV light before leaving the SR-2000. The UV chamber was ~3 ft long and 8 in. in diameter with the sample flowing concentric to a single high-intensity lamp (1500 W; 254 nm). The outer wall of the chamber was a reflector that refocused transmitted light into the sample. Power consumption for the SR-2000 was about 12 kW at startup and 6 kW in operation.

The pilot tests first assessed oxidation of specific known compounds in process water. These compounds are identified in Table 2. Measured quantities were placed in a 250-gal polyethylene vessel containing a nominal 100-gal of process water. Circulation through the SR-2000 was initiated with return to the storage container. Sodium hydroxide was added in most runs to make the solutions basic. Foaming caused by rapid recirculation of the solutions was a significant problem. A silicone-based antifoam agent (Scientific Polymers, Inc., SPI-30-M) was added in eight of ten trials. After the system stabilized, the UV light was turned on and power to the ozone generator was turned up. UV light was used in every trial. Measured ozone concentrations in the gas phase (Anseros Ozone Analyzer) were ~55 mg/L at 31 std. L/min (1.1 scfm), equivalent to 103 g O_3/h (5.4 lb/d).

Specialty Industrial Products determined COD using the closed reflux, colorimetric method (Standard Method 508C)[10]. A commercial laboratory determined BOD and TOC. We note that reported values of TOC at time zero were *much* lower than would be expected by either extrapolation of subsequent data points or by calculation based on measured quantities added. We attribute this fact to inadequate mitigation of foaming during instrumental analyses by the commercial laboratory.

Figure 2 shows changes in BOD with the ozone dose normalized against the initial COD. Normalization *compresses* each curve but does not change the fundamental *shape*. Except for Sorbac 80T, BODs generally increased indicating increased availability of the oxidation products for aerobic digestion. The BOD of the Sorbac 80T solution was high initially and fell rapidly as oxidation progressed. Ozone/UV treatment of Sipol LAL-21 and of diluted pond water increased BOD but only marginally. Full-strength DAF effluent (COD ~11,800 mg/L) was far too concentrated to be treated with the available ozone generation capacity; its BOD was essentially unchanged. Figure 2 also shows that ~0.5 mg O_3/mg COD was sufficient to increase BOD to its maximum levels. Further oxidation did not further increase BOD.

Figure 3 shows removal of COD by ozone/UV. Oxidation of Sipoest 1025DT and Sorbac 80T was relatively slow. The substrate was oxidized rapidly in all other single-component trials and in diluted pond water. Complete oxidation required 2 to 4 g O_3/g COD. Figure 4 shows removal of TOC by ozone/UV treatment. Patterns were similar to those observed with COD except that all reactions were somewhat slower and used more ozone.

The BOD/COD ratio is a viable measure of the *relative* biodegradability of an organic mixture. Figure 5 shows how ozone/UV changed the BOD/COD ratios and illustrates three distinct patterns. The BOD/COD ratio of Sorbac 80T (sorbitan monotallate) fell as the ozone dose increased; i.e., BOD was consumed more rapidly than COD. BOD/COD ratios of pond water and of Sipol LAL-21 (polyoxyethylene lauryl ether) were essentially unchanged by ozone/UV. BOD/COD ratios of POE(9) nonylphenol (polyoxyethylene (9) nonylphenol), Sipol L61 (EO/PO copolymer), Seaquat 091 (oleyl imidazoline diethyl sulphate quaternary amine), and Sipoest 1025DT (polyoxypropylene (1025) ditallate) increased progressively with ozone dose until BODs were comparable to CODs. Comparisons with Figures 2 and 3 show that the major effect was progressive consumption of COD rather than progressive growth of BOD. The highest *ratios* of BOD to COD were observed with 1 to 2 g of O_3/g of COD.

Figure 6 shows changes in the TOC/COD ratio with ozone dose. In all cases, COD was consumed faster than TOC. This indicates that oxidation (addition of oxygen) took place at faster rates than mineralization to carbon dioxide and water.

Figures 7 and 8 show plots of ozone consumption vs ozone dose and illustrate changes in the efficiency of the ozone consumption as a function of substrate and extent of reaction.

The pilot tests provided useful but not rigorous kinetic data. Several factors needed for kinetic measurements were not controlled. Ozone generation and the heat of the UV lamp increased solution temperatures by about 20°C in the course of a 3-h run; higher temperatures increase reaction rates but reduce the solubility and stability of ozone in water. Acids produced by oxidation and aeration shifted the pH of the unbuffered solutions by up to 4 pH units. Competitive oxidation of organic by-products would further complicate the kinetics.

Under controlled conditions, oxidation of substrate was expected to show pseudo-first order kinetics. The mechanistic sequence expressed by

$$O_{3\,(gas)} \underset{k_{-1}}{\overset{k_1}{\Longleftrightarrow}} O_{3(liquid)} \qquad (1)$$

$$O_{3(liquid)} + \text{Substrate} \overset{k_2}{\Longrightarrow} \text{Products} \qquad (2)$$

leads to rate laws of the form

$$-\frac{\delta[\text{Substrate}]}{\delta\ \text{Time}} = \frac{k_1\ k_2\ [O_{3(gas)}][\text{Substrate}]}{k_{-1} + k_2\ [\text{Substrate}]} \qquad (3)$$

where k_1, k_{-1}, and k_2 represent rate constants and brackets indicate concentration. Ozone concentrations in the gas phase remained nearly constant (pseudo zero-order). If $k_{-1} > k_2$ [Substrate], disappearance of Substrate will tend toward first order kinetics. Pseudo-first-order rate constants calculated for loss of COD and of TOC are collected in Table 4.

Ultrafiltration (UF)

In June, 1995, with ambient temperatures near 30°C, DAF effluent was passed through a Millipore Minitan laboratory ultrafiltration system. A 0.45 µm membrane had no effect on COD; a "10K MWCL" (10,000 Dalton Molecular Weight Cut-Off Limit) membrane reduced the COD from 11,800 to 5490 mg/L (50%) yielding a clear, colorless permeate. This result suggested that ultrafiltration might be an effective method to remove surfactants from wastewater and reinforced the importance of minimizing contact between suspended solids and fresh water (ie, rain and wash water) in which they might dissolve.

In December, 1995, pilot scale tests were conducted using a 1000 MWCL membrane filter (Osmonics Type SEPA-VF Model 815PT1) in a Sun River Innovations Model 5mUF-8 ultrafiltration system. Nominal pumping rates were 80 gallons/minute with ~10% of the throughput expected to permeate through the membrane as product. The system was fed with DAF effluent. Ambient daytime temperatures were ~10°C; overnight lows reached -7°C.

A 5 µm bag-type prefilter plugged within ~20 minutes; a 25 µm prefilter allowed prolonged operation. In both cases the permeate was clear with a pale yellow color. Feed averaged 14,000 mg/L as COD; retentate averaged 14,900 mg/L as COD. Permeate averaged 9,800 mg/L as COD (a 30% reduction) and 1350 mg/L as BOD.

Lower-than-expected rejection rates were attributed in part to lower-than-expected ambient temperatures which reduced surfactant aggregation and in part to composition of the wastestream at the time of the tests.

Gas Chromatography/Mass Spectroscopy (GC-MS) Characterization

The six compounds and effluent pond water[11] used in the pilot study were characterized by GC-MS. Gas chromatograms are shown as Figures 9 through 15. Mass spectral data are collected as Appendix 4. The compounds were injected as the undiluted liquids; pond effluent was extracted with Freon (1,1,2-trichloro-1,2,2-trifluoroethane) and injected as the extract. The gas chromatograph was a Hewlett Packard HP5890 with a glass capillary column; the mass spectrometer was a Hewlett Packard HP5970. The temperature of the injector was 250°C; column temperature ramped from 80°C to 250°C over 20 minutes; mass spectral data were recorded for mass/charge ratios between 40 and 550.

Gas chromatography showed each sample to be a complex mixture reflecting natural variations both in the fatty acid/fatty alcohol moiety and in the polymer moiety.[12]

Mass spectra of compounds extracted from pond effluent did not allow rigorous identification. Various comparisons of compounds extracted from pond effluent with those of the six available reference compounds were inconclusive.

Comparison of mass spectra found 36 peaks present in Pond Effluent but absent in Sipol L61; only the peak at mass/charge = 68 (6.1% relative intensity) exceeded 1.6% relative intensity. Twenty-three peaks were present in Sipol L61 but absent in Pond Effluent; three had relative intensities greater than 2% (m/e = 100 at 2.4%; m/e = 150 at 2.3%; m/e = 307 at 2.1%). About 254 significant peaks appeared both in Pond Effluent and in Sipol L61; six major peaks showed large differences in relative intensity (m/e = 66, 85, 101, 103, 151, and 153).

Comparison of mass spectra found 65 peaks present in Pond Effluent but absent in POE(9) Nonylphenol; all were small. The nonylphenol showed 117 peaks which were absent in Pond Effluent; only those at m/e = 46 (3.0%) and 65 (5.9%) had relative intensities >2%. About 196 peaks appeared in both Pond Effluent and in the nonylphenol; eight major peaks showed large differences in relative intensity (m/e = 45, 85, 101, 103, 107, 135, 151, and 153).

Comparison of mass spectra found 122 peaks present in Pond Effluent but absent in Sorbac 80T; peaks at m/e = 116, 118, 132, and 155 were significant; all others were small. Sorbac 80T showed 36 peaks which were absent in Pond Effluent; all had relative intensities <2%. About 171 peaks appeared in both Pond Effluent and in Sorbac 80T; nine major peaks showed large differences in relative intensity (m/e = 41, 55, 66, 85, 101, 103, 105, 151, and 153).

Comparison of mass spectra found 90 peaks present in Pond Effluent but absent in Sipol LAL-21; peaks at m/e = 134 (3.0%) and 179 (2.1%) were significant; all others were small. LAL-21 showed 122 peaks which were absent in Pond Effluent; all except m/e = 72 (3.7%) had relative intensities <2%. About 202 peaks appeared in both Pond Effluent and in LAL-21; seventeen major peaks showed large differences in relative intensity (m/e = 41, 43, 45, 55, 56, 57, 66, 67, 70, 71, 83, 98, 101, 103, 111, 151, and 153).

DISCUSSION

The biodegradability of surfactants in general and of nonionic surfactants in particular has been widely studied because of the potential of surfactants to substantially impact the environment. Typical of these studies are those by Kravetz.[13] Both Swisher[14] and Talmage[15] provide extensive compilations of these prior studies. While reported results, even for the same compounds, are *extremely* varied reflecting different conditions, methods, and interests of the investigators, there is near consensus that:

1. Alcohol ethoxylates with predominantly linear alkyl chains exhibit a high degree of

biodegradability under most test procedures. Biodegradation is retarded by a high degree of alkyl chain branching and by secondary alkyl structure [Talmage, p.3; Swisher, p.696]. Within the range generally utilized in detergent formulations, ethoxylate chain length has little effect on the rate or extent of biodegradation. Rates generally decrease slightly with increased chain length; above 20 EO units the rate of degradation is retarded [Talmage, p.20].

2. Linear alkyl ethoxylates degrade by hydrolysis of the ether linkage at the hydrophile-hydrophobe bond followed by oxidation of the alkyl and polyoxyethylene moieties [Talmage, p.35]. Polyoxyethylene chains are more resistant to microbial degradation than the alkyl moiety [Talmage, p.48]. Carbons of the C-chain are consumed much more rapidly than carbons of the polyoxyethylene chain [Swisher, p. 692]. Biodegradation of unsubstituted polyethylene glycols proceeds by stepwise removal of monomer units from the end of the polymer. Generally, biodegradation is facile [Swisher, p. 680].

3. Toxicity increases with an increase in the alkyl chain length, decreases with an increase in the ethoxylate chain length, and decreases with methyl branching of the alkyl chain [Talmage, p.4].

4. Substitution of PO or higher analogs for EO units retards biodegradation. Single and double polypropylene oxide groups are degradable but PO groupings greater than four do not appear to be biodegradable [Naylor[16] as cited by Talmage, p.45][Swisher, pp. 497 and 692].

5. Alkylphenol hydrophobes with either linear or branched alkyl groups markedly retard biodegradation [Swisher, p. 692]. The ultimate biodegradation of alkylphenol ethoxylates, especially with longer EO chains, is slow and uncertain [Swisher, p. 714].

6. Biodegradation of alkyl ethoxylates is much slower under anaerobic conditions than when oxygen is abundant [Talmage, p.50].

7. High surfactant concentrations may inhibit or damage bacteria making them unable to accomplish a degradation which might occur readily at lower concentrations [Swisher, p. 181].

8. Nutrient availability effects microbial ability to degrade organics. Ratios of N:P:COD should be about 5:1:100 although these requirements can be sustained by the sludge itself over extended periods without replenishment. Optimum levels of iron are about 10 ppm [Swisher, p. 272].

9. Many surfactants are biodegradable only after biological acclimation. Acclimation includes adaptive behavior by bioorganisms already present (which can be relatively

food source (which is relatively slow if it occurs at all) [Swisher, p.160].

Kravetz makes the important distinction between primary and ultimate biodegradability. Primary degradation results in loss of surfactant properties such as foaming while ultimate degradation is the conversion to carbon dioxide and water. Primary degradation of alkylethoxylates often is complete within a few days but ultimate degradation (significant loss of COD) may take many days. With alkyl phenol ethoxylates, even primary biodegradation usually is very slow.

The two volumes edited by Schick[17, 18] provide extensive information on the manufacture, physical chemistry, and uses of nonionic surfactants.

CONCLUSIONS and RECOMMENDATIONS

Key issues impacting performance of the wastewater treatment system are solubility and biodegradability. Polyethyloxylates manufactured by Specialty Industrial Products are intended specifically to enhance water solubility. In addition, their very presence is likely to enhance the aqueous solubility of otherwise insoluble coproducts.

The DAF system efficiently removes suspended solids and marginally soluble compounds which are adsorbed on bentonite clay used with the DAF. Removal of emulsifiers and marginally soluble compounds should be enhanced by reducing the volume of water (rain and wash water) they contact.

Water soluble compounds pass through the DAF and clarifier. If these soluble compounds are to be removed at all, it must be either by biodegradation or by a physical/chemical method of which ozonation and ultrafiltration are two examples.

Several products are both water soluble and well known to resist biodegradation.These include alkyl phenol ethoxylates (APEs) and polypropylene derivatives. Biological treatment is highly unlikely to degrade these compounds. The only options are source reduction or an effective physical/chemical treatment.

Alkyl ethoxylates are entirely different. Alkyl ethoxylates are widely regarded as easily biodegradable. Failure of the plant's treatment system to degrade alkyl ethoxylates is the likely result of three factors acting in concert. First and foremost, required nutrients, mainly nitrogen and phosphorous but also trace elements (iron, zinc, manganese etc), are likely to be absent in the treatment system. Second, microbes capable of degrading alkyl ethoxylates have either been killed by biotoxins or have failed to acclimate. Failure to acclimate often indicates that fluctuations in composition or concentration are too extreme. Third, and less likely, surfactant concentrations may be so high as to damage the microbes. Les Grandy at Clemson University or other experts should be able to recommend a nutrient regimen and offer expert advice on the other issues.

Of the limited set of reference compounds available, the compounds extracted from pond effluent appeared most like Sipol LAL-21, polyoxyethylene lauryl ether. The effects of ozone/UV on Pond Effluent and on Sipol LAL-21 were similar and distinctly different form those of the other five compounds tested. Pond Effluent peak shapes in the gas chromatographs were extremely sharp like those of LAL-21. Absent definitive analyses, this assignment is little more than speculation.

SUMMARY

The new owners of a surfactant manufacturing plant wanted to triple production but were limited by the plant's wastewater treatment capacity. Mass balance calculations indicated that little aerobic biodegradation was occurring in the plant's wastewater treatment system. Literature reviews and laboratory tests confirmed that as much as 60% of the plant's products might resist aerobic biodegradation. Overall chemical losses, both solid and aqueous, were estimated at ~3.8% of theoretical. Organic loadings to the wastewater treatment system were ~170 kg/d of which ~50 kg/d reached the biological treatment system. Pollution prevention measures have allowed a >20% increase in production levels with a 30% decrease in effluent volume and no net increase in discharge of COD. A new dissolved air floatation (DAF) system removes ~70% of the organic loading. Sludge volumes are lower by an order of magnitude than with the clarifier/drum-filter process it replaced.

Key issues impacting performance of the wastewater treatment system are solubility and biodegradability. Polyethyloxylates manufactured at the plant are intended specifically to enhance water solubility. The DAF system efficiently removes suspended solids and marginally soluble compounds which are adsorbed on bentonite clay used with the DAF. Water-soluble compounds pass through the DAF and clarifier. If these soluble compounds are to be removed at all, it must be either by biodegradation or by a physical/chemical method of which ozonation and ultrafiltration are two examples.

A 1000 MWCL membrane further reduced the COD by ~30% but was less effective than anticipated in rejecting dissolved surfactants.

Pilot-scale tests showed that ozone/UV treatment significantly increased the bioavailability of five of six compounds tested. In every case, COD was consumed more rapidly than TOC indicating that oxidation of organic substrates took place at faster rates than mineralization to carbon dioxide and water. About 0.5 mg O_3/mg COD was sufficient to increase BOD to the highest levels achieved. The highest *ratios* of BOD to COD required 1 to 2 g O_3/g COD. Ozone use ranged from ~1 g up to ~9 g O_3/g COD and from ~4 g up to ~33 g O_3/g of TOC.

Clearly, ozone/UV treatment would benefit wastewater treatment both by enhancing biodegradability and by direct destruction of COD. A nominal load of 20,000 L/d at 6,000 mg/L as COD (DAF effluent) and an ozone demand of 0.5 mg O_3/mg COD would require ~60 kg/d (132 lb/d) of ozone.

Many plant products are both water soluble and well known to resist biodegradation.These include alkyl phenol ethoxylates (APEs) and derivatives of EO/PO copolymers. Biological treatment is highly unlikely to degrade these compounds. The only options are further source reduction or an effective physical/chemical treatment.

Alkyl ethoxylates are entirely different. Alkyl ethoxylates are widely regarded as readily biodegradable. Failure of the plant's treatment system to degrade alkyl ethoxylates is the likely result of three factors acting in concert. First and foremost, required nutrients, mainly nitrogen and phosphorous but also trace elements (iron, zinc, manganese etc) are likely to be absent in the treatment system. Second, microbes capable of degrading alkyl ethoxylates have either been killed by biotoxins or have failed to acclimate. Failure to acclimate often indicates that fluctuations in composition or concentration are too extreme. Third, and less likely, surfactant concentrations may be so high as to damage the microbes.

INVENTIONS

No inventions were made or reported as a result of this CRADA.

COMMERCIALIZATION POSSIBILITIES

Addition of air to enhance biodegradation is standard industrial practice. Addition of pure oxygen to further accelerate biodegradation is growing as waste treatment operators recognize the tradeoffs between the added cost of oxygen and the cost-savings which can result from higher through-put. Other practitioners have recognized the potential value of ozone for enhancing the biodegradability of recalcitrant compounds; however, practical commercial use is not likely until the unit cost of ozone generation falls substantially.

PLANS FOR FUTURE COLLABORATION

There are no immediate plans for future collaboration.

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2. Dr. Craig D. Adams was a member of the Department of Environmental Systems Engineering. Clemson University, Clemson, South Carolina, at the time of this study. He is currently at the University of Missouri-Rolla, Rolla, Missouri.

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11. The effluent sample was collected on June 15, 1995.

12. Coconut oil fatty acids are typically ~50% C12, 15-20% C14, and 5-10% each of C8, C10, C16, and C18. Much of the C18 is usually unsaturated. Tallow fatty acids are typically ~66% C18 and 33% C16 with a few percent of C14. About 2/3 of the C18 is unsaturated, mainly oleic. Ethylene oxide- and propylene oxide-derived polymers typically are complex mixtures of compounds varying in the length of the polymer chain.

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Table 1. Typical wastewater analyses.

At start of project (10/94)

	COD	O&G	BOD	TSS
Aeration basin	20,450	317	8,100	1,540
Clarifier effluent	8,500	137		772
Pond effluent	8,200	105		733
Floc tank effluent	3,600	130		8

Effluent volume 23,000 L/d (before treatment)

After installation of the DAF system (5/95)

	COD	O&G	BOD	TSS
DAF-in	22,820	780	6,690	3,840
DAF-out	6,960	47	747	86
Pond effluent	10,840			
Floc tank effluent	5,820			

Effluent volume 15,000 L/d (before treatment)

where COD = chemical oxygen demand (mg/L)
O&G = oil and grease (mg/L)
BOD = biological oxygen demand (mg/L)
TSS = total suspended solids (mg/L)
DAF = dissolved air flotation

Table 2. Experimental matrix for pilot-scale ozone/UV tests.

Component	Initial concentration COD (mg/L)	Initial concentration Substrate (mg/L)	Initial pH	Antifoam	Peroxide
Sipoest 1025DT	110	105	10.2	No	No
Sorbac 80T	120	108	10.3	Yes	No
Seaquat 091	240	115	5.6	Yes	No
POE(9) nonylphenol	220	98	5.6	Yes	No
Sipol L61	350	109	10.2	No	No
Sipol LAL-21	360	137	9.9	Yes	No
Pond effluent 1	320	-	9.8	Yes	No
Pond effluent 2	280	-	10.8	Yes	Yes
DAF effluent 1	12000	-	10.3	Yes	No
DAF effluent 2	11670	-	10.2	Yes	Yes

Single-component compounds were as follows

- Sipoest 1025DT (CAS Registry No. 68648-12-4)
  Chemical name: Polyoxypropylene (1025) ditallate

- Sorbac 80T (CAS Registry No. 61791-48-8)
  Chemical name: Sorbitan monotallate

- Seaquat 091 (CAS Registry No. 68954-59-6)
  Chemical name: Oleyl imidazoline diethyl sulphate quaternary amine

- POE(9) nonylphenol (CAS Registry No. 9016-45-0)
  Chemical name: Polyethyleneoxide (9) nonylphenol

- Sipol L61 (CAS Registry No. 9003-11-0)
  Chemical name: Polyoxyethylene - polyoxypropylene - polyoxyethylene copolymer

- Sipol LAL-21 (CAS Registry No. 9002-92-0)
  Chemical name: Polyoxyethylene lauryl ether

Table 3. Results of pilot-scale ozone/UV studies.

Sample ID	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
Tap water	6.0	10	18	3.7

Sipoest 1025DT (CAS 68648-12-4)
Polypropylene oxide (1025) ditallate
Add 39.8 g to 100 gal of tap water (105 mg/L)
Add 48 ml of 50% NaOH

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
1025-1	0	30.6	n/a	1.1	10.2	110	38	14
1025-2	1260	35.6	n/a	1.1	9.2	100	3	31
1025-3	3600	43.3	n/a	1.1	6.3	80	48	37
1025-4	9180	53.9	n/a	1.1	7.0	30	14	12

Sorbac 80T (CAS 61791-48-8)
Sorbitan monotallate (Batch 502-8330)
Add 40.9 g to 100 gal of tap water (108 mg/L)
Add 70 ml 50% NaOH
Add 8 ml SPI-30-M silicone-based antifoam (Scientific Polymers Inc.)

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
SB80T-1	0	27.2	n/a	1.1	10.3	120	133	10
SB80T-2	1440	33.3	n/a	1.1	9.5	170	102	42
SB80T-3	3720	41.1	n/a	1.1	6.9	90	51	38
SB80T-4	8880	48.9	n/a	1.1	7.3	50	5	7

Seaquat 091 (Lot CS-6403; CAS 68954-59-6)
Des quat oleic imidazoline, quaternary ammonium salt
Add 43.5 g to 100 gal of tap water (115 mg/L)
Add 10 ml SPI-30-M silicone-based antifoam (Scientific Polymers, Inc.)

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
SQ91-1	0	29.4	n/a	1.1	5.6	240	<2	57
SQ91-2	1320	35.6	n/a	1.1	4.1	230	50	62
SQ91-3	3780	40.6	n/a	1.1	3.3	130	52	56
SQ91-4	8220	50.0	n/a	1.1	3.4	90	43	33

POE(9) nonylphenol (CAS 9016-45-9; Batch 504-8598)

Add 37.2 g to a nominal 100 gal of tap water (98 mg/L)

Add 7 ml SPI-30-M silicone-based antifoam (Scientific Polymers Inc.)

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
NP95-1	0	27.8	60	1.1	5.6	220	26	56
NP95-2	1260	33.3	60	1.1	4.6	150	67	61
NP95-3	3660	40.6	54	1.1	3.4	70	76	48
NP95-4	9480	49.4	50	1.1	5.2	10	8	7

EOPO block polymer (CAS 9003-11-0)

Sipol L61 (Batch 412-8128)

Add 41.1 g to a nominal 100 gal of tap water (109 mg/L)

Add 20 ml 50% NaOH

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
EOPO-1	0	28.9	n/a	1.1	10.2	350	10	59
EOPO-2	1320	33.3	55	1.1	8.8	330	60	60
EOPO-3	6060	47.8	58	1.1	6.8	120	60	38
EOPO-4	10620	52.2	49	1.1	7.2	10	12	9

Sipol LAL-21 (Batch 408-7701)

Poly(oxyethylene) lauryl ether (CAS 9002-92-0)

Add 51.7 g to 100 gal of tap water (137 mg/L)

Add 9 ml SPI-30-M silicone-based antifoam (Scientific Polymers, Inc.)

Add 40 g solid NaOH pellets

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
LAL21-1	0	27.2	n/a	1.1	9.9	360	16	42
LAL21-2	1140	32.2	n/a	1.1	9.1	470	24	61
LAL21-3	3480	38.3	n/a	1.1	6.8	230	23	56
LAL21-4	7020	46.7	n/a	1.1	6.6	190	17	46

7 gal of pond effluent from floc tank

Dilute to 100 gal with tap water

Add 20 g NaOH pellets

Add 20 ml SPI-30-M silicone-based antifoam (Scientific Polymers, Inc.)

Sample ID	**Elapsed** Time (s)	**Temp** (°C)	**Ozone** (g/m^3)	**Oxygen** (scfm)	**pH**	**COD** (mg/L)	**BOD** (mg/L)	**TOC** (mg/L)
Pond1-1	0	30.0	n/a	1.1	9.8	320	<2	74
Pond1-2	900	32.2	n/a	1.1	9.1	360	16	74
Pond1-3	2700	38.3	n/a	1.1	7.0	270	16	63
Pond1-4	5400	44.4	n/a	1.1	6.7	180	18	46

125 gal DAF effluent

Add 50 g solid NaOH and 300 mL 50% NaOH

Add 75 ml SPI-30-M silicone-based antifoam (Scientific Polymers, Inc.)

Sample ID	**Elapsed** Time (s)	**Temp** (°C)	**Ozone** (g/m^3)	**Oxygen** (scfm)	**pH**	**COD** (mg/L)	**BOD** (mg/L)	**TOC** (mg/L)
DAF1-1	0	30.6	n/a	1.1	10.3	12000	704	3310
DAF1-2	4440	42.8	n/a	1.1	8.9	11930	n/a	n/a
DAF1-3	7800	48.9	n/a	1.1	8.2	11320	693	3120

100 gal of DAF effluent

Add 350 ml 50% NaOH

Add 100 ml SPI-30-M silicone-based antifoam (Scientific Polymers, Inc.)

Meter 6 ml/min of 35% hydrogen peroxide into container.

Sample ID	**Elapsed** Time (s)	**Temp** (°C)	**Ozone** (g/m^3)	**Oxygen** (scfm)	**pH**	**COD** (mg/L)	**BOD** (mg/L)	**TOC** (mg/L)
DAF2-1	0	31.1	n/a	1.1	10.2	11670	845	3160
DAF2-2	2100	38.9	n/a	1.0	9.5	11540	715	2980
DAF2-3	5580	46.7	n/a	1.1	8.5	10470	716	2760
DAF2-4	7500	48.9	n/a	1.1	7.8	10300	700	3000

8 gal of pond effluent from discharge basin

Dilute to about 100 gal with tap water

Add 200 ml 50% NaOH

Add 20 ml SPI-30-M silicone-based antifoam (Scientific Polymers, Inc.)

Meter 6 ml/min of 35% hydrogen peroxide into tote.

Sample ID	Elapsed Time (s)	Temp (°C)	Ozone (g/m^3)	Oxygen (scfm)	pH	COD (mg/L)	BOD (mg/L)	TOC (mg/L)
Pond2-1	0	30.0	n/a	1.1	10.8	140	<2	64
Pond2-2	1320	32.2	n/a	1.1	10.7	260	<2	70
Pond2-3	3420	38.3	n/a	1.1	10.4	240	<2	68
Pond2-4	7140	48.3	n/a	1.1	9.8	250	<2	68

Table 4. Pseudo first-order rate constants.

Fitting data to: $COD = COD_o * \exp(-k*t)$

O_3/COD	COD_o	$-10^4 * k$	(g O_3/g O_2)	r
Sipoest 1025DT	119	1.45	4.4	0.989
Sorbac 80T	124	1.00	6.2	0.995 (delete point 2)
Seaquat 091	243	1.27	2.5	0.972
POE(9) nonylphenol	225	3.27	1.0	1.000
Sipol L61	481	3.31	0.5	0.962
Sipol LAL-21	344	0.91	2.4	0.973 (delete point 2)
Pond effluent 1	412	1.54	1.2	1.000 (delete point 1)
DAF-1	12094	0.07	31	0.872
DAF-2	11783	0.19	12	0.974

Fitting data to: $TOC = TOC_o * \exp(-k*t)$

O_3/TOC	TOC_o	$-10^4 * k$	(g O_3 /g C)	r
Sipoest 1025DT	45.0	1.35	12	0.905 (delete point 1)
Sorbac 80T	74.0	2.56	4.1	0.968 (delete point 1)
Seaquat 091	74.0	0.95	11	0.979 (delete point 1)
POE(9) nonylphenol	102.9	2.76	2.7	0.983 (delete point 1)
Sipol L61	72.7	1.74	6.1	0.943
Sipol LAL-21	65.2	0.49	24	0.994 (delete point 1)
Pond effluent 1	77.7	0.92	11	0.981

where
COD = chemical oxygen demand (mg/L)
TOC = total organic carbon (mg/L)
k = pseudo first-order rate constant (s^{-1})
t = elapsed time (s)
O_3/COD = ozone demand for consumption of first one-half of COD
O_3/TOC = ozone demand for consumption of first one-half of TOC

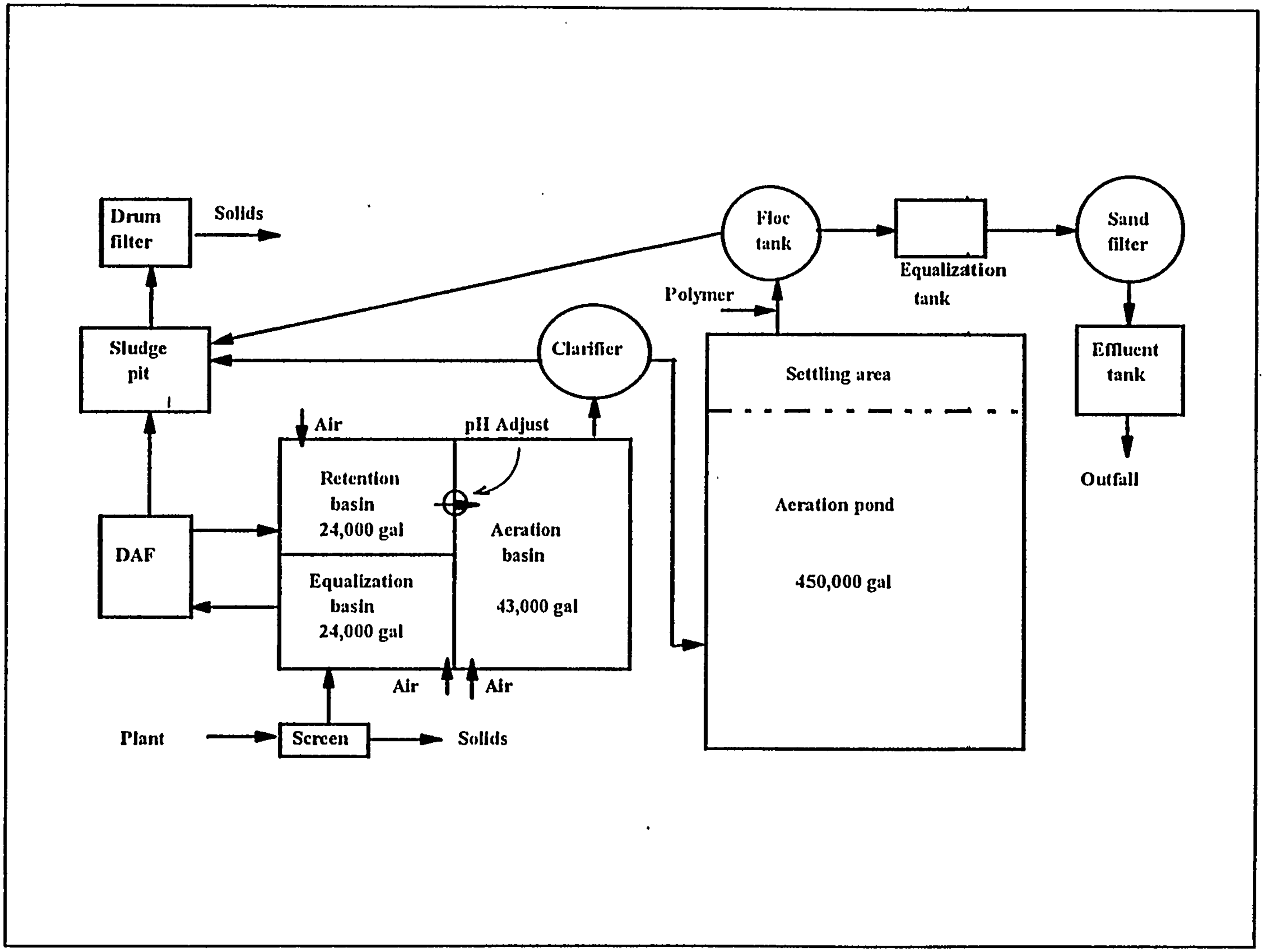

Figure 1. Schematic of the existing wastewater treatment system.

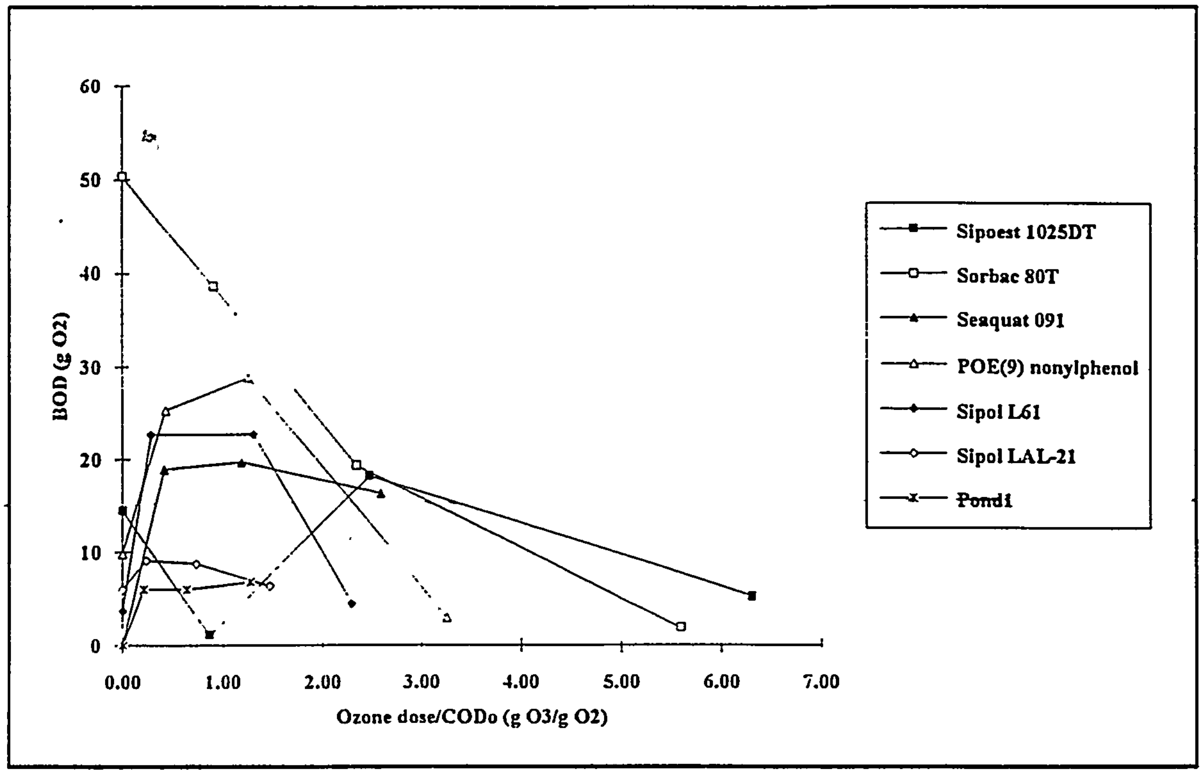

Figure 2. Plots of BOD vs ozone dose/initial COD.

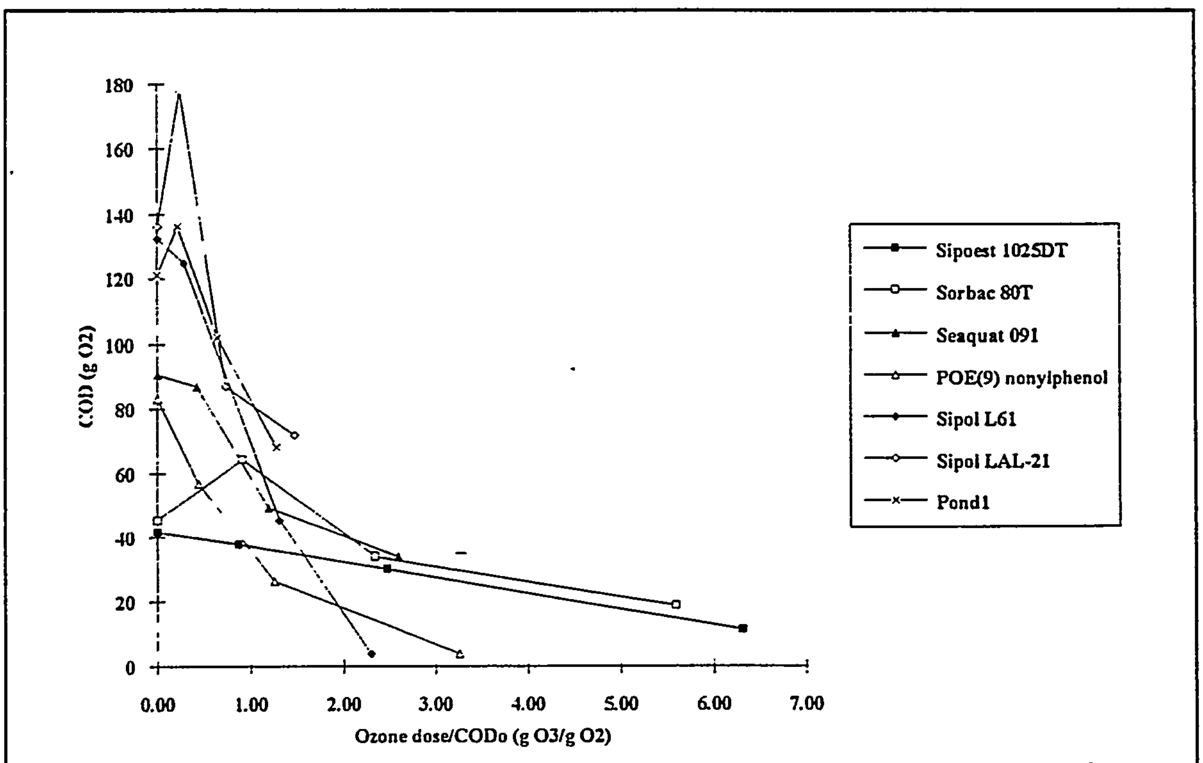

Figure 3. Plots of COD vs ozone dose/initial COD.

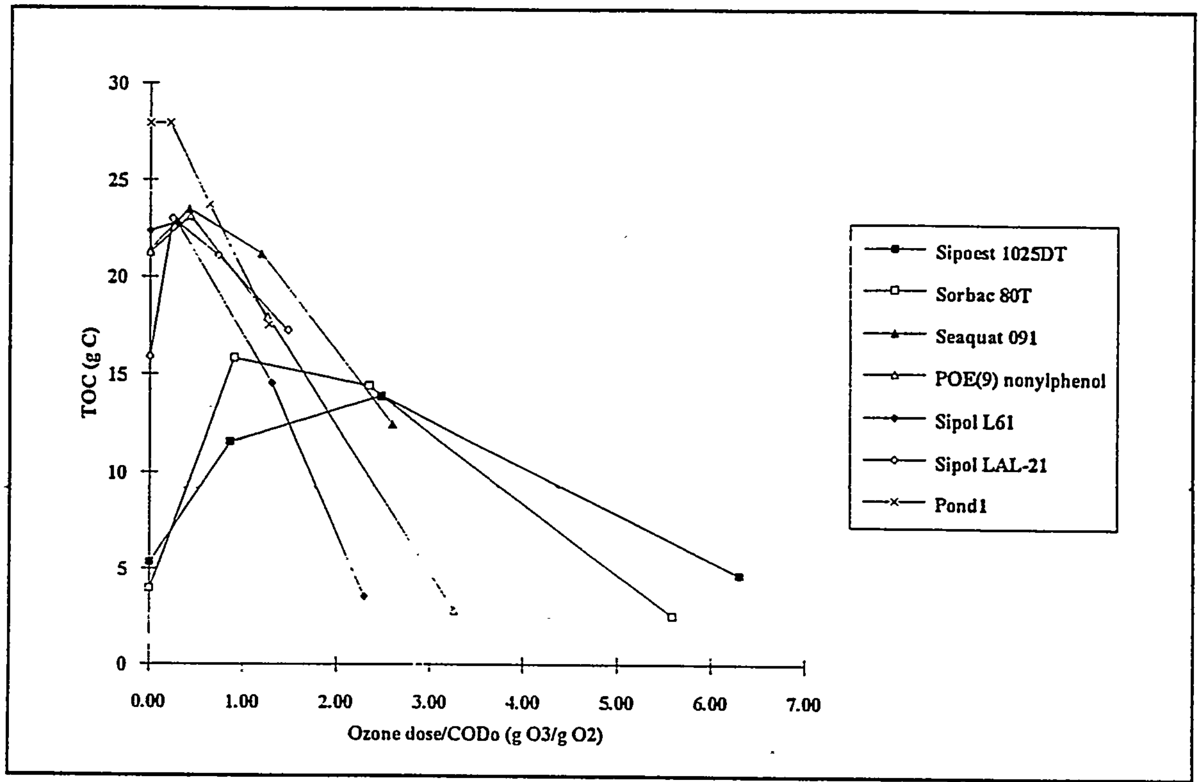

Figure 4. Plots of TOC vs ozone dose/initial COD.

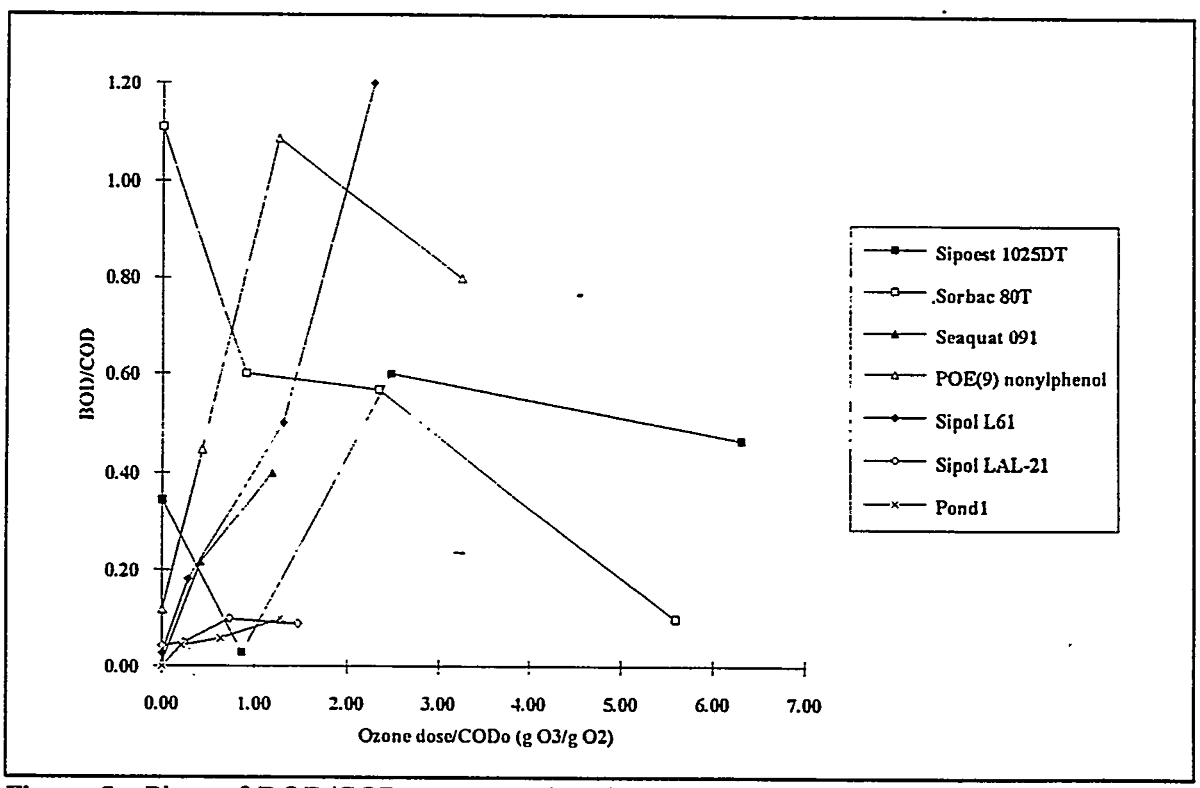

Figure 5. Plots of BOD/COD vs ozone dose/initial COD.

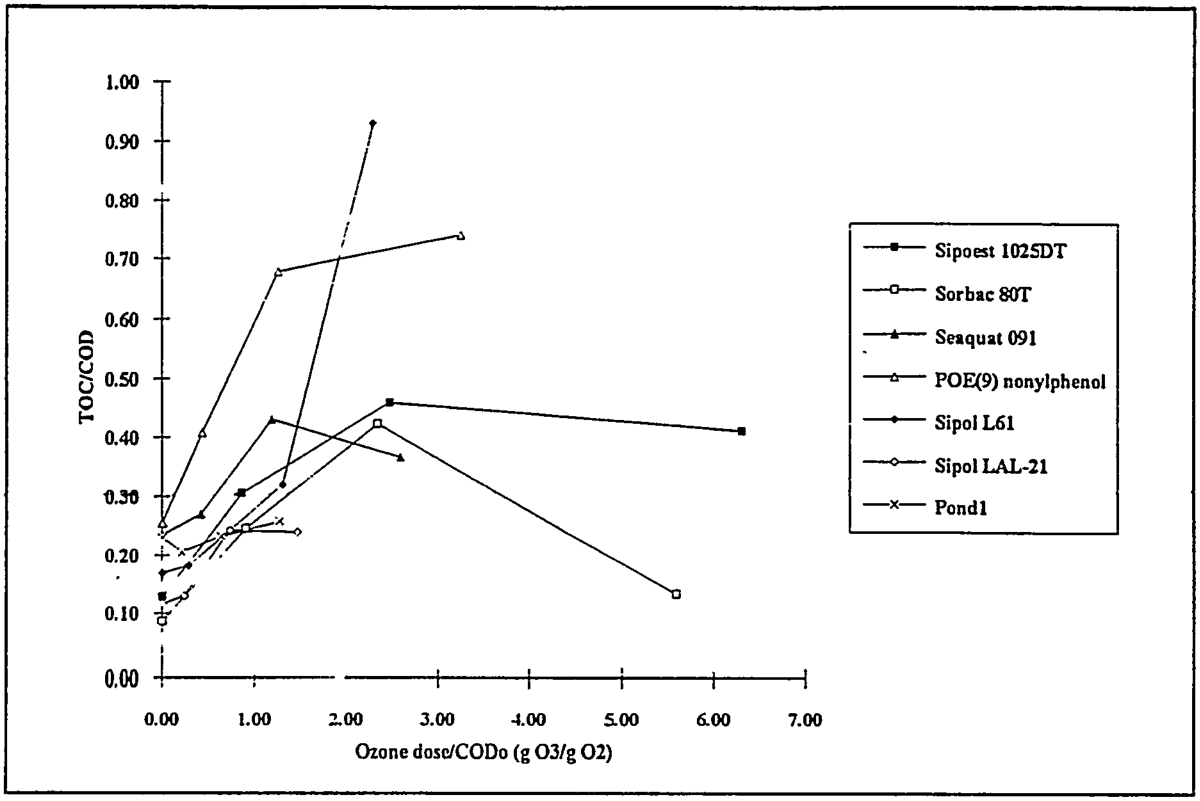

Figure 6. Plots of TOC/COD vs ozone dose/initial COD.

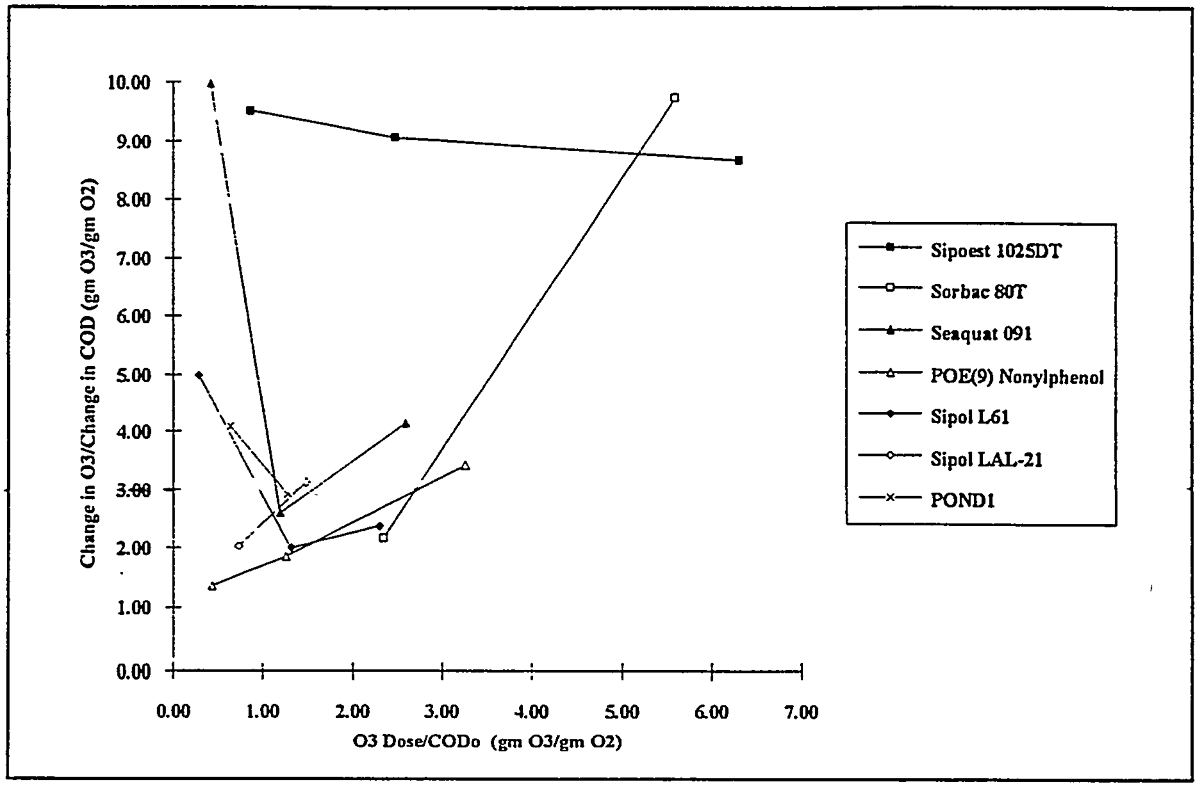

Figure 7. Plots of Change in O3/Change in COD vs Ozone Dose/Initial COD.

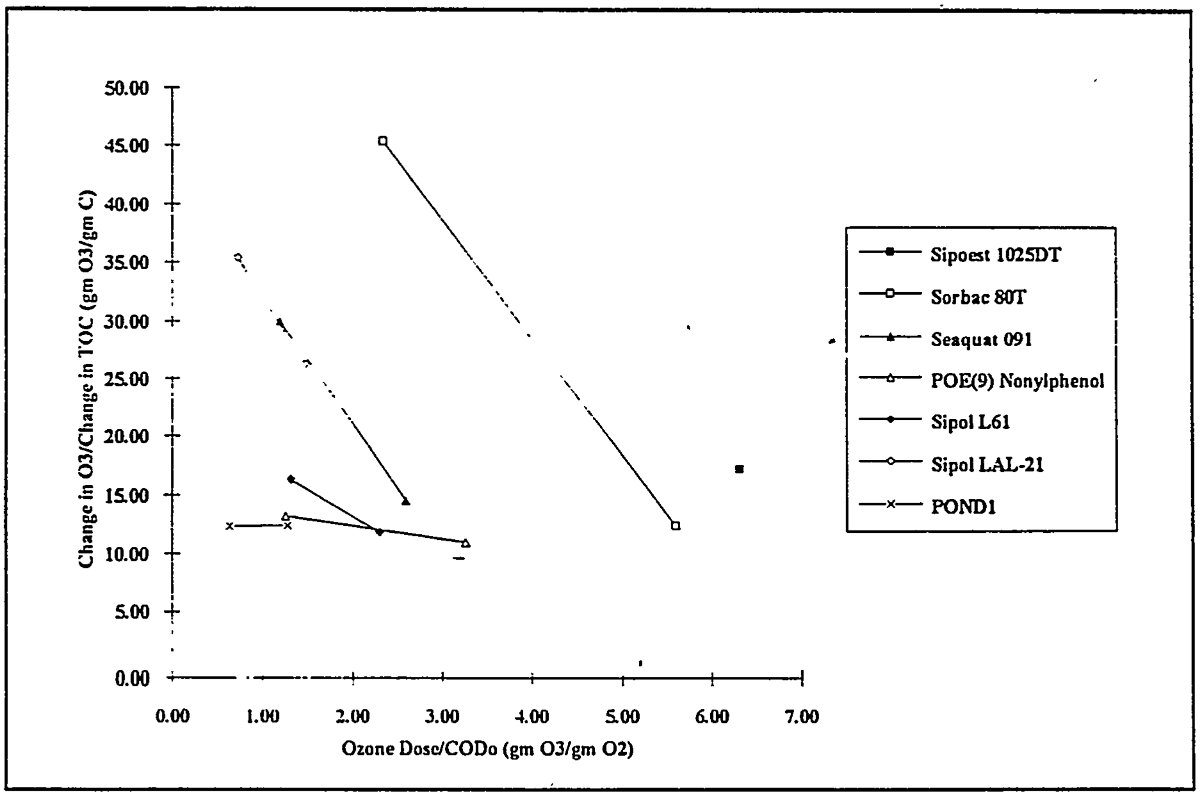

Figure 8. Plots of Change in Ozone/Change in TOC vs Ozone Dose/Initial COD.

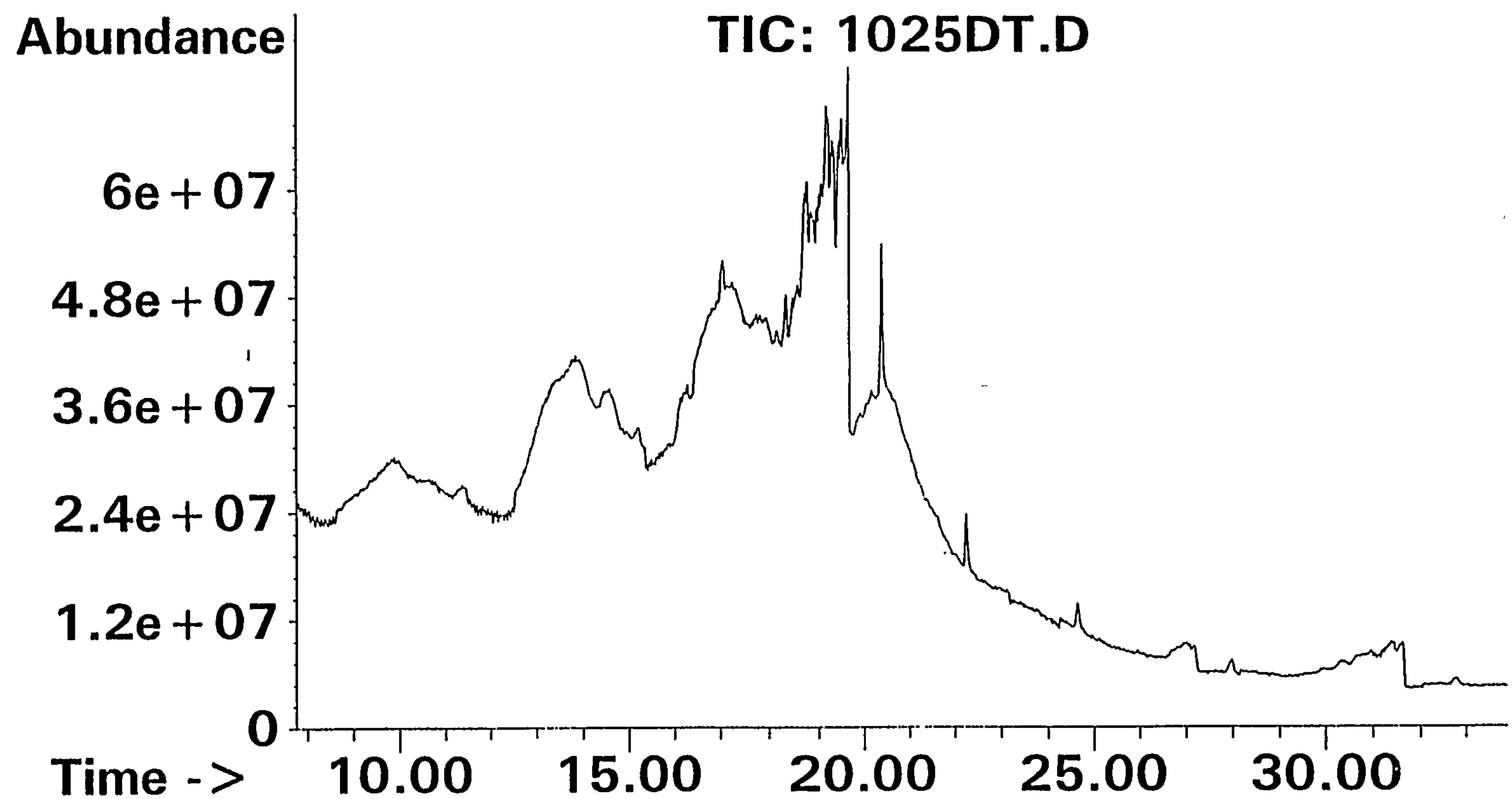

Figure 9. Gas chromatogram for Sipoest 1025DT (polyoxypropylene (1025)ditallate).

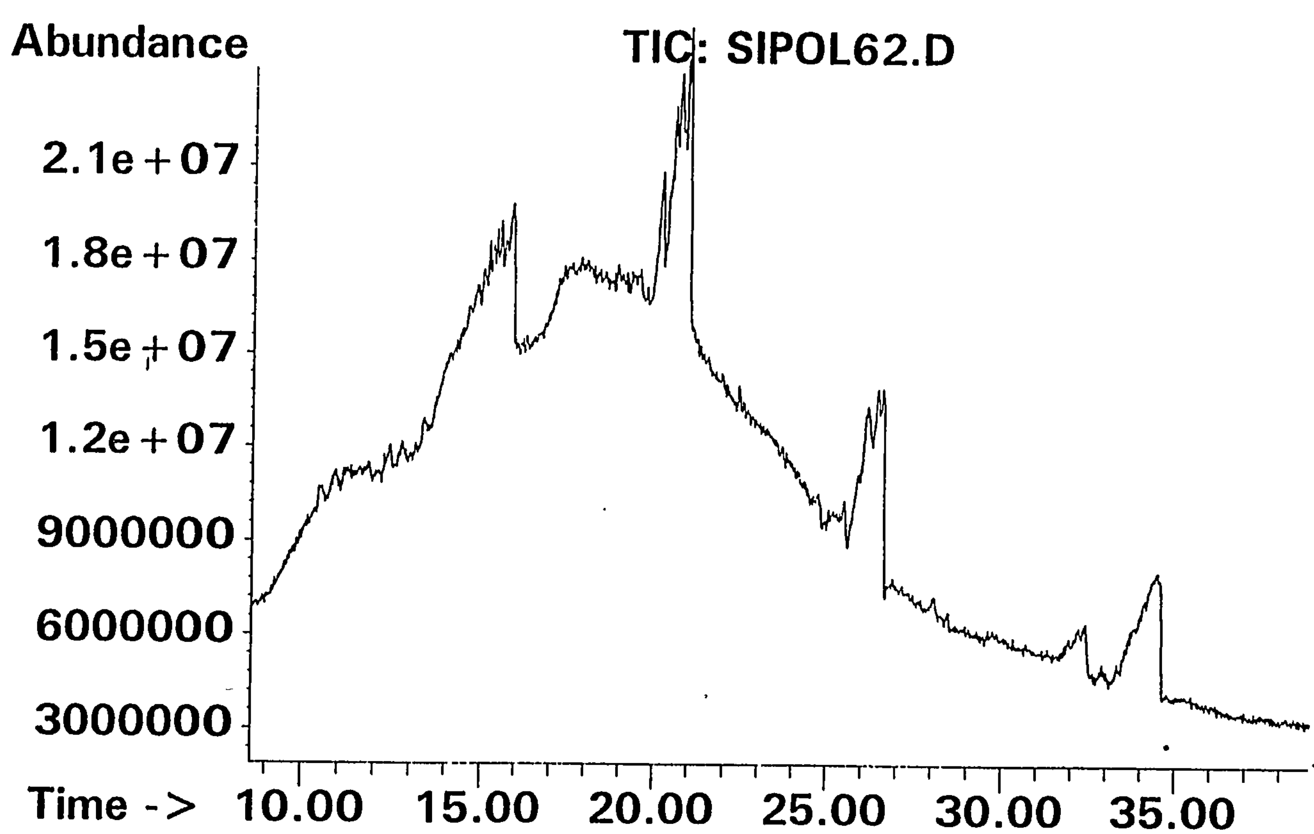

Figure 10. Gas chromatogram for Sipol L 61 (polyoxyethylene-polyoxypropylene-polyoxyethene copolymer).

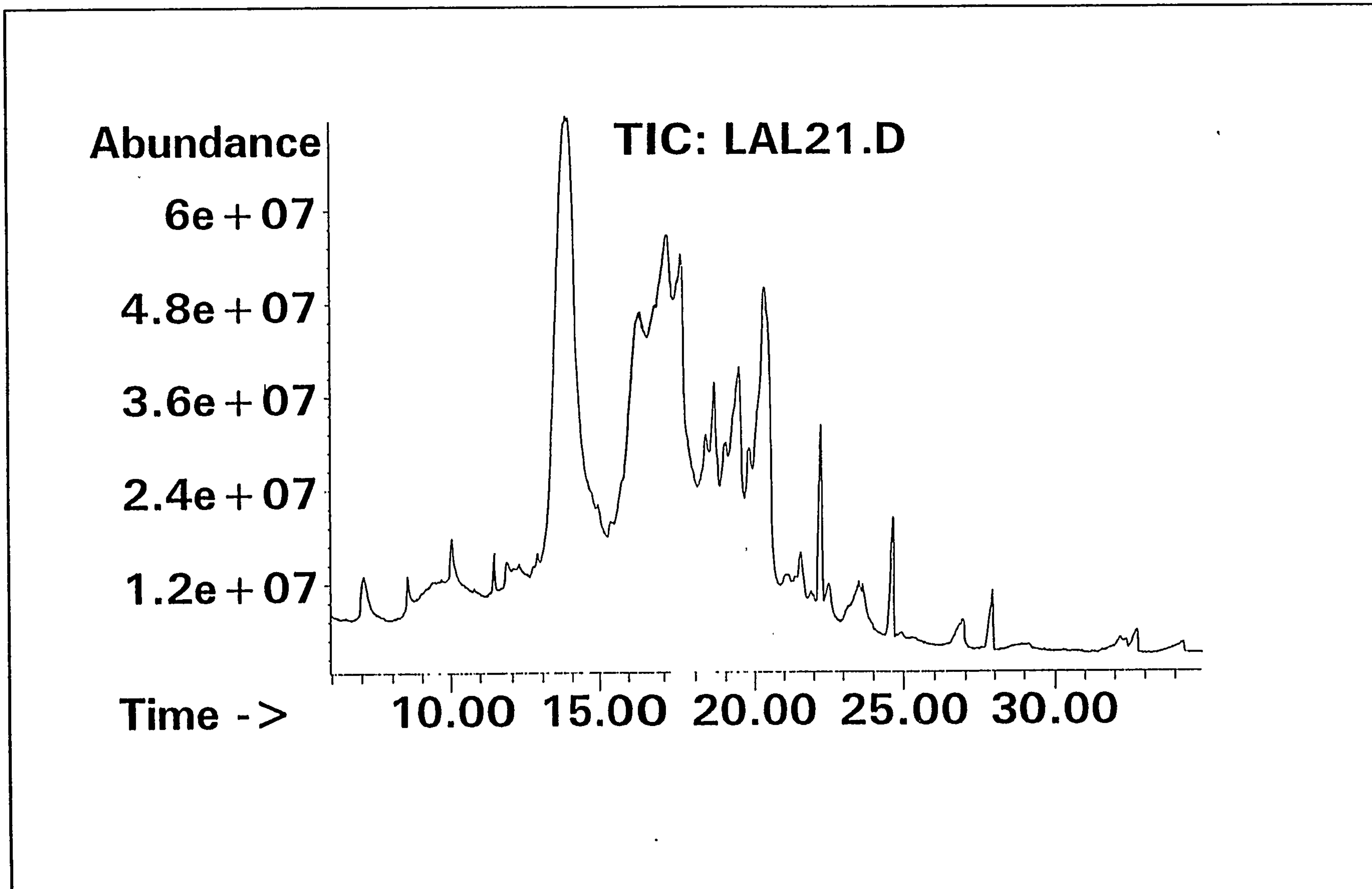

Figure 11. Gas chromatogram for Sipol LAL-21 (polyoxyethylene lauryl ether).

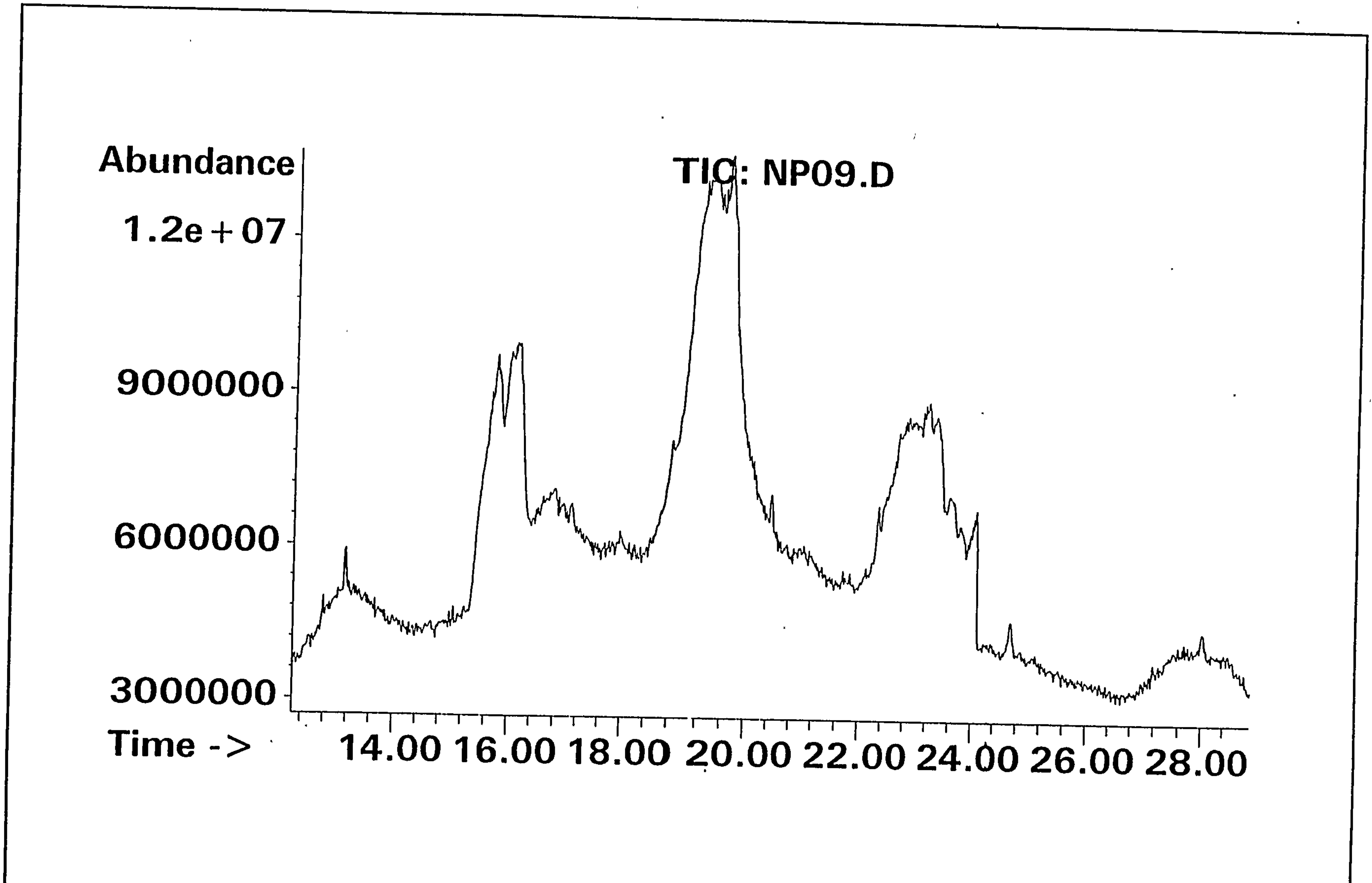

Figure 12. Gas chromatogram for POE(9) nonylphenol (polyoxyethylene (9) nonylphenol).

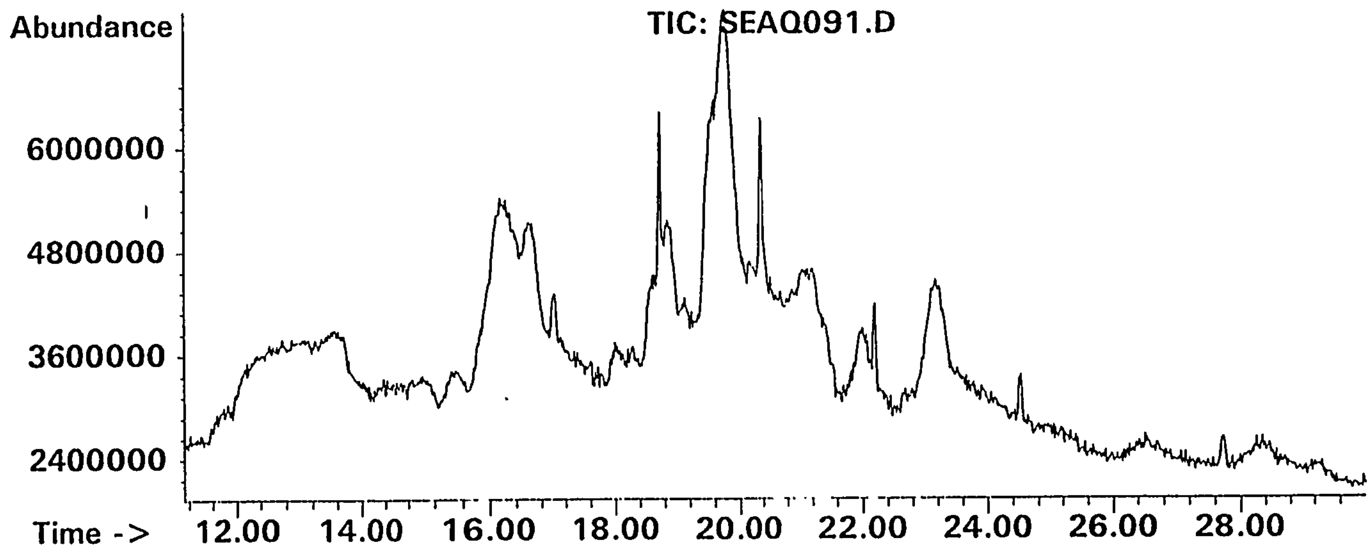

Figure 13. Gas chromatogram for Seaquat 091 (oleyl imidazoline diethyl sulphate quaternary amine).

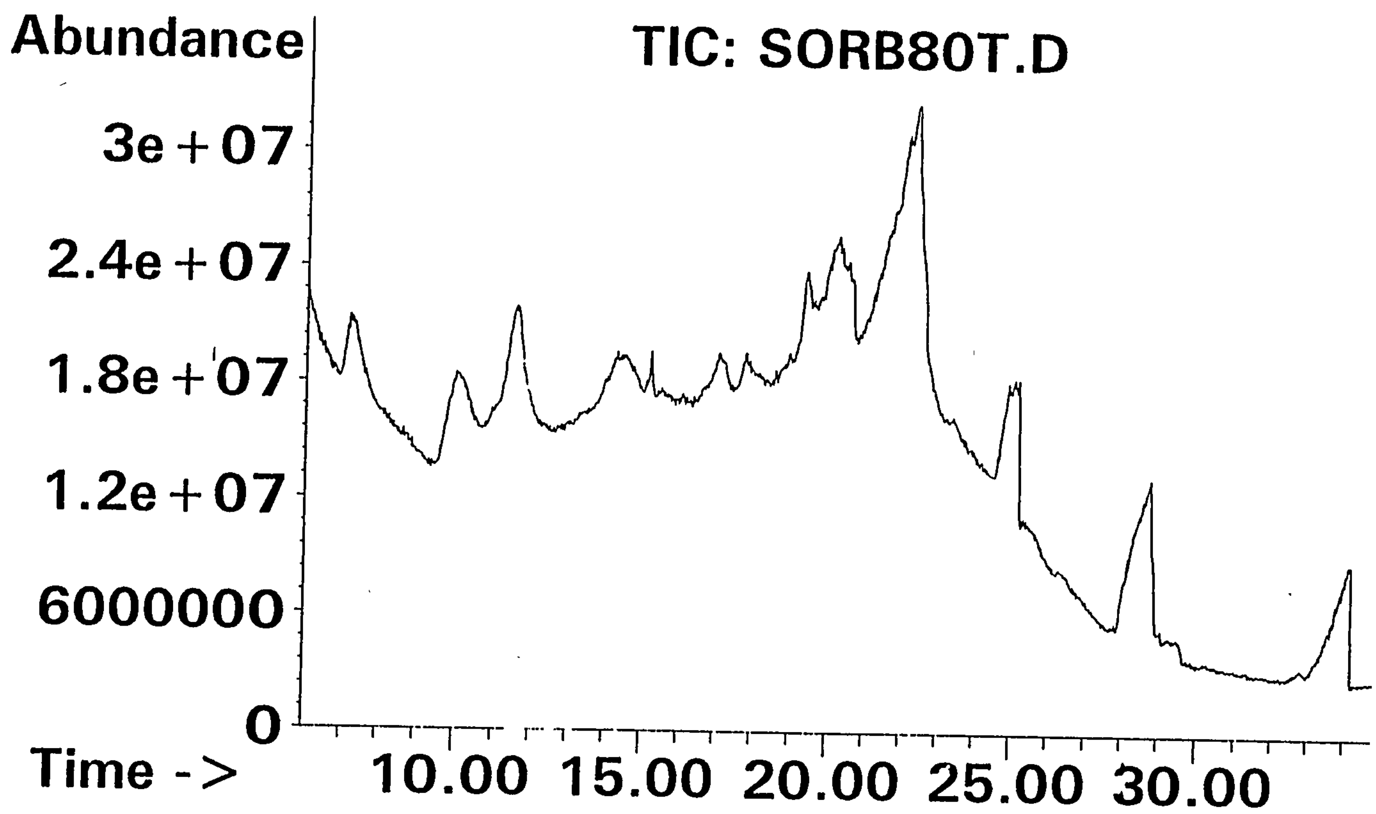

Figure 14. Gas chromatogram for Sorbac 80T (sorbitan monotallate).

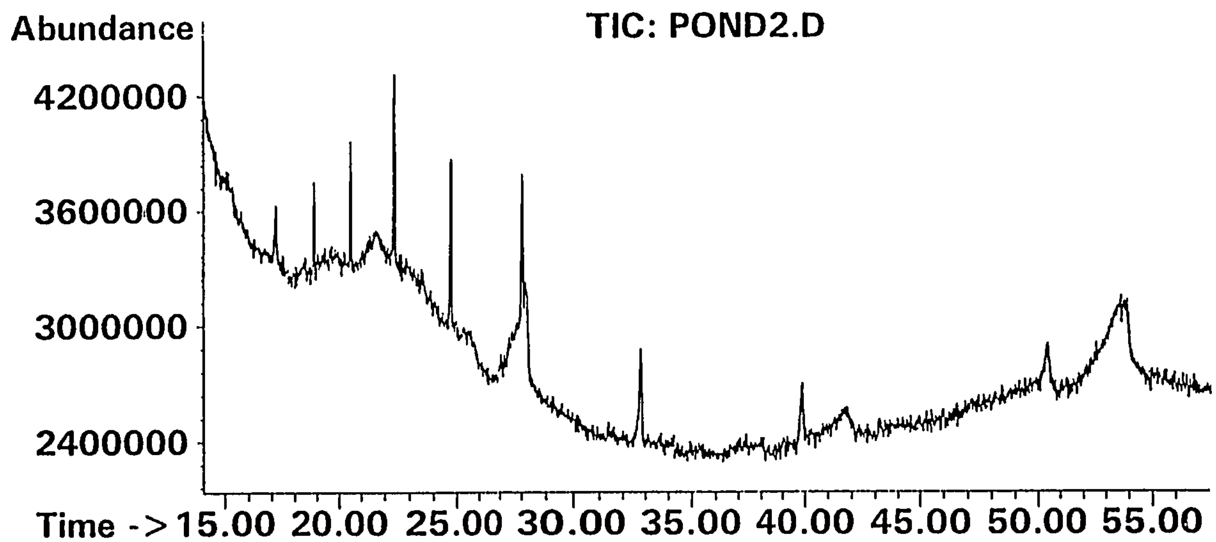

Figure 15. Gas chromatogram for the freon extract of Pond Effluent (06-13-95).

Appendix 1. Participant names and addresses

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Appendix 2. Raw material consumption (January - June, 1994)

Compound	Amount (kg)	Cumulative % of Total	Description	Biodegrad -ability
Sipol PPG 1025	89600	3.13	Polypropylene Glycol 1025	Poor
Laurastat 92	57700	5.15	Oleyl imidazoline diethyl sulfate quaternary amine	Poor
Sipol PPG 2025	26400	6.07	Polypropylene Glycol 2025	Poor
Sipol DSP 32(80)	17100	6.67	80% POE (32) Distyrene Phenol	Poor
NP 1.5	14900	7.19	Nonylphenol 1.5	Poor
Dow Antifoam 1500	1300	7.23	Distyrene phenol EO	Poor
GIV-Guard DXN	900	7.26	Biocide/Fungicide	Poor
Noedol 25-3	22600	8.05	C12-15 2' alcohol ethoxylated (3 moles EO)	Moderate
Tergitol 15-S-9	500	8.07	C11-15 2'alcohol ethoxylated (9 moles EO)	Moderate
Varisoft-Accosoft	7700	8.34	Hydrogenated tallow diamidamine methyl sulfate	Unk
Mineral Spirit 66	7300	8.60		Unk
Dequest 2010	6000	8.81	Diphosphonic acid	Unk
Dequest 2000	5400	8.99	Phosphonic acid	Unk
Raycalube PC	4500	9.15	Polyester emulsion	Unk
Dicyandiamide	1700	9.21	C2N4H4	Unk
Hexamine Tetramine	1200	9.25		Unk
Alcogum L-31	50	9.25		Unk
Sorbitol (70%)	679800	33.01	C6 Polyol similar to Glucose, MW 182.2 d 1.49	Good
Tall Oil Fatty Acid	468200	49.37	Rosin, oleic acid, linoleic acid	Good
Stearic Acid	361800	62.01	C-18 MW 284.5 mp 71.2 d 0.94	Good
Oleic Acid	315900	73.05	C-18 MW 282.5 mp 16.3 d 0.89	Good
Palmitic Acid	173200	79.10	C-16 MW 256.4 mp 63 d 0.85	Good
Coconut Fatty Acid	156500	84.57	Glyceride Mixture	Good
Tallow Fatty Acid	86000	87.57	Oleic, palmitic, stearic, lineolic (as glycerides)	Good
Oleyl Amine (30%)	44300	89.12	C18-NH2	Good
Soya Oil	44000	90.66	Glycerides of Oleic, Linoleic, linolenic, etc	Good
Ethoxylated Methyl Alcohol	43300	92.17		Good

Butyl Alcohol	37700	93.49	MW 74	Good
Cetyl Stearyl Alcohol	32000	94.61	C-16/C-18	Good
Polyethylene	17600	95.22		Good
Diethylene Glycol	15500	95.76		Good
Diethylenetriamine	13800	96.25	MW 103.2	Good
Myristic Acid	11500	96.65	C-14 MW 228.4 mp 58 d 0.84	Good
2-Ethyl Hexanol	8800	96.96		Good
Hydrogenated Tallow Glyceride	8000	97.24		Good
Glycerine	6800	97.47		Good
Urea	5300	97.66		Good
Isopropanol	4400	97.81		Good
Surfac OI-24	4000	97.95	Oleyl Imidazoline/C18	Good
Stearyl Alcohol	3000	98.06	C-18 mw 270.5 mp 59 d 0.81	Good
Propylene Glycol	2000	98.13		Good
Methane Sulfonic Acid (70%)	2000	98.20		Good
Acetic Acid	1500	98.25		Good
Triethanolamine	500	98.27		Good
Phosphoric Anhydride	15100	98.79		NA
Sodium Hydroxide (50%)	13000	99.25		NA
Hypophosphorous Acid	6500	99.48		NA
Potassium Hydroxide (45%)	6000	99.69		NA
Sulfamic Acid	5700	99.88	H2N-SO3H	NA
Hydrogen Peroxide	2500	99.97		NA
Phosphoric Acid (85%)	800	100.00		NA
Total Raw Materials	**2861850**			

Appendix 3. Products manufactured (January - June, 1994)

Compound	Amount (kg)	Cumulative % of Total	Description	Biodegrad-ability
Sorbac 40	204017	7.68	Sorbitan Mono Palmitate	Poor (5%)
SIPOTRIG CO200/50	137901	12.88	Ethyloxylated Triglyceride/50% POE (200) Castor	Poor (12%)
SIPOTRIG HCO200/50%	14301	13.41	50% POE (200) Hydrogenated Castor	Poor (12%)
CIBAPHASOL	24516	14.34	Ammonium Nonoxyl (1-5) Sulphate (APE family)	Poor (0%)
SIPOLUBE 136	304628	25.81	Proprietary Lubricant/Polypropylene Tufting Lube	Poor
Sorbac 80I	124487	30.50	Sorbitan Fatty Acid Ester/Sorbitan Mono Tofoate	Poor
SIPOLUBE NABL	69934	33.13	Proprietary LubricantNeat Applied Beaming Lube	Poor
SIPOEST PEG600 DT	67769	35.68	PEG 600 Ditallate	Poor
Sorbac 60K	59724	37.93	Sorbitan Mono Stearate	Poor
SIPOEST PPG 1025DT	59030	40.15	PPG 1025 Ditallate	Poor
Sorbac 20	45618	41.87	Sorbitan Mono Laurate	Poor
Sorbac 80EP	43652	43.52	Sorbitan Mono Oleate	Poor
AP20+ AP20U	38195	44.95	Ethoxylated Alkyl Phenol	Poor
SIPOLUBE 152	37147	46.35	Proprietary Lubricant/Polypropylene Short Staple Spin Lube	Poor
Sorbac 85	29962	47.48	Sorbitan Tri Oleate	Poor
Sorbac 60	25805	48.45	Sorbitan Mono Stearate	Poor
SIPOEST L61DO	16753	49.08	L61 Dioleate (PEG/PPG mono and di esters)	Poor
SIPOEST PPG 2025DT	11631	49.52	PPG 2025 Ditallate	Poor
SIPOLUBE 1100	10469	49.92	Proprietary Lubricant/Polypropylene Tufting Lube	Poor
Sipol DNP 150/40%	8989	50.25	40% POE (150) Dinonyl Phenol (APE)	Poor
Sipol NP30-70%	7968	50.55	70% POE (30) Nonyl Phenol (APE)	Poor
SIPOEST PPG 1025DS	7482	50.84	PPG 1025 Distearate	Poor
SIPOEST PEG 600DO K	4290	51.00	PEG 600 Dioleate	Poor
SIPOEST L61DS	3269	51.12	L61 Distearate (Distearate of PEG/PPG block copolymer)	Poor
Sorbac 83	19272	51.85	Sorbitan Sesquioleate	Mod (43%)
Sorbac 65K	19794	52.59	Sorbitan Tri Stearate	Mod (30%)
Sipamine SAM 5070	19622	53.33	70% POE (50) Stearylamine	Variable

FLAKED	120582	57.87	Proprietary	Unk
SIPOLUBE GS1031	103476	61.77	Proprietary Lubricant	Unk
SIPOMULSE 1065	97501	65.44	Sorbac 40 + Ethoxylated Castor Oil	Unk
SIPOLUBE 670	57249	67.60	Proprietary Lubricant	Unk
SIPOWAX P FLAKE	47738	69.39	Cetyl/Stearyl/Ethoxylate Blend	Unk
SIPOWAX D	43402	71.03	Cetyl/Stearyl/Ethoxylate Ether Blend	Unk
SIPOPH 06P	32416	72.25	Phosphated Alcohols, Un-neutralized	Unk
SIPOTUFT 99NP	26620	73.25		Unk
SIPOMULSE 1097	20494	74.02		Unk
SIPOWAX G	19068	74.74	Cetyl/Stearyl/Ethoxylate Sorbitan Ester Blend	Unk
SIPOSOFT 30HD	18902	75.45	Proprietary Textile Softener	Unk
SIPOMULSE 1011	17978	76.13		Unk
SIPOQUEST 1042	16571	76.75	Textile Bleach Bath Assistant	Unk
SIPOWET 1095	5330	76 95	Proprietary Wetting Agent	Unk
SIPOMULSE 1156	4631	77.13		Unk
SIPOSOFT 53	4540	77.30	Proprietary Textile Softener	Unk
SIPOWET 1074	4086	77.45	Proprietary Wetting Agent	Unk
SIPOLUBE NOH1066	3269	77.58	Proprietary Lubricant/Processing Aid for Nylon Carpet	Unk
SIPOWET 1153	1022	77.61	Proprietary Wetting Agent	Unk
SOPIC MO9	118252	82.07	Fatty Acid Ethoxylate/PEG 400 Mono Oleate (C9=C9)	Good
TOFA 9	82460	85.17	Tall Oil Fatty Acid	Good
SIPOIC ML-9	52372	87.15	PEG 400 Mono Laurate	Good
SQ0919	42290	88.74	PEG 400 Mono and Ditallate	Good
SIPOEST Me 0912	38613	90.19	Methoxy (PEG 400) Laurate (C12) (Methyl-capped PEG ester)	Good
MSB (SA-8)	34177	91.48	PEG 400 Monostearate	Good
SIPOEST D600DT	28257	92.54	PEG Ditallate	Good
SIPOEST IBT	25592	93.51	Fatty Acid Ester (Isobutyl Tallate)	Good
SIPOEST NBS	23345	94.39	N-Butyl Stearate	Good
SIPOEST 165K	21338	95.19	Glycerol Mono Stearate (Ethyloxylated Glycerine)	Good
SIPOEST NBS-K	18414	95.88	N-Butyl Stearate	Good

ESTER 5	15083	96.45		Good
SIPOPH 0613	14723	97.01	Phosphated Alcohols, Un-neutralized	Good
SIPOIC 2-L	12712	97.48	Fatty Acid Ethoxylate	Good
TOFA 13	11764	97.93		Good
SIPOEST DI0412	11681	98.37	PEG 200 Laurate	Good
SIPOEST 143M	9343	98.72	Fatty Acid Ester	Good
SIPOPHOS 9NP	5448	98.92	Phosphated PEG 9 Nonyl Phenol	Good
SIPOEST Me 0919	4250	99.08	Methoxy (PEG 400) Oleate	Good
SIPOPH 0208	4078	99.24	PEG 6 Ethyl Hexyl phosphate	Good
SIPOPHOS DA-6	3782	99.38	POE 6 Nonyl Phenyl Ether Phosphate	Good
SIPOSTAT2-2EHK	2951	99.49	Phos POE(2) 2-Ethyl Hexyl Alc,K+ antistat.	Good
IRGAPEL V	7446	99.77	Mineral Spirits and Oleic Acid	
Sipol TDA 8-90%	6075	100.00	POE (8) Branched Tridecyl Alcohol	
Total Finished Product	**2655546**			

Appendix 4. Mass spectral data.

Mass spectral data for Sipoest 1025DT.

Time (min)	1025DT	1025DT	1025DT	1025DT	1025DT
Start	12.59	16.06	18.25	20.23	22.16
End	15.50	18.18	19.70	20.50	22.37
m/z	Relative Intensity (%)				
41.1	55.58	69.54	71.89	66.47	55.18
42.1	35.43	43.99	44.71	38.17	33:35
43.0	100.00	100.00	100.00	100.00	100.00
44.0	32.74	33.43	42.76	22.60	18.25
45.0	64.89	82.43	83.08	64.95	50.17
46.0	3.65	4.47	4.61	2.42	1.93
47.0	3.09	3.14	3.77	2.98	3.84
50.1	2.14	1.94	1.95	1.75	2.58
51.0	2.70	3.04	3.44	3.06	4.36
52.1	1.33	1.30	1.34	1.25	1.71
53.1	5.08	5.49	6.18	5.63	6.65
54.1	3.16	3.58	4.30	4.60	4.55
55.1	17.00	21.43	27.68	24.83	24.53
56.1	6.31	7.56	9.18	7.06	6.84
57.1	25.01	30.40	32.34	25.15	18.19
58.1	11.24	13.60	14.61	10.28	7.15
59.1	54.79	77.09	76.80	64.91	33.02
60.1	6.58	9.10	11.91	8.86	6.87
61.1	2.84	3.45	4.10	2.70	2.36
63.1			1.08		1.52
64.1			1.25	1.19	1.79
65.1	1.50	1.87	2.29	2.22	2.85
66.0	1.67	1.32	1.39	1.30	1.81
67.1	3.55	4.47	5.43	5.66	5.49
68.1	2.79	3.06	3.78	3.16	3.10
69.1	6.55	9.41	13.04	12.12	14.38
70.1	2.61	3.02	3.65	2.72	2.50
71.1	4.49	5.45	6.84	4.82	4.35
72.1	2.22	2.91	1.74	2.21	
73.1	10.29	18.40	73.89	34.36	43.97
74.1	2.92	4.02	9.43	4.33	5.10
75.1	2.10	2.71	5.29	2.97	3.95
77.1	1.92	2.32	3.30	2.95	4.08
78.1					1.01
79.1	2.00	2.45	3.26	2.79	3.04

80.1			1.06		1.13
81.1	3.24	3.86	5.52	4.70	4.30
82.1	1.50	1.65	2.16	1.71	1.55
83.1	2.59	3.30	4.69	3.97	3.39
84.1	1.50	1.67	2.38	1.77	1.36
85.1	3.98	4.70	6.66	5.04	4.76
86.1	1.27	1.11	1.99		
87.1	16.11	24.74	27.64	23.59	9.43
88.1	1.08	1.51	1.76	1.38	
89.1			1.14		
91.1			1.27	1.20	1.66
95.1	1.41	2.16	3.22	2.72	3.18
96.1			1.35	1.09	
97.1	1.39	2.08	2.82	2.27	1.81
98.1		1.04	1.59	1.13	
99.1	1.18	1.71	2.51	1.77	1.51
100.1		1.16	1.64	1.09	1.03
101.1	5.86	7.39	9.50	6.56	3.98
103.1	2.05	1.92	2.36	1.46	1.09
111.1			1.07		
113.1		1.35	2.21	1.77	2.12
114.2			1.01		
115.1	1.17	2.16	2.80	1.92	1.33
117.1	0.77	1.47	2.05	1.35	
127.2			0.85	0.68	0.77
131.1	0.50		1.12		
133.1	0.38	0.82	1.81	1.35	1.83
139.2					0.42
141.2					0.53
145.1	0.43	0.86	1.36	1.04	1.21
147.2	0.54	1.39	13.60	3.87	5.06
148.2			2.19		
149.1			1.30		
151.1	0.48		2.78	1.25	2.09
157.2				0.32	0.51
159.2	0.22	0.35			
163.2	0.23	0.39	0.71	0.62	0.81
169.2	0.12		0.26	0.20	0.29
171.3		0.18	0.40	0.23	0.41
175.2	0.15	0.21	0.30	0.25	0.38
177.2			0.24	0.21	0.29
181.3				0.21	
183.2					0.29

185.3		0.26	0.30	0.35	0.36
187.2					0.28
189.2	0.14	0.40	0.51	0.37	
191.2			0.40		0.35
193.2	0.13				0.33
195.2			0.35	0.29	0.48
197.2				0.20	
199.2					0.23
201.3				0.16	0.20
203.2				0.13	0.19
207.3	0.19	0.44	3.43	1.07	1.60
213.2					0.33
217.4				0.11	
221.3	0.09	0.31	2.43	0.74	0.81
225.3	0.11	0.36	3.71	0.78	1.38
229.3					0.20
231.2			0.11	0.09	0.18
233.2			0.09	0.08	0.13
236.3					0.11
237.3	0.05			0.08	
238.3	0.06				
239.2	0.06	0.07	0.13	0.08	0.17
241.2		0.06		0.05	0.15
242.9				0.05	
243.8		0.06			
245.7	0.05	0.06	0.07		0.18
247.4		0.06		0.12	
249.2			0.16	0.13	0.14
251.3		0.07	0.16	0.09	0.16
252.9	0.06	0.07		0.10	
255.4	0.06		0.08	0.09	0.17
259.2		0.06	0.08	0.08	0.14
261.2	0.05				
261.8				0.04	
265.4			0.37	0.15	0.19
267.2	0.06	0.10	0.69	0.30	0.28
269.5	0.06		0.27		0.15
271.5		0.06	0.07	0.11	0.13
272.4	0.05				
273.3	0.05				0.10
275.4	0.05			0.09	0.10
277.0					0.09
281.7	0.09	0.34	2.90	0.87	1.02

285.5				0.16	
287.8				0.07	0.15
289.4	0.05			0.06	
291.1			0.05	0.06	0.08
294.3					0.08
295.2				0.11	0.09
299.7	0.06	0.11	1.67	0.39	0.26
304.4	0.04			0.04	
305.2	0.04	0.04		0.04	0.10
306.8		0.04			
307.5			0.05	0.05	
308.6					0.08
309.3	0.05			0.04	
311.3		0.04	0.06	0.03	0.07
312.0		0.04			
313.7	0.03			0.04	0.08
315.0					0.08
316.6	0.03	0.03			0.07
318.2			0.03	0.04	
319.3			0.04	0.03	
320.1					0.06
321.1					0.07
325.3	0.04	0.06	0.21	0.16	0.23
327.7	0.06	0.07	0.28	0.11	0.20
329.1	0.05		0.14		
332.0				0.04	0.06
333.3			0.04	0.04	
334.1					0.04
335.0	0.04				
335.8	0.04				
341.8	0.04	0.07	0.43	0.27	0.24
345.2	0.04				0.09
345.9	0.04				0.08
347.2				0.05	
349.2			0.04	0.03	0.05
350.8					0.05
355.8	0.06	0.10	0.56	0.31	0.24
356.9				0.12	
359.7			0.14	0.07	
361.2					0.09
363.1				0.04	
363.9		0.03			
364.7		0.03			

365.4					0.06
367.5	0.03				
368.1	0.03				
369.5			0.07	0.04	
370.6				0.03	
373.6	0.03	0.05	0.49	0.09	0.16
376.4	0.03				
379.8					0.06
382.9	0.03	0.03		0.04	0.06
383.9			0.05		
385.2		0.03	0.06		0.06
386.1	0.03		0.05	0.03	0.06
387.1	0.03		0.05	0.04	
389.1		0.03			0.06
390.0			0.04		
391.1		0.03			0.05
392.9	0.03				0.05
394.0			0.03	0.04	0.05
397.1	0.03				0.04
399.1			0.06		0.06
402.0	0.04	0.05	0.17	0.13	0.08
403.0	0.04		0.12	0.08	0.08
403.8	0.03	0.04			
405.7	0.03				
410.2				0.03	
412.0				0.03	
416.0	0.02	0.04	0.17	0.08	0.09
419.5	0.02				0.05
420.3	0.03			0.02	0.04
421.3		0.02		0.02	
423.7				0.02	
425.2		0.02			
430.1	0.04	0.05	0.21	0.11	0.07
430.6					0.08
431.4				0.05	
436.0	0.02	0.02			0.03
437.4	0.02				0.03
438.2		0.02		0.02	0.04
442.1		0.02	0.02	0.03	
443.4					0.04
444.4	0.02				0.04
445.5				0.03	
448.1	0.02	0.02	0.04	0.03	

448.4			0.04		
449.8			0.03	0.02	0.04
451.0					0.04
451.9	0.02	0.02	0.03		
453.6		0.02		0.02	0.04
456.6	0.02				
457.9	0.02				0.04
460.0	0.02		0.05		0.04
461.2			0.08	0.04	
461.7	0.02	0.03	0.09	0.06	0.05
465.1	0.02				
466.3	0.02			0.04	
467.2		0.02			
469.2			0.02		0.03
470.3			0.02		0.04
472.9	0.02				
475.0		0.02	0.04	0.03	0.05
476.2	0.02	0.02	0.06	0.03	0.06
477.1			0.05	0.03	
478.4	0.02			0.03	
480.2					0.07
481.3					0.05
482.7	0.02	0.02			
483.5				0.02	
484.4					0.04
486.2					0.03
487.4	0.02				0.03
489.3	0.02	0.02	0.05	0.02	
490.8					0.04
491.7			0.04	0.02	
493.0				0.02	
494.2		0.02			
496.1	0.02	0.02		0.01	
496.9	0.01				0.03
498.7				0.02	
501.0	0.02				0.03
502.6					0.03
504.1	0.02	0.03	0.10	0.03	
504.4				0.04	
505.2			0.06		0.04
507.2				0.02	0.03
510.5				0.02	
512.1	0.02	0.01			0.03

516.6		0.01		0.02	
517.5		0.01			0.03
518.2	0.02		0.02		
520.3			0.03		0.03
522.2	0.01	0.01	0.02	0.02	0.03
523.9			0.02		
524.8		0.01			
526.1	0.01				
526.8					0.04
527.9	0.01			0.01	
530.1				0.01	
533.2					0.03
534.1			0.04		
535.1	0.02		0.04	0.02	
535.8		0.02	0.05		
536.9		0.02	0.04	0.03	
539.4					0.04
540.1	0.02	0.01		0.02	0.03
541.6			0.02		
542.9		0.01			0.03
544.5				0.02	
545.0				0.01	
546.1	0.02				
547.7		0.01			
549.8			0.02		

<u>Mass spectral data for Sipol L61.</u>

Time (min)	Sipol L61	Sipol L61	Sipol L61	Sipol L61
Start	13.82	20.01	25.71	33.35
End	15.97	21.13	26.73	34.69
m/z	Relative Intensity (%)			
41.11	19.05	10.01	5.09	5.14
42.11	14.94	8.14	5.08	5.41
43.05	100.00	71.72	34.30	28.66
44.05	24.73	17.83	15.61	14.00
45.05	36.19	16.37	10.41	10.02
46.09	2.35	1.59	1.51	2.13
47.03	2.88	2.46	3.03	3.91
47.95				1.48
49.08	1.16	1.09	1.25	1.89

50.04	2.02	1.67	1.85	2.84
51.05	6.86	6.82	5.39	7.13
52.10				1.59
53.09	1.94	1.49	1.47	1.98
54.10	1.17		1.07	1.61
55.09	3.16	2.00	1.72	2.30
56.11	2.36	1.52	1.32	1.87
57.09	13.06	6.97	3.98	4.34
58.13	7.21	3.63	2.73	2.84
59.13	42.69	23.31	9.36	8.26
60.05	3.99	2.58	1.96	2.45
61.05	2.81	1.69	1.64	2.27
62.06	1.24	1.01	1.31	1.79
63.08	1.68	1.52	1.56	2.13
64.03	6.62	7.19	5.70	7.48
65.05	6.10	6.70	4.78	5.79
66.02	1.15		1.10	1.86
67.04	1.25	1.05	1.23	1.29
69.01	23.29	24.08	19.13	23.54
70.06	1.54	1.22	1.28	1.78
71.09	2.09	1.57	1.42	1.91
72.15	1.83			
73.10	62.60	100.00	100.00	100.00
74.10	7.04	9.20	9.43	9.87
75.09	8.20	8.41	7.83	9.23
76.05	1.56	1.40	1.50	2.06
77.03	5.34	5.71	4.98	6.06
78.01	1.20	1.14	1.22	1.80
79.00	3.83	3.18	4.08	3.61
80.03	1.13		1.18	1.52
81.04	2.74	3.22	3.79	4.03
82.01	1.25	1.17	1.37	1.84
83.05	1.99	1.68	1.59	2.25
84.00	1.05			
85.04	3.18	2.72	2.25	2.87
86.06	1.52	1.05	1.25	1.72
87.06	27.39	18.91	6.58	5.42
88.04	2.79	2.07	1.48	2.08
89.06	3.91	2.80	2.21	3.03
90.08	1.18		1.05	1.39
91.04	2.21	1.93	1.69	2.27
93.08	1.75	1.52	1.39	2.01
94.04	1.42	1.17	1.34	1.53

95.00	16.42	18.49	13.52	17.22
96.01	1.61	1.85	2.36	2.80
97.01	2.90	2.76	2.22	2.96
98.00	1.03			
99.08	2.52	2.42	1.57	2.20
100.01	2.67	2.31	1.96	2.72
101.05	12.97	7.77	4.06	4.37
102.04	2.04	1.28	1.17	1.64
103.06	4.76	2.03	1.82	2.33
104.05	1.39		1.08	1.58
104.98	1.15		1.10	1.57
106.05				1.43
107.08	1.26	1.13	1.25	1.80
108.05	1.85	1.88	1.65	2.51
109.06	3.21	3.45	2.76	3.63
110.03			1.01	1.46
111.03	1.68	1.51	1.42	1.97
111.98	1.03		1.18	1.43
112.99	16.18	18.27	13.59	18.34
114.03	2.35	1.82	1.44	2.16
115.04	4.32	3.80	2.67	3.74
116.00	1.34			1.37
117.03	3.51	3.24	2.16	2.83
117.95				1.33
119.01	2.66	2.68	2.62	3.63
120.03	1.05			1.47
121.00	1.94	2.03	1.80	2.57
122.01	1.26	1.18	1.21	1.67
123.04	1.66	1.54	1.61	2.20
124.10				1.02
125.04	1.93	1.82	1.82	2.56
126.05	1.53	1.58	1.49	2.23
127.01	3.01	3.46	3.27	4.46
128.00	1.50	1.58	1.51	2.30
128.99	1.57	1.52	1.16	1.69
130.99	4.56	4.60	3.98	5.42
132.05			1.03	1.62
133.00	21.27	27.69	24.39	36.43
134.01	1.44	1.63	1.79	2.58
135.04	1.56	1.65	1.70	2.37
135.95				1.35
137.04	1.64	1.78	1.93	2.78
138.02	1.03		1.02	1.41

139.03	3.55	3.71	3.23	4.40
140.04	1.15	1.15	1.21	1.75
141.01	2.43	2.90	2.84	3.44
143.04	1.63	1.55	1.48	2.00
144.03	1.93	1.97	1.75	2.66
144.98	15.18	19.25	16.38	23.24
146.03	1.75	1.85	1.64	2.41
147.05	14.11	31.19	41.65	55.02
148.04	2.71	4.98	6.59	9.16
149.04	2.07	3.45	4.52	5.74
150.03	1.91	2.16	2.22	2.98
151.01	4.95	7.25	8.65	10.90
152.03	1.20	1.49	1.78	2.39
153.00	1.94	2.16	2.36	2.89
155.04	1.12	1.16	1.36	1.76
156.03			1.00	1.35
157.03	2.55	3.06	2.67	3.59
158.05	1.05	1.16	1.12	1.59
159.03	3.52	3.83	3.37	4.09
160.00				1.27
160.99	2.15	1.98	1.86	2.23
161.98		1.02	1.12	1.49
162.99	14.27	18.91	18.51	21.54
163.98	1.55	1.81	1.97	2.39
164.96	1.34	1.52	1.68	2.13
165.95				1.25
167.00	1.20	1.19	1.25	1.59
168.00				1.12
168.99	2.89	3.04	3.02	3.37
170.01	1.16	1.10	1.12	1.56
171.03	1.57	1.75	1.68	2.01
172.00	1.32	1.31	1.45	1.49
173.01	1.47	1.51	1.42	1.55
174.00			1.02	1.18
175.01	3.25	3.72	3.68	4.21
176.01	1.23	1.48	1.59	2.02
177.03	3.23	4.37	4.95	5.30
177.95		1.09	1.36	1.60
178.99	1.42	1.69	2.18	2.35
179.90				1.06
180.99	2.53	2.93	3.02	3.19
181.98			1.01	1.20
182.98	2.79	3.42	3.52	3.68

184.98	3.17	3.72	3.52	3.79
186.00				1.17
187.00	2.46	2.73	2.82	2.76
187.99	1.14	1.19	1.21	1.32
189.01	4.75	5.25	4.43	3.90
190.01	1.38	1.42	1.49	1.28
191.00	2.87	3.99	5.99	5.19
192.00		1.20	1.66	1.66
193.03	1.59	2.13	3.19	3.15
194.00	1.85	2.31	2.55	2.73
194.98	6.33	8.63	8.49	7.90
195.99	1.07	1.19	1.32	1.35
196.98	4.93	7.16	6.64	5.67
197.90			1.02	1.07
198.95	1.17	1.17	1.18	1.06
199.98		1.05	1.12	1.19
200.98	1.84	2.06	1.93	1.78
203.01	1.95	2.61	2.13	1.98
204.99	1.65	2.54	2.95	2.31
206.00	1.10	1.31	1.25	1.18
207.01	12.37	26.58	45.22	29.08
208.00	2.67	5.43	9.32	6.32
209.00	3.34	5.81	8.68	5.65
210.03		1.31	1.76	1.56
210.98	2.53	3.65	4.65	3.30
211.99	1.00	1.14	1.34	1.16
213.00	4.22	5.58	5.29	3.85
213.98	2.42	2.89	2.39	1.94
214.99	2.43	3.04	2.71	2.23
217.00	1.32	1.52	1.37	1.16
218.00		1.03		
219.00	2.10	2.74	2.35	2.02
221.03	8.62	21.21	26.79	15.19
222.05	2.58	5.81	7.39	4.26
223.04	2.50	4.80	5.52	3.38
223.90				1.09
225.05	17.37	37.99	41.87	20.78
226.06	4.36	8.78	9.56	5.25
227.03	4.57	7.87	8.19	4.50
228.00	1.15	1.67	1.77	1.29
228.98	1.79	2.18	2.00	1.42
230.98	2.24	3.12	2.63	1.58
232.98	2.44	3.38	2.56	1.70

234.98	1.64	2.07	1.80	1.12
236.99	1.86	2.57	2:14	1.40
237.98	1.07	1.17	1.01	
239.00	4.11	5.50	3.65	2.33
240.00		1.15		
240.99	2.73	3.56	2.66	1.85
242.00		1.04		
242.97	1.35	1.57	1.36	
244.95	2.03	2.75	1.86	1.20
246.98	1.19	1.90	1.06	
248.98	1.72	2.28	2.03	1.28
250.00		1.04		
250.98	1.87	2.57	2.07	1.41
251.95		1.03		
252.99	2.25	2.90	2.09	1.24
254.00	1.11	1.19		
255.01	1.81	2.11	1.68	1.06
257.00	2.72	3.50	1.98	1.08
258.00	1.17	1.40		
258.96	3.71	5.33	2.80	1.43
260.00		1.06		
261.00	1.86	2.68	1.48	
262.62	1.52	1.03	1.24	
262.95		1.87		
264.00		1.07		
264.98	2.67	4.52	3.39	1.86
265.98	1.05	1.55	1.22	
266.98	3.69	7.63	6.18	3.13
267.96	1.58	2.61	2.14	1.28
268.98	2.63	4.37	2.93	1.58
270.00		1.26		
270.97	2.21	3.15	1.74	
273.02	1.80	2.23	1.16	
274.93	2.41	3.31	1.65	
276.98	1.58	1.86	1.02	
278.98	1.86	2.98	1.74	
280.96	19.12	42.94	24.71	9.33
281.99	6.59	14.45	7.97	2.99
282.99	6.24	12.09	6.49	2.53
284.23	1.66	3.11	1.64	2.12
284.98	4.92	8.47	5.00	
286.00	1.64	2.71	1.59	
286.95	1.96	3.05	1.51	

288.95	1.66	2.21		
291.00	1.18	1.53		
292.98	1.28	1.64		
295.05	2.86	6.12	2.35	
296.03	1.07	2.15		
296.98	1.74	2.75		
299.00	18.75	44.86	13.90	2.09
300.00	6.12	13.94	4.36	
300.98	3.99	7.57	2.47	
301.98	1.23	2.13		
303.02	3.51	5.07	1.44	
304.00		1.26		
305.00	2.21	2.90		
307.00	1.70	2.43		
308.98	1.55	1.94		
311.05		1.17		
313.00		1.08		
318.95	1.21	1.37		
321.00	1.64	1.50		
323.00	1.45	1.78		
324.98	3.01	4.78	1.65	0.91
325.98	1.16	1.62		
326.97	3.32	4.77	1.57	
328.00	1.10	1.54		
329.00	1.38	1.87		
336.95	1.17	1.16		
339.00	1.60	2.09		
341.03	4.38	6.71	1.94	0.95
341.98	1.68	2.44		
342.98	1.81	2.41		
345.05	1.32	1.52		
346.98	2.21	2.32		
348.93	1.11	1.05		
355.01	6.43	9.96	2.04	0.96
356.05	2.55	3.82		
357.03	2.33	3.13		
359.00	2.33	2.59		
368.98	1.08	1.10		
373.03	5.17	6.44	1.04	
374.08	1.88	2.28		
375.03	1.53	1.74		
376.98	1.24	1.15		
385.00		0.73		

400.93	1.96	2.11	0.68
415.00	1.11	1.23	
429.07	1.27	1.46	0.38
441.00		0.33	
446.95		0.32	
460.90		0.41	
474.95		0.29	
503.00	0.22	0.29	
518.85	0.22	0.17	
534.95		0.21	

Mass spectral data for POE(9) nonylphenol (NP09).

Time (min)	NP09	NP09	NP09
Start	15.21	18.89	22.33
End	16.38	20.01	24.21
m/z	Relative Intensity (%)		
41.10	48.62	22.07	22.68
42.10	13.80	6.11	8.07
43.05	50.57	31.91	43.44
44.05	27.37	10.36	20.47
45.05	40.35	30.80	46.90
46.07	3.39	1.53	3.00
47.00	3.65	1.75	3.70
47.98	1.81		1.57
48.63	1.25		1.11
49.15	1.86		
50.08	3.63	1.34	2.59
51.05	7.92	3.35	5.52
52.10	3.34	1.05	1.82
53.08	7.44	2.50	3.46
54.05	2.76		1.64
55.10	16.98	6.70	8.10
56.10	4.29	1.76	2.79
57.10	10.42	6.41	9.72
58.12	6.90	2.72	4.28
59.13	13.90	8.55	10.06
60.08	3.72	1.36	2.60
61.05	2.88	1.05	2.23
62.03	2.55		1.61
63.08	4.67	1.56	2.45
64.00	4.66	2.44	4.73

65.07	11.85	4.45	5.89
66.02	3.88	1.16	1.97
67.10	3.30	1.24	2.42
67.95	2.18		1.26
69.05	11.43	7.36	13.85
70.08	2.59	1.13	2.22
71.12	3.74	2.43	4.47
72.05	2.49		
73.10	30.02	100.00	100.00
74.10	3.80	4.94	7.58
75.10	5.99	3.33	6.46
76.10	2.59	1.23	2.14
77.05	20.43	7.78	9.53
78.07	5.28	2.71	3.85
79.05	8.11	3.50	5.72
80.03	2.19		1.71
81.00	3.60	1.63	4.30
81.98	1.90		1.64
83.05	2.47	1.10	2.37
84.13	1.11		1.41
85.03	3.43	1.65	3.64
86.03	2.26		1.81
87.05	8.62	6.49	8.96
88.08	2.95	1.53	2.83
89.07	6.38	3.34	5.57
90.05	2.47	2.13	3.20
91.07	18.43	9.14	11.69
92.07	3.66	1.67	2.84
93.07	3.83	1.47	2.53
94.02	4.46	1.28	2.01
95.00	12.47	5.81	9.85
95.93	1.97		2.37
97.07	2.37	1.10	2.27
98.00	1.61		
99.07	2.06	1.04	2.05
100.00	2.08	1.00	1.99
101.03	4.37	2.52	4.33
102.05	3.05	1.39	2.27
103.07	8.12	3.82	6.21
104.05	2.83	1.53	2.81
105.08	6.06	3.33	5.51
106.07	1.58	1.75	3.58
107.10	68.44	14.02	15.72

108.08	6.87	1.91	2.83
109.05	2.57	1.31	2.44
110.10	1.30		1.33
110.98	1.76		1.67
111.95	1.34		1.26
112.98	5.84	4.55	8.78
113.95	1.37		1.64
115.05	7.27	5.09	6.93
116.07	2.87	1.80	2.77
117.07	4.19	3.56	5.71
118.05	2.72	1.79	3.21
119.05	11.66	4.40	6.60
120.08	5.34	1.70	3.72
121.05	47.33	7.03	11.62
122.03	5.33	1.11	2.12
123.05	2.19		1.77
123.95			1.05
125.03	1.71		1.80
126.08	1.44		1.63
126.98	3.28	1.91	3.44
127.98	2.79	1.84	2.89
129.03	2.18	1.42	2.41
130.10	1.07		1.35
131.02	5.78	2.93	6.44
132.05	3.12	1.27	2.43
133.00	15.72	11.15	22.67
134.08	14.11	3.39	7.24
135.03	100.00	13.42	19.04
136.07	11.18	1.81	2.95
137.03	2.49		2.10
138.00	1.50		1.23
138.98	2.14	1.27	2.61
140.00	1.34		1.27
141.00	2.08	1.34	2.58
142.05	1.19		1.05
142.98	1.23		1.71
143.95	2.03		1.87
144.97	7.60	6.38	11.77
146.02	2.37	1.14	2.18
147.05	8.25	12.06	33.74
148.03	3.98	2.54	7.23
149.05	47.87	6.42	7.78
150.02	6.96	1.44	2.49

151.03	2.89	3.74	6.00
152.00	1.44		1.61
152.95			1.99
154.00	1.23		
155.10	1.17		1.39
157.02	1.94	1.14	2.22
158.00	1.47		1.37
159.02	2.66	1.73	3.13
159.98	1.27		1.42
161.02	3.32	1.85	4.51
161.98	2.91		1.80
163.00	35.14	7.38	11.32
164.03	4.79		1.64
165.02	1.64	5.37	2.11
166.03	1.01		1.08
167.00			1.04
168.10	1.04		
168.93	1.71		1.93
170.98	1.18		1.36
171.95			1.21
173.03	1.45		1.49
173.95			1.08
175.03	2.51	1.91	3.66
176.00	1.80		1.54
177.05	15.80	2.33	4.03
178.07	2.86	1.15	1.32
179.00	1.68	18.87	2.90
180.00		2.51	1.08
181.02	1.41	1.15	1.91
182.98	1.70	1.17	2.14
185.00	1.48	1.09	1.98
186.98	1.39	1.04	1.93
187.95			1.01
189.03	2.41	1.81	2.63
190.03	1.23		1.08
191.05	7.96	2.03	3.61
192.10	1.50		1.31
193.03	1.42	14.00	2.80
194.03	1.31	2.51	1.62
194.92	2.58	2.53	4.02
196.95	2.01	1.96	2.93
199.85	1.01		
201.00	1.26		1.33

202.98	1.48		1.39
205.03	2.03	1.03	1.84
207.02	3.55	28.91	15.86
208.00	1.39	4.03	3.67
208.98	1.33	1.74	3.93
210.00			1.05
210.93	1.39		2.09
212.93	1.79	1.47	2.36
213.93	1.17		1.16
214.93	1.06		1.41
218.98	1.99		1.41
220.05	3.96		
221.05	2.05	16.54	8.97
222.03		3.26	2.74
223.00	1.07	1.49	6.52
224.05			1.30
225.05	2.49	3.53	10.67
226.05		1.13	2.98
227.00	1.32	1.24	2.58
230.93	1.10		1.11
233.00	1.27	1.04	1.25
235.10		5.17	
236.10		1.12	
237.08	0.95		3.96
238.10			1.20
238.93	1.00	1.01	1.42
241.03	1.04	0.76	1.11
243.00	0.80		
248.00	1.08		
249.05		1.96	
251.03	0.83		7.71
252.05			1.90
252.90	0.96		1.12
256.15	0.72		
259.00	0.87		
263.05		1.39	
264.90	0.63		3.47
266.10			1.01
266.93		1.13	2.05
268.90	0.84		1.07
275.00	0.79		
279.10			1.25
280.97	1.46	3.21	5.76

281.98		1.07	1.85
282.95			1.58
284.98	0.85		1.34
289.95	0.48		
292.15		0.79	
292.90	0.52		
293.65	0.56		
295.23	0.53	0.50	
298.93	0.63	0.90	1.32
302.85	0.54		
306.25	0.41		
306.90		0.25	
309.03	0.47	0.23	
310.00		0.19	
310.95		0.20	
312.15	0.51		
315.20	0.49	0.15	
316.05	0.39		
318.30		0.13	
318.90		0.14	
321.90	0.55		
325.03	0.52	0.39	0.60
327.02	0.43	0.35	0.58
334.40	0.47		
335.10		0.17	
337.00	0.51		
339.30	0.42		
340.93	0.44	0.44	0.79
344.70	0.45	0.19	
345.95	0.42		
346.85		0.19	
349.75	0.45		
354.88	0.42	0.49	0.69
356.05			0.45
356.75	0.42		
358.85	0.41		
360.90		0.12	
362.95		0.12	
364.75	0.33		
365.50	0.36		
367.18	0.31	0.14	
369.10		0.13	
370.75	0.31		

372.80	0.34	0.16	
373.30			0.26
374.60			0.26
375.20		0.12	
377.50	0.36		
378.83	0.32	0.11	
379.57	0.33	0.13	0.26
384.00	0.31		
385.03	0.34	0.13	
387.93	0.30	0.12	
388.95			0.25
390.25	0.29		
392.00		0.13	
393.15	0.29		
394.90	0.29		
397.10		0.14	
399.28	0.39		0.30
400.95		0.20	0.31
404.95	0.34		
405.75	0.29		
406.70		0.10	
408.90		0.10	
410.45	0.30		
411.95		0.08	
413.25		0.09	
414.87	0.32	0.09	0.23
415.85		0.08	
418.35	0.28		
419.13	0.26	0.11	
420.90	0.28	0.10	
424.40	0.32		
426.80		0.09	
428.03		0.09	0.22
428.90	0.25		0.23
430.10			0.20
431.00	0.26	0.13	
432.60	0.25		
435.35		0.09	0.20
436.75	0.28	0.10	
439.50		0.08	
440.40	0.29		
441.05		0.09	
444.60	0.28		

445.25		0.08	
446.85		0.08	0.21
448.05			0.19
450.00	0.25		
452.20		0.08	
454.10		0.08	
454.78	0.22	0.08	
456.15		0.08	
456.85	0.23		
458.90			0.17
459.85		0.10	
461.65			0.18
463.05		0.08	
465.40	0.24	0.07	
467.15	0.28		0.18
468.70		0.09	
471.20			0.19
472.20		0.08	
473.20		0.08	
475.40	0.26		
477.20			0.17
477.85		0.09	
479.20	0.23		
481.40		0.08	
484.15	0.22		
485.00	0.22		
486.58		0.07	0.15
488.75	0.22		
490.05		0.07	
491.00	0.22		
493.55		0.08	0.15
496.45	0.25		
498.15		0.07	0.16
502.05		0.07	
503.15	0.24		
504.95			0.15
506.23	0.26	0.07	
510.50			0.13
511.20		0.06	
511.95		0.06	
513.00	0.23		
516.80		0.06	
519.25		0.07	

521.80			0.13
522.70			0.12
523.70	0.20		
525.50		0.06	
528.30			0.12
529.45	0.19		
531.75		0.07	0.12
532.70		0.07	
536.10		0.05	
538.80	0.18		
540.85		0.07	
542.10		0.06	
544.65		0.06	
547.75		0.05	
549.28	0.17		0.12

Mass spectral data for Sipol LAL21.

Time (min)	LAL21	LAL21	LAL21	LAL21	LAL21	LAL21	LAL21	LAL21	LAL21	LAL21	LAL21
Start	13.08	12.99	15.68	16.56	17.33	18.48	19.10	19.93	22.09	24.46	27.66
End	20.77	15.11	16.50	17.33	18.01	18.69	19.55	20.61	22.33	24.72	27.99
m/z	Relative Intensity (%)										
41.1	91.20	100.00	100.00	87.90	77.23	60.93	80.61	54.78	23.39	21.02	19.24
42.1	27.08	30.94	27.58	23.34	22.77	18.48	23.23	16.30	8.62	8.17	8.32
43.1	100.00	98.44	98.91	100.00	94.36	68.37	100.00	70.74	31.54	27.97	23.49
44.1	23.33	25.13	20.71	16.30	21.59	16.98	21.60	16.70	11.35	10.74	9.86
45.1	68.46	63.48	43.70	58.39	80.05	40.67	68.80	61.89	25.60	19.32	16.49
46.1		2.73	2.12	2.06	2.68	1.85	2.65	2.04	1.29	1.25	1.42
47.1		3.03	2.93	1.67	2.66	2.73	2.87	2.71	1.72	1.76	2.10
48.0											1.07
49.2											1.14
50.1	1.09		1.08				1.16			1.08	1.54
51.0	2.35	2.07	2.31	1.63	2.18	2.03	2.49	1.58	1.46	1.63	2.18
52.1		1.06	1.09				6.47				1.14
53.1	7.33	7.99	7.73	6.27	6.18	5.01	7.62	4.31	2.59	2.79	3.04
54.1		11.20	10.24	7.33	7.25	6.76	64.04	4.95	2.87	2.45	2.55
55.1	73.13	86.22	80.80	64.59	58.35	51.54	23.74	40.77	18.38	15.85	12.49
56.1	34.82	50.96	36.43	27.95	24.94	19.60	74.91	15.16	6.03	5.05	4.31
57.1	67.69	55.29	64.59	87.93	68.25	41.93	9.89	57.15	16.50	12.55	9.14
58.1	10.61	11.91	8.51	7.73	9.71	7.15	9.91	7.91	3.76	3.15	2.79
59.1	7.33	5.19	7.68	4.09	7.09	6.22	6.50	7.27	4.26	3.61	3.13
60.0	6.83	4.85	11.16	3.75	8.79	4.41	3.35	4.20	2.39	2.25	2.07
61.0	2.73	1.82	2.81	1.67	3.18	2.31	1.65	2.53	1.46	1.35	1.41
62.1								1.51			1.14
63.1	6.68	1.23	6.39	19.65	5.86	3.03	7.22	2.30	1.07	1.17	1.35
64.0	1.46		1.36	1.25	1.40	1.32	1.85	1.15	1.04	1.05	1.47
65.1	2.48	2.11	2.45	1.89	2.31	2.11	2.96	1.76	1.46	1.39	1.67

66.1	2.16	2.14	2.09	1.71	2.14	1.63	2.35	1.58		1.01	1.49
67.1	14.25	15.95	15.49	11.87	11.89	10.27	13.79	8.79	4.40	4.03	3.54
68.1	16.88	21.81	18.33	13.96	13.29	10.72	14.55	9.00	3.58	2.93	2.38
69.1	51.02	62.85	58.06	43.51	40.17	36.64	44.69	25 73	11.22	9.74	7.45
70.1	30.65	47.56	33.47	23.01	20.78	17.80	19.46	10.62	4.06	3.57	2.50
71.1	34.12	20.50	31.79	50.35	37.36	21.33	43.52	32.37	9.39	6.97	4.47
72.1		1.35	2.80	4.68	1.68		5.84	4.85			
73.1	75.20	49.04	52.24	37.13	100.00	100.00	82.00	100.00	100.00	100.00	100.00
74.1		3.57	4.83	3.53	7.56	8.04	7.24	6.77	7.88	8.90	8.99
75.1		5.49	6.35	9.98	6.63	6.68	8.93	7 96	5.77	5.69	5.82
76.1			1.11		1.47	1.11	1.84	1 25			1.12
77.1	5.21	2.44	4.95	2.59	4.80	4.77	7.71	7.97	3.72	3.15	2.98
79.1	3.56	2.90	3.41	2.62	3.37	3.30	1.01	2.86	2.18	2.25	1.01
79.1											2.09
80.1		1.17	1.48	1.14	1.61	1.45	4.22	1.38		1.18	1.21
81.1	10.85	9.62	10.64	8.28	10.30	9.76	2.03	8.92	5.56	5.12	4.01
82.1	22.89	26.97	24.42	20.14	21.56	15.42	13.11	13.65	4.44	3.44	2.29
83.1	39.45	50.25	47.19	34.41	29.90	29.79	24.72	18.21	7.05	5.78	3.70
84.1	19.12	27.11	21.42	14.77	13.50	13.59	35.06	7.86	3.20	2.78	1.92
85.1	24.77	13.14	22.24	36.48	27.87	16.18	13.78	23.27	7.99	5.79	4.20
86.1	4.47	2.83	3.40	3.86	4.26	5.46	33.08	4.39	2.34	1.95	1.75
87.1	7.63	5.61	6.74	3.80	8.53	7.94	5.20	7.51	4.36	4.51	3.41
88.1	2.93	2.70	2.14	1.41	3.44	2.57	8.10	2.73	1.56	1.53	1.31
89.1	6.58	5.54	3.40	2.25	7.16	5.17	2.90	10.32	3.38	2.85	2.09
90.1		1.15			1.45		7.65	1.83			
91.1	4.75	1.34	1.66	4.73	10.93	2.35	1.80	6.06	1.88	1.41	1.44
93.1	1.45		1.25		1.46	1.44	13.69	1.29		1.09	1.19
94.1	1.23		1.08		1.36	1.26	1.14	1.12			
95.1	8.14	5.77	7.40	6.19	8.66	7.61	2.15	7.56	4.38	3.71	2.99
96.1	11.91	11.98	11.87	10.08	12.12	8.87	1.76	9.89	3.34	2.73	1.78

97.2	32.50	37.57	39.43	32.24	25.60	27 75	11.26	16.67	5.87	4.76	2.88
98.2	13.56	16.43	14.07	10.66	10.18	12.58	14.91	7.95	3.33	2.80	1.88
99.2	8.15	3.86	6.68	11.30	9.26	7.09	29.98	7.86	3.46	3.24	2.30
100.1	2.16	1.21	1.87	1.99	2.48	1.90	11.47	1.96	1.28	1.17	1.07
101.1	3.71	2.29	3.57	2.09	4.08	3.30	11.06	4.43	2.09	2.12	1.54
102.1	1.94	1.90	1.74		1.95	1.97	3.02	1.40		1.01	
103.1	2.74	1.68	2.33	1.50	2.95	3.00	4.60	2.96	1.90	1.58	1.54
104.1	1.40				1.19	2.50	2.12	1.49			
105.1						1.10	3.84				
107.1	1.79		1.14		1.42	1.71	1.73	3.07	1.32	1.07	
108.2					1.04	1.02	1.16	1.02			
109.1	3.61	2.18	2.83	2.88	4.43	3.05	3.07	4.25	1.92	1.93	1.20
110.2	5.77	5.16	5.65	5.02	6.29	4.44	1.44	5.43	1.87	1.48	1.19
111.2	19.05	20.42	22.62	21.26	15.28	16.46	5.63	10.49	3.27	2.90	1.55
112.2	8.12	9.54	9.25	7.23	6.07	7.15	7.41	4.19	1.88	1.61	1.24
113.1	6.63	2.99	5.57	8.19	7.39	5.91	17.61	6.35	3.43	2.91	2.24
114.1	1.48		1.16	1.40	1.80	1.44	7.16	1.30			
115.1	2.49	1.22	3.20	1.50	3.20	2.81	9.61	1.93	1.46	1.43	1.32
116.1	1.15				1.78	1.44	2.15	1.00			
117.1	1.93		1.45	1.49	1.99	2.91	3.14	2.02	1.87	2.06	1.82
118.1	1.13						1.46	3.42	1.01		
119.1	1.52	1.05	1.13		1.72	1.53	2.71	1.54	1.12	1.22	1.33
120.1										1.05	
121.1	1.60		1.27		1.45	1.92	1.48	1.81	1.39	1.44	1.16
123.1	2.51	1.28	1.80	1.92	3.39	2.23	1.99	3.28	1.51	1.31	1.04
124.2	3.32	2.25	3.17	2.82	3.96	2.96	2.98	4.02	1.27	1.02	
125.2	7.89	7.57	10.58	8.08	6.01	8.60	1.35	4.29	2.01	1.70	1.16
126.2	4.05	3.99	5.28	3.48	3.02	4.69	4.49	2.19	1.16	1.05	
127.2	3.21	1.54	2.68	3.82	3.53	3.01	5.30	2.97	1.76	1.52	1.21
128.1	1.32		1.14	1.30	1.49	1.21	8.89	1.14			

129.1	2.77	1.35	4.94	1.41	4.03	2.05	4.61	2.23	1.16	1.16	
131.1	2.12		2.14	1.14	1.78	3.15	5.29	2.16	3.02	3.24	1.71
132.1						2.14	2.14	1.20			
133.1	4.05	1.72	3.48	2.36	4.28	5.90	2.92	4.50	4.38	4.45	3.22
135.2	1.78		1.00		1.02	1.58	3.44	5.67	1.82	1.20	
137.1	2.03	1.03	1.55	1.46	2.63	2.08	1.26	2.61	1.39	1.18	
138.2	2.82	1.57	2.71	2.09	3.23	3.01	6.59	3.57	1.18		
139.2	3.51	2.64	4.47	3.13	3.05	4.41	2.40	2.39	1.35	1.22	
140.2	7.23	9.79	6.50	8.93	6.07	4.15	1.04	2.64	1.05	1.05	
141.2	2.70	1.91	2.20	2.51	3.21	2.71	3.97	2.11	1.51	1.26	
143.1	1.61	1.01	2.32		1.89	1.70	5.48	1.28			
144.2						1.03	4.98				
145.1	3.56	1.81	3.30	2.27	3.84	4.40	4.03	3.69	2.91	2.69	1.75
147.1	6.55	2.01	5.91	3.12	4.03	19.98	4.54	11.65	30.53	39.42	36.91
148.1	1.40		1.27			3.39	1.04	2.13	5.10	6.52	5.87
149.1	1.36		1.35		1.25	2.71	2.05	1.70	3.45	4.07	3.76
151.1	3.56	1.69	3.54	2.02	2.62	8.70	1.15	4.65	9.45	10.20	9.19
152.1	1.20		1.41			2.33	5.56	1.30	1.99	1.91	1.92
153.1	1.54		2.21	1.17	1.36	2.86	6.99	1.35	1.52	1.44	1.25
154.2			1.61			1.80	1.57				
155.2	1.52		1.41	1.14	1.82	2.14	1.68	1.60	1.38	1.07	
157.1	1.88		4.84	1.13	1.73	1.73	1.06	1.46	1.01	1.08	
159.1	1.02		1.02		1.12	1.26	4.07	1.04	1.35		
161.1						1.24	2.20				
163.1	2.96	1.49	3.04	2.27	3.35	3.93	2.15	2.97	2.29	1.87	1.24
165.2								1.32			
166.2	2.86		1.04	2.23	4.87	1.90	1.29	8.95	1.03		
167.2	1.17		1.22	1.06	1.41	1.46	2.58	2.07			
168.2	4.63	3.49	7.91	8.46	3.84	2.45	1.39	1.75		0.87	
169.2	2.39	1.50	2.73	3.42	2.94	2.02	2.11	1.84	1.03	1.31	

171.2	1.23		2.17	1.18	1.49	1.38	1.55	1.02			
175.1	1.01		1.06		1.06	1.32	1.35				0.68
177.1						1.13	4.45			0.74	0.58
181.1			1.10			1.44	1.31				0.58
183.2	2.48		1.58	3.01	4.23	4.84	4.16	3.07	1.56	1.02	0.64
185.2	1.52		1.33	1.73	3.06	1.61	1.54	1 39			
187.2			1.06	1.43	1.04		3.95			1.26	
189.1			1.14		1.05	1.41	2.37	1 01			
191.1	1.11		1.35			2.12	1.35	1.45	2.18	1.61	1.05
193.1						1.74	1.46	1.09	1.59	1.36	1.00
194.2								1.22	1.23		
195.1	1.41		1.61	1.39	1.53	2.14	1.10	1.54	1.76	1.23	
196.3	1.08		3.37	1.31		2.05	1.16				
197.2	1.52		1.43	2.22	3.51	1.53	2.48	1.68	0.98		
199.3	1.68		1.61	4.96	1.91		1.71	1.12			
200.3			1.92	1.07			1.01				
201.3						1.20	1.25				
205.2						1.11	1.01		1.53	1.10	
207.2	4.78	1.78	5.39	3.89	2.55	12.32	2.38	10.80	20.45	13.35	7.23
208.2	1.17		1.33			2.80	1.77	2.41	4.46	2.94	1.86
209.2	1.11		1.33			2.27	1.27	2.00	3.54	2.38	1.50
211.1	1.29		1.42	1.16	1.02	2.23	1.59	2.12	2.47	1.73	1.11
212.3					1.15		1.35				
213.2				0.92	1.11	1.01	3.08				
221.2	1.95		1.83	1.56		4.39	1.61	5.88	10.24	5.48	3.12
222.2						1.16	1.01	1.49	2.60	1.42	1.01
223.2								1.08	1.72		
225.2	4.35	1.67	4.69	3.64	1.81	10.81	1.21	12.24	20.59	10.67	5.61
226.2	1.11		1.22			2.32	2.36	2.87	4.64	2.55	1.51
227.1			1.03			1.68	0.45	1.99	2.93	1.53	1.23

233.1										0.21	
239.3	0.36			0.44			0.34	0.41	0.45	0.34	
241.2				0.34			0.33				0.39
243.9										0.17	
245.2				0.24			0.27				
249.1	0.34		0.41	0.33		0.52	0.41	0.49	0.73	0.53	0.48
251.1	0.34			0.31	0.28	0.52	0.28		0.66	0.58	0.44
253.1			0.37	0.29			0.86		0.43		0.40
255.2									0.28	0.31	
257.2				0.21			0.23				
258.3										0.15	
259.2				0.24	0.33		0.11		0.20		
260.2										0.15	
265.3						0.63	0.10	0.65		0.75	0.69
267.2	0.62		0.64	0.50	0.35	1.06	0.09	1.20	2.03	1.45	1.12
269.3				0.32	0.27		0.14				
271.2									0.49		
281.3	1.32	0.71	1.11	0.92	0.59	2.05	0.16	3.78	6.19	4.45	3.22
282.2								1.13	2.01	1.33	1.07
283.2									1.56	1.17	
285.2	0.62	0.48	0.61	0.45	0.34	1.04	0.15	1.13	1.79	1.39	1.03
293.3				0.09			0.15				
295.3										0.28	
297.2											0.35
299.3		0.37		0.33	0.19	0.59	0.11	1.57	2.06	0.84	0.60
300.3										0.39	
303.2				0.11	0.13		0.17		0.20	0.17	
304.3										0.14	
307.1									0.09		
308.4				0.07			0.11				

309.2						0.14	0.08				
309.8										0.15	0.21
311.1				0.07			0.09		0.11		
312.2				0.06			0.08			0.15	
314.5									0.11		
315.2				0.06	0.10	0.09	0.07			0.12	
317.3				0.06			0.06			0.14	
318.0										0.13	
319.6				0.07		0.08	0.12				
320.9				0.06			0.11				
325.3	0.20			0.13	0.11	0.36	0.06	0.35	0.55	0.50	0.30
326.4											0.36
327.3	0.25	0.22	0.27	0.21	0.17	0.33	0.07	0.36	0.56	0.47	0.38
329.3					0.12		0.06				
334.4				0.06			0.06				
339.2				0.08			0.07				
341.3	0.24	0.20	0.19	0.13	0.11	0.34	0.05	0.42	0.63	0.52	0.54
342.3											0.30
344.3					0.09		0.06				
345.2				0.07			0.06		0.16		
346.1					0.08		0.07				
347.3									0.12		
349.6				0.05			0.06				
351.3				0.05			0.04				
355.3	0.17	0.12		0.10	0.11	0.20	0.05	0.35	0.58	0.51	0.37
356.4	0.11						0.04	0.16			
357.4											0.27
359.3			0.10	0.08	0.10	0.14	0.04		0.23		
360.4	0.08						0.04				
362.9										0.14	

364.6				0.04			0.04				
365.5					0.07		0.05			0.11	
367.5									0.09		
368.3				0.05			0.04				
369.1				0.06	0.08		0.05				
373.3	0.09		0.10	0.08	0.08	0.16		0.18	0.35	0.27	0.26
374.2				0.05							0.21
376.9				0.04							
377.4	0.08				0.07			0.10			
379.3		0.07				0.09					
380.2				0.04							0.16
380.9										0.10	
382.7				0.05						0.10	
384.0											0.15
385.1			0.10		0.06	0.07			0.13		
387.4			0.09	0.05	0.06						
388.5				0.05						0.09	
389.2						0.08				0.11	0.21
390.5					0.06						
391.3				0.04		0.06					
392.5				0.04							
394.8				0.03							
395.5				0.03							
399.4			0.09							0.18	
401.3	0.13	0.12	0.10	0.12	0.08	0.23		0.17	0.33	0.34	0.33
402.5			0.11	0.07	0.07			0.11	0.20	0.18	
403.3									0.15		
405.3				0.05							
406.0				0.04							
406.6				0.04							

410.6				0.04						
411.9					0.06					
415.5	0.08	0.08	0.09	0.06	0.07	0.09	0.10	0.18	0.24	0.21
416.7	0.06					0.10		0.12	0.12	
417.4						0.08	0.06	0.09		0.17
418.3									0.09	
419.4				0.04				0.07		
421.7				0.03						
424.0				0.03	0.05					
426.7					0.05					
429.6	0.05			0.06		0.10	0.09	0.19	0.16	0.17
430.5				0.05				0.15	0.14	0.18
431.3	0.06				0.05		0.06	0.11		
433.5		0.05		0.04		0.08				
434.3			0.07					0.07		
435.8				0.04						
436.5				0.04	0.06					
437.5								0.05	0.08	
439.5						0.07				
440.7				0.03				0.06	0.09	0.16
443.0	0.05				0.05	0.06				
445.2			0.06	0.03						
445.9	0.05	0.05								
446.5								0.06		
447.8				0.04					0.07	0.17
451.6				0.03	0.04	0.06			0.08	
455.1				0.03						
458.1			0.06	0.03						
459.2						0.09			0.10	0.13
460.8				0.04		0.07				

461.6	0.07			0.05	0.05			0.11	0.13	0.13	0.13
463.1			0.06		0.05						0.13
464.0		0.05									0.12
465.3		0.05							0.09		
471.5				0.03							
472.3		0.04			0.05						
473.3				0.03					0.05		
474.3	0.04										
475.7	0.05					0.07			0.06	0.09	0.11
476.6								0.05	0.05	0.07	
477.7				0.03							
479.7									0.05		0.09
480.5									0.04		
481.4				0.03	0.04						
483.8											0.08
484.8	0.04										
485.5		0.04		0.03							0.08
487.4			0.06		0.04						
489.8				0.03		0.08		0.03		0.06	
490.5	0.03								0.05	0.07	
491.6				0.03					0.05		
493.4			0.05		0.04						
494.6				0.02	0.04						
496.5				0.03					0.04		
498.1		0.04			0.04						0.11
499.0	0.03										
501.1	0.03	0.04				0.05					
502.5		0.04									
503.5				0.02	0.04				0.06		
504.8				0.02							

506.2	0.04					0.05		0.04	0.05		0.12
509.1				0.02							
509.8				0.02							
510.5	0.04			0.02							
512.0	0.03				0.03	0.04					
512.6			0.04	0.02							
515.5									0.03		0.10
516.4		0.04		0.02	0.03						
517.2		0.04									
519.7					0.03				0.04		
520.6									0.04		
521.2	0.04			0.02					0.04	0.07	
522.6	0.03										0.11
523.4						0.04					
525.8				0.03							
526.5										0.08	0.10
527.4											0.10
529.1				0.02							
530.0	0.04	0.04			0.04						
533.1				0.03				0.03			
535.5			0.04	0.02	0.04			0.03	0.08		
536.5			0.05			0.05					
537.4									0.06		0.10
538.5									0.05		
539.4	0.03	0.03				0.04					
541.7			0.04								0.10
544.9				0.02							
547.1		0.03			0.03			0.04			
549.8	0.03			0.03					0.05	0.07	

Mass spectral data for Seaquest 091.

Time (min)	Seaq091	Seaq091	Seaq091	Seaq091	Seaq091	Seaq091
Start	15.72	18.391	19.27	20.217	20.627	21.608
End	16.872	19.236	20.089	20.456	21.608	22.521
m/z	Relative Intensity (%)					
41.1	100.00	83.41	86.38	73.07	77.91	78.97
42.1	33.64	32.35	30.91	30.92	34.04	35.24
43.1	99.12	100.00	100.00	97.13	100.00	100.00
44.1	27.67	27.44	25.82	28.00	34.35	37.70
45.1	54.76	61.77	84.05	61.04	66.80	71.11
46.1	2.69	2.96	3.00	2.65	3.37	3.89
47.0	3.85	4.40	4.32	4.90	6.31	6.65
48.0	1.15	1.17		1.10	1.16	1.66
49.0	1.41	1.46	1.21	1.35	1.72	2.04
50.0	3.03	2.88	2.43	2.64	3.37	3.96
51.0	4.49	4.51	3.78	4.34	5.42	5.57
52.1	2.44	2.24	1.89	2.14	2.58	2.72
53.0	10.09	9.04	8.19	8.16	9.28	9.23
54.1	7.74	7.19	6.72	6.76	7.42	7.42
55.1	46.40	43.99	43.34	40.40	42.24	39.53
56.1	13.97	11.86	12.42	11.63	11.51	11.63
57.1	30.52	29.62	33.37	30.91	28.62	28.34
58.1	4.98	6.54	6.44	6.87	7.27	7.00
59.1	4.95	6.64	6.73	7.56	7.53	7.13
60.1	4.27	5.36	4.46	5.39	6.81	5.72
61.1	2.51	2.70	2.63	3.56	3.14	3.09
62.1	1.44	1.61	1.73	1.65	1.85	2.25
63.1	3.98	3.24	1.96	2.04	2.70	2.78
64.0	1.79	2.07	1.62	2.01	2.30	2.64

65.1	3.18	3.21	2.79	3.05	3.64	3.63
66.0	2.20	2.25	1.95	2.17	2.61	2.83
67.0	8.84	8.60	8.37	8.09	9.10	8.33
68.1	5.76	5.30	5.13	5.10	5.39	5.23
69.0	18.19	17.90	17.17	17.34	18.08	17.05
70.1	6.14	5.21	5.15	5.07	4.88	4.76
71.1	9.99	10.18	11.31	10.70	10.23	9.73
72.0	1.31					
73.1	31.96	70.37	69.91	100.00	92.86	74.84
74.1	3.50	6.35	5.77	8.61	8.22	6.92
75.0	5.17	6.90	8.90	7.93	8.58	8.52
76.0	1.30	1.40	1.34	1.46	1.59	1.82
77.0	4.65	5.26	5.77	5.63	6.56	6.85
78.1	1.34	1.46	1.23	1.04	1.67	1.79
79.1	3.74	3.98	3.70	4.00	4.70	4.58
80.1	1.56	1.56	1.43	1.63	1.99	2.22
81.0	4.94	5.58	5.52	6.12	6.86	6.62
82.1	4.02	3.53	3.69	3.43	3.37	3.48
83.1	6.69	6.48	6.28	6.38	6.11	5.66
84.0	3.00	2.73	2.74	2.93	2.86	2.72
85.0	6.16	7.16	7.22	7.28	7.19	7.18
86.1	1.89	2.13	2.08	2.26	2.54	2.58
87.0	2.58	3.93	3.81	4.64	4.78	4.18
88.0	1.16	1.43	1.23	1.36	1.67	1.70
89.0	1.51	2.25	2.83	2.25	2.54	2.73
90.0					1.03	
91.0	1.83	1.92	1.76	1.81	2.11	2.26
92.0					1.06	
93.1	1.31	1.53	1.31	1.47	1.71	1.84
94.0		1.26		1.04	1.32	1.42

95.1	3.15	3.56	3.38	3.82	3.96	3.85
96.1	2.01	2.03	2.13	2.00	2.11	2.20
97.1	3.86	3.70	3.65	3.83	3.59	3 39
98.1	1.99	2.03	1.83	2.11	2.21	2.22
99.1	2.37	2.84	2.62	3.12	3.28	3.11
100.1	1.08	1.35	1.00	1.34	1.42	1.50
101.0	1.50	2.04	1.84	1 99	2.21	2.27
102.0		1.08			1.16	1.23
103.0	1.18	1.54	1.26	1.51	1.55	1.69
105.0		1.05		1.12	1.23	1.20
107.0	1.14	1.11	1.19	1.15	1.44	1.54
108.1					1.05	
109.0	1.26	1.41	1.34	1.43	1.60	1.59
110.0	1.11	1.17	1.11	1.06	1.27	
111.1	1.94	1.84	1.85	1.93	1.90	1.90
112.1	1.23	1.23		1.24	1.24	1.40
113.0	1.59	2.06	1.90	1.95	2.31	2.32
114.2						1.04
115.0	1.17	1.37	1.17	1.45	1.61	1.70
117.1		1.11		1.16	1.33	1.25
119.0				1.07	1.04	
121.0		1.01		1.17	1.03	
123.1					1.20	1.06
124.0						1.08
125.0	1.03	1.08			1.28	1.29
127.1		1.18	1.07	1.16	1.27	1.28
129.1				1.01		1.09
131.0		1.04		1.12	1.26	1.31
133.0	1.08	1.64	1.40	1.72	2.01	1.99
137.1					1.10	1.04

139.0						1.11
145.0		1.15		1.08	1.28	1.29
147.1	1.49	5.53	5.84	10.08	10.10	5.34
148.0		1.19	1.16	1.88	2.02	1.46
149.0		1.12	1.03	1.29	1.61	1.20
151.0	1.20	2.22	1.82	3.17	2.87	2.47
152.2						1.15
163.0					1.01	1.06
165.2	0.53					
175.2		0.51				
177.1		0.48				
183.2	0.52		0.63	0.78	0.79	
191.0	I	0.69				
193.0		0.56		0.62		
195.1	0.43					
207.0	0.75	1.68	1.58	2.56	2.63	1.80
221.0		1.03	1.07	1.53	1.82	1.01
225.1	0.47	1.36	1.46	2.35	2.49	1.39
240.0	0.28					
241.1			0.26			
244.8	0.28					
249.0	0.28			0.30	0.37	0.37
251.0		0.35	0.26			0.37
252.1			0.26			
265.0			0.28			0.47
266.9	0.32	0.54	0.51			0.40
267.2						0.38
281.1	0.37	1.12	1.11	1.73	1.95	1.21
285.1		0.53				
294.4	0.21					

298.1	0.20					
299.1	0.21			0.68	0.72	0.53
313.0	0.19		0.16			
314.5			0.16			
316.2	0.20					
321.8					0.27	
323.0					0.26	
325.1	0.21		0.16	0.33		0.35
325.9						
326.9	0.22	0.34			0.27	0.39
328.0			0.14			
329.1			0.14			
336.8	'					
341.0		0.31	0.29	0.43	0.39	0.33
344.8	0.17					
346.0	0.16					
346.8	0.16					
353.1	0.15					
353.9	0.16					
355.1		0.30	0.28	0.32	0.49	0.27
356.1		0.21		0.26		0.23
369.0						0.22
370.0				0.14		
371.6	0.13					
373.2			0.18	0.18	0.30	
374.8	0.12				0.20	0.23
379.7	0.11					
384.2						
385.0		0.15				
386.2		0.13				

386.7		0.13				
387.7						
389.9	0.12					
390.6	0.11					
391.4				0.14		
392.9						0.21
395.6	0.11		0.11			
397.9						
398.9		0.15		0.16		
399.1						
400.0	0.11					0.20
401.0	0.11	0.17	0.14	0.16	0.23	0.19
402.8	0.12					
409.1			0.11			
412.1	0.11					
413.3						0.19
414.5		0.15				
415.3						0.18
416.1						
417.6					0.10	
422.5	0.11			0.11		
426.6						
427.4	0.10					
429.2					0.14	
430.1				0.15		0.14
431.0			0.09			
433.2			0.08			
436.3	0.11					
440.2	0.10					
443.5					0.10	

444.4		0.12				
446.0						0.14
448.2				0.09	0.11	
451.1						0.13
452.5			0.08			
456.0						0.13
457.0					0.10	
457.9	0.08					
460.4				0.09		
461.1	0.08	0.08		0.09		
464.2	0.07	0.10				
466.8		0.09				
467.8			0.05			
468.7						
469.5					0.09	
471.5				0.09		
472.3					0.10	0.15
474.9	0.08		0.05			
477.5		0.08				
483.1						
483.9			0.05			
485.9						
487.0	0.08			0.08		0.11
488.2		0.07			0.08	
489.9	0.07					
493.7		0.08	0.05			0.10
497.0					0.07	
505.1	0.07	0.07				
507.5			0.05			
508.2			0.06		0.06	

512.7				0.10		0.08		
514.8								
518.6	0.05							
522.5		0.06			0.07	0.08		
524.8					0.07			
527.2		0.06				0.08		
530.9				0.12				
531.9								
533.1			0.04	0.09				
537.1	0.07							
537.8			0.03					
539.1								
541.6		0.06						
542.1								
543.1					0.05			
544.4		0.07				0.09		
546.4	0.07				0.05	0.08		

Mass spectral data for Sorbac 80T.

Time (min)	Sorbac80T	Sorbac80T	Sorbac80T	Sorbac80T	Sorbac80T	Sorbac80T	Sorbac80T	Sorbac80T
Start	6.638	9.557	10.956	19.711	20.889	24.507	27.647	33.143
End	7.816	10.598	12.134	20.684	22.852	25.275	28.961	34.389
m/z	Relative Intensity (%)							
41.1	76.03	100.00	100.00	29.80	77.16	25.49	25.77	19.51
42.1	34.73	39.94	35.87	10.54	21.43	9.59	10.72	8.91
43.1	64.69	87.27	79.13	49.77	100.00	43.96	36.67	22.47
44.1	100.00	90.76	75.74	23.02	37.29	24.04	25.51	17.01
45.1	16.52	18.80	19.02	15.34	25.91	12.48	12.81	10.39
46.1	5.81	4.96	3.84	1.48	2.20	1.34	1.64	1.60

47.0	28.54	9.11	5.39	4.28	5.38	2.75	3.34	3.34
48.1	1.38	1.32	1.06					1.14
49.0	9.47	3.34	2.06	1.00	1.40		1.37	1.64
50.1	16.59	7.14	5.20	1.81	2.76	1.69	2.39	2.52
51.1	4.50	6.97	7.36	4.75	7.96	4.35	5.13	4.18
52.1	2.17	3.25	3.41		1.77		1.40	1.71
53.1	8.56	14.85	15.44	4 47	9.93	3.84	4.39	3 73
54.1	7.44	11.14	11.88	4.88	14.41	3.50	3.55	2.91
55.1	37.74	55.30	52.78	20.33	58.28	16.70	14.33	9.53
56.1	28.54	28.81	22.34	6.35	16.72	4.93	4.77	3.46
57.1	34.93	36.65	40.45	11.89	26.08	10.27	8.87	5 74
58.1	7.39	7.62	8.69	2.98	4.79	3.15	2.83	2.33
59.1	3.81	3.73	3.97	7.58	10.79	5.66	5.03	3.81
60.1	5.97	11.01	10.02	6.28	14.41	4.24	4.23	3.30
61.1	1.89	2.33	2.22	1.78	3.01	1.26	1.47	1.57
62.1	3.15	1.84	1.52	1.16	1.69		1.18	1.13
63.1	1.44	1.88	2.07	1.82	2.45	1.18	1.48	1.65
64.1		1.63	1.77	3.56	5.85	3.06	3.42	2.67
65.1		4.22	5.59	4.12	7.66	3.46	3.59	2.68
66.1	30.32	10.29	7.45	1.71	3.02	1.24	1.58	1.65
67.1	10.24	14.45	17.07	7.37	19.42	4.98	4.22	3.15
68.1	18.39	14.65	14.03	4.70	11.32	2.98	2.90	2.40
69.1	15.43	23.89	27.12	21.51	48.08	16.56	15.92	10.50
70.1	17.07	29.60	29.24	4.44	11.85	3.21	3.04	2.23
71.1	9.00	11.47	11.88	4.29	9.30	4.43	3.53	2.49
72.2	4.66	5.86	4.13					
73.1	6.27	20.85	28.93	100.00	94.62	100.00	100.00	100.00
74.1	1.59	3.03	3.59	9.20	9.22	8.99	9.04	9.11
75.1	1.23	2.28	2.69	6.34	7.79	5.77	6.03	5.73
76.1					1.30		1.13	1.32

77.1	2.15	4.45	5.58	5.05	7.93	4.00	4.19	3.46
78.1	4.57	2.53	2.24	1.12	1.95	1.01	1.13	1.30
79.1	4.09	8.22	9.21	7.47	11.30	4.16	3.87	2.74
80.1	2.79	3.57	3.11	2.07	3.72	1.43	1.48	1.30
81.1	14.38	24.22	35.87	12.48	20.94	6.92	6.15	4.17
82.1	13.65	10.54	12.75	3.86	9.32	2.58	2.19	1.69
83.1	7.81	17 40	18.39	5.80	16.77	4.22	3.38	2.33
84.1	9.60	10.21	9.62	3.31	9.28	2.32	2.02	1.51
85.1	55.89	19.52	13.61	4.71	8.25	3.64	3.54	2.49
86.1	3.55	5.43	9.01	1.84	2.71	1.31	1.40	1.30
87.1	17.65	6.47	4.87	2.86	4.76	2.14	2.29	1.93
88.1		1.00			1.21			
89.1		1.10	1.05	1.29	2.22	1.20	1.40	1.19
91.1	1.11	2.08	2.45	1.89	3.66	1.84	1.77	1.51
92.1			1.03	1.29	1.51			
93.1	1.20	2.84	3.10	1.55	3.10	1.37	1.39	1.32
94.1	1.56	3.21	3.03	1.49	2.90	1.20	1.14	1.05
95.1	5.05	8.16	9.36	8.58	16.94	7.42	6.83	4.02
96.1	4.67	4.36	5.07	3.57	8.75	2.36	2.04	1.57
97.1	3.06	5.80	5.78	3.93	11.75	3.07	2.47	1.84
98.2	4.36	6.02	5.48	2.37	6.71	1.81	1.61	
99.1	2.37	2.38	2.40	1.74	3.39	1.52	1.52	1.28
100.1			2.41	1.23	2.53	1.12	1.27	1.25
101.0	89.37	22.76	10.50	2.27	4.05	1.74	1.72	1.52
102.1					1.11			
103.1	53.08	13.12	6.19	1.01	1.55		1.17	1.12
105.1	9.02	2.99	1.77		1.66		1.03	
107.1		2.43	2.03	1.31	2.32	1.24	1.28	1.05
108.1		1.40	1.55	1.02	2.07		1.12	
109.1	1.05	1.70	2.17	2.13	4.72	2.28	1.74	1.23

110.1	1.07	2.99	1.77	1.52	4.22	1.29	1.30	1.03
111.1		2.48	2.74	1.92	5.30	1.71	1.43	1.16
112.2		2.06	2.45	1.14	2.84			
113.1	1.32	1.93	2.30	5.19	9.80	5.09	4.90	2.95
114.2	1.16	1.05			2.33			1.01
115.1		1.07	1.35	1.32	2.62	1.27	1.43	
116.1	9.59	2.65	1.45					
117.1	3.76	1.49	1.07	1.31	1.86	1.33	1.37	1.49
118.0	3.41	1.23						
119.0	3.32	1.41	1.19	1.29	2.44	1.20	1.36	1.13
120.1				1.09	1.42			
121.1	1.39	1.77	2.60	1.51	2.61	1.31	1.31	1.21
122.1					1.40			
123.1		1.44	1.44	1.25	3.01	1.15	1.09	1.08
124.1		1.01	1.60		2.27			
125.1		1.28	1.31	1.28	3.04	1.26	1.17	1.05
126.1					1.79		1.00	1.00
127.1				1.40	3.08	1.36	1.44	1.21
128.1				1.09	1.81		1.17	
129.1					1.76			
131.1				1.61	2.42	1.63	1.83	1.57
132.0	2.36	1.02						
133.1				6.01	11.01	6.70	6.93	4.43
133.2		1.47	1.70					
134.1	1.76				1.47			
135.2				1.17	2.06	1.09	1.14	
137.1				1.07	2.27		1.06	
138.1					1.76			
139.1				1.44	2.83	1.24	1.28	1.04
140.2					1.07			

141.1					1.78	1.02	1.08	
143.1					1.19			
145.1		1.13	1.32	4.12	7.24	4.09	4.25	2.87
147.1		1.38	1.98	10.56	11.93	15.37	19.78	22.73
148.2				1.95	2.79	2.71	3.53	4.04
149.2				1.67	2.15	1.85	2.28	2.50
150.2					1.34			
151.1	43.54	11.22	5.86	4.24	4.79	4.21	4.35	4.78
152.2			1.25	1.01	1.59		1.10	1.21
153.1	27.91	7.15	3.57	1.02	1.67	1.00	1.10	1.21
155.0	4.59	1.47						
157.1					1.47			
159.1					1.47		1.02	
161.1					1.34			
163.1			1.12	3.35	6.10	3.35	3.62	2.34
165.2					1.27			
169.1	0.84				1.55			
175.1					1.58	0.91	1.02	
177.1					1.47	0.92	1.16	
179.1					1.04			
181.1		0.52	0.47		1.34			
183.1					1.25			
185.1					1.54			
187.1					1.10			
189.1			0.53		1.65		1.02	
191.0		0.58		1.07	1.49	1.14	1.37	1.33
193.1	0.33				1.15			1.00
195.0	0.32			1.37	2.43	1.47	1.63	1.25
197.1					1.62	1.01	1.19	
205.1							1.03	1.02

207.1	0.65	1.38	1.76	7.19	7.47	8.33	9.78	9.86
208.0				1.60	1.71	1.82	2.28	2.46
209.1				1.47	1.71	1.68	1.92	1.95
211.0				1.04	1 29	1.03	1.26	1.24
213.1					1 57		1.14	
221.1				4.21	4.84	5.93	7.72	7.35
222.1				1 20	1 68	1.62	2.16	2.19
223.1					1.38	1.27	1.60	1.61
225.1	0.58	1.55	2.22	9.81	8.60	11.01	11.85	11.11
226.1				2.27	2.14	2.65	2 99	2.95
227.0				1.73	1.90	1.86	2.24	2.16
239.1	0.33	0.36			1.30			0.55
241.1					0.95			
249.0						0.58		0.65
251.1			0.33		0.86	0.67		
253.1		0.30				0.54		
254.5	0.27							
255.2		0.28						
264.3					1.24			
265.0					1.24	1.09	1.33	1.29
267.1	0.30	0.55		1.54	1.74	2.04	2.65	2.44
269.1							1.12	
281.1	0.42	1.17	1.55	7.79	7.68	11.10	12.05	9.45
282.1				2.65	2.78	3.55	4.07	3.42
283.1				2.24	2.38	2.90	3.39	2.57
285.0	0.35	0.69		2.10	2.07	2.22	2.37	2.03
295.1					1.02	1.28	1.55	
299.1		0.79	1.12	7.67	7.11	10.10	10.47	6.59
300.2	0.23			2.38	2.22	3.21	3.35	1.94
301.1				1.36	1.45	1.73	1.87	

304.1	0.23							
311.1						0.35		
315.2	0.19							
317.1	0.22							
318.6	0.21							
325.1					1.18	1.37	1.38	0.89
327.0		0.40	0.51	1.17	1.33	1.50	1.36	1.05
330.0	0.19							
330.7	0.19							
341.1		0.52	0.64	2.27	2.20	2.79	2.37	1.56
342.1	0.20					1.02		
343.4	0.19							
349.3	0.18							
350.1	0.19							
355.1	0.19	0.42	0.54	3.78	3.71	4.54	3.43	1.71
356.1				1.44	1.48	1.76	1.38	
357.1				1.09	1.17	1.36	1.01	
359.1	0.19	0.31		1.14	1.18	1.34		
373.2	0.20	0.33	0.42	2.67	3.01	4.45	2.32	1.04
374.1	0.17				1.10	1.53	0.94	
375.1						1.10		
377.0		0.26						
381.2	0.15							
385.0	0.15					0.40		
387.1						0.27		
389.1					0.38			
389.8	0.16							
395.2	0.15							
399.1						0.64		
401.0		0.32	0.42	1.39	1.55	1.73	1.04	0.46

402.7	0 16							0.32
409.8	0.15							
415.1	0 14	0.23	0.38	1.25	1.22	0.99		0.30
416.2						0.45		0.25
429.1		0.21	0.32	1.37	2.29	1.51	0.68	0.26
430.1	0 14	0.18			1.03	0.66		0.23
431.0	0 14							0.22
433.0								0.19
445.0		0.15						
447.1					0.36	0.20	0.16	
448.5	0.16							0.11
449.1		0.16						
451.1			0.15			0.11		
453.2			0.12					
455.2	0.13							
459.0					0.40	0.34	0.21	
461.0		0.14		0.84	0.64	0.40	0.24	0.18
462.1								0.17
470.9		0.15						
473.5	0.12							
475.1				0.52	0.41	0.26	0.14	0.14
476.3	0.11		0.12					
477.0					0.25	0.14	0.12	
479.0	0.11							0.14
480.8						0.06		
482.2		0.11						
487.9	0.11	0.10						
489.2		0.10	0.11		0.31	0.15	0.08	0.13
490.0						0.11		
491.2	0.11				0.19	0.11	0.08	

494.3		0.10						0.12
498.7		0.09						
503.1	0.12		0.10	0.36	0.39	0.26	0.09	
504.2						0.15		
505.2					0.23			
506.2							0.08	0.11
507.0	0.11		0.09					0.12
512.1		0.11						
513.9		0.10						
515.7	0.10							
517.1					0.17	0.08		0.11
519.1					0.23	0.11	0.10	
521.1		0.10			0.17			0.10
525.0	0.10							
527.2								0.10
529.4		0.10					0.09	
531.1	0.09		0.09					
532.9		0.09		0.22	0.19	0.11		
535.1				0.18	0.36	0.18	0.10	
535.9							0.08	
536.9				0.17	0.22	0.11		0.12
537.5			0.09					
538.3		0.09						
539.1						0.08		
539.9								0.11
540.6	0.09							
543.0	0.10							
545.1						0.04		
547.3			0.08			0.04		
548.1								0.11

548.8			0.07				0.10		0.05	

Mass spectral data for Pond Effluent.

Time (min)	Pond201	Pond202	Pond203	Pond204	Pond205	Pond206	Pond207	Pond208	Pond209	Pond210
Start	16.91	18.53	20.20	22 13	24.50	26.79	32.47	39.52	50.02	52.46
End	17 37	19.21	20.75	22.66	24.96	28.48	33.00	40.13	50.63	54.30
m/z	Relative Intensity (%)									
41.1	1.67	1.55	2.29	2.28	2.36	2.62	1.21	0.74	0.62	0.58
42.2	1.68	1.71	2.25	2.37	2.80	3.25	3.22	2.64	2.40	2.51
43.1	6.22	6.21	7.62	7.45	8.62	9.40	9.01	6.34	4.78	5.33
44.1	14.94	17.95	21.34	24.86	34.42	44.63	57.19	50.91	49.48	53.53
45.1	2.57	2.81	3.73	4.28	5.46	6.52	7.03	6.06	5.88	6.21
46.1									1.12	1.15
47.1	14.56	14.37	14.40	14.53	15.17	15.73	14.76	10.13	7.93	7.77
48.1	0.23	0.42	0.44	0.54	0.79	0.98	1.17	0.91	0.87	0.91
49.1	5.03	4.86	4.69	4.81	4.89	4.94	4.41	2.87	2.06	2.01
50.1	8.25	8.14	7.74	7.87	7.77	7.83	7.13	4.49	3.04	2.88
51.1	0.93	1.20	1.29	1.39	1.69	2.12	2.32	1.74	1.39	1.43
52.1	0.28	0.35	0.37	0.36	0.50	0.65	0.74	0.53	0.44	0.45
53.1	0.44	0.48	0.53	0.55	0.74	0.86	0.97	0.75	0.63	0.64
54.1	0.37	0.40	0.45	0.48	0.61	0.69	0.80	0.60	0.53	0.53
55.1	0.58	0.71	0.87	0.87	0.91	1.16	1.05	0.79	0.67	0.69
56.1	0.42	0.45	0.57	0.62	0.70	0.84	0.86	0.67	0.49	0.54
57.1	1.23	1.17	1.64	1.65	1.79	1.97	1.62	1.09	0.88	0.93
58.2	1.02	1.02	1.27	1.46	1.58	1.75	1.60	1.12	0.89	0.97
59.1	4.25	3.67	5.31	5.67	5.64	6.21	5.05	3.77	3.49	3.68
60.1	0.48	0.53	0.72	0.70	0.91	1.06	1.13	0.91	0.82	0.87
61.0	0.83	0.88	1.03	1.16	1.53	1.83	2.09	1.74	1.80	1.95
62.1	1.64	1.67	1.77	1.76	1.84	1.98	1.95	1.31	0.99	1.01

63.1	0.51	0.55	0.66	0.71	0.90	1.05	1.16	0.99	0.87	0.89
64.1	0.75	1.02	1.16	1.27	1.55	1.86	2.07	1.62	1.42	1.42
65.0								1.66	1.47	1.53
66.0	20.38	19.90	19.56	19.64	19.30	19.13	17.00	10.40	6.81	6.56
67.1	1.03	1.12	1.18	1.18	1.44	1.52	1.57	1.11	0.95	0.97
68.0	6.77	6.52	6.41	6.42	6.57	6.61	5 95	3.84	2.62	2.50
69.1	3.20	4.03	4.51	4.55	5.50	6.22	6 48	4.72	3.78	3.86
70.1	0.89	0.92	0.92	0.94	1.07	1.22	1.19	0.94	0.68	0.68
71.2	0.41	0.54	0.62	0.70	0.81	1.04	1.01	0.80	0.72	0.75
73.1	11.51	17.36	22.50	27.97	42.50	54.17	46.67	30.25	31.03	36.26
74.1	1.45	1.98	2.47	3.06	4.42	5.49	5 16	3.52	3.56	4.03
75.1	1.46	2.03	2.55	3.13	4.50	5.81	6.49	5.40	5.51	6.02
76.1	0.34	0.43	0.49	0.56	0.80	0.97	1 17	0.92	0.92	0.93
77.1	1.25	1.72	2.00	2.43	3.30	4.22	4.75	4.17	4.01	4.33
78.1	3.42	3.40	3.48	3.67	3.79	4.04	3.84	2.64	2.12	2.11
79.1	2.24	3.02	4.18	5.98	8.76	11.29	14 99	13.88	14.33	15.78
80.0	1.44	1.53	1.66	1.89	2.25	2.50	2.78	2.29	2.08	2.14
81.1	2.14	2.86	3.60	4.97	6.29	8.20	10.18	8.89	9.27	10.35
82.0	5.40	5.48	5.47	5.66	6.18	6.42	6.26	4.52	3.68	3.89
83.1	0.41	0.78	0.92	0.96	1.27	1.52	1.58	1.28	1.18	1.26
84.1	4.51	4.44	4.24	4.00	4.03	4.19	3.78	2.20	1.51	1.45
85.1	46.58	45.73	45.24	46.23	45.76	46.18	40.83	26.46	18.84	18.26
86.1	1.43	1.74	1.46	1.73	1.79	1.79	1.91	1.34	0.93	1.04
87.1	15.96	15.68	16.76	17.26	17.00	17.73	14.90	9.88	7.53	7.53
88.1	0.54	0.58	0.73	0.92	1.21	1.50	1.68	1.45	1.47	1.59
89.1	0.45	0.63	0.85	1.13	1.73	2.29	2.92	2.66	2.84	3.16
90.0	0.19	0.28	0.33	0.37	0.51	0.65	0.76	0.64	0.62	0.67
91.1	0.77	0.88	1.04	1.09	1.29	1.56	1.82	1.45	1.23	1.25
92.1	0.27	0.33	0.39	0.36	0.43	0.52	0.60	0.49	0.37	0.37
93.0	0.36	0.46	0.52	0.57	0.71	0.83	0.90	0.74	0.58	0.61

94.1	0.87	0.93	0.99	1.08	1.33	1.47	1.74	1.32	1.13	1.19
95.1	1.38	2.09	2.31	2.41	2.98	3.42	3.59	2.49	2.08	2.11
96.1	1.05	1.66	2.45	4.15	6.67	9.46	13.41	13.10	15.41	17.46
97.1	1.66	1.79	1.96	2.23	2.63	3.08	2.85	1.38	0.38	0.50
98.1	0.45	0.44	0.51	0.57	0.75	0.91	0.94	0.81	0.74	0.80
99.1	0.99	1.08	1.17	1.15	1.25	1.36	1.32	0.88	0.67	0.68
101.0	100.00	100.00	100.00	100.00	100.00	100.00	88.27	55.46	38.11	36.41
103.0	62.23	62.21	61.72	62.98	62.72	64.40	57.24	37.17	26.83	26.16
104.1	0.83	1.21	1.11	1.43	1.78	2.04	2.33	1.81	1.70	1.70
105.0	10.27	10.42	10.43	10.69	11.14	11.17	10.44	7.13	5.48	5.38
106.1	0.45	0.52	0.61	0.65	0.72	0.93	0.98	0.86	0.70	0.73
107.0	0.33	0.41	0.44	0.54	0.63	0.88	1.01	0.84	0.76	0.80
108.1	0.27	0.36	0.39	0.42	0.53	0.60	0.67	0.52	0.45	0.44
109.1	0.41	0.52	0.59	0.61	0.78	0.87	0.87	0.68	0.59	0.58
110.0	0.02	0.27	0.31	0.35	0.41	0.56	0.59	0.50	0.44	0.44
111.0	0.36	0.45	0.55	0.53	0.72	0.83	0.86	0.71	0.62	0.64
112.1	0.26	0.33	0.38	0.51	0.69	0.76	0.97	0.73	0.58	0.62
113.1	1.82	2.45	2.79	2.80	3.24	3.62	3.53	2.48	1.95	1.90
114.1	0.37	0.40	0.51	0.52	0.64	0.74	0.77	0.51	0.44	0.45
115.1	0.18	0.60	1.58	2.04	2.77	3.29	3.80	3.33	3.30	3.52
116.1	12.62	12.51	12.30	12.34	12.30	12.24	10.92	6.89	4.54	4.25
117.0	5.06	5.13	5.55	5.73	6.02	6.43	5.75	4.09	3.16	3.23
118.0	4.43	4.44	4.37	4.48	4.64	4.78	4.53	2.89	2.05	2.01
119.0	4.57	4.86	5.13	5.68	6.48	7.39	7.96	6.44	5.85	6.04
120.1	0.20	0.31	0.47	0.50	0.70	0.88	1.05	0.90	0.82	0.90
121.0	1.68	1.85	1.88	1.93	2.19	2.37	2.43	1.78	1.47	1.48
122.0	0.26	0.33	0.37	0.38	0.53	0.63	0.67	0.56	0.48	0.47
123.1	0.47	0.63	0.67	0.68	0.95	1.07	1.21	0.95	0.89	0.89
124.1	0.22	0.25	0.25	0.33	0.32	0.48	0.51	0.36	0.31	0.29
125.1	0.38	0.54	0.61	0.75	0.95	1.28	1.52	1.35	1.32	1.42

126.1	0.29	0.38	0.44	0.50	0.75	0.81	0.91	0.70	0.65	0.68
127.0	0.40	0.54	0.64	0.70	1.04	1.04	1.03	0.80	0.67	0.68
128.0	0.22	0.28	0.33	0.35	0.55	0.49	0.47	0.37	0.30	0.31
129.1	0.27	0.34	0.41	0.44	0.58	0.61	0.62	0.51	0.41	0.42
130.1	0.21	0.19	0.26	0.28	0.32	0.32	0.33	0.31	0.25	0.23
131.1	0.60	0.92	1.04	1.25	1.83	2.02	1.91	1.41	1.25	1.33
132.0	3.71	3.72	3.80	3.93	4.75	4.39	4.20	2.95	2.21	2.15
133.1	2.17	3.70	4.75	6.45	10.54	12.38	15.17	13.44	13.73	14.56
134.0	2.39	2.69	2.69	2.94	3.96	3.77	4.13	3.13	2.86	2.80
135.0	0.46	0.65	0.79	1.02	1.67	1.99	2.61	2.36	2.42	2.52
136.0	0.52	0.59	0.62	0.67	1.01	0.95	1.06	0.81	0.69	0.70
137.1	0.54	0.75	0.95	1.22	2.32	2.85	3.92	3.94	4.24	4.47
138.1	0.28	0.34	0.38	0.43	0.67	0.76	0.91	0.79	0.79	0.82
139.1	0.49	0.64	0.75	0.76	1.10	1.13	1.25	1.00	0.84	0.88
140.1	0.25	0.35	0.38	0.43	0.61	0.66	0.78	0.58	0.55	0.54
141.1	0.35	0.55	0.63	0.68	0.92	0.98	0.91	0.76	0.63	0.62
142.0	0.10	0.16	0.20	0.20	0.23	0.32	0.21	0.18	0.19	0.19
143.0	0.31	0.37	0.44	0.46	0.62	0.67	0.76	0.54	0.42	0.43
144.0	0.26	0.35	0.42	0.43	0.57	0.58	0.62	0.42	0.33	0.32
145.1	1.35	1.92	2.26	2.37	3.30	3.39	3.14	2.16	1.60	1.70
146.1	0.19	0.12	0.14	0.25	0.11	0.12	0.21	0.30	0.28	0.28
147.1	2.81	5.29	7.38	9.68	18.09	23.04	18.07	10.95	10.74	12.24
148.1	0.70	1.05	1.44	1.82	3.40	4.21	3.57	2.25	2.08	2.36
149.1	0.69	1.06	1.31	1.64	2.83	3.45	3.39	2.49	2.44	2.70
151.0	83.02	84.90	86.44	86.66	100.00	88.12	76.69	48.59	30.64	28.07
153.0	53.22	54.79	55.09	55.99	64.93	56.35	49.84	30.80	19.83	17.95
154.0	1.47	1.50	1.52	1.62	2.02	1.82	1.78	1.16	0.84	0.79
155.0	8.37	8.86	9.11	9.39	10.45	9.40	8.73	5.57	3.73	3.47
156.0	0.40	0.45	0.50	0.54	0.64	0.69	0.79	0.53	0.42	0.41
157.1	0.34	0.46	0.61	0.60	0.86	0.81	0.88	0.64	0.48	0.48

158.1	0.18	0.25	0.30	0.30	0.43	0.45	0.51	0.32	0.23	0.24
159.1	0.46	0.56	0.66	0.66	0.95	1.02	1.03	0.74	0.63	0.67
160.0	0.14	0.19	0.25	0.27	0.38	0.36	0.33	0.29	0.25	0.21
161.0	0.39	0.50	0.63	0.90	1.50	1.70	2.09	1.94	1.95	1.95
162.1	0.22	0.28	0.33	0.40	0.61	0.82	0.99	0.90	0.86	0.84
163.0	1.36	2.17	2.54	3.11	4.65	5.05	5.77	4.78	4.27	4.41
164.0	0.26	0.36	0.46	0.52	0.87	0.98	1.15	0.98	0.89	0.92
165.0	0.28	0.42	0.58	0.77	1.33	1.54	2.08	1.83	1.80	1.93
166.0	0.12	0.14	0.23	0.25	0.43	0.49	0.60	0.51	0.49	0.47
166.9	0.97	1.01	1.03	1.04	1.41	1.32	1.39	0.93	0.74	0.72
168.0	0.14	0.22	0.24	0.25	0.40	0.39	0.41	0.34	0.29	0.26
169.0	1.05	1.17	1.21	1.23	1.48	1.42	1.34	0.86	0.63	0.60
170.1	0.14	0.23	0.26	0.26	0.38	0.38	0.38	0.25	0.21	0.17
171.0	0.41	0.48	0.56	0.52	0.69	0.65	0.67	0.42	0.30	0.30
172.0	0.18	0.23	0.28	0.30	0.44	0.41	0.45	0.30	0.22	0.19
173.1	0.19	0.28	0.31	0.34	0.46	0.46	0.43	0.29	0.25	0.23
174.1	0.12	0.18	0.20	0.20	0.26	0.31	0.23	0.20	0.13	0.14
175.1	0.36	0.49	0.64	0.67	0.93	0.97	1.01	0.80	0.60	0.63
176.1	0.20	0.34	0.42	0.62	1.01	1.22	1.67	1.56	1.52	1.56
177.0	0.47	0.81	1.23	1.90	3.63	4.50	6.23	5.97	6.16	6.45
178.0	0.20	0.33	0.46	0.71	1.44	1.96	2.89	2.86	2.99	3.16
179.0	0.32	0.52	0.84	1.27	3.04	4.25	6.66	6.83	7.48	7.89
180.0	0.17	0.29	0.34	0.41	0.78	0.96	1.33	1.35	1.35	1.43
181.0	0.39	0.51	0.59	0.70	1.18	1.27	1.50	1.34	1.29	1.30
182.1	0.15	0.22	0.24	0.30	0.40	0.43	0.44	0.40	0.33	0.34
183.0	0.28	0.40	0.47	0.52	0.77	0.76	0.79	0.59	0.43	0.48
184.1	0.10	0.14	0.16	0.12	0.19	0.24	0.18	0.18	0.12	0.10
185.0	0.34	0.45	0.55	0.49	0.71	0.73	0.79	0.61	0.44	0.41
186.0	0.24	0.24	0.28	0.28	0.35	0.34	0.37	0.22	0.16	0.14
187.0	0.43	0.56	0.64	0.62	0.88	0.87	0.87	0.65	0.45	0.48

188.1	0.26	0.31	0.37	0.39	0.55	0.48	0.52	0.34	0.22	0.19
189.1	0.51	0.60	0.72	0.84	1.20	1.28	1.38	1.10	0.98	0.98
190.1	0.22	0.26	0.33	0.28	0.29	0.24	0.28	0.18	0.04	0.05
191.1	0.80	1.40	2.16	3.95	7.53	9.19	12.53	11.88	11.92	12.36
192.1	0.26	0.41	0.63	0.95	1.81	2.21	2.93	2.71	2.69	2.79
193.1	0.64	1.05	1.50	2.30	4.25	5.13	6.79	6.19	6.05	6.29
194.0	0.30	0.44	0.58	0.73	1.18	1.36	1.67	1.48	1.36	1.38
195.0	0.52	0.81	1.01	1.17	1.73	1.94	2.07	1.69	1.52	1.56
196.0	0.11	0.18	0.20	0.25	0.35	0.45	0.51	0.41	0.34	0.33
197.0	0.32	0.51	0.64	0.69	0.97	1.03	1.13	0.83	0.70	0.68
198.0	0.10	0.14	0.15	0.17	0.30	0.29	0.27	0.22	0.16	0.20
199.0	0.25	0.20	0.23	0.25	0.40	0.38	0.40	0.33	0.26	0.25
200.1	0.14	0.18	0.19	0.20	0.30	0.27	0.22	0.13	0.15	0.14
201.0	0.24	0.33	0.37	0.38	0.48	0.54	0.56	0.45	0.33	0.31
202.0	0.06	0.07	0.11	0.12	0.14	0.19	0.14	0.08	0.09	0.07
203.0	0.32	0.42	0.48	0.51	0.69	0.83	0.90	0.69	0.60	0.56
204.0	0.10	0.15	0.18	0.21	0.26	0.32	0.35	0.31	0.22	0.23
205.1	0.26	0.45	0.60	0.76	1.12	1.50	1.50	1.07	0.95	1.05
207.1	4.23	8.70	15.14	28.48	52.34	75.53	100.00	100.00	100.00	100.00
208.1	0.97	2.00	3.34	6.18	10.92	16.14	21.82	20.37	21.10	21.85
209.1	0.74	1.40	2.33	4.25	7.09	9.87	13.19	12.75	12.65	12.91
210.1	0.16	0.33	0.49	0.80	1.26	1.80	2.34	2.13	2.13	2.16
211.0	0.70	1.13	1.41	1.93	3.01	4.13	4.83	4.49	4.52	4.72
212.0	0.23	0.39	0.44	0.51	0.77	1.00	1.22	0.94	0.91	0.93
213.0	0.36	0.64	0.76	0.79	1.02	1.24	1.34	1.05	0.86	0.84
214.1	0.15	0.25	0.25	0.30	0.35	0.40	0.43	0.33	0.21	0.24
215.0	0.23	0.34	0.44	0.49	0.68	0.83	0.88	0.74	0.60	0.60
216.1	0.06	0.10	0.15	0.16	0.18	0.27	0.30	0.21	0.15	0.16
217.0	0.22	0.27	0.35	0.36	0.43	0.51	0.50	0.42	0.33	0.32
218.1	0.10	0.14	0.17	0.21	0.23	0.28	0.32	0.17	0.20	0.19

219.0	0.32	0.43	0.51	0 55	0.68	0.87	0.92	0.65	0.52	0.51
220.0	0.08	0.14	0.08	0.14	0.11	0.17	0.19	0.32	0.23	0.26
221.1	0.99	2.00	2.87	3.89	6.63	10.25	7.34	4.07	4.04	4.77
222.1	0.34	0.63	0.86	1 09	1.80	2.74	1.97	1.16	1.12	1.30
223.1	0.35	0 62	0.83	1.02	1.58	2.22	1.79	1.17	1.14	1.22
224.1	0.10	0 14	0.16	0 14	0.13	0.11	0.26	0.24	0.23	0.13
225.1	1.88	2 94	4.36	5.81	9.65	13.05	9.51	5.58	5.26	5.89
226.1	0.52	0 73	1.10	1.42	2.44	3.32	2.35	1.40	1.30	1.49
227.1	0.42	0.66	0.89	1.14	1.82	2.39	1.87	1.20	1.11	1.25
228.0	0.09	0.14	0.18	0.27	0.43	0.54	0.43	0.32	0.25	0.28
229.0	0.20	0 30	0.34	0.41	0.54	0.67	0.62	0.45	0.42	0.40
230.1	0.07	0.11	0.12	0.14	0.15	0.17	0.24	0.11	0.08	0.08
231.0	0.16	0.27	0.32	0.34	0.36	0.43	0.42	0.25	0.22	0.19
232.1	0.06	0 10	0.10	0.14	0.11	0.15	0.14	0.08	0.05	0.06
232.9	0.30	0 41	0.45	0.47	0.54	0.68	0.68	0.48	0.36	0.34
234.0	0.05	0.09	0.12	0.10	0.13	0.13	0.15	0.13	0.11	0.16
235.0	0.38	0.50	0.53	0.55	0.72	0.95	1.05	0.83	0.72	0.69
236.0	0.12	0.20	0.20	0.23	0.29	0.36	0.42	0.37	0.28	0.30
237.0	0.17	0.29	0.34	0.41	0.50	0.60	0.66	0.50	0.40	0.40
238.0	0.15	0.21	0.26	0.29	0.36	0.43	0.39	0.34	0.24	0.21
239.1	0.25	0.32	0.40	0.42	0.59	0.67	0.62	0.39	0.30	0.33
240.0	0.06	0.10	0.14	0.15	0.17	0.21	0.15	0.07	0.09	0.05
241.0	0.14	0.26	0.30	0.31	0.39	0.43	0.43	0.26	0.18	0.17
243.0	0.04	0.12	0.17	0.14	0.18	0.18	0.14	0.05	0.07	0.05
245.0	0.08	0.16	0.18	0.20	0.22	0.21	0.25	0.15	0.07	0.09
247.1	0.06	0.08	0.20	0.18	0.18	0.22	0.13	0.11		0.08
248.1	0.05	0.08	0.13	0.15	0.12	0.22	0.20	0.14	0.19	0.16
249.0	0.31	0.43	0.57	0.75	1.18	1.48	1.78	1.53	1.40	1.50
250.0	0.11	0.22	0.24	0.31	0.44	0.61	0.73	0.64	0.57	0:58
251.0	0.25	0.38	0.47	0.74	0.86	1.19	1.28	1.03	0.99	1.04

252.0	0.21	0.29	0.36	0.43	0.55	0.76	0.91	0.79	0.73	0.73
253.0	0.20	0.34	0.44	0.50	0.74	1.00	1.19	1.16	1.12	1.15
254.0	0.23	0.32	0.37	0.39	0.52	0.65	0.81	0.63	0.56	0.52
255.0	0.16	0.22	0.24	0.30	0.42	0.50	0.55	0.44	0.37	0.40
256.1	0.03	0.10	0.07	0.05	0.13	0.14	0.11	0.06	0.06	0.05
257.1	0.10	0.21	0.25	0.25	0.28	0.37	0.28	0.25	0.17	0.15
259.1	0.11	0.21	0.27	0.22	0.33	0.37	0.32	0.19	0.15	0.10
261.0	0.04	0.07	0.11	0.16	0.15	0.18	0.11	0.04	0.04	0.05
263.0		0.14	0.15	0.14	0.24	0.27	0.18	0.09	0.10	0.09
265.1	0.25	0.44	0.63	0.92	1.33	1.81	1.93	1.50	1.43	1.51
266.1	0.07	0.16	0.22	0.31	0.41	0.65	0.65	0.52	0.48	0.52
267.1	0.59	1.01	1.39	1.80	2.94	4.01	4.05	3.14	2.97	3.18
268.0	0.35	0.48	0.60	0.73	1.09	1.40	1.34	1.12	0.95	0.97
269.0	0.29	0.42	0.52	0.65	1.02	1.30	1.27	0.97	0.90	0.94
270.0	0.39	0.47	0.51	0.54	0.71	0.82	0.79	0.61	0.43	0.42
271.1	0.20	0.31	0.37	0.47	0.61	0.79	0.79	0.67	0.57	0.59
272.0	0.14	0.17	0.21	0.23	0.36	0.38	0.31	0.24	0.18	0.17
273.0	0.04	0.10	0.13	0.16	0.25	0.24	0.28	0.18	0.16	0.16
275.0	0.09	0.17	0.22	0.23	0.24	0.28	0.23	0.15	0.11	0.11
277.0		0.08	0.12	0.10	0.15	0.19	0.16	0.04	0.05	0.06
279.0	0.07	0.22	0.31	0.36	0.61	0.80	0.67	0.36	0.38	0.41
281.1	1.93	3.59	5.20	7.53	13.03	18.29	18.63	14.75	13.97	14.94
282.1	0.58	1.09	1.60	2.33	3.87	5.62	5.67	4.40	4.44	4.58
283.1	0.47	0.81	1.20	1.66	2.79	3.93	3.90	2.96	2.97	3.10
284.1	0.15	0.24	0.36	0.50	0.76	1.04	1.01	0.81	0.75	0.77
285.1	0.60	0.89	1.15	1.55	2.50	3.23	3.18	2.61	2.56	2.62
286.0	0.20	0.29	0.38	0.49	0.76	0.99	0.97	0.76	0.71	0.76
287.1	0.14	0.24	0.33	0.41	0.57	0.71	0.77	0.57	0.52	0.54
288.1		0.03	0.05	0.07	0.08	0.13	0.07	0.07	0.06	0.10
289.0	0.09	0.15	0.21	0.26	0.35	0.47	0.55	0.38	0.32	0.33

291.1		0.04	0.06	0.06	0.05	0.07	0.05	0.05	0.04	0.04
293.0		0.07	0.05	0.08	0.09	0.14	0.07	0.05		0.05
295.1	0.12	0.30	0.44	0.59	1.02	1.65	1.20	0.67	0.67	0.81
296.1		0.09	0.14	0.21	0.41	0.58	0.40	0.20	0.23	0.29
297.0	0.04	0.14	0.21	0.23	0.37	0.54	0.42	0.26	0.25	0.29
298.1		0.05	0.04	0.06	0.05	0.06	0.04	0.07	0.04	0.05
299.1	0.77	1.35	2.19	3.11	5.65	8.25	5.38	3.10	3.10	3.59
300.2	0.22	0.44	0.66	1.02	1.74	2.58	1.76	0.97	0.96	1.13
301.1	0.16	0.34	0.48	0.71	1.18	1.67	1.19	0.73	0.68	0.78
302.1	0.03	0.06	0.09	0.13	0.26	0.44	0.27	0.15	0.11	0.19
303.1	0.09	0.16	0.27	0.28	0.42	0.47	0.36	0.21	0.20	0.18
305.0		0.07	0.09	0.14	0.16	0.14	0.10		0.04	
309.1		0.05	0.09	0.12	0.21	0.25	0.24	0.20	0.22	0.22
311.0		0.03	0.07	0.09	0.17	0.18	0.11	0.08	0.11	0.11
313.0			0.05	0.04	0.10	0.09	0.10	0.06	0.06	0.07
323.1	0.03	0.16	0.22	0.25	0.40	0.47	0.36	0.32	0.30	0.29
324.1		0.03	0.05	0.08	0.07	0.12	0.12	0.05	0.04	0.05
325.1	0.20	0.38	0.54	0.58	0.91	1.16	1.05	0.70	0.63	0.67
326.1	0.06	0.13	0.17	0.24	0.35	0.49	0.39	0.25	0.27	0.27
327.1	0.29	0.47	0.64	0.75	1.18	1.51	1.44	0.98	0.90	0.99
328.0	0.06	0.13	0.19	0.26	0.39	0.52	0.51	0.35	0.30	0.35
329.0	0.06	0.13	0.18	0.26	0.39	0.50	0.44	0.31	0.25	0.30
339.1		0.07	0.11	0.19	0.33	0.48	0.37	0.16	0.23	0.23
340.1			0.07	0.07	0.09	0.14	0.17	0.06	0.05	0.05
341.1	0.43	0.76	1.06	1.33	2.08	2.97	2.46	1.66	1.56	1.74
342.1	0.10	0.27	0.39	0.46	0.74	1.06	0.90	0.60	0.54	0.61
343.1	0.08	0.23	0.33	0.39	0.60	0.82	0.72	0.53	0.45	0.49
344.1		0.03	0.08	0.07	0.13	0.19	0.10	0.04	0.05	0.09
345.0		0.15	0.21	0.27	0.44	0.52	0.56	0.40	0.32	0.36
346.1			0.03	0.04	0.11	0.11	0.06	0.08	0.07	0.05

347.1		0.05	0.06	0.07	0.11	0.10	0.09	0.04	0.07	0.04
355.1	0.58	1.26	1.76	2.29	3.66	5.25	4.62	2.95	2.75	2.99
356.1	0.27	0.46	0.68	0.89	1.36	2.00	1.75	1.06	0.99	1.12
357.1	0.15	0.37	0.49	0.58	0.96	1.40	1.19	0.82	0.72	0.80
358.1		0.07	0.18	0.16	0.27	0.46	0.30	0.19	0.18	0.21
359.1	0.18	0.28	0.34	0.44	0.70	0.88	0.71	0.48	0.45	0.49
360.1	0.04	0.05	0.07	0.11	0.14	0.22	0.11	0.07	0.06	0.12
361.1	0.04	0.05	0.04	0.10	0.10	0.13	0.06		0.05	0.05
369.1		0.03	0.07	0.10	0.24	0.47	0.28	0.06	0.13	0.17
373.1	0.16	0.36	0.60	0.87	1.79	2.89	1.72	1.05	1.02	1.20
374.2	0.03	0.11	0.20	0.33	0.70	1.09	0.63	0.33	0.36	0.46
375.1		0.08	0.13	0.23	0.49	0.74	0.38	0.17	0.20	0.32
399.0	0.03	0.09	0.15	0.15	0.28	0.40	0.32	0.07	0.09	0.17
401.0	0.25	0.35	0.45	0.54	0.80	1.14	0.10	0.64	0.58	0.63
402.0	0.05	0.08	0.16	0.18	0.34		0.90	0.16	0.19	0.25
403.0	0.07	0.05	0.08	0.13	0.22		0.33	0.09	0.12	0.14
415.1	0.10	0.23	0.32	0.39	0.67		0.68	0.45	0.41	
416.1	0.03		0.08	0.11	0.24		0.17	0.10	0.10	
429.1	0.20	0.38	0.55	0.74	1.13		1.52	0.82	0.74	
430.1	0.04	0.13	0.24	0.36	0.53		0.69	0.33	0.37	
431.2		0.07	0.18	0.26	0.35		0.45	0.20	0.22	
433.1			0.03	0.04	0.07					
459.1			0.03		0.05					
461.1			0.09		0.12		0.07		0.03	
475.1					0.10		0.07	0.04	0.03	
476.0								0.01		
503.2			0.05				0.14	0.07	0.05	
504.2			0.01				0.04	0.01	0	
505.0			0.01				0.01			
535.3			0.01							