AN ABSTRACT OF THE THESIS OF

Murray Hackett for the degree of Master of Science in
Toxicology presented on April 27, 1987.

Title: The Determination of Selected Polychlorinated
Dibenzo-p-dioxins and Dibenzofurans in Environmental
Samples from Sites Associated with the use of Chlorophenolic
Wood Preservatives

Abstract Approved: __________________________
Kenneth J. Williamson

Polychlorinated dibenzo-p-dioxins (PCDD's) and
dibenzofurans (PCDF's) are environmental pollutants associ-
ated with the production and use of a number of industrial
chemicals. In addition, PCDD's and PCDF's are produced
during low temperature combustion of wastes containing
polyvinylchloride (PVC), chlorophenols, and a number of
other chemical precursors.

A significant source of environmental contamination
by PCDD/PCDF in Oregon has been the use of technical
grades of pentachlorophenol (t-PCP) and 2,3,4,6-
tetrachlorophenol, and their sodium and potassium salts.
These compounds have been used extensively by the lumber
industry as wood preservatives since the 1930's.

Environmental samples from five sites in Oregon and Washington State were screened for 21 selected PCDD/PCDF isomers. These included the most toxic laterally substituted isomers, that is those with chlorines in the 2,3,7, and 8 positions, but lacking substituents in one or more of the peri positions. The samples were taken from sediments, soil, wood shavings from pressure treated lumber, diptank sludge, fresh crystalline t-PCP, and tissues from bovines and equines exposed to these chemicals in the environment. Three of the Oregon sites were associated with chlorophenate salts used to prevent "sapstain" in finished lumber. The fourth Oregon site served as a control. The Eagle Harbor, Washington, site was located near a pressure treatment facility long known to be a point source for creosote in Eagle Harbor.

The soil and sediment samples were analyzed for PCDD/PCDF with the intent of finding evidence for in-situ degradation, and perhaps acclimated microorganisms capable of degrading these stable and persistent compounds. No significant evidence of such processes occurring under natural conditions was discovered. This tends to support other work which suggests these compounds are highly refractory to microbiological processes.
The Determination of Selected Polychlorinated Dibenzo-p-dioxins and Dibenzofurans in Environmental Samples from Sites Associated with the use of Chlorophenolic Wood Preservatives

by

Murray Hackett

A THESIS

submitted to Oregon State University

in partial fulfillment of the requirements for the degree of

Master of Science

Completed April 27, 1987
Commencement June 1987
Approved:

Redacted for Privacy

Professor of Civil Engineering in charge of major

Redacted for Privacy

Chairman of Department of Toxicology

Redacted for Privacy

Dean of the Graduate School

Date thesis is presented April 27, 1987

Typed by the researcher for Murray Hackett
ACKNOWLEDGMENTS

This study was made possible by the cooperation and assistance of many individuals and several organizations. The Environmental Protection Agency, The National Science Foundation, and the Department of Civil Engineering at OSU are acknowledged for research support. The Department of Chemistry at Oregon State provided a Tartar Fellowship during the summer of 1985.

Partial support for analytical standards and supplies was provided by the Graduate Research Council, Oregon State University. The U.S. EPA Environmental Research Laboratory at Duluth, Minnesota and the University of Wisconsin at Superior, Wisconsin are acknowledged for their analytical support. Although most of the analytical work was carried out at EPA ERL Duluth, Oregon State University is solely responsible for the content of this thesis.

Specific individuals and other organizations to be acknowledged include:

Oregon State University, Department of Civil Engineering
Dr. Kenneth Williamson, Dr. Sandra Woods

Oregon State University, Department of Agricultural Chemistry
Dr. Max Deinzer, Dr. James Laramee, Mr. Brian Arbogast, Dr. Ian Tinsley, Mr. Rod Inman, Dr. Donald Buhler
Oregon State University, Department of Chemistry
Dr. John Westall, Dr. James Krueger

Oregon State University, School of Pharmacy
Dr. Robert Larson

Oregon State University, Department of Soil Science
Dr. John Baham

Oregon State University, School of Veterinary Medicine
Dr. Nancy Kerkvliet, Dr. Bruce Hultgren, Dr. Wayne Schmotzer

Oregon Department of Environmental Quality
Mr. Jeff Dresser, Mr. Larry Patterson

U.S. EPA, ERL Duluth, Minnesota
Dr. Norbert Jaworski, Mr. Brian Butterworth, Mr. Douglas Kuehl, Dr. Gilman Veith, Dr. Philip Cook, Ms. Barbara Halligan

U.S. EPA, ERL Newport, Oregon
Dr. Donald Baumgartner
Dr. Larry Smith

Northrop Environmental Inc, Corvallis, Oregon
Mr. Glen Wilson

Center For Lake Superior Environmental Studies, University of Wisconsin, Superior, Wisconsin
Dr. Donald Bahnick, Dr. Raymond Hanson, Mr. Kenneth Johnson, Ms. Darcy Johnson, Ms. Sandra Neumann, Ms. Marie Larsen, Mr. Larry Holland, Mr. William DeVita, Mr. Chris Sauer
Oregon Department of Environmental Quality
Mr. Jeff Dresser, Mr. Larry Patterson

Oregon Health Division
Mr. Michael Heumann

Crist, Stewart, Lowe & Maurer, Attorneys at Law
Mr. John Lowe
Mr. Thomas Rastetter

Anderson Development Co.
Adrian, Michigan

Chapman Chemical Co.
Memphis, Tennessee

Reichold Chemical Co.
Tacoma, Washington
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction</td>
<td>1</td>
</tr>
<tr>
<td>Materials and Methods</td>
<td>7</td>
</tr>
<tr>
<td>I. Eagle Harbor Site</td>
<td>14</td>
</tr>
<tr>
<td>II. Arabian Horse Farm, Adjacent to Sawmill Site 1</td>
<td>18</td>
</tr>
<tr>
<td>III. Sawmill Site Number 2</td>
<td>23</td>
</tr>
<tr>
<td>IV. Sawmill Site Number 3</td>
<td>29</td>
</tr>
<tr>
<td>V. Control Site</td>
<td>31</td>
</tr>
<tr>
<td>Overall Summary and Conclusions</td>
<td>33</td>
</tr>
<tr>
<td>References</td>
<td>71</td>
</tr>
<tr>
<td>Appendix A: TCDD Equivalent Factors</td>
<td>78</td>
</tr>
<tr>
<td>Appendix B: Sample cleanup methods for Soil/Sediment</td>
<td>79</td>
</tr>
<tr>
<td>Appendix C: Sample cleanup methods for Biological Tissues</td>
<td>86</td>
</tr>
<tr>
<td>Appendix D: Internal Standards</td>
<td>89</td>
</tr>
<tr>
<td>Appendix E: HRGC/GCMS Operating Parameters</td>
<td>90</td>
</tr>
<tr>
<td>Appendix F: Source Code for Computer Programs used to Quantify Samples</td>
<td>94</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>--------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>1.</td>
<td>Sampling Locations, Eagle Harbor Site</td>
</tr>
<tr>
<td>2.</td>
<td>Sampling Locations, Sawmill Site 2</td>
</tr>
<tr>
<td>3.</td>
<td>Chemical Structures of Pentachlorophenol, 2,3,4,6-Tetrachlorophenol, 1,2,3,6,7,8-HxCDD, 1,2,3,4,7,8-HxCDF, 2-nonachlorophenoxyphenol</td>
</tr>
<tr>
<td>4.</td>
<td>Two Eagle Harbor Sediment Samples Compared to an Industry Composite Sample of t-PCP, Congener Group Total Concentrations normalized to OCDD</td>
</tr>
<tr>
<td>5.</td>
<td>Sample 222 Compared to Mean Values of four PCDD Isomers in t-PCP and Flyash</td>
</tr>
<tr>
<td>6.</td>
<td>Mass Chromatograms of HxCDD's in Eagle Harbor, t-PCP and Flyash</td>
</tr>
<tr>
<td>7.</td>
<td>Mean Values of four Selected PCDD/PCDF from Table 9 Compared to Sample 223</td>
</tr>
<tr>
<td>8.</td>
<td>Mean Values of four Selected PCDD/PCDF from Table 9 Compared to Mean Values from Table 8</td>
</tr>
<tr>
<td>9.</td>
<td>Schematic Diagram Showing Outline of Analytical Method for PCDD/PCDF</td>
</tr>
<tr>
<td>Table</td>
<td>Description</td>
</tr>
<tr>
<td>-------</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>1.</td>
<td>Descriptions of Tissue Samples</td>
</tr>
<tr>
<td>2.</td>
<td>Descriptions of Soil/Sediment/Other Samples</td>
</tr>
<tr>
<td>3.</td>
<td>Results, Isomer Specific Analyses of Two Samples of Technical Pentachlorophenol</td>
</tr>
<tr>
<td>4.</td>
<td>Results, Congener Group Analyses of Two Samples of Technical Pentachlorophenol compared with Industry Composite Values</td>
</tr>
<tr>
<td>5.</td>
<td>Results, Isomer Specific Analyses of Eagle Harbor Samples</td>
</tr>
<tr>
<td>6.</td>
<td>Results, Congener Group Analyses of Eagle Harbor Samples</td>
</tr>
<tr>
<td>7.</td>
<td>Results, Isomer Specific Analyses, Vicinity of Site 2</td>
</tr>
<tr>
<td>7a.</td>
<td>Results, Congener Group Analyses, Soil Core, Site 2</td>
</tr>
<tr>
<td>7b.</td>
<td>Results, isomer specific analyses of sludge from Na-pentachlorophenate diptank, Site 2, concentrations normalized to OCDD</td>
</tr>
<tr>
<td>8.</td>
<td>Results, Isomer Specific Analyses, Farm Near Site 3</td>
</tr>
<tr>
<td>9.</td>
<td>Results, Isomer Specific Analyses, Beavercreek OR Control Site</td>
</tr>
<tr>
<td>10.</td>
<td>Results, Isomer Specific Analyses, Equine Control Tissues</td>
</tr>
<tr>
<td>11.</td>
<td>Results, Isomer Specific Analyses, Stallion From Arabian Horse Farm</td>
</tr>
</tbody>
</table>
12. Results, Contaminated Wood Chips, Arabian Horse Farm

13. Results, Isomer Specific Analyses, Tissues from Stillborn Foal, Arabian Horse Farm; Bull from Farm Near Site 2

14. Results, Isomer Specific Analysis of Soil Sample from Arabian Horse Farm

15. Results, Congener Group Analyses, Stillborn Foal, Arabian Horse Farm

16. Results, Congener Group Analyses, Mare from Arabian Horse Farm; Bull from Farm Near Site 2

17. Results, Six Replicates of a Contaminated Fish from the Petenwell Reservoir in Wisconsin

18. Results, six replicates of a reference sediment from northern Minnesota known to Contain Low ppt Levels of 2,3,7,8-TCDD

19. Statistical Summary of Analytical Precision for Data Summarized in Table 17, Fish

20. Statistical Summary of Analytical Precision for Data Shown in Table 18, Sediments
The Determination of Selected Polychlorinated Dibenzo-p-dioxins and Dibenzofurans in Environmental Samples from Sites Associated with the use of Chlorophenolic Wood Preservatives

INTRODUCTION

The purpose of the work was to determine the extent of off-site contamination by polychlorinated dibenzo-p-dioxins (PCDD's) and dibenzofurans (PCDF's) at several sites in Oregon and Washington associated with the use of technical grades of pentachlorophenol (t-PCP) and/or 2,3,4,6-tetrachlorophenol. PCDD's and PCDF's are the most toxic, and likely the most environmentally persistent, contaminants present in commercial formulations of these products (1).

From measured spatial distributions of these compounds, descriptions of the environmental fate, transport and degradation properties of PCDD's/PCDF's would be proposed based on data from several "real world" sites of contamination.
Despite the wide interest in these compounds both within the scientific community and society at large, relatively few papers have been published with respect to dioxin/furan residues at sites contaminated with t-PCP. Most of these papers have been from Europe.

Isomer specific data has, as of this writing, been very limited; for example, see references (16) and (17). At present, there are a number of studies presently being conducted under EPA and other federal funding which should help expand knowledge concerning the environmental behavior of PCDD's/PCDF's associated with t-PCP and other sources, such as the combustion of PVC (polyvinylchloride) (54).

Pentachlorophenol has often been cited as the second most common biocide in the United States (18), (19). Commercial formulations of t-PCP or tetrachlorophenol consist of the chlorophenol dissolved in an organic solvent, or the potassium or sodium salts dissolved in water, or other polar solvent system. Penta has also been applied as an aerosol under conditions of heat and high pressure. Railroad ties, heavy laminated beams, and telephone poles are typically impregnated with penta at pressure treatment facilities. "Dip tanks" of aqueous chlorophenate ion are used as an anti-stain treatment for finished lumber.

It has found use as a wood preservative, fungicide
and slimacide, to mention only a few of many applications. Largely as a result of work by Jansson et al. (2), and Rappe and coworkers (3)(4), the Swedish government has banned commercial grades of penta- and tetrachlorophenol for most of the applications for which these chemicals have been used in this country. Due to regulatory pressure, many wood treatment facilities have switched over to technical 2,3,4,6-tetrachlorophenol based formulations in recent years. The literature is ambiguous as to whether or not the tetrachlorophenol formulations have a lower PCDD/PCDF content than those based on pentachlorophenol (16), (17), (19).

The acute toxicities of technical grade tetra- and pentachlorophenol formulations are very similar, with respect to fish. They both have 96 hour LC-50 values on the order of 0.10 mg/liter (ppm) for Coho salmon (56).

The selection of sampling sites was made on the basis of both scientific and regulatory interest. The sediment samples from Eagle Harbor, Washington were provided by EPA Region 10. This site was adjacent to a wood treatment plant which has used t-PCP or its salts. Sites 1, 2, and 3 were selected based on past sampling for chlorophenols carried out by the Oregon Department of Environmental Quality (DEQ). These sites were adjacent to
sawmills which have treated lumber using chlorophenate diptanks located on-site. Because of limited time and funding, only a small number of samples could be analyzed. PCDD/PCDF determinations are extremely expensive in terms of manual labor required, the cost of analytical standards, and the costs of the instrumentation. For this reason, no formal, statistically-based, sampling protocol was found which would have allowed the collection of an economically realistic number of samples (20), (21). Sample selection was therefore based on "best" judgement, depending on the hypothesis being tested. This is relevant to samples from Site 2, where an attempt was made to determine the relative contributions of runoff from a lumber yard versus combustion from a nearby incinerator.

All tissue samples analyzed using mass spectrometry are listed in Table 1. Soil, sediment and wood shaving samples are listed in Table 2. The sample numbers correspond to the numbers used in the remaining Tables, which contain all the quantitative GC-MS data gathered for this thesis. Recently, it has become common to report PCDD/PCDF concentrations as "TCDD Equivalent Units". For readers who wish to convert the data to these units, Appendix A shows the conversion factors currently being used by EPA and CDC (Centers for Disease Control) to perform such calc-
ulations (12)(13).

For purposes of reference, the chemical structures for pentachlorophenol, 2,3,4,6-tetrachlorophenol, 1,2,3,6,7,8-HxCDD, 1,2,3,4,7,8-HxCDF and 2-nonachlorophenoxy phenol are shown in Figure 3.

Technical pentachlorophenol has been manufactured using two different processes: the direct chlorination of phenol using aluminum trichloride as a catalyst, and the treatment of hexachlorobenzene with strong base, followed by acid. The former process is the only one used in the United States. Of the two methods, the former also produces lower concentrations of PCDD/PCDF (19). The resulting chlorophenol then can be reacted with NaOH or KOH to form the sodium or potassium salt, if a water soluble product is desired. The total dioxin content and the specific isomers present varies depending on the reaction conditions existing during manufacture. Considerable differences exist between the phenols and their salts. The sodium and/or potassium salts have been observed to have a higher overall PCDD/PCDF content and a wider range of isomers present (19) (22).

The contaminants present in t-PCP in the highest concentration (1 to 5 %) are the phenoxy phenols, also called predioxins or isopredioxins, depending on the location of the phenolic OH group. These compounds are of much lower
toxicity than the toxic PCDD's/PCDF's (1). They are of interest to the present study in that the analytical methods used had to be effective in removing these compounds without converting them to PCDD/PCDF. The reaction pathways postulated for this conversion, as well as other pathways of dioxin/furan formation from chlorophenolic precursors, are reviewed in reference (19). The chemistry and toxicology of the phenoxyphenols are also discussed in references (22), (23) and (24).
MATERIALS AND METHODS

1) Sample Collection and Storage

Samples were collected in new, solvent-washed, amber glass bottles supplied by VWR. Their caps were teflon lined. Tissue samples were frozen immediately after collection, and thawed prior to sample preparation. Soil or sediment samples were frozen or kept in a 10 C cold room until sample preparation. Samples shipped from OSU to ERL Duluth, Minnesota, were sent overnight express mail in insulated containers, cooled with dry ice.

2) Sample Preparation

The sample preparation scheme for tissues is described in Appendix B. Where it differs from tissues, the sample preparation for soil/sediments/wood chips is described in Appendix C. For further information on sources of supplies, activation of reagents, and quality assurance/quality control, readers are urged to consult the final versions of references (42) and (60). They are expected to be published sometime during the summer of 1987, after an external peer review scheduled for June, 1987.

Briefly, the sample cleanup involved the removal of
bulk matrix and interferences with strong acid/strong base, silica gel, silver nitrate on silica, and chromatography using alumina and carbon dispersed on silica gel. This process is shown schematically in Figure 9.

3) Gas Chromatography/Mass Spectrometry

All samples listed in Tables 1 and 2 were analyzed for PCDD/PCDF using either capillary GC/low resolution mass spectrometry (HRGC/LRMS) or capillary GC/high resolution mass spectrometry (HRGC/HRMS). All isomer specific data were generated using HRGC/HRMS. For isomer specific work, representative samples were run on both a 30 M DB5 and a 60 M SP2330 to insure the correct identification of individual PCDD/PCDF. Isomer assignments within a congener group (based on the number of chlorines attached) were based on a combination of labeled internal standards and a well defined qualitative standard known to contain all the compounds shown in Tables 3-18. Relative retention times assigned were also checked against literature values (26), (27), (28).

The GC/MS operating parameters are given in detail in Appendix E. The compositions of the internal standard solutions are given in Appendix D. In general, the approach used corresponds to the description of isotope dilution mass
spectrometry given by Millard (29). It was assumed that all native PCDD/PCDF within a given congener group had the same response relative to the labeled analog used to quantify isomers within that group. Samples were quantified based on the labeled compounds in internal standard solution A. This solution was added to the sample prior to extraction. Internal standard solution B was added to the microvial prior to sample injection into the GC/MS. Solution B was used to calculate recoveries of the labeled compounds in solution A. Three computer programs were written in order to generate response factors and quantify samples. The BASIC code for these programs is given in Appendix F, along with a more detailed summary of their structure and function. The key equations for quantitation and recovery are given as:

1) \[ C_n = \frac{A_n \cdot C_l}{A_l \cdot RRF} \]

Where:
- \( C_n \) = concentration of analyte, pg/g
- \( C_l \) = concentration of label standard spiked into sample
- \( A_n \) = peak area of natural ion
- \( A_l \) = peak area of labeled ion
- \( RRF = \frac{R_n}{R_l} \), relative response
- \( R = \) absolute response of ion, ADC counts/pg

2) \[ \%REC = \frac{C_{l, measured} \times 100}{C_{l, spiked}} \]

Where:
- \( C_{l, measured} = \frac{A_l \cdot C_{334}}{A_{334} \cdot RF} \)
- \( C_{334} \) = concentration of I.S. B
- \( A_{334} = \) area of I.S. B
- \( RF = \frac{R}{R_{334}} \)
The internal standard method used was superior to methods based on external calibration curves in that losses occurring at various stages in the cleanup, and changes in the instrument's sensitivity were all compensated for. The only major source of error which was not compensated for was the difference in extraction efficiency which would be expected for labeled surrogates spiked into a sample immediately prior to extraction and more tightly bound, weathered native compound (65). Weathered dioxin residues would be expected to be very tightly bound to their sample matrices, when organic carbon content is significant.

4) Quality Control

Of the 24 compounds presently listed in Tables 3 to 18 and the computer programs, the majority are substituted in all four of the lateral 2,3,7 and 8 positions. These are the most toxic isomers, except for OCDF and OCDD, which are nearly devoid of biological activity (30). However, OCDD may be of utility with respect to identifying sources. Other compounds on the list were included because of their demonstrated bioaccumulative potential in fish. Two isomers on the list are present for reasons which are not relevant
to this study, 1,2,3,4-TCDD and 1,3,4,6,7-PCDF.

Many of the toxic isomers coelute with other, less toxic PCDD/PCDF. The situation is drastically simplified in biological tissues, which show a strong preference for retaining only isomers substituted in at least 3 of the 4 lateral ring positions. A number of recent publications describing PCDD/PCDF residues in human adipose tissue have found only compounds substituted in all four 2,3,7, and 8 positions (31), (32), (33). The situation is more complex in soils, sediments and contaminated wood shavings, where potentially any of the PCDD/PCDF isomers may exist.

Other compounds have been documented to interfere with PCDD/PCDF determinations, including planar PCB's, diphenyl ethers, certain chlorinated naphthalenes and biphenylenes (35), and chlorinated xanthenes and xanthones (36).

Avoidance of false positives requires retention time data from at least two capillary columns and correct ion ratios for at least two ions within the molecular ion cluster. A close look at retention time data for all 75 PCDD's and 135 PCDF's, collected at ERL Duluth on the 30 M DB5 and the 60 M SP2330 capillary columns, requires two caveats with respect to the "isomer specificity" of the data. Of the 24 compounds listed in Tables 3 to 18, all can be identified with two exceptions, if data
from both capillary columns is used. One exception is that the 1,2,3,7,8-TCDF isomer coelutes with 1,2,3,4,8-TCDF on both columns. A contribution by the latter isomer cannot be ruled out, particularly in the soil/sediment data. The second exception is that 1,2,6,9-TCDF was shown to elute on the SP2330 as a shoulder, 7 seconds earlier, than 2,3,7,8-TCDF. Thus one cannot completely rule out a contribution by the former isomer.

Limitations on the availability of HRMS instrumentation made it impossible to run every single sample on two columns. Alternatively, selected samples from groups appearing to contain the same cross section of isomers on one column were confirmed, and if necessary, requantified on the second column. All samples with positives in the tetra- and penta-congener groups were run on two columns; these groups presented the greatest problems with single column data. Because only a limited number of replicate samples were run, due to the high cost per sample, it is difficult to adequately describe the analytical precision of the data (34). To help address this question, five replicates of a reference tissue and six of a reference sediment were analyzed for PCDD/PCDF. The data are presented in Tables 17 and 18. The statistical evaluation of the data with respect to analytical precision are presented in Tables
19 and 20. These results compare favorably with what has been achieved in other laboratories (34). Precision is often poor for OCDD measurements due to the ubiquitous nature of the compound; it was almost always observed in laboratory blanks, along with 1,2,3,4,6,7,8-HpCDD. All values reported here have been background corrected based on levels found in the set reagent/glassware blank, with the single exception of the data in Table 17. The blank values are shown explicitly, in this one instance. The precision indicated by the fish data in Tables 17 and 19 is better than what is normally achieved. Unfortunately, the glassware cleaning procedure which was largely responsible for these results did not lend itself to routine use. Although the data were reported as positive if the blank was significantly lower, the author believes that any value for OCDD under 150 parts per trillion (ppt) has very little meaning for in this study. Other laboratories have reported blank levels of OCDD as high as the low parts per billion (ppb) (34).
I. EAGLE HARBOR SITE

1) Introduction

Eagle Harbor is a small inlet in western Puget Sound with a history of contamination by a variety of chemical pollutants (37), (38). The proximity of Eagle Harbor to a wood treatment plant, which has used creosote and t-PCP, suggested that in addition to the high concentrations of PAH's and nitrogenous aromatic compounds known to be present at the ppm level, PCDD/PCDF would also be present. The site was of interest as a possible location to study in-situ biodegradation. It first had to be determined, however, that PCDD/PCDF was in fact present.

2) Results

The data for PCDD/PCDF concentrations are shown in Tables 3 and 4. Figure 6 shows the HxCDD mass chromatograms, on a DB5 column, for an Eagle Harbor Sediment, t-PCP, and fly ash from a MSWI (Municipal Solid Waste Incinerator) located in the eastern United States. Figure 4 shows two Eagle Harbor Sediment Samples compared to literature values for t-PCP congener group total concentrations.
3) Discussion

As shown in Figure 4, when congener group totals are compared among two Eagle Harbor sediment samples and an industry composite sample of t-PCP (14), the three sets of concentration values are quite similar when normalized to OCDD concentration.

The isomer specific data in Table 5 indicates an interesting difference between the sediments and commercial t-PCP formulations described in the literature (16) and in Tables 3 and 4. The most toxic single component of the PCDD/PCDF fraction from t-PCP is probably the 1,2,3,6,7,8-HxCDD isomer. This is also the HxCDD isomer which is reported to be present in the highest concentration of the 10 possible isomers, in all t-PCP formulations for which the author has seen isomer specific data. For example, see reference (14). Significantly different distributions have been observed for the chlorophenate salts, however. Miles et al. (16) have published data indicating the major components for the salts to be the 1,2,4,6,7,9/1,2,4,6,8,9 and 1,2,3,6,7,9/1,2,3,6,8,9 isomer pairs. The major component in the sediments was observed to be the 1,2,4,6,7,9/1,2,4,6,8,9 pair, which coelutes on both of the capillary columns used in this study. The next largest component was observed to be the 1,2,3,6,7,9/1,2,3,6,8,9
isomer pair. Samples of fly ash from waste incinerators which have been analyzed at ERL Duluth also show these two isomer pairs as major peaks in the HxCDD congener group (39). The mass chromatograms in Figure 6 show these peaks for the different samples discussed above. Preliminary data from Oregon and Washington collected as part of the EPA's National Dioxin Study suggests that 2,3,7,8-TCDD is rare in Pacific Northwest watersheds, quite unlike the widespread dispersion of this compound which has been observed east of the Mississippi River (40). This would lend support to the observation that a specific point source is responsible for the PCDD/PCDF in Eagle Harbor. The absence of 2,3,7,8-TCDD, and any other tetrachlorodioxin isomers also tends to argue against contributions from nonpoint sources such as combustion.

4) Conclusions

The overall pattern of PCDD/PCDF isomers present in the sediments more strongly resembles that expected from Na-PCP or K-PCP salts than that observed for combustion of municipal solid waste or the laboratory scale pyrolysis of chlorophenols or chlorophenates (2), (4), (39). The absence of control site samples makes the extent of
contributions from combustion, if any, and/or airborne transport difficult to estimate.

No evidence of selective degradation of any PCDD/PCDF was observed, if one accepts the premise that these compounds had as their source some combination of pentachlorophenol/pentachlorophenate. It appears that the PCDD/PCDF residues in Eagle Harbor have not undergone any significant in-situ degradation, as would be evidenced by selective degradation of the 6 and 7 chlorine compounds. These would presumably be more subject to microbial degradation than a fully substituted compound such as OCDD.

The much higher concentrations of creosote related compounds, including a variety of PAH's and heterocyclic compounds known to be carcinogenic (37)(64), suggests that PCDD/PCDF does not contribute significantly to the overall toxicity of the sediments.
II. ARABIAN HORSE FARM
ADJACENT TO SAWMILL SITE 1

1) Introduction

Sawmill Site 1 contained a diptank on-site. A farm was located next to this mill which maintained a herd of 15 to 20 Arabian horses. Most of these animals became ill during the period 1981-1985. A local veterinarian attributed much of the herd's problems to t-PCP exposure. No link was ever found between the use of t-PCP at the adjacent mill and animal illness. However, a source of t-PCP exposure was discovered, and residue analysis confirmed the presence of elevated levels of PCP and PCDD/PCDF in the horses. Tissue samples, wood chips and soil samples were collected in order to determine the source and extent of PCDD/PCDF contamination on the farm. Tissue samples were collected at necropsy from two mature horses and a stillborn foal. These animals died during or shortly after the period of time in which they were exposed to wood chips, used for bedding, which were highly contaminated with t-PCP. The cause of death was attributed by the OSU Veterinary Diagnostic Laboratory to t-PCP in one instance, the mare described later in this section (44). There was no connection between the toxic wood chips and the mill adjacent to the farm property.
The number of successful births on this farm dropped from normal levels in the 1970's to virtually zero during 1981-1985. The contaminated wood chips were later traced by the Oregon Department of Environmental Quality to shavings from the surface of pressure treated "glulam" beams used in heavy construction. All wood chips measured by DEQ to contain more than 600 ppm pentachlorophenol were removed from Clackamas County farms in the late summer and fall of 1984. The same sample of wood chips shown in Table 12 was measured by Columbia Laboratories (Corbett, OR) to contain 2770 ppm pentachlorophenol (44). Sampling for chlorinated phenols carried out privately by the farm's owners and by the DEQ showed either not detectable or low levels of these compounds, with the exception of the wood chips.

2) Results

The PCDD/PCDF data for tissue samples collected from horses living on the farm are shown in Tables 11, 13, 15 and 16. The data for contaminated wood chips, used for animal bedding, are shown in Table 12. Data for a soil sample collected from the barn, in which the wood chips were used, are summarized in Table 14. Data from four equine control tissues, provided by Dr. Bruce Hultgren at
the OSU School of Veterinary Medicine, are shown in Table 10.

In addition, several soil samples were screened semi-quantitatively using capillary GC with electron capture. These samples were collected by the author in May, 1985 from areas of the farm which potentially could receive drainage from the nearby sawmill's logging yard. Results were negative, except for low ppt (parts per trillion) traces of the always present OCDD. No mass spectrometry based analyses were carried out on these samples, so they were not listed in Table 2.

3) Discussion

The horses on this farm began to develop a variety of illnesses, later attributed to t-PCP exposure (43), in 1981. These included laminitis, colic, respiratory problems, reproductive problems, blood disorders and mortality. Poor management, tansy, heavy metals, SCIDS, and other possible confounding factors were ruled out as causes of death with respect to the Arabian mare for which the most information was gathered (44). The PCDD/PCDF results for this animal's liver are shown in Table 16, Sample 9. These results are about two orders of magnitude higher than background levels suggested by the data in Table 10. The liver and adipose tissue from another animal from the same farm, shown in
Table 11, yielded similar results. Tissues collected from a stillborn foal, conceived roughly three months prior to removal of the tainted chips from the premises, also showed elevated levels of PCDD/PCDF. The mare discussed above, and other horses on the farm, contained elevated levels of chlorophenols in their blood (43).

Tissues collected from a bull known to have been exposed to t-PCP containing runoff, but not to contaminated bedding or feed, are shown as Samples 420, 421, and 422 in Tables 13 and 16. This bull belonged to a farm near Sawmill Site 2. The PCDD/PCDF residues found in this animal's liver are slightly higher than those reported for control tissues in Table 10. Residues measured in the bull's liver may be useful as a "positive control" with which to compare the Arabian Horse farm data.

4) Conclusions

The only point source of PCDD/PCDF contamination discovered was the wood chips described above. The DEQ had sampled other areas along the border of the mill with the road separating the farm from the mill property. The DEQ results were negative for chlorophenols (45). The residue analyses for PCDD/PCDF, in tissues from horses exposed to highly contaminated wood chips, tend to
support the etiology described in Dr. Wayne Schmotzer's final case report on the mare (44). According to this report, the mare died as a result of exposure to t-PCP and/or its more toxic dimeric contaminants.

As has been observed for human adipose tissue (32), and for cattle (50), only 2,3,7,8-substituted isomers were retained in the tissues of the exposed horses. As one would expect, given the much longer toxicokinetic halflife of PCDD/PCDF when compared to PCP (1)(47), these compounds were retained long after higher levels of chlorophenols had been excreted. Thus, it would follow that negative results for chlorophenols should not be used to rule out exposure to PCDD/PCDF contained in commercial chlorophenol formulations.
III. SAWMILL SITE NUMBER 2

1) Introduction

Sawmill Site 2 was of interest because of: 1) its location next to a stream which at one time served as a spawning area for salmon (45), 2) extensive DEQ records regarding PCP levels in the stream and other areas adjacent to the mill property, and 3) the presence of an abandoned incinerator which presumably burned t-PCP containing waste when it was in operation. Soil and sediment samples were collected from various locations adjacent to the mill property, including the stream mentioned above, a logging yard and its drainage ditch, farmland which received runoff from the logging yard, diptank sludge, and tissues from cattle exposed to PCDD/PCDF containing runoff.

2) Results

The data from sampling locations adjacent to Sawmill Site 2 are presented in Tables 7, 7a, and 7b. All samples from the area were positive for PCDD/PCDF. These results can be compared with those from a nearby community which the Oregon Health Division chose as a control site for an epidemiological study related to t-PCP exposure (51). These "control" values are summarized
in Table 9, and discussed in more detail in Part V.

The relative locations of the different samples discussed are shown in Figure 2.

Full scan mass spectra of crude extracts from Sample 12 suggested the presence of a variety of polyhalogenated compounds, in addition to PCDD/PCDF and PCP. No attempt was made to assign structures to these spectra, however.

3) Discussion

Site 2 had a long and well documented history of t-PCP contamination in adjacent drainages and in the stream shown in Figure 2 (52). Most Site 2 samples contained higher concentrations of PCDD/PCDF than what was observed in the Control Site samples. Sample number 223, which consisted of high TOC sediment collected upstream from Site 2, contained PCDD/PCDF levels comparable to those observed in the Control Site samples, as shown in Figure 7. Samples collected downstream from the mill, particularly from portions of the stream in closest proximity to the diptank operation (Sample 222), contained high concentrations of PCDD/PCDF. Sample 222 was one of five samples which showed very low level traces of 2,3,7,8-TCDD, in addition to the highest levels of total dioxins recorded in the present paper for any soil/sediment sample. The levels
of PCDD/PCDF recorded for Sample 222 were expected based on DEQ records of PCP concentrations in the water a few yards downstream from this point (52). Dioxins are extremely hydrophobic compounds, with water solubilities on the order of 12 parts per trillion (57), (58). Similar compounds have been observed to collect at interfaces and are believed to equilibrate rapidly in the environment between organic matter and water (63). Figure 5 compares sample 222 to the mean values calculated by averaging the data for t-PCP in Table 3, and also to flyash from a MSWI. The four PCDD isomers selected for this comparison were chosen based on their toxicity or presence in t-PCP. Note the similarity shown by t-PCP and sample 222. In general, flyash samples have a lower relative amount of OCDD present than samples contaminated by t-PCP. The values shown in Figure 5 were normalized to OCDD concentration in order to emphasize this point.

The samples collected from the drainage ditch shown in Figure 2, on the opposite side of the mill property from Sample 222, were highest in concentration adjacent to the lumber yard. Concentrations of PCDD/PCDF were observed to decline as one moved downstream along the ditch towards the confluence with the stream. Samples 204 and 205 were collected from a field on the opposite side of the road
bordering the logging yard, across the street from an oil distributor. These samples were quite high in PCDD/PCDF, containing low levels of 2,3,7,8-TCDD and 1,2,3,7,8-PCDD, two compounds not normally associated with t-PCP or its salts (54). However, the data in Table 7b, which shows the concentrations of PCDD/PCDF in diptank sludge collected from Site 2 in 1984, indicated the presence of these two isomers. Note that the levels in Table 7b are presented as normalized concentrations relative to OCDD. It was not possible to be absolutely quantitative with this sample, due to large changes in volume which took place during storage. Perhaps not coincidentally, the teepee burner was located near the oil distributor mentioned above, roughly two hundred yards from where Samples 204 and 205 were taken. According to DEQ sources, the burning of wood waste containing chlorophenols has been, and continues to be, a common practice in Oregon. The formation of PCDD/PCDF from the pyrolysis of chlorophenols and chlorophenates has been well documented (60)(42). Residues of the two above mentioned isomers were found in Samples 80, 218, and 222. Several other samples which were negative for 2,3,7,8-TCDD were positive for 1,2,3,7,8-PCDD. These were Samples 55, 92, 202, 214, and 221.
The recent findings by Hagenmaier (61) and Miller et al. are very relevant to the results presented herein. Hagenmaier has found measurable traces of 2,3,7,8-TCDD in several tetra- and penta-substituted phenols/phenates manufactured in Europe. To what extent this may be true of similar products produced in this country is uncertain.

Miller et al. have shown that under laboratory conditions, OCDD will preferentially photodegrade to 2,3,7,8-substituted isomers when it is bound to soil. This is very different from what has been observed in solution. In solution, the predominant photodegradation pathway for OCDD is the loss of the lateral chlorines and retention of those in the 1,4,6, and 9 positions (62). This has obvious implications for the hundreds of sites, similar to Site 2 in this study, where OCDD is present in soils at ppb to ppm levels.

4) Conclusions

Higher than background levels of PCDD/PCDF were found in soil and stream sediment adjacent to Sawmill Site 2, which contained a diptank on-site. However, several of these samples contained isomers which, up to now, were not believed to be present in the diptank solution which was observed by DEQ to be the point source of PCP pollution in the stream.
described above and in Figure 2. The combustion of chlorophenol containing waste and its airborne transport is suggested as one plausible hypothesis to explain the presence of 2,3,7,8-TCDD and 1,2,3,7,8-PCDD (41) (54). Another possibility, particularly for Sample 222, is a direct contribution by diptank runoff, as indicated by the presence of both above mentioned isomers in diptank sludge described in Table 7b. In light of the findings of Hagenmaier and Miller discussed in the previous section, it would seem that there are enough potential sources of 2,3,7,8-substituted isomers that it is not possible to draw any firm conclusions from the Site 2 data with respect to separating out contributions from OCDD photolysis, direct contributions by t-PCP salts, or combustion of t-PCP containing wood waste.
IV. SAWMILL SITE 3

1) Introduction

Several soil samples from public and private lands adjacent to Sawmill Site 3 were screened using capillary EC-GC with negative results, except for low ppt traces of OCDD. Samples collected from areas subject to runoff from the mill were collected from one farm whose manager had complained to state authorities about contamination from the mill. The mill used a chlorophenate diptank on-site.

2) Results

The results for PCDD/PCDF determinations from samples collected from the farm are shown in Table 8. The samples were collected based on best judgement as to the most likely locations to detect PCDD/PCDF. In this case, it meant low elevation areas most likely to receive runoff from the mill.

3) Discussion

The results shown in Table 8 are too close to those shown in Table 9, for the Control Site, to discern any difference. The mean PCDD/PCDF values for four selected
isomers, detected in every sample shown in Table 8 and Table 9, are shown in Figure 7. If one accepts the idea the Control Site samples are legitimate control values, then it would follow that the values in Table 8 indicate background levels. Although EC-GC was employed as a semi-quantitative screening tool, external calibration curves suggested a sensitivity roughly equal to that achieved by the HRGC-HRMS instrument used for the mass spectrometry based analyses.

4) Conclusions

The areas tested near Sawmill Site 3 did not show PCDD/PCDF levels significantly different from the Control Site.
1) Introduction

The community of Beavercreek, Oregon was chosen as a control community based on the recommendation of the DEQ and the Oregon Health Division. It was located in the same region of Oregon as sites 1, 2 and 3, but did not have any sawmills within several miles.

2) Results

The results are presented in Table 9. It should be noted that sample 402 was obviously mislabeled. The bottle contained what appeared to be dry soil, although it was labeled as stream sediment. Table 9 indicates a background level in the low ppt range for several PCDD/PCDF isomers, and high ppt levels of OCDD.

3) Discussion

Beavercreek was chosen as a control site for reasons already noted. It should be stated explicitly both with respect to residue analysis and epidemiology that to use Beavercreek as a "control" is to compare one "exposed" community with other "exposed" communities. Objections to this approach for epidemiological studies have been
raised at recent conferences addressing the subject of human exposure to PCDD/PCDF (55)(31)(33). For purposes of this study, the author is uncertain as to the validity of using the data in Table 9 as a yardstick against which to compare the rest of the Oregon data. EC-GC screening of samples gathered from a variety of sites in and around OSU and nearby farms failed to turn up any trace of PCDD/PCDF, with the usual exception of low ppt traces of OCDD.

In support of the data, it was very similar to the upstream sample results for the stream next to Site 2 (sample 223), as discussed in Part III. Not enough is known about the background levels of PCDD/PCDF in the Willamette Valley to address this question with any certainty. The sawdust dealer which distributed the tainted wood chips discussed in Part II was located in Beavercreek, Oregon. It is unknown if any connection exists between this fact and the measurable traces of PCDD/PCDF found in environmental samples from that community, as shown in Table 9. These levels are well below any which might be of human health concern, according to the most widely cited risk estimates for residential soils (59). According to DEQ sources, t-PCP was used in past decades all over the valley to control weeds. This might be another possible source for well dispersed background levels of PCDD/PCDF.
OVERALL SUMMARY AND CONCLUSIONS

The results indicate that isolated areas of high parts per trillion to parts per billion PCDD/PCDF contamination are associated with sites where chlorophenols or their salts are used, or burned without any precautions to insure sufficiently high temperatures exist to destroy PCDD/PCDF. A well dispersed low parts per trillion background level of four, five, six, and seven chlorine PCDD's and PCDF's was observed to be superimposed over residues from obvious point source discharges, in the northern Willamette Valley. At all sites studied, OCDD, a compound of low biological activity, was present in higher concentrations. Evidence for such secondary sources was not found in sediment samples from Eagle Harbor, Washington.

Equines exposed to ppb levels of PCDD/PCDF in t-PCP contaminated wood chips over a period of roughly four years accumulated significant residues of these compounds in their liver and adipose tissues.

No evidence of significant naturally occurring degradative processes was suggested by any of the soil or sediment data. PCDD/PCDF, although apparently mobil enough to contaminate areas surrounding facilities where chlorophenolic products have been used, have been observed to be
extremely persistent and refractory compounds under natural conditions. The patterns of laterally substituted PCDD/PCDF isomers present in environmental samples were, in general, quite similar to that expected based on the content of the original chlorophenol/chlorophenate formulations released into the environment.
<table>
<thead>
<tr>
<th>OSU no.</th>
<th>% lipid</th>
<th>Description, including date collected</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NR*</td>
<td>adipose, stillborn foal, Arabian horse farm, 3-29-85</td>
</tr>
<tr>
<td>3</td>
<td>NA</td>
<td>whole blood, stillborn foal, Arabians horse farm, 3-29-85</td>
</tr>
<tr>
<td>4</td>
<td>NR*</td>
<td>liver, stillborn foal, Arabian horse farm, 3-29-85</td>
</tr>
<tr>
<td>5</td>
<td>NR*</td>
<td>placenta, stillborn foal, Arabian horse farm, 3-29-85</td>
</tr>
<tr>
<td>6</td>
<td>NR*</td>
<td>spleen, stillborn foal, Arabian horse farm, 3-29-85</td>
</tr>
<tr>
<td>7</td>
<td>NR*</td>
<td>thymus, stillborn foal, Arabian horse farm, 3-29-85</td>
</tr>
<tr>
<td>9</td>
<td>NR*</td>
<td>liver, &quot;Caraa&quot; (Arabian mare), Arabian horse farm, collected at necropsy, OSU Vet. Med., 5-23-83</td>
</tr>
<tr>
<td>420</td>
<td>NR</td>
<td>heart (composite of muscle/adipose), bull, farm near sawmill site 2, 5-13-85</td>
</tr>
<tr>
<td>421</td>
<td>NR</td>
<td>liver, bull, 5-13-85</td>
</tr>
<tr>
<td>422</td>
<td>NR</td>
<td>muscle, bull, 5-13-85</td>
</tr>
<tr>
<td>501</td>
<td>3</td>
<td>liver, &quot;grey mare control&quot;, received from Dr. Hultgren OSU Vet. Med., 9-10-86</td>
</tr>
<tr>
<td>502</td>
<td>83</td>
<td>adipose, &quot;grey mare control&quot;, received from Dr. Hultgren OSU Vet. Med., 9-10-86</td>
</tr>
<tr>
<td>504</td>
<td>2</td>
<td>liver, &quot;13 yr old mare control&quot;, received from Dr. Hultgren OSU Vet. Med., 9-10-86</td>
</tr>
<tr>
<td>505</td>
<td>91</td>
<td>adipose, &quot;13 yr old mare control&quot;, received from Dr. Hultgren, OSU Vet. Med., 9-10-86</td>
</tr>
<tr>
<td>506</td>
<td>77</td>
<td>adipose, &quot;Coyns Fortune&quot; (stallion), Arabian horse farm, collected at necropsy, OSU Vet. Med., October 1985</td>
</tr>
</tbody>
</table>

NR* not recorded due to insufficient sample, sample lost or damaged
NA not applicable
### Table 2

**Descriptions of Soil/Sediment/Other Samples**

<table>
<thead>
<tr>
<th>OSU no.</th>
<th>% Moisture</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EH#1</td>
<td>58</td>
<td>Eagle Harbor, WA sediment, received from EPA Region 10, April 1985</td>
</tr>
<tr>
<td>EH#2</td>
<td>67</td>
<td>Eagle Harbor, WA sediment, received from EPA Region 10, April 1985</td>
</tr>
<tr>
<td>EH05-6</td>
<td>54</td>
<td>Eagle Harbor, WA sediment, received from EPA Newport, OR Environmental Res. Lab., 8-28-85</td>
</tr>
<tr>
<td>EH2</td>
<td>37</td>
<td>Eagle Harbor, WA sediment, received from EPA Newport, OR Environmental Res. Lab., dated 8-9-85, received 9-24-85</td>
</tr>
<tr>
<td>Reichold NA</td>
<td></td>
<td>crystalline technical grade pentachlorophenol &quot;4-9-162&quot;, gift from Reichold Chemical Co., Tacoma WA</td>
</tr>
<tr>
<td>Aldrich NA</td>
<td></td>
<td>crystalline technical grade pentachlorophenol, lot no. CCO22487, gift of Dr. Nancy Kerkyliet, OSU Vet. Med. School</td>
</tr>
<tr>
<td>11</td>
<td>NA</td>
<td>diptank sludge from mill, Site 2, collected by DEQ in 1984</td>
</tr>
<tr>
<td>12</td>
<td>44</td>
<td>soil collected from drainage ditch between road and lumber yard, see Figure 2, 2-12-85, Site 2</td>
</tr>
<tr>
<td>33</td>
<td>NA</td>
<td>wood chips, from &quot;Carra's&quot; stall, Columbia Labs no. B604, Arabian horse farm, 6-84</td>
</tr>
<tr>
<td>53</td>
<td>19</td>
<td>surface soil collected from underneath easternmost stall in barn, Arabian horse farm, 5-10-85</td>
</tr>
<tr>
<td>55</td>
<td>56</td>
<td>surface soil collected from drainage ditch between Road and lumber yard, see Figure 2, 5-10-85, Site 2</td>
</tr>
<tr>
<td>80</td>
<td>25</td>
<td>surface soil collected from drainage ditch between Road and lumber yard, see Figure 2, 5-10-85, Site 2</td>
</tr>
<tr>
<td>92</td>
<td>28</td>
<td>surface soil collected from drainage ditch between Road and lumber yard, see Figure 2, 5-10-85, Site 2</td>
</tr>
</tbody>
</table>
(Table 2, continued)

202 24  surface sediment collected from drainage ditch at Road 150 ft upstream of confluence with Stream, 6-13-85, Site 2

203 27  same location as 202, samples are not exact duplicates, surface ditch sediment, 6-13-85, Site 2

204 25  middle of field across street from Oil Company, 6-13-85 dry soil, Site 2

205 31  surface sediment from ditch across street from Oil Company, 6-13-85, Site 2

207 16  Stream, 10-20 cm sediment core, middle of creek, 10 ft south of 13275 access rd. culvert, 6-13-85, Site 2

208 27  Stream, 2-10 cm sediment core, middle of creek, 10 ft south of 13275 access rd. culvert, same location as 207, 6-13-85

209 24  Stream, surface sediment, 20 ft north of 13275 access rd culvert, 6-13-85, Site 2

210 26  Stream, 100 yds south of Road, confluence ditch surface sediment from middle of creek, 6-13-87, Site 2

211 23  same as 210 except sampled east side of Stream, 2 ft from bank, 6-13-85, Site 2

214 36  beginning of drainage ditch between Road and lumber yard, see Figure 2, 6-13-85, Site 2

215  NR*  surface soil, to depth of 7.6 cm, from ditch draining Avison lumber yard, drains into larger ditch running along Road see Figure 2, 6-13-85

216  NR*  same location as 215, 7.6-15.2 cm depth, see Figure 2, 6-13-85, Site 2

217 41  110 ft upstream from confluence with Road ditch, small ditch draining lumber yard, see Figure 2, 6-13-85, Site 2

218 47  surface soil on bank of Road, ditch adjacent to farm property, 25 ft upstream from driveway, 5-13-85, Site 2

219 23  farm property, surface soil, field adjacent to Road, ditch, center of field, 6-13-85, site 2

220 21  same as 219, but corner of field closest to trailer, 6-13-85, Site 2
(Table 2, continued)

221 28  
same as 219, but extreme NW corner of property, adjacent to Road, ditch, 6-13-85, Site 2

222 34  
Stream east of culvert next to Crown Zellerbach easement, surface sediment, adjacent to mill, 6-13-85

223 23  
control surface sediment upstream from mill, Stream, 20 ft east of continuation of Crown Zellerbach easement, 6-13-85, Site 2

401 38  
Beaver Creek control sample, "stream sediment beside rd", received from OSU 8-28-85

402 8 **  
Beaver Creek control sample, "ditch sediment ", received from OSU 8-28-85

403 8  
Beaver Creek control sample, "agricultural soil", received from OSU 8-28-85

404 46  
Beaver Creek control sample, "64 core top", received from OSU 8-28-85

405 35  
Beaver Creek control sample, "64 core bottom", received from OSU 8-28-85

407 34  
Farm near site 3, "agricultural soil, flood plain", received from OSU 8-29-85

408 25  
Farm near site 3, "sediment sample, stagnant pond", received from OSU 8-29-85

409 60  
Farm near site 3, "sediment sample...", received from OSU 8-29-85

410 27  
Farm near site 3, "sediment sample, moving water above stagnant pool", received from OSU 8-29-85

** not recorded due to insufficient sample

** sample appeared to be dry soil when received for analysis, contrary to label on bottle
Table 3

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in two Samples of Technical Pentachlorophenol

<table>
<thead>
<tr>
<th>n</th>
<th>isomer</th>
<th>sample, units are microgram/gram of t-PCP (Reichold*)</th>
<th>(Aldrich**)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>nd(0.10)</td>
<td>nd(0.10)</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>nd(0.07)</td>
<td>nd(0.15)</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(0.07)</td>
<td>nd(0.15)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>nd(0.05)</td>
<td>nd(0.08)</td>
</tr>
<tr>
<td>6</td>
<td>12467-PCDF</td>
<td>nd(0.01)</td>
<td>nd(0.14)</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>1.10</td>
<td>1.61</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
<td>nd(0.07)</td>
<td>nd(0.14)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>0.30</td>
<td>0.48</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>0.47</td>
<td>0.63</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>nd(0.11)</td>
<td>nd(0.15)</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
<td>1.43</td>
<td>nd(0.08)</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
<td>nd(0.04)</td>
<td>nd(0.04)</td>
</tr>
<tr>
<td>14</td>
<td>123678-HxCDF</td>
<td>0.55</td>
<td>nd(0.01)</td>
</tr>
<tr>
<td>15</td>
<td>234678-HxCDF</td>
<td>0.32</td>
<td>0.62</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>0.62</td>
<td>0.13</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDD</td>
<td>nd(0.07)</td>
<td>nd(0.10)</td>
</tr>
<tr>
<td>18</td>
<td>123679-HxCDF</td>
<td>0.30</td>
<td>12.66</td>
</tr>
<tr>
<td>19</td>
<td>123789-HxCDD</td>
<td>0.51</td>
<td>0.22</td>
</tr>
<tr>
<td>20</td>
<td>1234678-HpCDF</td>
<td>8.32</td>
<td>39.50</td>
</tr>
<tr>
<td>21</td>
<td>1234789-HpCDF</td>
<td>nd(0.67)</td>
<td>0.41</td>
</tr>
<tr>
<td>22</td>
<td>1234678-HpCDD</td>
<td>83.1</td>
<td>157</td>
</tr>
<tr>
<td>23</td>
<td>OCDF</td>
<td>4.97</td>
<td>210</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>1500</td>
<td>1100</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

NR = data not recorded

* only documentation with 1 lb can was "4-9-162" stamped on the top

** lot no. CCO22487, gift of Dr. Nancy Kerkvliet, OSU School of Veterinary Medicine
Table 4

Summary Table of Results, Total Congener Group
Concentrations of PCDD, PCDF found in two Samples
of Technical Pentachlorophenol Compared with an
Industry Composite Sample

<table>
<thead>
<tr>
<th>Congener Group</th>
<th>sample, units are microgram/gram of t-PCP</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Reichold)</td>
<td>(Aldrich)</td>
<td>(from reference (14))</td>
</tr>
<tr>
<td>TCDF***</td>
<td>nd(0.10)</td>
<td>5.42</td>
<td>NR</td>
</tr>
<tr>
<td>PCDF</td>
<td>6.05</td>
<td>3.20</td>
<td>nd(2.0)</td>
</tr>
<tr>
<td>HxCDF</td>
<td>18.0</td>
<td>52.5</td>
<td>57</td>
</tr>
<tr>
<td>HpCDF</td>
<td>24.3</td>
<td>158</td>
<td>130</td>
</tr>
<tr>
<td>OCDF</td>
<td>4.97</td>
<td>210</td>
<td>90</td>
</tr>
<tr>
<td>TCDD***</td>
<td>nd(0.06)</td>
<td>nd(0.083)</td>
<td>NR</td>
</tr>
<tr>
<td>PCDD</td>
<td>nd(0.11)</td>
<td>nd(6.15)</td>
<td>nd(1.0)</td>
</tr>
<tr>
<td>HxCDD</td>
<td>21.0</td>
<td>29.2</td>
<td>15.0</td>
</tr>
<tr>
<td>HpCDD</td>
<td>138</td>
<td>221</td>
<td>410</td>
</tr>
<tr>
<td>OCDD</td>
<td>1500</td>
<td>1100</td>
<td>1500</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

NR = not reported in publication, presumably not detected

*** DOES NOT include any contributions from 2,3,7,8-TCDF
or 2,3,7,8-TCDD. These isomers were not found in either
t-PCP sample at the detection limits stated
in Table 1.
Table 5
Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Eagle Harbor Sediments

<table>
<thead>
<tr>
<th>n</th>
<th>isomer</th>
<th>(EH#1)</th>
<th>(EH#2)</th>
<th>(EH05-6)</th>
<th>(EH2*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2378-TCDF***</td>
<td>nd(2)</td>
<td>nd(3)</td>
<td>nd(2)</td>
<td>nd(6)</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>nd(2)</td>
<td>nd(3)</td>
<td>nd(2)</td>
<td>nd(6)</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(2)</td>
<td>nd(3)</td>
<td>nd(2)</td>
<td>nd(10)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD***</td>
<td>nd(8)</td>
<td>nd(12)</td>
<td>nd(4)</td>
<td>nd(2)</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>nd(6)</td>
<td>nd(64)</td>
<td>nd(8)</td>
<td>nd(6)</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
<td>nd(6)</td>
<td>nd(64)</td>
<td>nd(8)</td>
<td>nd(6)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>nd(6)</td>
<td>nd(64)</td>
<td>nd(8)</td>
<td>nd(6)</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>nd(6)</td>
<td>nd(64)</td>
<td>nd(8)</td>
<td>nd(6)</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>nd(6)</td>
<td>nd(75)</td>
<td>nd(4)</td>
<td>5</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
<td>nd(5)</td>
<td>nd(8)</td>
<td>nd(6)</td>
<td>nd(8)</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
<td>nd(5)</td>
<td>nd(8)</td>
<td>nd(6)</td>
<td>nd(3)</td>
</tr>
<tr>
<td>14</td>
<td>123678-HxCDF</td>
<td>nd(5)</td>
<td>nd(8)</td>
<td>nd(6)</td>
<td>nd(3)</td>
</tr>
<tr>
<td>15</td>
<td>234678-HxCDF</td>
<td>nd(5)</td>
<td>nd(8)</td>
<td>nd(6)</td>
<td>nd(3)</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>nd(5)</td>
<td>nd(8)</td>
<td>nd(6)</td>
<td>nd(3)</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDD</td>
<td>nd(12)</td>
<td>nd(20)</td>
<td>nd(25)</td>
<td>nd(4)</td>
</tr>
<tr>
<td>18</td>
<td>123678-HxCDD</td>
<td>nd(12)</td>
<td>nd(20)</td>
<td>nd(25)</td>
<td>16</td>
</tr>
<tr>
<td>19</td>
<td>123789-HxCDD</td>
<td>nd(12)</td>
<td>nd(20)</td>
<td>nd(25)</td>
<td>nd(20)</td>
</tr>
<tr>
<td>20</td>
<td>1234678-HpCDF</td>
<td>440</td>
<td>790</td>
<td>225</td>
<td>58</td>
</tr>
<tr>
<td>21</td>
<td>1234789-HpCDF</td>
<td>nd(20)</td>
<td>nd(25)</td>
<td>nd(30)</td>
<td>nd(10)</td>
</tr>
<tr>
<td>22</td>
<td>1234678-HpCDD</td>
<td>1450</td>
<td>2370</td>
<td>800</td>
<td>420</td>
</tr>
<tr>
<td>23</td>
<td>OCDF</td>
<td>980</td>
<td>1440</td>
<td>350</td>
<td>250</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>37000</td>
<td>42000</td>
<td>6050</td>
<td>4500</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded
* samples received OSU during April 85
** sample dated 8-9-85, received ERLD 9-24-85

*** DOES NOT include any contributions from 2,3,7,8-TCDD or 2,3,7,8-TCDF. These isomers were NOT found in any Eagle Harbor samples.
Table 6

Summary Table of Results, Total Congener Group
Concentrations of PCDD, PCDF found in
Eagle Harbor Sediments

<table>
<thead>
<tr>
<th>Congener Group</th>
<th>Sample, units are pg/gram dryweight</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(EH#1*)</td>
</tr>
<tr>
<td>TCDF***</td>
<td>nd(2)</td>
</tr>
<tr>
<td>PCDF</td>
<td>nd(6)</td>
</tr>
<tr>
<td>HxCDF</td>
<td>207</td>
</tr>
<tr>
<td>HpCDF</td>
<td>980</td>
</tr>
<tr>
<td>OCDF</td>
<td>980</td>
</tr>
<tr>
<td>TCDD***</td>
<td>nd(8)</td>
</tr>
<tr>
<td>PCDD</td>
<td>nd(6)</td>
</tr>
<tr>
<td>HxCDD</td>
<td>67</td>
</tr>
<tr>
<td>HpCDD</td>
<td>4400</td>
</tr>
<tr>
<td>OCDD</td>
<td>37000</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

* sample received OSU during April 85
** sample dated 8-9-85, received ERLD 9-24-85
*** DOES NOT include any contributions from 2,3,7,8-TCDF or 2,3,7,8-TCDD. These isomers were not found in any Eagle Harbor Samples, at the detection limits stated in Table 5.
Table 7

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF from Vicinity of Sawmill Site 2*

<table>
<thead>
<tr>
<th>n</th>
<th>isomer</th>
<th>Sample, units are pg/gram dry weight</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(12)</td>
</tr>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>nd(51)</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>nd(1.6)</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(1.6)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>nd(12)</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>nd(1.2)</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>123</td>
</tr>
<tr>
<td>8</td>
<td>12357-PCDF</td>
<td>nd(50)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>163</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>nd(1.2)</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>nd(151)</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
<td>116</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>14</td>
<td>134678-HxCDF</td>
<td>157</td>
</tr>
<tr>
<td>15</td>
<td>1234678-HxCDF</td>
<td>126</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDD</td>
<td>nd(2.1)</td>
</tr>
<tr>
<td>18</td>
<td>123678-HxCDD</td>
<td>3250</td>
</tr>
<tr>
<td>19</td>
<td>123789-HxCDD</td>
<td>678</td>
</tr>
<tr>
<td>20</td>
<td>1234678-HpCDF</td>
<td>1810</td>
</tr>
<tr>
<td>21</td>
<td>1234789-HpCDF</td>
<td>2580</td>
</tr>
<tr>
<td>22</td>
<td>1234678-HpCDD</td>
<td>20600</td>
</tr>
<tr>
<td>23</td>
<td>OCDF</td>
<td>569</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>68100</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded due to poor recoveries

‡ samples collected in on May 10 and June 13, 1985
# sample collected on February 12, 1985
<table>
<thead>
<tr>
<th>Sample, units are pg/gram dry weight</th>
<th>(92)</th>
<th>(209)</th>
<th>(211)</th>
<th>(214)</th>
<th>(217)</th>
<th>(220)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2379-TCDF</td>
<td>nd(50)</td>
<td>nd(2.0)</td>
<td>nd(5.1)</td>
<td>nd(8.0)</td>
<td>nd(0.5)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>2 2367-TCDF</td>
<td>nd(4.8)</td>
<td>nd(0.4)</td>
<td>nd(1.0)</td>
<td>nd(1.2)</td>
<td>nd(0.5)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>3 3467-TCDF</td>
<td>nd(2.6)</td>
<td>nd(0.4)</td>
<td>nd(2.0)</td>
<td>nd(0.9)</td>
<td>nd(0.5)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>4 1234-TCDI</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5 2378-TCDI</td>
<td>nd(0.5)</td>
<td>nd(0.6)</td>
<td>nd(2.4)</td>
<td>nd(4.9)</td>
<td>nd(1.1)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>6 13467-PCDF</td>
<td>nd(1.0)</td>
<td>nd(0.4)</td>
<td>nd(0.9)</td>
<td>nd(0.7)</td>
<td>nd(0.3)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>7 12378-PCDF</td>
<td>nd(68)</td>
<td>nd(2.1)</td>
<td>nd(5.7)</td>
<td>nd(13)</td>
<td>nd(0.6)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>8 12367-PCDF</td>
<td>nd(1.0)</td>
<td>nd(0.4)</td>
<td>nd(0.9)</td>
<td>nd(0.7)</td>
<td>nd(0.3)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>9 23478-PCDF</td>
<td>42</td>
<td>1.3</td>
<td>nd(10)</td>
<td>11</td>
<td>nd(0.3)</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>10 23467-PCDF</td>
<td>61</td>
<td>2.8</td>
<td>nd(13)</td>
<td>16</td>
<td>nd(0.3)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>11 12378-PCDD</td>
<td>110</td>
<td>nd(4.2)</td>
<td>nd(9.6)</td>
<td>22</td>
<td>nd(1.1)</td>
<td>nd(1.6)</td>
</tr>
<tr>
<td>12 123478-HxCDF</td>
<td>47</td>
<td>2.5</td>
<td>nd(6.0)</td>
<td>18</td>
<td>nd(1.0)</td>
<td>nd(1.8)</td>
</tr>
<tr>
<td>13 123467-HxCDF</td>
<td>nd(1.6)</td>
<td>nd(0.7)</td>
<td>nd(1.3)</td>
<td>nd(0.9)</td>
<td>nd(0.5)</td>
<td>nd(0.3)</td>
</tr>
<tr>
<td>14 123678-HxCDF</td>
<td>74</td>
<td>2.6</td>
<td>nd(2.0)</td>
<td>nd(1.3)</td>
<td>nd(0.5)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>15 234678-HxCDF</td>
<td>61</td>
<td>2.7</td>
<td>5.0</td>
<td>15</td>
<td>nd(0.5)</td>
<td>nd(0.8)</td>
</tr>
<tr>
<td>16 123789-HxCDF</td>
<td>20</td>
<td>nd(3.0)</td>
<td>nd(3.3)</td>
<td>5.8</td>
<td>nd(0.5)</td>
<td>nd(0.8)</td>
</tr>
<tr>
<td>17 123478-HxCDD</td>
<td>nd(9.2)</td>
<td>nd(6.6)</td>
<td>nd(5.9)</td>
<td>nd(49)</td>
<td>nd(3.7)</td>
<td>nd(4.1)</td>
</tr>
<tr>
<td>18 123678-HxCDD</td>
<td>1090</td>
<td>34</td>
<td>57</td>
<td>233</td>
<td>nd(26)</td>
<td>6.1</td>
</tr>
<tr>
<td>19 123789-HxCDD</td>
<td>253</td>
<td>5.7</td>
<td>8.9</td>
<td>52</td>
<td>nd(3.1)</td>
<td>nd(2.7)</td>
</tr>
<tr>
<td>20 123467-HpCDF</td>
<td>803</td>
<td>87</td>
<td>163</td>
<td>207</td>
<td>98</td>
<td>21</td>
</tr>
<tr>
<td>21 123478-HpCDF</td>
<td>17</td>
<td>nd(5.2)</td>
<td>nd(10)</td>
<td>nd(7.2)</td>
<td>nd(27)</td>
<td>nd(4.2)</td>
</tr>
<tr>
<td>22 123467-BhpCDD</td>
<td>8770</td>
<td>548</td>
<td>860</td>
<td>2560</td>
<td>716</td>
<td>136</td>
</tr>
<tr>
<td>23 OCDF</td>
<td>253</td>
<td>55</td>
<td>83</td>
<td>66</td>
<td>NR*</td>
<td>NR*</td>
</tr>
<tr>
<td>24 OCDD</td>
<td>29900</td>
<td>6240</td>
<td>5500</td>
<td>13400</td>
<td>NR*</td>
<td>NR*</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded
NR* = data not recorded due to poor recoveries
* samples collected on June 13, 1985
** sample collected on May 10, 1985
Summary Table of Results, Biosignificant Isomers of PCDD, PCDF from Vicinity of Sawmill Site 2

<table>
<thead>
<tr>
<th>n</th>
<th>Sample, units are pg/gram dry weight</th>
<th>(218)</th>
<th>(219)</th>
<th>(221)</th>
<th>(222)</th>
<th>(223)</th>
<th>(80)**</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>50</td>
<td>nd(1.5)</td>
<td>nd(12.5)</td>
<td>120</td>
<td>nd(0.7)</td>
<td>20</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>1.5</td>
<td>nd(0.7)</td>
<td>nd(1.2)</td>
<td>16</td>
<td>nd(0.7)</td>
<td>nd(6.9)</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>1.2</td>
<td>nd(0.7)</td>
<td>0.5</td>
<td>17</td>
<td>nd(1.1)</td>
<td>nd(3.7)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>3.0</td>
<td>nd(1.7)</td>
<td>nd(0.5)</td>
<td>2.0</td>
<td>nd(1.5)</td>
<td>0.5</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>nd(2.0)</td>
<td>nd(1.2)</td>
<td>nd(0.3)</td>
<td>nd(1.8)</td>
<td>nd(1.2)</td>
<td>nd(1.6)</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>159</td>
<td>nd(1.2)</td>
<td>nd(26)</td>
<td>252</td>
<td>nd(1.2)</td>
<td>37</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
<td>nd(2.0)</td>
<td>nd(1.2)</td>
<td>nd(0.3)</td>
<td>nd(1.8)</td>
<td>nd(1.2)</td>
<td>nd(1.6)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>179</td>
<td>nd(1.2)</td>
<td>11</td>
<td>127</td>
<td>nd(1.2)</td>
<td>37</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>308</td>
<td>nd(1.2)</td>
<td>17</td>
<td>524</td>
<td>nd(1.2)</td>
<td>53</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>441</td>
<td>nd(3.5)</td>
<td>27</td>
<td>250</td>
<td>nd(4.9)</td>
<td>152</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
<td>223</td>
<td>nd(1.9)</td>
<td>15</td>
<td>293</td>
<td>nd(1.6)</td>
<td>33</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
<td>nd(3.1)</td>
<td>nd(1.9)</td>
<td>nd(0.6)</td>
<td>nd(2.9)</td>
<td>nd(1.6)</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>14</td>
<td>123467-HxCDF</td>
<td>314</td>
<td>nd(1.9)</td>
<td>24</td>
<td>315</td>
<td>nd(1.6)</td>
<td>78</td>
</tr>
<tr>
<td>15</td>
<td>23478-PCDF</td>
<td>323</td>
<td>nd(1.9)</td>
<td>17</td>
<td>320</td>
<td>nd(1.6)</td>
<td>53</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>115</td>
<td>nd(1.9)</td>
<td>nd(12)</td>
<td>143</td>
<td>nd(1.6)</td>
<td>12</td>
</tr>
<tr>
<td>17</td>
<td>123478-PCDD</td>
<td>nd(546)</td>
<td>nd(4.2)</td>
<td>nd(2.9)</td>
<td>612</td>
<td>nd(6.1)</td>
<td>76</td>
</tr>
<tr>
<td>18</td>
<td>123678-HxCDD</td>
<td>4800</td>
<td>nd(21)</td>
<td>284</td>
<td>5100</td>
<td>nd(23)</td>
<td>830</td>
</tr>
<tr>
<td>19</td>
<td>123798-HxCDD</td>
<td>1140</td>
<td>nd(4.2)</td>
<td>54</td>
<td>908</td>
<td>nd(12)</td>
<td>326</td>
</tr>
<tr>
<td>20</td>
<td>1234678-HpCDF</td>
<td>3690</td>
<td>10</td>
<td>348</td>
<td>7170</td>
<td>22</td>
<td>844</td>
</tr>
<tr>
<td>21</td>
<td>1234789-HpcCDF</td>
<td>57</td>
<td>nd(4.1)</td>
<td>nd(3.6)</td>
<td>221</td>
<td>nd(3.4)</td>
<td>20</td>
</tr>
<tr>
<td>22</td>
<td>1234678-HpCDD</td>
<td>46100</td>
<td>70</td>
<td>3180</td>
<td>77000</td>
<td>158</td>
<td>9440</td>
</tr>
<tr>
<td>23</td>
<td>OCDF</td>
<td>893</td>
<td>nd(11)</td>
<td>nd(142)</td>
<td>2000</td>
<td>nd(30)</td>
<td>296</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>218000</td>
<td>600</td>
<td>13400</td>
<td>650000</td>
<td>1200</td>
<td>51800</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

** sample collected on May 10, 1985

Estimated concentration based on FID data
Summary Table of Results, Biosignificant Isomers of PCDD, PCDF from Vicinity of Sawmill Site 2*

<table>
<thead>
<tr>
<th>Sample</th>
<th>Units are pg/gram dry weight</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(203)</td>
<td>(204)</td>
<td>(205)</td>
<td>(210)</td>
</tr>
<tr>
<td>1 2378-TCDF</td>
<td>nd(1.0)</td>
<td>5.5</td>
<td>28</td>
<td>nd(0.8)</td>
</tr>
<tr>
<td>2 2367-TCDF</td>
<td>nd(0.2)</td>
<td>2.3</td>
<td>nd(3.6)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>3 3467-TCDF</td>
<td>nd(0.2)</td>
<td>nd(0.9)</td>
<td>nd(2.4)</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>4 1234-TCDD</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5 2378-TCDD</td>
<td>nd(0.5)</td>
<td>3.0</td>
<td>7.2</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>6 13467-PCDF</td>
<td>nd(0.2)</td>
<td>nd(4.0)</td>
<td>nd(5.0)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>7 12378-PCDF</td>
<td>nd(0.5)</td>
<td>nd(13)</td>
<td>57</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>8 12367-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(5.0)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>9 23478-PCDF</td>
<td>nd(0.3)</td>
<td>10</td>
<td>74</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>10 23467-PCDF</td>
<td>nd(0.2)</td>
<td>22</td>
<td>105</td>
<td>1.1</td>
</tr>
<tr>
<td>11 12378-PCDD</td>
<td>nd(2.0)</td>
<td>25</td>
<td>120</td>
<td>nd(1.8)</td>
</tr>
<tr>
<td>12 123478-HxCDF</td>
<td>1.3</td>
<td>15</td>
<td>92</td>
<td>nd(2.2)</td>
</tr>
<tr>
<td>13 123478-HxCDF</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
<td>65</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>14 123678-HxCDF</td>
<td>nd(2.3)</td>
<td>19</td>
<td>92</td>
<td>3.0</td>
</tr>
<tr>
<td>15 234678-HxCDF</td>
<td>0.9</td>
<td>16</td>
<td>86</td>
<td>1.8</td>
</tr>
<tr>
<td>16 123799-HxCDF</td>
<td>nd(0.4)</td>
<td>4.9</td>
<td>40</td>
<td>nd(0.8)</td>
</tr>
<tr>
<td>17 123478-HxCDD</td>
<td>nd(0.9)</td>
<td>nd(1.3)</td>
<td>100</td>
<td>nd(1.0)</td>
</tr>
<tr>
<td>18 123678-HxCDD</td>
<td>10</td>
<td>250</td>
<td>2340</td>
<td>28</td>
</tr>
<tr>
<td>19 123789-HxCDD</td>
<td>4.3</td>
<td>72</td>
<td>371</td>
<td>nd(8.0)</td>
</tr>
<tr>
<td>20 1234678-HpCDF</td>
<td>25</td>
<td>300</td>
<td>1500</td>
<td>36</td>
</tr>
<tr>
<td>21 1234789-HpCDF</td>
<td>nd(0.9)</td>
<td>10</td>
<td>43</td>
<td>nd(1.4)</td>
</tr>
<tr>
<td>22 1234678-HpCDD</td>
<td>183</td>
<td>1900</td>
<td>7000</td>
<td>437</td>
</tr>
<tr>
<td>23 OCDF</td>
<td>32</td>
<td>232</td>
<td>649</td>
<td>32</td>
</tr>
<tr>
<td>24 OCDD</td>
<td>5820</td>
<td>14000</td>
<td>72000*</td>
<td>2500</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

* samples collected on June 13, 1985

* Estimated concentration based on FID data
Table 7a

Summary Table of Results, Total Congener Group
Concentrations of PCDD, PCDF found in Soil Core
From Sawmill Site 2

<table>
<thead>
<tr>
<th>Congener Group</th>
<th>sample, units are pg/gram wet weight as received</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(215)                                      (216)</td>
</tr>
<tr>
<td>TCDF***</td>
<td>nd(2.0)                                   nd(5.0)</td>
</tr>
<tr>
<td>PCDF</td>
<td>nd(5.0)                                   nd(20)</td>
</tr>
<tr>
<td>HxCDF</td>
<td>NR                                         NR</td>
</tr>
<tr>
<td>HpCDF</td>
<td>NR                                         NR</td>
</tr>
<tr>
<td>OCDF</td>
<td>NR                                         NR</td>
</tr>
<tr>
<td>TCDD***</td>
<td>nd(1.0)                                   nd(5.0)</td>
</tr>
<tr>
<td>PCDD</td>
<td>76                                         nd(30)</td>
</tr>
<tr>
<td>HxCDD</td>
<td>1700                                       10</td>
</tr>
<tr>
<td>HpCDD</td>
<td>5400                                       400</td>
</tr>
<tr>
<td>OCDD</td>
<td>30000                                      2900</td>
</tr>
</tbody>
</table>

Note that these samples are reported as wet weight concentrations, due to insufficient sample present for % moisture determination

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

NR = not reported

*** DOES NOT include any contributions from 2,3,7,8-TCDF or 2,3,7,8-TCDD. These isomers were not found in either core sample at the detection limits indicated

‡ Samples collected on June 13, 1985
Table 7b
Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Diptank Sludge Collected From Site 2

<table>
<thead>
<tr>
<th>n</th>
<th>isomer</th>
<th>Sample, units are dimensionless*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>0.51</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>0.087</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(0.0010)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>0.0033</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>NR</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>0.20</td>
</tr>
<tr>
<td>8</td>
<td>12357-PCDF</td>
<td>nd(0.0050)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>0.28</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>0.80</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>0.22</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
<td>nd(0.008)</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
<td>nd(0.008)</td>
</tr>
<tr>
<td>14</td>
<td>123678-HxCDF</td>
<td>nd(0.008)</td>
</tr>
<tr>
<td>15</td>
<td>234678-HxCDF</td>
<td>11</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>1.3</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDD</td>
<td>nd(0.01)</td>
</tr>
<tr>
<td>18</td>
<td>123578-HxCDD</td>
<td>19</td>
</tr>
<tr>
<td>19</td>
<td>123789-HxCDD</td>
<td>3.2</td>
</tr>
<tr>
<td>20</td>
<td>1234789-HpCDF</td>
<td>3.9</td>
</tr>
<tr>
<td>21</td>
<td>1234789-HpCDF</td>
<td>2.5</td>
</tr>
<tr>
<td>22</td>
<td>1234789-HpCDD</td>
<td>770</td>
</tr>
<tr>
<td>23</td>
<td>OCDF</td>
<td>100</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>10000</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

* Concentrations have been normalized to a scale with OCDD = 10000 dimensionless units. It was not possible to assign absolute concentrations to this sample.
Table 8

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found at Farm near Sawmill Site 3

<table>
<thead>
<tr>
<th>Sample, units are pg/gram dry weight</th>
<th>(407)</th>
<th>(407)</th>
<th>(408)</th>
<th>(409)</th>
<th>(410)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2378-TCDF</td>
<td>nd(1)</td>
<td>nd(1.6)</td>
<td>nd(0.9)</td>
<td>nd(2)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>2 2367-TCDF</td>
<td>nd(1)</td>
<td>0.5</td>
<td>nd(0.2)</td>
<td>nd(1.4)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>3 3467-TCDF</td>
<td>nd(1)</td>
<td>nd(0.6)</td>
<td>nd(0.2)</td>
<td>nd(0.9)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>4 1234-TCDD</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5 2378-TCDD</td>
<td>nd(2)</td>
<td>nd(4.4)</td>
<td>nd(0.8)</td>
<td>nd(0.6)</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>6 13467-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>7 12378-PCDF</td>
<td>nd(0.3)</td>
<td>nd(0.2)</td>
<td>nd(1.2)</td>
<td>nd(0.7)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>8 12367-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>9 23478-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.4)</td>
<td>nd(1.1)</td>
<td>nd(0.4)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>10 23467-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.6)</td>
<td>nd(2.2)</td>
<td>nd(0.4)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>11 12378-PCDD</td>
<td>nd(0.6)</td>
<td>nd(1.5)</td>
<td>nd(1.5)</td>
<td>nd(2.6)</td>
<td>nd(1.4)</td>
</tr>
<tr>
<td>12 123478-HxCDF</td>
<td>nd(0.4)</td>
<td>nd(2.0)</td>
<td>1.7</td>
<td>nd(2.2)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>13 123467-HxCDF</td>
<td>nd(0.4)</td>
<td>nd(0.4)</td>
<td>nd(0.3)</td>
<td>nd(0.4)</td>
<td>nd(0.2)</td>
</tr>
<tr>
<td>14 123678-HxCDF</td>
<td>nd(0.4)</td>
<td>nd(0.4)</td>
<td>nd(4.3)</td>
<td>nd(0.4)</td>
<td>nd(0.3)</td>
</tr>
<tr>
<td>15 234678-HxCDF</td>
<td>nd(0.4)</td>
<td>nd(0.4)</td>
<td>3.8</td>
<td>nd(0.4)</td>
<td>nd(0.3)</td>
</tr>
<tr>
<td>16 123789-HxCDF</td>
<td>nd(0.4)</td>
<td>nd(0.4)</td>
<td>nd(3.0)</td>
<td>nd(0.7)</td>
<td>nd(0.3)</td>
</tr>
<tr>
<td>17 123478-HxCDD</td>
<td>nd(0.7)</td>
<td>nd(1.1)</td>
<td>nd(0.8)</td>
<td>nd(0.9)</td>
<td>nd(1.4)</td>
</tr>
<tr>
<td>18 123678-HxCDD</td>
<td>nd(8)</td>
<td>5.5</td>
<td>29</td>
<td>14</td>
<td>nd(17)</td>
</tr>
<tr>
<td>19 123789-HxCDD</td>
<td>1.1</td>
<td>2.3</td>
<td>5.8</td>
<td>3.5</td>
<td>nd(1.1)</td>
</tr>
<tr>
<td>20 1234678-HpCDF</td>
<td>6.7</td>
<td>6.3</td>
<td>120</td>
<td>23</td>
<td>17</td>
</tr>
<tr>
<td>21 1234789-HpCDF</td>
<td>nd(1.2)</td>
<td>nd(1.5)</td>
<td>nd(3.6)</td>
<td>nd(1.1)</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>22 1234678-HpCDD</td>
<td>38.8</td>
<td>36.9</td>
<td>876</td>
<td>128</td>
<td>174</td>
</tr>
<tr>
<td>23 OCDF</td>
<td>nd(14)</td>
<td>9.2</td>
<td>91</td>
<td>34</td>
<td>12</td>
</tr>
<tr>
<td>24 OCDD</td>
<td>532</td>
<td>334</td>
<td>16100</td>
<td>1890</td>
<td>4010</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

* samples collected during July 1985
Table 9

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found at Beaver Creek Control Sites

<table>
<thead>
<tr>
<th>Sample, units are pg/gram dry weight</th>
<th>(401)</th>
<th>(402)</th>
<th>(402)</th>
<th>(403)</th>
<th>(404)</th>
<th>(405)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n isomer</td>
<td>nd(0.5)</td>
<td>nd(0.5)</td>
<td>nd(0.5)</td>
<td>nd(0.5)</td>
<td>nd(0.5)</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>1 2378-TCDF</td>
<td>nd(0.8)</td>
<td>nd(0.8)</td>
<td>nd(1.5)</td>
<td>nd(0.7)</td>
<td>nd(2.3)</td>
<td></td>
</tr>
<tr>
<td>2 2367-TCDF</td>
<td>nd(0.6)</td>
<td>nd(0.8)</td>
<td>nd(1.4)</td>
<td>nd(0.9)</td>
<td>0.4</td>
<td>0.7</td>
</tr>
<tr>
<td>3 3467-TCDF</td>
<td>nd(0.3)</td>
<td>nd(0.8)</td>
<td>nd(0.3)</td>
<td>nd(0.6)</td>
<td>nd(0.2)</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>4 13467-PCDF</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5 12378-PCDF</td>
<td>nd(0.5)</td>
<td>nd(1.3)</td>
<td>0.9</td>
<td>nd(1.1)</td>
<td>nd(1.5)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>6 13467-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
<td>nd(0.3)</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
</tr>
<tr>
<td>7 12378-PCDF</td>
<td>nd(0.6)</td>
<td>nd(1.3)</td>
<td>0.9</td>
<td>nd(1.1)</td>
<td>nd(1.5)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>8 12378-PCDF</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
<td>nd(0.3)</td>
<td>nd(0.2)</td>
<td>nd(0.2)</td>
<td>nd(0.3)</td>
</tr>
<tr>
<td>9 12378-PCDF</td>
<td>nd(0.6)</td>
<td>nd(1.3)</td>
<td>0.9</td>
<td>nd(1.1)</td>
<td>nd(1.5)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>10 12378-PCDF</td>
<td>nd(0.9)</td>
<td>1.6</td>
<td>nd(6.2)</td>
<td>nd(2.8)</td>
<td>nd(1.3)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>11 12378-PCDF</td>
<td>nd(1.1)</td>
<td>nd(3.3)</td>
<td>nd(1.5)</td>
<td>nd(1.2)</td>
<td>0.8</td>
<td>nd(1.6)</td>
</tr>
<tr>
<td>12 123467-PCDF</td>
<td>nd(1.9)</td>
<td>2.7</td>
<td>3.6</td>
<td>nd(0.3)</td>
<td>nd(0.4)</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>13 123467-HxCDF</td>
<td>nd(0.4)</td>
<td>nd(0.6)</td>
<td>nd(0.4)</td>
<td>nd(4.1)</td>
<td>1.6</td>
<td>nd(0.7)</td>
</tr>
<tr>
<td>14 23678-TCDF</td>
<td>nd(0.5)</td>
<td>nd(2.9)</td>
<td>2.6</td>
<td>nd(2.3)</td>
<td>nd(3.6)</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>15 23678-TCDF</td>
<td>nd(0.6)</td>
<td>nd(3.2)</td>
<td>nd(3.7)</td>
<td>nd(1.4)</td>
<td>3.5</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>16 23678-TCDF</td>
<td>nd(0.4)</td>
<td>nd(2.9)</td>
<td>nd(2.3)</td>
<td>nd(1.5)</td>
<td>nd(2.4)</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>17 23678-TCDF</td>
<td>nd(1.4)</td>
<td>1.3</td>
<td>1.7</td>
<td>nd(0.4)</td>
<td>nd(2.1)</td>
<td>nd(1.4)</td>
</tr>
<tr>
<td>18 23678-TCDF</td>
<td>nd(4.7)</td>
<td>10</td>
<td>14</td>
<td>4.3</td>
<td>18</td>
<td>nd(7.6)</td>
</tr>
<tr>
<td>19 123467-PCDF</td>
<td>nd(1.8)</td>
<td>4.2</td>
<td>6.5</td>
<td>2.4</td>
<td>nd(3.2)</td>
<td>nd(1.4)</td>
</tr>
<tr>
<td>20 123467-PCDF</td>
<td>3.6</td>
<td>32</td>
<td>49</td>
<td>15</td>
<td>64</td>
<td>nd(9.5)</td>
</tr>
<tr>
<td>21 123467-PCDF</td>
<td>nd(1.2)</td>
<td>1.2</td>
<td>nd(5.0)</td>
<td>nd(0.4)</td>
<td>nd(3.1)</td>
<td>nd(1.0)</td>
</tr>
<tr>
<td>22 123467-PCDF</td>
<td>19</td>
<td>151</td>
<td>218</td>
<td>62</td>
<td>683</td>
<td>nd(46)</td>
</tr>
<tr>
<td>23 OCDF</td>
<td>nd(18)</td>
<td>71</td>
<td>66</td>
<td>32</td>
<td>54</td>
<td>nd(16)</td>
</tr>
<tr>
<td>24 OCDD</td>
<td>296</td>
<td>1290</td>
<td>1630</td>
<td>536</td>
<td>18000</td>
<td>595</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

* samples received from OSU via Federal Express 8-29-85, collected under supervision of S. Woods and K.J. Williamson
Table 10
Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Control Equine Tissue from Western Oregon and Western Washington

<table>
<thead>
<tr>
<th>Sample, units are pg/gram wet weight of homogenized tissue</th>
<th>Isomer</th>
<th>(501)</th>
<th>(502)</th>
<th>(502)</th>
<th>(504)</th>
<th>(505)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>isomer</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
<td>nd(0.5)</td>
<td>nd(0.2)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
<td>nd(0.5)</td>
<td>nd(0.2)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
<td>nd(0.5)</td>
<td>nd(0.2)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDF</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>nd(1.0)</td>
<td>nd(1.3)</td>
<td>nd(1.1)</td>
<td>nd(1.1)</td>
<td>nd(1.5)</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>nd(0.7)</td>
<td>nd(0.7)</td>
<td>nd(1.6)</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>nd(0.7)</td>
<td>nd(0.7)</td>
<td>nd(1.5)</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
<td>nd(0.7)</td>
<td>nd(0.7)</td>
<td>nd(1.6)</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>nd(0.7)</td>
<td>nd(0.7)</td>
<td>nd(1.6)</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>nd(0.7)</td>
<td>nd(0.7)</td>
<td>nd(1.6)</td>
<td>nd(0.4)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>nd(2.6)</td>
<td>nd(6.1)</td>
<td>nd(5.8)</td>
<td>nd(1.8)</td>
<td>nd(5.5)</td>
</tr>
<tr>
<td>12</td>
<td>13467-HxCDF</td>
<td>nd(2.2)</td>
<td>nd(2.3)</td>
<td>nd(6.1)</td>
<td>nd(1.7)</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>13</td>
<td>12378-HxCDF</td>
<td>nd(2.2)</td>
<td>nd(2.3)</td>
<td>nd(6.1)</td>
<td>nd(1.7)</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>14</td>
<td>12367-HxCDF</td>
<td>nd(2.2)</td>
<td>nd(2.3)</td>
<td>nd(6.1)</td>
<td>nd(1.7)</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>15</td>
<td>23467-HxCDF</td>
<td>nd(2.2)</td>
<td>nd(2.3)</td>
<td>nd(6.1)</td>
<td>nd(1.7)</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>nd(2.2)</td>
<td>nd(2.3)</td>
<td>nd(6.1)</td>
<td>nd(1.7)</td>
<td>nd(2.4)</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDF</td>
<td>nd(7.5)</td>
<td>nd(5.1)</td>
<td>nd(3.9)</td>
<td>nd(4.6)</td>
<td>nd(4.5)</td>
</tr>
<tr>
<td>18</td>
<td>123467-HxCDF</td>
<td>nd(7.5)</td>
<td>nd(5.1)</td>
<td>nd(3.9)</td>
<td>nd(4.6)</td>
<td>nd(4.5)</td>
</tr>
<tr>
<td>19</td>
<td>123789-HxCDF</td>
<td>nd(7.5)</td>
<td>nd(5.1)</td>
<td>nd(3.9)</td>
<td>nd(4.6)</td>
<td>nd(4.5)</td>
</tr>
<tr>
<td>20</td>
<td>1234789-HpCDF</td>
<td>nd(2.2)</td>
<td>nd(2.2)</td>
<td>nd(4.3)</td>
<td>nd(4.4)</td>
<td>nd(1.2)</td>
</tr>
<tr>
<td>21</td>
<td>1234678-HpCDF</td>
<td>nd(2.2)</td>
<td>nd(2.2)</td>
<td>nd(4.3)</td>
<td>nd(4.4)</td>
<td>nd(1.2)</td>
</tr>
<tr>
<td>22</td>
<td>1234789-HpCDF</td>
<td>nd(5.0)</td>
<td>nd(2.0)</td>
<td>nd(1.2)</td>
<td>nd(2.0)</td>
<td>nd(1.2)</td>
</tr>
<tr>
<td>23</td>
<td>23789-HpCDF</td>
<td>nd(4.1)</td>
<td>nd(8.4)</td>
<td>nd(10)</td>
<td>nd(3.4)</td>
<td>nd(4.9)</td>
</tr>
<tr>
<td>24</td>
<td>1234789-HpCDF</td>
<td>nd(4.1)</td>
<td>nd(8.4)</td>
<td>nd(10)</td>
<td>nd(3.4)</td>
<td>nd(4.9)</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

* samples received from Dr. Hultgren at OSU School of Veterinary Medicine on September 10, 1986
Table II

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Tissues Collected From "Coyne's Fortune", Arabian horse farm

<table>
<thead>
<tr>
<th>Sample</th>
<th>units are pg/gram wet weight of homogenized tissue</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(506)</td>
</tr>
<tr>
<td>1</td>
<td>2378-TCDF</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
</tr>
<tr>
<td>9</td>
<td>23467-PCDF</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
</tr>
<tr>
<td>14</td>
<td>123678-HxCDF</td>
</tr>
<tr>
<td>15</td>
<td>234678-HxCDF</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDD</td>
</tr>
<tr>
<td>18</td>
<td>123789-HxCDD</td>
</tr>
<tr>
<td>19</td>
<td>1234678-HpCDF</td>
</tr>
<tr>
<td>20</td>
<td>1234678-HpCDF</td>
</tr>
<tr>
<td>21</td>
<td>1234678-HpCDF</td>
</tr>
<tr>
<td>22</td>
<td>OCDF</td>
</tr>
<tr>
<td>23</td>
<td>OCDD</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

† samples collected during necropsy at OSU School of Veterinary Medicine, March 1986
Table 12

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Wood Chips taken from Arabian horse farm

<p>| Sample, units are nanogram/gram of wood chips, wet weight as received |
|-----------------------------|--------------------------------|</p>
<table>
<thead>
<tr>
<th>n</th>
<th>isomer</th>
<th>units</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>nd(0.007)</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>0.066</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(0.007)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>nd(0.019)</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>nd(0.008)</td>
</tr>
<tr>
<td>7</td>
<td>12347-PCDF</td>
<td>1.450</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
<td>nd(0.008)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>1.000</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>1.600</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>21.80</td>
</tr>
<tr>
<td>12</td>
<td>123478-5-HxCDF</td>
<td>4.020</td>
</tr>
<tr>
<td>13</td>
<td>123467-5-HxCDF</td>
<td>nd(0.020)</td>
</tr>
<tr>
<td>14</td>
<td>123678-5-HxCDF</td>
<td>2.780</td>
</tr>
<tr>
<td>15</td>
<td>234678-5-HxCDF</td>
<td>2.330</td>
</tr>
<tr>
<td>16</td>
<td>123789-5-HxCDF</td>
<td>nd(0.023)</td>
</tr>
<tr>
<td>17</td>
<td>123478-5-HxCDD</td>
<td>nd(0.021)</td>
</tr>
<tr>
<td>18</td>
<td>123678-5-HxCDD</td>
<td>30.90</td>
</tr>
<tr>
<td>19</td>
<td>123789-5-HxCDD</td>
<td>3.530</td>
</tr>
<tr>
<td>20</td>
<td>1234678-5-HpCDF</td>
<td>43.90</td>
</tr>
<tr>
<td>21</td>
<td>1234789-5-HpCDF</td>
<td>2.550</td>
</tr>
<tr>
<td>22</td>
<td>1234678-5-HpCDD</td>
<td>1170</td>
</tr>
<tr>
<td>23</td>
<td>OCDF</td>
<td>714</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>28000</td>
</tr>
</tbody>
</table>

**nd** = not detected at S/N 2.5 corresponding to the quantity in parentheses

**NR** = data not recorded
Table 13

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Tissues Collected From Stillborn Foal, Arabian horse farm*, and bull from farm near Sawmill Site 2 **

<table>
<thead>
<tr>
<th>n</th>
<th>isomer</th>
<th>(3)</th>
<th>(4)</th>
<th>(420)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2378-TCDF</td>
<td>nd(0.2)</td>
<td>nd(0.5)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>2</td>
<td>2367-TCDF</td>
<td>nd(0.2)</td>
<td>nd(0.5)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>3</td>
<td>3467-TCDF</td>
<td>nd(0.2)</td>
<td>nd(0.5)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>4</td>
<td>1234-TCDD</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>5</td>
<td>2378-TCDD</td>
<td>nd(0.2)</td>
<td>nd(0.6)</td>
<td>nd(0.5)</td>
</tr>
<tr>
<td>6</td>
<td>13467-PCDF</td>
<td>nd(0.2)</td>
<td>nd(1.4)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>7</td>
<td>12378-PCDF</td>
<td>nd(0.2)</td>
<td>nd(1.4)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>8</td>
<td>12367-PCDF</td>
<td>nd(0.2)</td>
<td>nd(1.4)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>9</td>
<td>23478-PCDF</td>
<td>nd(0.2)</td>
<td>nd(1.4)</td>
<td>1.8</td>
</tr>
<tr>
<td>10</td>
<td>23467-PCDF</td>
<td>nd(0.2)</td>
<td>nd(1.4)</td>
<td>nd(0.4)</td>
</tr>
<tr>
<td>11</td>
<td>12378-PCDD</td>
<td>nd(0.6)</td>
<td>nd(6.2)</td>
<td>nd(13)</td>
</tr>
<tr>
<td>12</td>
<td>123478-HxCDF</td>
<td>nd(0.8)</td>
<td>nd(1.8)</td>
<td>2.0</td>
</tr>
<tr>
<td>13</td>
<td>123467-HxCDF</td>
<td>nd(0.8)</td>
<td>nd(1.8)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>14</td>
<td>123678-HxCDF</td>
<td>nd(0.8)</td>
<td>nd(1.8)</td>
<td>1.1</td>
</tr>
<tr>
<td>15</td>
<td>234678-HxCDF</td>
<td>nd(0.8)</td>
<td>nd(1.8)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>16</td>
<td>123789-HxCDF</td>
<td>nd(0.8)</td>
<td>nd(1.8)</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>17</td>
<td>123478-HxCDD</td>
<td>nd(1.5)</td>
<td>nd(3.3)</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>18</td>
<td>123678-HxCDD</td>
<td>nd(1.5)</td>
<td>18</td>
<td>15</td>
</tr>
<tr>
<td>19</td>
<td>123789-HxCDD</td>
<td>nd(1.5)</td>
<td>nd(2.3)</td>
<td>nd(0.9)</td>
</tr>
<tr>
<td>20</td>
<td>1234678-HPCDF</td>
<td>nd(1.1)</td>
<td>nd(12.6)</td>
<td>nd(6.7)</td>
</tr>
<tr>
<td>21</td>
<td>1234678-HPCDF</td>
<td>nd(1.1)</td>
<td>nd(2.2)</td>
<td>nd(0.8)</td>
</tr>
<tr>
<td>22</td>
<td>1234678-HPcDD</td>
<td>3.4</td>
<td>24</td>
<td>21</td>
</tr>
<tr>
<td>23</td>
<td>OCFD</td>
<td>2.8</td>
<td>nd(5.1)</td>
<td>nd(1.3)</td>
</tr>
<tr>
<td>24</td>
<td>OCDD</td>
<td>19</td>
<td>180</td>
<td>50</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

* tissues collected by attending veterinarian, March 3, 1985
** tissue collected May 13, 1985
<table>
<thead>
<tr>
<th>Sample, units are pg/gram dry weight (53)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>7</td>
</tr>
<tr>
<td>8</td>
</tr>
<tr>
<td>9</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>11</td>
</tr>
<tr>
<td>12</td>
</tr>
<tr>
<td>13</td>
</tr>
<tr>
<td>14</td>
</tr>
<tr>
<td>15</td>
</tr>
<tr>
<td>16</td>
</tr>
<tr>
<td>17</td>
</tr>
<tr>
<td>18</td>
</tr>
<tr>
<td>19</td>
</tr>
<tr>
<td>20</td>
</tr>
<tr>
<td>21</td>
</tr>
<tr>
<td>22</td>
</tr>
<tr>
<td>23</td>
</tr>
<tr>
<td>24</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses
NR = data not recorded

soil collected May 10, 1985
Table 15

Summary Table of Results, Total Congener Group
Concentrations of PCDD, PCDF found in
Tissues from Stillborn Foal, Arabian horse far

<table>
<thead>
<tr>
<th>Congener Group</th>
<th>sample, units are pg/gram wet weight</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(1) (4) (5) (7) (6)</td>
</tr>
<tr>
<td>TCDF***</td>
<td>nd(0.5) nd(6.0) nd(1.0) nd(2.0) nd(2.0)</td>
</tr>
<tr>
<td>PCDF</td>
<td>nd(2.0) nd(0.5) nd(2.0) nd(1.0) nd(3.0)</td>
</tr>
<tr>
<td>HxCDF</td>
<td>nd(10) nd(10) nd(4.0) nd(100) nd(17)</td>
</tr>
<tr>
<td>HpCDF</td>
<td>NR NR NR NR NR</td>
</tr>
<tr>
<td>OCDF</td>
<td>NR NR NR NR NR</td>
</tr>
<tr>
<td>TCDD***</td>
<td>nd(0.5) nd(7.0) nd(1.0) nd(1.0) nd(9.0)</td>
</tr>
<tr>
<td>PCDD</td>
<td>nd(54) nd(13) nd(7.0) nd(3.0) nd(3.0)</td>
</tr>
<tr>
<td>HxCDD</td>
<td>110 20 nd(12) 50 110</td>
</tr>
<tr>
<td>HpCDD</td>
<td>110 20 49 62 280</td>
</tr>
<tr>
<td>OCDD</td>
<td>360 150 490 230 3000</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

* samples collected on March 29, 1985

*** DOES NOT include any contributions from 2,3,7,8-TCDF
or 2,3,7,8-TCDD. These isomers were not found in any animal tissues from the Molalla area analyzed in this study.
Table 16

Summary Table of Results, Total Congener Group
Concentrations of PCDD, PCDF found in
Tissues from Mare and Bull**

<table>
<thead>
<tr>
<th>Congener Group</th>
<th>sample, units are pg/gram wet weight</th>
<th>(9)</th>
<th>(421)</th>
<th>(422)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCDF***</td>
<td>nd(3.6)</td>
<td>nd(3.0)</td>
<td>nd(3.0)</td>
<td></td>
</tr>
<tr>
<td>PCDF</td>
<td>nd(3.0)</td>
<td>nd(3.0)</td>
<td>nd(3.0)</td>
<td></td>
</tr>
<tr>
<td>HxCDF</td>
<td>nd(50)</td>
<td>nd(15)</td>
<td>nd(93)</td>
<td></td>
</tr>
<tr>
<td>HpCDF</td>
<td>200</td>
<td>nd(40)</td>
<td>nd(40)</td>
<td></td>
</tr>
<tr>
<td>OCDF</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td></td>
</tr>
<tr>
<td>TCDD***</td>
<td>nd(18)</td>
<td>nd(30)</td>
<td>nd(5)</td>
<td></td>
</tr>
<tr>
<td>PCDD</td>
<td>nd(2.0)</td>
<td>nd(17)</td>
<td>nd(18)</td>
<td></td>
</tr>
<tr>
<td>HxCDD</td>
<td>2000</td>
<td>nd(50)</td>
<td>nd(35)</td>
<td></td>
</tr>
<tr>
<td>HpCDD</td>
<td>1900</td>
<td>50</td>
<td>nd(20)</td>
<td></td>
</tr>
<tr>
<td>OCDD</td>
<td>19000</td>
<td>1700</td>
<td>142</td>
<td></td>
</tr>
</tbody>
</table>

*nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

** sample from Arabian horse farm collected May 23, 1983 at necropsy

*** sample from farm near Sawmill Site 2 collected May 13, 1983

**** DOES NOT include any contributions from 2,3,7,8-TCDF or 2,3,7,8-TCDD. These isomers were not found in any animal tissues from the Molalla area analyzed in this study.
Table 17

Summary Table of Results, Replicate Analyses for Selected Isomers, Fish Tissue Sample (carp) From the Petenwell Reservoir, Wisconsin

<table>
<thead>
<tr>
<th>isomer</th>
<th>Units are pg/gram wet weight of tissue</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(REP1)</td>
</tr>
<tr>
<td>2378-TCDF</td>
<td>15</td>
</tr>
<tr>
<td>1234-TCDD$</td>
<td>200</td>
</tr>
<tr>
<td>2378-TCDD</td>
<td>59</td>
</tr>
<tr>
<td>12378-PCDF</td>
<td>1.1</td>
</tr>
<tr>
<td>12378-PCDD</td>
<td>4</td>
</tr>
<tr>
<td>123678-HxCDD</td>
<td>9</td>
</tr>
<tr>
<td>1234678-HpCDD</td>
<td>12</td>
</tr>
<tr>
<td>OCDD**</td>
<td>26</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

\$ laboratory artifact

\** low level of OCDD in blank was only achieved by nonstandard glassware cleaning procedure employed for this set; values have not been corrected for background
Table 18
Summary Table of Results, Replicate Analyses of a Control Lake Sediment From Northern Minnesota Known to be Contaminated with Low ppt Levels of 2,3,7,8-TCDD

<table>
<thead>
<tr>
<th>isomer</th>
<th>Units are pg/gram wet weight of sediment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(REP1)</td>
</tr>
<tr>
<td>2378-TCDF</td>
<td>nd(2.1)</td>
</tr>
<tr>
<td>1234-TCDD</td>
<td>NR</td>
</tr>
<tr>
<td>2378-TCDD</td>
<td>4.5</td>
</tr>
<tr>
<td>12378-PCDF</td>
<td>nd(0.6)</td>
</tr>
<tr>
<td>12378-PCDD</td>
<td>nd(2.1)</td>
</tr>
<tr>
<td>123678-HxCDD</td>
<td>nd(1.9)</td>
</tr>
<tr>
<td>1234678-HpCDD**</td>
<td>21</td>
</tr>
<tr>
<td>OCDD**</td>
<td>129</td>
</tr>
</tbody>
</table>

nd = not detected at S/N 2.5 corresponding to the quantity in parentheses

NR = not reported

** does not differ significantly from blank values at the time these replicates were analyzed
Table 19

Statistical Summary of Fish Replicate Data
(from Table 17)

<table>
<thead>
<tr>
<th>isomer</th>
<th>(n)</th>
<th>(mean)</th>
<th>(%RSD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2378-TCDF</td>
<td>5</td>
<td>14.2</td>
<td>3.2</td>
</tr>
<tr>
<td>1234-TCDD</td>
<td>5</td>
<td>172</td>
<td>13</td>
</tr>
<tr>
<td>2378-TCDD</td>
<td>5</td>
<td>55</td>
<td>9.0</td>
</tr>
<tr>
<td>12378-PCDF</td>
<td>5</td>
<td>1.2</td>
<td>16</td>
</tr>
<tr>
<td>12378-PCDD</td>
<td>5</td>
<td>3.4</td>
<td>16</td>
</tr>
<tr>
<td>123678-HxCDD</td>
<td>5</td>
<td>7.4</td>
<td>15</td>
</tr>
<tr>
<td>1234678-HpCDD</td>
<td>5</td>
<td>12</td>
<td>3.8</td>
</tr>
<tr>
<td>OCDD</td>
<td>5</td>
<td>15</td>
<td>31</td>
</tr>
</tbody>
</table>

Table 20

Statistical Summary of Sediment Replicate Data
(from Table 18)

<table>
<thead>
<tr>
<th>isomer</th>
<th>(n)</th>
<th>(mean)</th>
<th>(%RSD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2378-TCDF</td>
<td>6</td>
<td>nd(1.2)</td>
<td>52</td>
</tr>
<tr>
<td>1234-TCDD</td>
<td>6</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>2378-TCDD</td>
<td>6</td>
<td>4.7</td>
<td>11</td>
</tr>
<tr>
<td>12378-PCDF</td>
<td>6</td>
<td>nd(0.7)</td>
<td>38</td>
</tr>
<tr>
<td>12378-PCDD</td>
<td>5</td>
<td>nd(2.6)</td>
<td>37</td>
</tr>
<tr>
<td>123678-HxCDD</td>
<td>6</td>
<td>nd(2.0)</td>
<td>33</td>
</tr>
<tr>
<td>1234678-HpCDD</td>
<td>6</td>
<td>25</td>
<td>22</td>
</tr>
<tr>
<td>OCDD</td>
<td>6</td>
<td>166</td>
<td>32</td>
</tr>
</tbody>
</table>
Figure 1: Sampling Locations for Eagle Harbor Site (taken, with permission, from Swartz et al., Toxicity of sediment from Eagle Harbor, Washington to the Infaunal Amphipod, Rhepoxynius Abronius, Environ. Sci. Technol., in press)
Figure 2: Sketch of Sampling Locations, Site 2
(scale is approximately 1 inch = 725 feet)
Figure 3

Chemical Structures of Some Compounds Found in t-PCP
Figure 4

Two Eagle Harbor Sediment Samples Compared to Industry Composite Values for PCDD/PCDF in t-PCP Taken from Reference 14, Congener Group Total Concentrations, Normalized to OCDD
Figure 5: Sample 222 Compared to Concentrations of Four Selected PCDD's Found in t-PCP and Flyash (the values for t-PCP were calculated by averaging the two samples shown in Table 3)
Figure 6

Mass Chromatograms for HxCDD's in a Typical Sample of t-PCP, Flyash from a MSWI (Municipal Solid Waste Incinerator), and an Eagle Harbor Sediment (data was collected on a 30 meter x 0.32 mm DB5 capillary column, monitoring m/z 389.8156)
Isomer Assignment Key to Labels Shown in Figure 6

A. 1,2,4,6,7,9/1,2,4,6,8,9-HxCDD
B. 1,2,3,4,6,8-HxCDD
C. 1,2,3,6,7,9/1,2,3,6,8,9-HxCDD
D. 1,2,3,4,6,9-HxCDD
E. 1,2,3,4,7,8-HxCDD
F. 1,2,3,6,7,8-HxCDD
G. 1,2,3,7,8,9/1,2,3,4,6,7-HxCDD
Figure 7: Mean Values for Positives for Four Selected Isomers of PCDD/PCDF Shown in Table 9 Compared with Those Found in Sample 223 (Table 9 values were used as background control values)
Figure 8: Mean Values for Positives in Table 9 Compared with Table 8 for Four Selected Isomers of PCDD/PCDF (Table 9 values were used as background control values)
Figure 9

Diagram in Flow Chart Form Outlining the Analytical Scheme, modified from that presented by Tondeur in Reference (12)
REFERENCES


17) Hagenmaier, H., Berchtold, A. (1985). Analysis of waste from PCP-na-production for PCDD and PCDF. Poster presentation at Dioxins 85, 5th International Symposium on Chlorinated Dioxins and Related Compounds, Bayreuth, FRG September 16-19, 1985. The authors are from the University of Tubingen, FRG.


39) Kuehl, D.W., EPA ERL Duluth, Minnesota, unpublished data.


44) Schmotzer, W.O., DVM. Case Summary, Arabian mare OSU VTH #183-002-739, and supporting records.

45) Oregon Department of Environmental Quality, Northwest Regional Office, unpublished records of sampling for chlorophenols carried out at Publishers Paper sawmill, Liberal, Oregon.


52) Oregon Department of Environmental Quality, Northwest Regional Office, unpublished monitoring data from the vicinity of Avison Lumber Co., Molalla, Oregon.


56) Oregon Department of Environmental Quality, unpublished bioassay data provided by northwest regional office.


61) Hagenmaier, H. (1986). The determination of 2,3,7,8-Tetrachlorodibenzo-p-dioxin in commercial chlorophenols and related products. Fresenius' Z. Anal. Chem. 325: 603-606. (This paper is written in English.)


APPENDICES
APPENDIX A

2,3,7,8-TCDD "Toxicity Equivalent Factors" or TEF's
Currently used by EPA and CDC for Dioxin Risk
Assessments*

<table>
<thead>
<tr>
<th>compound(s)</th>
<th>TEF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3,7,8-TCDD</td>
<td>1.00</td>
</tr>
<tr>
<td>1,2,3,7,8-PCDD</td>
<td>0.20</td>
</tr>
<tr>
<td>1,2,3,6,7,8-HxCDD</td>
<td>0.04</td>
</tr>
<tr>
<td>1,2,3,7,8,9-HxCDD</td>
<td>0.04</td>
</tr>
<tr>
<td>1,2,3,4,7,8-HxCDD</td>
<td>0.04</td>
</tr>
<tr>
<td>1,2,3,4,6,7,8-HpCDD</td>
<td>0.001</td>
</tr>
<tr>
<td>other TCDD**</td>
<td>0.01</td>
</tr>
<tr>
<td>other PCDD**</td>
<td>0.002</td>
</tr>
<tr>
<td>other HxCDD**</td>
<td>0.0004</td>
</tr>
<tr>
<td>other HpCDD**</td>
<td>0.00001</td>
</tr>
<tr>
<td>OCDD</td>
<td>0.0</td>
</tr>
</tbody>
</table>

| 2,3,7,8-TCDF           | 0.10 |
| 1,2,3,7,8-PCDF         | 0.10 |
| 2,3,4,7,8-PCDF         | 0.10 |
| 1,2,3,6,7,8-HxCDF      | 0.01 |
| 1,2,3,7,8,9-HxCDF      | 0.01 |
| 1,2,3,4,7,8-HxCDF      | 0.01 |
| 2,3,4,6,7,8-HxCDF      | 0.01 |
| 1,2,3,4,6,7,8-HpCDF    | 0.001|
| 1,2,3,4,7,8,9-HpCDF    | 0.001|
| other TCDF**           | 0.001|
| other PCDF**           | 0.001|
| other HxCDF**          | 0.0001|
| other HpCDF**          | 0.00001|
| OCDF                   | 0.0  |

* taken from references (12) and (13)

** compounds which are not substituted in all four 2,3,7, and 8 positions
APPENDIX B

Sample Cleanup Methods for Soils, Sediments and Other Particulates

This appendix describes the sample preparation method for soils, and sediments. It is based on modifications of procedures used by EPA ERLD (60). These procedures are based on a combination of earlier work by Nestrick and Lamparski (7), Langhorst and Shadoff (8), Stalling et al. (9) and Buser (10). The bulk matrix removal column, using 50% silica gel/H2SO4, v/v, and the silver nitrate column, are based on the two Dow Chemical Co. references above.

As with the tissue methods described in Appendix C, the core of the procedure is the carbon column chromatography developed primarily by David Stalling, Larry Smith and coworkers at the U.S. Fish and Wildlife Columbia National Fisheries Laboratory. This step, more than any other, allows the separation of planar aromatics from environmental coextractives and interferences often present at several orders of magnitude higher concentration than the analytes of interest. This is particularly important in light of the 1000 X concentration of the toluene used to elute the PCDD/PCDF fraction from the carbon.
Reagents

1) All solvents were Burdick and Jackson (Muskegon, Michigan) distilled in glass, high purity grade; methylene chloride, benzene, carbon tetrachloride, hexane, isoctane, toluene, acetone and methanol.

2) The following reagents were used in preparing the cleanup columns described in this appendix:

- silica gel 60, 80-100 mesh, Merck Darmstadt (Germany)
- aluminum oxide 90, 70-230 mesh, Merck Darmstadt (Germany)
- Super-A activated carbon, AX-21, Anderson Development Co. Adrian, Michigan
- disposable pasteur pipets, 5.25 inch borosilicate glass, Kimball, Toledo, Ohio
- Anhydrous sodium sulfate, course, granular, J. T. Baker
- Ultrex concentrated sulfuric acid, J. T. Baker, Jackson Tennessee
- potassium hydroxide, pellets, high purity grade, Aldridge Chemical Co., Milwaukee, Wisconsin
- copper, granular, 20-30 mesh, J. T. Baker
- Whatman glass fiber filter paper, 15 cm, W. R. Balston (United Kingdom)
- sodium hydroxide, pellets, ACS reagent grade, J. T. Baker
- silver nitrate, ACS reagent grade, J. T. Baker
Notes on preparation of reagents and glassware

1) Activated silica was prepared by soxhlet extraction of silica gel 60 overnight in methanol. The solvent washed silica was then dried for eight hours in a fume hood. After the batch was free of solvent vapors, it was placed in a vacuum oven at 125 C overnight. It was then transferred to a 120 C oven and left until use (60).

2) Basic alumina was soxhlet extracted with methanol (60). dried the same as described above for silica, and left in a 120 C oven until columns were are prepared. The complete columns were activated for 24 hours at 225 C prior to use.

3) The activated carbon reagent was prepared by blending 10 grams AX-21 carbon with 200 grams activated silica; 200 mg of this mixture was used for each column. The columns themselves were fabricated from disposable pasteur pipets, as described in reference (60).

4) Silver nitrate on silica was prepared as described in reference (7), with the exception that the slow heating described by Lamparski and Nestrick at Dow Chemical was carried out in a vacume oven, not in a tube furnace under nitrogen. Extreme care must be used in the preparation of this reagent to avoid reducing the silver ion to metallic silver.

5) Potassium silicate was prepared by dissolving 56 grams of KOH in 300 ml methanol. The mixture was heated to 60 C, 100 grams of silica gel were added; then left to stir for an hour. The reagent was dried as described above for silica gel, then left in a 120 C oven until use. This procedure was based on that of the Dow Chemical Co. (7).

6) All glassware was repeatedly solvent washed with acetone, hexane and methylene chloride prior to use. Soxhlet extractors were assembled empty and allowed to reflux for at least 12 hours with methylene chloride prior to use. After a set of samples suspected to contain high levels of PCDD/PCDF was prepared, all glassware was soaked for 15 minutes in a hot solution of 10N KOH in methanol, 50/50 v/v. This has proven effective in removing residual PCDD/PCDF. The treated glassware was then put through ERLD's normal
washing procedure consisting of sonic cleaning in detergent solution, rinse with filtered tapwater, followed by a final rinse in acetone before the glassware was returned to the shelf.

Procedure

1) An appropriate amount of sample was weighed out. This was to a certain extent dependent on prior knowledge, if any, of the site in question. In practice, this varied from 1 to 20 grams, wet weight as received. A 1.0 gram aliquot of the sample was placed in a disposable aluminum pan and baked at 105-110°C for 18-24 hours. The sample dry weight was determined by difference.

   The portion of the sample weighed out for analysis was spread out evenly over a piece of glass fiber filter paper, placed on a stainless steel screen, and left to dry over night in a fume hood. For dry soils, this step was omitted. The partially dried sample was mixed with roughly an equal amount of course sodium sulfate in a conveniently sized beaker; the mixture was placed in an all glass soxhlet thimble with a course (70-100 micron) frit. Prior to adding the sample, the frit was covered with about 1.0 cm of solvent washed unactivated silical gel. This facilitated cleaning the thimbles by preventing sample from being trapped within the frit itself. The loaded thimble was spiked with 100 or 200 ul of the labeled internal standard solution described in Appendix D. A plug of solvent extracted glass wool was placed on top of the sample, to keep all sample particles within the thimble during the extraction. The loaded thimble was placed in the soxhlet apparatus and extracted for 24-30 hours with 50/50 (by volume) methylene chloride/benzene, 250 ml total volume. The extraction flask contained 5.0 grams of fresh copper shavings for relatively clean samples. Up to 20 grams of copper was used for sulfur rich anaerobic sediments.

2) The crude extract was poured through a funnel, containing glass wool covered with 20 grams of sodium sulfate, into a 500 ml Kuderna Danish (KD) apparatus containing 5.0 ml of isoocctane. The funnel was precleaned with 100 ml of hexane prior to being used with the sample. The extracting solvent was boiled off over a steam bath, leaving the concentrated residue in isoocctane.
3) The lower tube was separated from the KD and the sample transferred to the bulk matrix removal column with several 1 to 2 ml washes of hexane. The KD was washed twice with hexane, the wash being deposited in the column. Allowing each wash to drain until only a cm or so of solvent remains above the top layer, the column was eluted twice with 100 ml of 5% benzene in hexane. All washes and both 100 ml fractions were drained into a 500 ml KD apparatus.

The column itself was prepared as follows:

a) A solvent washed liquid chromatography column, 30 cm X 2.5 cm with a 300 ml reservoir and teflon stopcock, was packed with a plug of glass wool. This was followed, from bottom to top, by 2 grams of activated silica, 2 grams of potassium silicate, 2 grams of silica, 10 grams of 44% sulfuric acid on silica, 4 grams silica, and 2 grams Na2SO4.

b) The sulfuric acid/silica was prepared by slowly adding 4.0 ml of Ultrex (J.T. Baker) grade acid to 6 grams of activated silica while the silica was still hot. This operation was performed in a hood, as large amounts of highly irritating fumes were given off. The potassium silicate was prepared according to the procedure in reference (60).

c) The column was washed with 100 ml of 5% benzene in hexane and the wash discarded prior to adding the sample.

d) The eluate from the column was concentrated to 5.0 ml, leaving the sample in isooctane. The sample was concentrated further, down to about 2.0 ml, under a gentle stream of filtered air over a heated water bath.

4) A column (20 cm X 1 cm with 50 ml reservoir) containing 10% silver nitrate on silica was prepared. This reagent was kept in a heated vacuum dessicator over "Drierite" until immediately prior to use. The prepared column should be kept under hexane until the sample is applied. The sample was applied to the column, followed by three 0.5 to 1.0 ml hexane washes. The column was then eluted with 50 ml of 5% benzene in hexane. All eluate was retained in a 100 ml pair flask. The silver ion serves to complex compounds containing olefinic bonds (11).
visible residual pigmented materials which survived the bulk matrix column were removed at this point, including an as yet unidentified yellow-green oil which coeluted with the dioxin fraction on both alumina and activated carbon. Silver nitrate chromatography has a reputation for being tricky in practice, and has fallen out of favor in some labs doing dioxin work for this reason. This worker has found it to be the only method described in the literature which effectively removes the above described material. If left in the sample, these pigments often have the effect of ruining capillary columns after only a few injections. It was found in all anaerobic sediments and many soils analyzed during this study.

5) The sample was applied to an alumina column (60) with three 1 ml washes of hexane. The column was eluted with 4.0 ml of carbon tetrachloride, which was discarded. This fraction contained PCB's and polychlorinated napthalenes. The alumina column was then placed such that it drained directly into a reservoir attached to a carbon column. The PCDD/PCDF fraction was eluted off the alumina with 8.0 ml of methylene chloride, which drained into the carbon column. The reservoir was washed three times with 0.5 ml of methylene chloride. The carbon and alumina columns were made from disposable pasteur pipets. The details of their construction, activation of reagents, etc. are discussed in reference (60).

6) The carbon column was eluted in the forward direction with 15 ml of methylene chloride, followed by 15 ml of 25% (by volume) benzene in methylene chloride. These fractions were discarded. The column was "flipped", reattached to its reservoir, and eluted with 20 ml of toluene. This fraction contains PCDD/PCDF and was retained in a 25 ml pear flask.

7) The pear flask was placed, using a specially fabricated rack, in a warm water bath and the toluene evaporated under a gentle stream of pure air until only about 50 ul remained. This was transferred with a microliter syringe to a tapered microvial of about 300 ul capacity. The pear flask was carefully washed with 30-50 ul amounts of toluene, until the microvial was filled to a reasonable volume. The sample was stored in the microvial, with a teflon lined cap, frozen,
until shortly before GC-MS analysis. Prior to GC-MS analysis, the toluene is evaporated at room temperature. The "dry" microvial was then brought to a final volume of 20 ul with 10 ul of internal standard B (see Appendix D) and 10 ul of toluene.
This appendix describes the different approach required for the cleanup of mammalian tissues, particularly liver and adipose tissue. It was discovered that the sulfuric acid/celite column (42) used at ERLD to clean up fish tissues was inadequate to deal with samples containing more than 5.0 grams of extractable lipid. This left a choice between gel permeation chromatography (5) and a separatory funnel type cleanup, similar to that employed by the Brehm Laboratory at Wright State University (6).

The separatory funnel method was chosen due to its relative simplicity. The reagents and procedures used were much the same as those described in Appendix B. Only the steps which differ will be described here.
1) Frozen bovine and equine tissues were thawed out and weighed. If sufficient tissue existed, 2.0 grams was set aside for a % lipid determination. PCDD/PCDF determinations are often reported on a lipid basis, like most hydrophobic environmental pollutants. The 2.0 gram subsample was mixed with sufficient sodium sulfate to dry the tissue, loaded into a liquid chromatography column, and slowly eluted with 50 ml of methylene chloride, which drained into a pre-weighed disposable aluminum pan. The % lipid was calculated based on the weights of the tissue, pan, and pan plus extracted lipid.

2) In a 100 ml beaker, 20 grams or all remaining sample was weighed out and mixed with sufficient sodium sulfate to dry the sample. All tissues had to be cut up with a solvent washed scissors and ground by hand, using a mortar and pestle. The meat grinders used for fish samples at ERLD were not effective against the more tendonous, tough, stringy tissues analyzed in this study. A Soxhlet thimble was loaded with half the sample, spiked with 100 ul of internal standard solution, loaded with the remaining sample, covered with a plug of glass wool, and loaded into the extractor. The sample was extracted for 24 hours in hexane/methylene chloride, 50/50 v/v, 250 ml total volume.

3) The crude extract was quantitatively transferred with several hexane washes to a KD containing 3.0 to 5.0 ml isooctane. The extracting solvent was removed by heating over a steam bath. The sample was then transferred to a 500 ml separatory funnel with sufficient hexane washes to bring the total solvent volume to about 200 ml. The hexane phase was then washed, with 5 to 8 minutes of vigorous shaking each, with the following reagents:

a) 10-15 ml of Ultrex sulfuric acid, repeated until all visible color was removed. With liver, it was necessary to dilute the acid 50% with millipore water. Undiluted sulfuric acid was observed to form a thick, intractable gel with equine liver samples. Care must be taken to cool the water/acid mixture before adding it to the separatory funnel, to avoid any unwanted chemical reactions.

b) three 50 ml washes with millipore water
c) two washes with 10 to 15 mls 0.5N NaOH

d) three 50 ml washes with millipore water

4) The hexane phase was then poured through a funnel containing glass wool and sodium sulfate, into a KD. The funnel was rinsed three times with 5 to 10 ml quantities of hexane. The hexane was boiled off, leaving the sample in 3 to 5 ml of isoctane. The sample was further concentrated and cleaned up with silver nitrate on silica and carbon on silica as described in Appendix B. The alumina column was omitted for tissues analyzed using high resolution mass spectrometry, but retained for samples analyzed on a quadrupole instrument.

Although messy, time consuming, and expensive when compared to the soil/sediment methods in Appendix B, the approach described here proved effective on tissue samples which were impossible to deal with using techniques already established for fish. The silver nitrate column was effective in removing lipid pigments which were refractory to the sulfuric acid treatment; these orange/yellow pigments were present in adipose tissue samples from equines. Although not visible in 200 ml of hexane, these samples took on an obvious orange/yellow tint when concentrated to 2.0 ml.
### APPENDIX D

#### Internal Standard A Concentrations

<table>
<thead>
<tr>
<th>Compound</th>
<th>Solution pg/ul</th>
<th>Sample ppt</th>
</tr>
</thead>
<tbody>
<tr>
<td>37C14 2,3,7,8-TCDD</td>
<td>5</td>
<td>25</td>
</tr>
<tr>
<td>13C6 1,2,3,4-TCDD</td>
<td>5</td>
<td>25</td>
</tr>
<tr>
<td>13C12 2,3,7,8-TCDF</td>
<td>5</td>
<td>25</td>
</tr>
<tr>
<td>13C12 1,2,3,7,8-PCDD</td>
<td>10</td>
<td>50</td>
</tr>
<tr>
<td>13C12 1,2,3,7,8-PCDF</td>
<td>10</td>
<td>50</td>
</tr>
<tr>
<td>13C12 1,2,3,4,7,8-HxCDD</td>
<td>20</td>
<td>100</td>
</tr>
<tr>
<td>13C12 1,2,3,4,7,8-HxCDF</td>
<td>20</td>
<td>100</td>
</tr>
<tr>
<td>13C12 1,2,3,4,6,7,8-HpCDD</td>
<td>20</td>
<td>100</td>
</tr>
<tr>
<td>13C12 1,2,3,4,6,7,8-HpCDF</td>
<td>20</td>
<td>100</td>
</tr>
<tr>
<td>13C12 OCDD</td>
<td>40</td>
<td>200</td>
</tr>
</tbody>
</table>

#### Internal Standard B Concentrations

<table>
<thead>
<tr>
<th>Compound</th>
<th>Solution pg/ul</th>
<th>Sample ppt</th>
</tr>
</thead>
<tbody>
<tr>
<td>13C12-1,2,3,4-TCDD</td>
<td>2000</td>
<td>100</td>
</tr>
</tbody>
</table>

* Assuming analysis on a 20 gram aliquot of sample, brought to a final volume of 20 ul.

The concentrations above are based on the assumption of 100 ul of internal standard A and 10 ul of internal standard B brought to a final sample volume of 20 ul.
APPENDIX E

GC-MS Operating Parameters

Data Acquisition:  Multiple Ion Selection of the Following Ions:

<table>
<thead>
<tr>
<th>Compounds</th>
<th>m/z Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCDF</td>
<td>303.9016, 305.8986</td>
</tr>
<tr>
<td>13C12-TCDF</td>
<td>317.9389</td>
</tr>
<tr>
<td>TCDD</td>
<td>319.8965, 321.8936</td>
</tr>
<tr>
<td>37C14-TCDD</td>
<td>327.8847</td>
</tr>
<tr>
<td>13C6-TCDD</td>
<td>327.9137</td>
</tr>
<tr>
<td>13C12-TCDD</td>
<td>333.9338</td>
</tr>
<tr>
<td>PCDF</td>
<td>339.8597, 341.8567</td>
</tr>
<tr>
<td>13C12-PCDF</td>
<td>351.9000</td>
</tr>
<tr>
<td>PCDD</td>
<td>355.8546, 357.8516</td>
</tr>
<tr>
<td>13C12-PCDD</td>
<td>367.8949</td>
</tr>
<tr>
<td>HxCDF</td>
<td>373.8207, 375.8178</td>
</tr>
<tr>
<td>13C12-HxCDF</td>
<td>385.8610</td>
</tr>
<tr>
<td>HxCDD</td>
<td>389.8156, 391.8127</td>
</tr>
<tr>
<td>13C12-HxCDD</td>
<td>401.8559</td>
</tr>
<tr>
<td>HpCDF</td>
<td>407.7817, 409.7788</td>
</tr>
<tr>
<td>13C12-HpCDF</td>
<td>419.8220</td>
</tr>
<tr>
<td>HpCDD</td>
<td>423.7766, 425.7737</td>
</tr>
<tr>
<td>13C12-HpCDD</td>
<td>435.8169</td>
</tr>
<tr>
<td>OCDF</td>
<td>443.7398, 445.7369</td>
</tr>
<tr>
<td>OCDD</td>
<td>457.7377, 459.7348</td>
</tr>
<tr>
<td>13C12-OCDD</td>
<td>471.775</td>
</tr>
</tbody>
</table>

Note: Nominal masses were used for low resolution MS

*The material in this appendix is taken almost entirely from reference (42), with slight modifications based on conditions specific to the work reported here.
Operating parameters for Finnigan-MAT 8230 mass spectrometer

Sample Introduction: Open split interface with fused silica transfer line inserted directly into source
Ionization: Electron Impact, 70eV, 1mA emission current
Source Pressure: 7 x 10^-6 torr
Ionizer Temperature: 250 °C
Mass Resolution: 5000, 10% valley
Scan Rate: 1 MIS cycle per second
GC Column: 30 m DB5, 60 m SP2330
Linear Velocity: 30 cm/sec Helium
Temperature Programs:
30 m DB5
- 120 H1, 120-160 at 20/min, 160-280 at 3/min, H10
60 m SP2330
- a) 120 H1, 120-200 at 20/min, 220-240 at 3/min, H65
- b) 120 H1, 120-200 at 20/min, 220-240 at 3/min, H45
Injector: split/splitless 300 °C

Operating parameters for Finnigan 4500 mass spectrometer

Sample Introduction: Insertion of fused silica capillary column directly into source
Ionization: Electron Impact, 70eV, .25 mA emission current
Source Pressure: 5 x 10^-6 torr
Ionizer Temperature: 150 °C
Mass Resolution: unit resolution over mass range 69-502
Scan Rate: 1 scan per second
GC Column: 30 m DB5, 60 m SP2330
Linear Velocity: 40 cm/sec Helium
Temperature Programs:
30 m DB5
- 100 H1, 100-200 at 12/min, 200-260 at 4/min, H30
60 m SP2330
- a) 120 H1, 100-175 at 12/min, 175-260 at 4/min, H35
- b) 120 H1, 100-175 at 12/min, 220-260 at 4/min, H25
Injector: split/splitless 300 °C
GC Column Performance

Resolution: The ion current profile for 13C6 1,2,3,4-TCDD and for 37Cl4 2,3,7,8-TCDD must be resolved by a resolution coefficient of 0.75 (87.5% resolved) or greater, see references (42) and (60).

Isomer Identification: The ion current profile for a natural isomer must maximize at the same time as the stable isotope labeled analog, or elute at the relative GC retention time of an isomer identified in one of the two Qualitative Standards available at ERL-Duluth.

Quality Assurance Requirement: Scan maxima may deviate by 2 scans.

Mass Spectrometer Performance
Mass Resolution
(8230 Instrument)

Mass resolution will be determined by analyzing for 13C6 1,2,3,4-TCDD and 37Cl4 2,3,7,8-TCDD at 2500, 5000, 7500 and 10,000 resolution and calibrating resolution with peak overlap between the two TCDD isomers.

Quality Assurance Requirement: 10% of set resolution

See reference (28) for more a more detailed description of this procedure.

Resolution was also determined statically at the beginning of each working day using methods described in the manufacturer's operating manual.
Quality Assurance Parameters

<table>
<thead>
<tr>
<th>Ion Ratio$ (± error)</th>
<th>Method Efficiency</th>
<th>Accuracy at 10 pg/g (+/-)</th>
<th>Precision at 10 pg/g (+/-)</th>
<th>S/N minimum</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCDD .76±.10</td>
<td>&gt;50%</td>
<td>+50%</td>
<td>+50%</td>
<td>2.5</td>
</tr>
<tr>
<td>PCDD 1.53±.15</td>
<td>&gt;35%</td>
<td>+50%</td>
<td>+50%</td>
<td>2.5</td>
</tr>
<tr>
<td>HxCDD 1.23±.15</td>
<td>&gt;35%</td>
<td>+100%</td>
<td>+100%</td>
<td>2.5</td>
</tr>
<tr>
<td>HpCDD 1.02±.15</td>
<td>&gt;35%</td>
<td>+100%</td>
<td>+100%</td>
<td>2.5</td>
</tr>
<tr>
<td>OCDD .88±.20</td>
<td>&gt;25%</td>
<td>+200%</td>
<td>+100%</td>
<td>2.5</td>
</tr>
<tr>
<td>TCDF .76±.10</td>
<td>&gt;50%</td>
<td>+50%</td>
<td>+50%</td>
<td>2.5</td>
</tr>
<tr>
<td>PCDF 1.53±.15</td>
<td>&gt;35%</td>
<td>+50%</td>
<td>+50%</td>
<td>2.5</td>
</tr>
<tr>
<td>HxCDF 1.23±.15</td>
<td>&gt;35%</td>
<td>+100%</td>
<td>+100%</td>
<td>2.5</td>
</tr>
<tr>
<td>HpCDF 1.02±.15</td>
<td>&gt;35%</td>
<td>+500%</td>
<td>+500</td>
<td>2.5</td>
</tr>
<tr>
<td>OCDF 1.53±.20</td>
<td>&gt;25%</td>
<td>+500%</td>
<td>+500</td>
<td>2.5</td>
</tr>
</tbody>
</table>

* Ratio of chlorine isotope pattern
APPENDIX F

Source Code for Computer Programs Used to Quantify Samples

This appendix consists of three BASIC computer programs used to quantify samples analyzed for PCCD/PCDF utilizing data generated by ERLD’s Finnigan-MAT 8230 high resolution mass spectrometer. RFACCTOR calculates response factors for the ions of interest. In addition, it also checks the “fit” of the users’ isomer assignments against libraries of known retention times. These libraries have, at the time of this writing, been created for the 30 meter X 0.32 mm DB5 and the 60 meter X 0.32 mm SP2330 columns.

DFQUANT reads the files generated by RFACCTOR, peak area/height and retention time data entered by the user, and libraries; it then combines this information to quantify the sample and send reports to a printer and/or disk drive.

QAD reads the output from DFQUANT and generates a short report, containing concentrations and detection limits only.

All programs are written in a hybrid of Microsoft IBM-PC BASIC and a newer language, Microsoft’s “Quick BASIC” compiler. At present, the chemists at ERLD must still enter their data manually. It is anticipated that in the near future both programs will be able to read and sort raw data files sent over modem or hardwire serial connection from the host PDP 11-24 to a VAX minicomputer or several IBM PC-AT’s. Earlier versions of both programs have been in use since July of 1986, on several IBM and compatible microcomputers. Previously, the individual chemist was required to reduce his data by hand. This was clumsy for 2,3,7,8-TCDD alone, but impossibly slow when screening for the 24 compounds currently in the program libraries. The PDP 11 based data system, which came with ERLD’s 8230, was inadequate to this task with existing software. Thus, the reason for writing data reduction software as part of my project. This source code will not run on a BASIC interpreter. It must be compiled with Quick BASIC into a stand alone EXE file or used within the Quick BASIC programming environment.

Examples of program output are included.

The linear regression routine used in RFACCTOR is based on that published by Wolfe and Koelling (15).
DEF FNCONVERT(X)
FNCONVERT = INT(X) + ((X - INT(X)) / .6000)
END DEF

DEF FNMINSEC(Y)
FNMINSEC = INT(Y) + ((Y - INT(Y)) * .6000)
END DEF

REM initialize variables
DEFINT I
DIM L3(20), N3(50), L4(20), N4(50), L1(20), L2(20), N1(50), N2(50)
DIM L5(20), L6(20), N5(50), N6(50)
DIM LP(20,20), LRT(20,20), NP(50,20), NRT(50,20), RFLC(50,20)
DIM RFL(20,20), RFN(50,20), RRFL(20,20), RRFN(50,20)
DIM RFA(20), RFA(20), RRFA(20), RRFNA(50)
DIM MRTA(50), LRTA(20), SUMNT(50), SUMLT(20), SUML(20)
DIM SUMN(50), SUMRL(20), SUMRN(50)
DIM RSDLRT(50), RSDRT(50), RSDRFN(50), RSDLR(50), RRRL(20)
DIM SUMSQN(50), SUMSSRN(50), SUMSSNT(50), RRTN(50)
DIM SUMSQR(20), SUMSRQL(20), SUMSRSL(20)
DIM VRF(20), VRNFL(20), VRNFL(20)
DIM VRFN(50), VRNFL(50), VNRT(50)
DIM ALYXE(30), BION(30), RBBT(30), LION(20), NIDN(50)
DIM DLRT(20,20), DLRTA(20), DNRT(50,20), DNRTA(50)
DIM BRT(30), DBRT(30), X(30), Y(30), EY(30), PRMS(30), LIB(30)

REM User must enter raw peak area and RT data interactively
CLS : PRINT : PRINT : KEY OFF
PRINT"Be sure and set the Caps Lock Key so that only"
PRINT"caps will be printed, otherwise things will not work!"
PRINT : PRINT
INPUT"Strike ENTER key when ready ... ", ANY$:
CLS : PRINT : PRINT
INPUT"How many Q series standards do you wish to average "; N
CLS
LABEL = 12 : REM Number of labeled ions, loop counter
NAT = 48 : REM Number of natural ions, loop counter
HALFNAT = 24 : REM Number of natural analytes

REM subroutines
GOSUB 1080 : REM Enter picograms/ul for Q Standards
GOSUB 280 : REM enter data, calculate RF and RRF values
GOSUB 3000 : REM average RF, RRF, RRT data for n standards
GOSUB 4000 : REM Standard Deviations, Q standards
GOSUB 5000 : REM Biosignificant standard
GOSUB 5500 : REM output user data to printer, check accuracy
GOSUB 6000 : REM linear regression routine for isomer identification
GOSUB 7000 : REM Output to printer, disk

PRINT : PRINT
PRINT "RFactor is now finished with your data."
BEEP : BEEP : BEEP

END

REM Subroutine: enter peak areas and RT's for Q Standards
FOR J = 1 TO N
REM
PRINT "Are you ready to enter data for Q Standard?"
PRINT : PRINT
INPUT "Strike ENTER key when ready...", ANY$;
CLS : PRINT : PRINT
PRINT "Which Q Standard is being used for this iteration?"
CLS
INPUT '1', '2', '3', '4', '5', or '6', "QQ
CLS
INPUT 'Enter peak areas for 2378 TCDF, 304 and 306'; NP(1,J), NP(2,J)
INPUT 'enter RT's for 304, 306'; NRT(1,J), NRT(2,J)
CLS
INPUT 'enter peak area for 13C12 2378 TCDF, 318'; LP(2,J)
INPUT 'enter RT for 13C12 2378 TCDF'; LRT(2,J)
CLS
INPUT 'enter peak areas for 1234 TCDD, 320 and 322'; NP(7,J), NP(8,J)
INPUT 'enter RT's for 320, 322'; NRT(7,J), NRT(8,J)
CLS
INPUT 'enter peak areas for 2378 TCDD, 320 and 322'; NP(9,J), NP(10,J)
INPUT 'enter RT's for 320, 322'; NRT(9,J), NRT(10,J)
CLS
INPUT 'enter peak area for 37CL4 2378 TCDD, 327.8847'; LP(4,J)
INPUT 'enter RT for 37CL4 2378 TCDD'; LRT(4,J)
CLS
INPUT 'enter peak area for 13C6 1234 TCDD, 327.9137'; LP(3,J)
INPUT 'enter RT for 13C6 1234 TCDD'; LRT(3,J)
CLS
INPUT 'enter peak area for 13C12 1234 TCDD, 334'; LP(1,J)
INPUT "enter RT for 13C12 1234 TCDD "; LRT(1,J)
CLS
INPUT "enter peak areas for 12378 PCDF, 340 and 342 "; NP(12,J), NP(14,J)
INPUT "enter RT's for 340, 342 "; NRT(13,J), NRT(14,J)
CLS
INPUT "enter peak area for 13C12 12378 PCDF, 352 "; LP(5,J)
INPUT "enter peak RT for 13C12 12378 PCDF "; LRT(5,J)
CLS
INPUT "enter peak areas for 12378 PCDD, 356 and 358 "; NP(21,J), NP(22,J)
INPUT "enter RT's for 356, 358 "; NRT(21,J), NRT(22,J)
CLS
INPUT "enter peak area for 13C12 12378 PCDD, 368 "; LP(6,J)
INPUT "enter RT for 13C12 12378 PCDD "; LRT(6,J)
CLS
INPUT "enter peak areas for 123478 HxCDF, 374 and 376 "; NP(23,J), NP(24,J)
INPUT "enter RT's for 374, 376 "; NRT(23,J), NRT(24,J)
CLS
INPUT "enter peak area for 13C12 123478 HxCDF, 386 "; LP(7,J)
INPUT "enter RT for 13C12 123478 HxCDF "; LRT(7,J)
CLS
INPUT "enter peak areas for 123678 HxCDD, 390 and 392 "; NP(35,J), NP(36,J)
INPUT "enter RT's for 390, 392 "; NRT(35,J), NRT(36,J)
CLS
INPUT "enter peak area for 13C12 123678 HxCDD, 402 "; LP(8,J)
INPUT "enter RT for 13C12 123678 HxCDD "; LRT(8,J)
CLS
INPUT "enter peak areas for 1234678 HpCDF, 408 and 410 "; NP(39,J), NP(40,J)
INPUT "enter RT's for 408, 410 "; NRT(39,J), NRT(40,J)
CLS
INPUT "enter peak area for 13C12 1234678 HpCDF, 420 "; LP(9,J)
INPUT "enter RT for 13C12 1234678 HpCDF "; LRT(9,J)
CLS
INPUT "enter peak areas for 1234678 HpCDF, 424, 426 "; NP(43,J), NP(44,J)
INPUT "enter RT for 424, 426 "; NRT(43,J), NRT(44,J)
CLS
INPUT "enter peak area for 13C12 1234678 HpCDF, 436 "; LP(10,J)
INPUT "enter RT for 13C12 1234678 HpCDF "; LRT(10,J)
CLS
INPUT "enter peak areas for OCDF, 444 and 446 "; NP(45,J), NP(46,J)
INPUT "enter RT's for 444, 446 "; NRT(45,J), NRT(46,J)
CLS
INPUT "enter peak area for 13C12 OCDF, 456 "; LP(11,J)
INPUT "enter RT for 13C12 OCDF "; LRT(11,J)
CLS
INPUT "enter peak areas for OCDD, 458 and 460 "; NP(47,J), NP(48,J)
INPUT "enter RT's for 458, 460 "; NRT(47,J), NRT(48,J)
CLS
INPUT "enter peak area for 13C12 OCDD, 472 "; LP(12,J)
INPUT "enter RT for 13C12 OCDD "; LRT(12,J)
CLS : REM add natural ions for biosig compounds not in Q standards
NP(3,J) = NP(1,J) : NP(5,J) = NP(1,J) : NP(4,J) = NP(2,J) : NP(6,J) = NP(2,J)
NP(11,J) = NP(13,J) : NP(15,J) = NP(13,J) : NP(17,J) = NP(13,J) : NP(19,J) = NP(13,J)
NP(12,J) = NP(14,J) : NP(16,J) = NP(14,J) : NP(18,J) = NP(14,J) : NP(20,J) = NP(14,J)
NP(25,J) = NP(23,J) : NP(27,J) = NP(23,J) : NP(26,J) = NP(24,J) : NP(28,J) = NP(24,J)
NP(29,J) = NP(22,J) : NP(31,J) = NP(25,J) : NP(33,J) = NP(27,J) : NP(35,J) = NP(29,J) : NP(37,J) = NP(31,J) : NP(39,J) = NP(33,J) : NP(41,J) = NP(35,J) : NP(43,J) = NP(37,J) : NP(45,J) = NP(39,J) : NP(47,J) = NP(41,J)

6DTO 2500

REM pg/ul for each Q standard, Q1-06
REM Subroutine: Enter concentrations for Q standards

REM Standard Q3
L3(1) = 100 : REM pg 13C12 1234 TCDD ion 334
L3(3) = 12.5 : REM pg 13C6 1234 TCDD ion 328
L3(4) = 12.5 : REM pg 37CL4 2378 TCDD ion 328
L3(2) = 12.5 : REM pg 13C12 2378 TCFD ion 318
L3(5) = 25 : REM pg 13C12 12378 PCDF ion 352
L3(6) = 25 : REM pg 13C12 12378 PCDD ion 368
L3(7) = 50 : REM pg 13C12 123478 HxCDF ion 328
L3(8) = 50 : REM pg 13C12 2378 PCDF ion 340
L3(9) = 50 : REM pg 13C12 123478 HxCDF ion 342
L3(11) = 100 : REM pg 13C12 12346789 OCDF ion 356

REM add natural ions for biosig compounds not in Q3 standard
N3(1) = 12.5 : REM pg nat 2378 TCFD ion 304
N3(2) = 12.5 : REM pg nat 2378 TCFD ion 306
N3(3) = 12.5 : REM pg nat 1234 TCDD ion 320
N3(4) = 2.5 : REM pg nat 1234 TCDD ion 322
N3(5) = 12.5 : REM pg nat 2378 TCFD ion 320
N3(6) = 12.5 : REM pg nat 2378 TCFD ion 322
N3(7) = 25 : REM pg nat 12378 HxCDF ion 304
N3(8) = 25 : REM pg nat 12378 HxCDF ion 306
N3(9) = 25 : REM pg nat 12378 HxCDF ion 320
N3(10) = 25 : REM pg nat 12378 HxCDF ion 322
N3(11) = 50 : REM pg nat 12378 HxCDF ion 340
N3(12) = 50 : REM pg nat 12378 HxCDF ion 342
N3(13) = 50 : REM pg nat 12378 HxCDF ion 356
N3(14) = 50 : REM pg nat 12378 HxCDF ion 358
N3(15) = 50 : REM pg nat 12378 HxCDF ion 374
N3(16) = 50 : REM pg nat 12378 HxCDF ion 376
N3(17) = 50 : REM pg nat 12378 HxCDF ion 390
N3(18) = 50 : REM pg nat 12378 HxCDF ion 392
N3(19) = 50 : REM pg nat 1234678 HxCDF ion 390
N3(20) = 50 : REM pg nat 1234678 HxCDF ion 392
N3(21) = 50 : REM pg nat 1234678 HxCDF ion 394
N3(22) = 50 : REM pg nat 1234678 HxCDF ion 400
N3(23) = 50 : REM pg nat 1234678 HxCDF ion 402
N3(24) = 50 : REM pg nat 1234678 HxCDF ion 404
N3(25) = 50 : REM pg nat 1234678 HxCDF ion 406
N3(26) = 50 : REM pg nat 1234678 HxCDF ion 408
N3(27) = 50 : REM pg nat 1234678 HxCDF ion 410
N3(28) = 50 : REM pg nat 1234678 HxCDF ion 412
N3(29) = 50 : REM pg nat 1234678 HxCDF ion 414
N3(30) = 50 : REM pg nat 1234678 HxCDF ion 416
N3(31) = 50 : REM pg nat 1234678 HxCDF ion 418
N3(32) = 50 : REM pg nat 1234678 HxCDF ion 420
N3(33) = 50 : REM pg nat 1234678 HxCDF ion 422
N3(34) = 50 : REM pg nat 1234678 HxCDF ion 424
N3(35) = 50 : REM pg nat 1234678 HxCDF ion 426
N3(36) = 50 : REM pg nat 1234678 HxCDF ion 428
N3(37) = 50 : REM pg nat 1234678 HxCDF ion 430
N3(38) = 50 : REM pg nat 1234678 HxCDF ion 432
N3(39) = 50 : REM pg nat 1234678 HxCDF ion 434
N3(40) = 50 : REM pg nat 1234678 HxCDF ion 436
N3(41) = 50 : REM pg nat 1234678 HxCDF ion 438
N3(42) = 50 : REM pg nat 1234678 HxCDF ion 440
N3(43) = 50 : REM pg nat 1234678 HxCDF ion 442
N3(44) = 50 : REM pg nat 1234678 HxCDF ion 444
N3(45) = 50 : REM pg nat 1234678 HxCDF ion 446
N3(46) = 50 : REM pg nat 1234678 HxCDF ion 448

REM add natural ions for biosig compounds not in Q3 standard
N3(3) = N3(1) : N3(5) = N3(1) : N3(4) = N3(2) : N3(6) = N3(2)
N3(12) = N3(14) : N3(16) = N3(14) : N3(18) = N3(14) : N3(20) = N3(14)
N3(33) = N3(35) : N3(34) = N3(36) : N3(37) = N3(35) : N3(38) = N3(36)
N3(41) = N3(39) : N3(42) = N3(40)

L4(1) = 100 : REM pg 13C12 1234 TCDD ion 334
1450 L4(3) = 25 : REM pg 13C6 1234 TCDD ion 328
1460 L4(4) = 25 : REM pg 37CL4 2378 TCDD ion 328
1470 L4(2) = 25 : REM pg 13C12 2378 TCDF ion 318
1480 L4(5) = 50 : REM pg 13C12 12378 PCDF ion 352
1490 L4(6) = 50 : REM pg 13C12 12378 PCDD ion 368
1500 L4(7) = 100 : REM pg 13C12 123478 HxCDF ion 386
1510 L4(8) = 100 : REM pg 13C12 123678 HxCDD ion 402
1520 L4(9) = 100 : REM pg 13C12 1234678 HxCDD ion 436
1530 L4(10) = 200 : REM pg 13C12 12346789 OCDF ion 456
1540 L4(11) = 200 : REM pg 13C12 12346789 OCDD ion 472
1550 L4(12) = 200 : REM pg 13C12 12346789 OCDD ion 472

1560 N4(1) = 25 : REM pg nat 2378 TCDF ion 304
1570 N4(2) = 25 : REM pg nat 2378 TCDF ion 306
1580 N4(7) = 5 : REM pg nat 1234 TCDD ion 320
1590 N4(8) = 5 : REM pg nat 1234 TCDD ion 322
1600 N4(9) = 25 : REM pg nat 2378 TCDD ion 320
1610 N4(10) = 25 : REM pg nat 2378 TCDD ion 322
1620 N4(13) = 50 : REM pg nat 12378 PCDF ion 338
1630 N4(14) = 50 : REM pg nat 12378 PCDF ion 342
1640 N4(21) = 50 : REM pg nat 12378 PCDD ion 356
1650 N4(22) = 50 : REM pg nat 12378 PCDD ion 358
1660 N4(23) = 100 : REM pg nat 123478 HxCDF ion 374
1670 N4(24) = 100 : REM pg nat 123478 HxCDF ion 376
1680 N4(35) = 100 : REM pg nat 123678 HxCDD ion 390
1690 N4(36) = 100 : REM pg nat 123678 HxCDD ion 392
1700 N4(39) = 100 : REM pg nat 1234578 HxCDF ion 408
1710 N4(40) = 100 : REM pg nat 1234678 HxCDD ion 410
1720 N4(43) = 100 : REM pg nat 1234678 HxCDD ion 424
1730 N4(44) = 100 : REM pg nat 1234678 HxCDD ion 426
1740 N4(47) = 200 : REM pg nat 1234679 OCDD ion 458
1750 N4(48) = 200 : REM pg nat 1234679 OCDD ion 460
1760 N4(45) = 200 : REM pg nat 1234679 OCDF ion 442
1770 N4(46) = 200 : REM pg nat 1234679 OCDF ion 446

1771 CLS : REM add natural ions for biosig compounds not in Q4 standard
1779 N4(41) = N4(39) : N4(42) = N4(40)

1780 REM standard Q2, picograms per microliter
1790 L2(1) = 100 : REM pg 13C12 1234 TCDD ion 334
1800 L2(2) = 12.5 : REM pg 13C12 1234 TCDD ion 328
1810 L2(4) = 12.5 : REM pg 37CL4 2378 TCDD ion 328
1820 L2(2) = 12.5 : REM pg 13C12 2378 TCDF ion 318
1830 L2(5) = 25 : REM pg 13C12 12378 PCDF ion 352
1840 L2(6) = 25 : REM pg 13C12 12378 PCDD ion 368
1850 L2(7) = 50 : REM pg 13C12 123478 HxCDF ion 386
1860 L2(8) = 50 : REM pg 13C12 123678 HxCDD ion 402
1870 L2(9) = 50 : REM pg 13C12 1234678 HxCDF ion 436
1880 L2(10) = 50 : REM pg 13C12 1234678 HPtCDD ion 436
1910 L2(1) = 100 : REM pg 13C12 2346789 OCDF ion 456
1920 L2(12) = 100 : REM pg 13C12 12346789 OCDD ion 472

1910 N2(1) = 5 : REM pg nat 2378 TCDF ion 304
1920 N2(2) = 5 : REM pg nat 2378 TCDF ion 306
1930 N2(7) = 2.5 : REM pg nat 1234 TCDD ion 320
1940 N2(8) = 2.5 : REM pg nat 1234 TCDD ion 322
1950 N2(9) = 5 : REM pg nat 2378 TCDD ion 320
1960 N2(10) = 5 : REM pg nat 2378 TCDD ion 322
1970 N2(13) = 10 : REM pg nat 12378 PCDF ion 340
1980 N2(14) = 10 : REM pg nat 12378 PCDD ion 342
1990 N2(21) = 10 : REM pg nat 123878 PCDD ion 356
2000 N2(22) = 10 : REM pg nat 12378 PCDD ion 358
2010 N2(23) = 20 : REM pg nat 123478 HxCDF ion 374
2020 N2(24) = 20 : REM pg nat 123478 HxCDF ion 376
2030 N2(25) = 20 : REM pg nat 123678 HxCDD ion 390
2040 N2(26) = 20 : REM pg nat 123678 HxCDD ion 392
2050 N2(27) = 20 : REM pg nat 123678 HxCDF ion 408
2060 N2(28) = 20 : REM pg nat 123678 HxCDF ion 410
2070 N2(29) = 20 : REM pg nat 123678 HxCDF ion 424
2080 N2(30) = 20 : REM pg nat 123678 HxCDF ion 426
2090 N2(31) = 40 : REM pg nat 12346789 OCDF ion 458
2100 N2(32) = 40 : REM pg nat 12346789 OCDF ion 450
2110 N2(33) = 40 : REM pg nat 12346789 OCDF ion 444
2120 N2(34) = 40 : REM pg nat 12346789 OCDF ion 446

2121 CLS : REM add natural ions for biosig compounds not in Q2 standard
2122 N2(3) = N2(1) : N2(5) = N2(1) : N2(4) = N2(2) : N2(6) = N2(2)
2124 N2(12) = N2(14) : N2(16) = N2(14) : N2(18) = N2(14) : N2(20) = N2(14)
2127 N2(33) = N2(35) : N2(34) = N2(36) : N2(37) = N2(35) : N2(38) = N2(36)
2128 N2(41) = N2(39) : N2(42) = N2(40)

2130 REM Standard Q1
2140 L1(1) = 100 : REM pg 13C12 1234 TCDD ion 334
2150 L1(3) = 12.5 : REM pg 13C6 1234 TCDD ion 328
2160 L1(4) = 12.5 : REM pg 37CL4 2378 TCDD ion 328
2170 L1(2) = 12.5 : REM pg 13C12 2378 TCDF ion 318
2180 L1(5) = 25 : REM pg 13C12 12378 PCDF ion 352
2190 L1(6) = 25 : REM pg 13C12 12378 PCDD ion 368
2200 L1(7) = 50 : REM pg 13C12 123478 HxCDF ion 386
2210 L1(8) = 50 : REM pg 13C12 123678 HxCDD ion 402
2220 L1(9) = 50 : REM pg 13C12 123478 HxCDF ion 420
2230 L1(10) = 50 : REM pg 13C12 12346789 OCDF ion 436
2240 L1(11) = 100 : REM pg 13C12 12346789 OCDD ion 456
2250 L1(12) = 100 : REM pg 13C12 12346789 OCDD ion 472

2270 N1(1) = 1 : REM pg nat 2378 TCDF ion 304
2280 N1(2) = 1 : REM pg nat 2378 TCDF ion 306
2290 N1(7) = 2.5 : REM pg nat 1234 TCDD ion 320
2300 N1(8) = 2.5 : REM pg nat 1234 TCDD ion 322
2310 N1(9) = 1 : REM pg nat 2378 TCDD ion 320
2320 N1(10) = 1 : REM pg nat 2378 TCDD ion 322
CLS : REM add natural ions for biosig compounds not in Dl standard

L5(1) = 100 : REM pg l3C12 1234 TCDD ion 334
L5(3) = 25 : REM pg l3C6 1234 TCDD ion 328
L5(4) = 25 : REM pg 37CL4 2378 TCDD ion 328
L5(2) = 25 : REM pg l3C12 2378 TCDF ion 318
L5(5) = 50 : REM pg l3C12 12378 PCDF ion 352
L5(6) = 50 : REM pg l3C12 12378 PCDD ion 368
L5(7) = 100 : REM pg l3C12 123478 HxCDF ion 374
L5(8) = 100 : REM pg l3C12 123678 HxCDD ion 380
L5(9) = 100 : REM pg l3C12 12378 HpCDF ion 386
L5(10) = 100 : REM pg l3C12 123678 HpCDD ion 392
L5(11) = 200 : REM pg l3C12 1234678 HpCDF ion 402
L5(12) = 200 : REM pg l3C12 1234678 HpCDD ion 408
CLS: REM add natural ions for biosig compounds not in Q5 standard
N5(41)= N5(39) : N5(42)= N5(40)

REM Q6

L5(1) = 100 : REM pg 13C12 1234 TCDD ion 334
L5(2) = 25 : REM pg 13C6 1234 TCDD ion 328
L5(4) = 25 : REM pg 37CL4 2378 TCDD ion 328
L5(6) = 25 : REM pg 13C12 2378 TCDF ion 318
L5(10) = 50 : REM pg 13C12 12378 PCDF ion 352
L5(11) = 50 : REM pg 13C12 12378 PCDD ion 368
L5(16) = 100 : REM pg 13C12 123478 HxCDF ion 386
L5(20) = 100 : REM pg 13C12 123478 HxCDD ion 392
L5(25) = 200 : REM pg 13C12 1234678 HpCDF ion 408
L5(26) = 200 : REM pg 13C12 1234678 HpCDD ion 424
L5(27) = 400 : REM pg 13C12 1234678 HpCDF ion 426
L5(28) = 400 : REM pg 13C12 1234678 HpCDD ion 460
L5(29) = 400 : REM pg 13C12 1234678 HpCDF ion 442
L5(30) = 400 : REM pg 13C12 1234678 HpCDD ion 446

N6(1) = 100 : REM pg nat 1234 TCDD ion 334
N6(2) = 100 : REM pg nat 1234 TCDD ion 328
N6(3) = 5 : REM pg nat 1234 TCDD ion 322
N6(4) = 5 : REM pg nat 1234 TCDD ion 320
N6(5) = 100 : REM pg nat 2378 TCDD ion 320
N6(6) = 100 : REM pg nat 2378 TCDD ion 322
N6(7) = 200 : REM pg nat 12378 PCDF ion 338
N6(8) = 200 : REM pg nat 12378 PCDF ion 342
N6(9) = 200 : REM pg nat 12378 PCDF ion 356
N6(10) = 200 : REM pg nat 12378 PCDD ion 358
N6(11) = 400 : REM pg nat 123478 HxCDF ion 374
N6(12) = 400 : REM pg nat 123478 HxCDF ion 376
N6(13) = 400 : REM pg nat 123478 HxCDD ion 390
N6(14) = 400 : REM pg nat 123478 HxCDD ion 392
N6(15) = 400 : REM pg nat 1234678 HpCDF ion 408
N6(16) = 400 : REM pg nat 1234678 HpCDF ion 410
N6(17) = 400 : REM pg nat 1234678 HpCDD ion 424
N6(18) = 400 : REM pg nat 1234678 HpCDD ion 426
N6(19) = 800 : REM pg nat 12346789 OCDD ion 458
N6(20) = 800 : REM pg nat 12346789 OCDD ion 460
N6(21) = 800 : REM pg nat 12346789 OCDF ion 442
N6(22) = 800 : REM pg nat 12346789 OCDF ion 446
CLS : REM add natural ions for biosig compounds not in QE standard
N6(3) = N6(1) : N6(5) = N6(1) : N6(4) = N6(2) : N6(6) = N6(2)
N6(12) = N6(14) : N6(16) = N6(14) : N6(18) = N6(14) : N6(20) = N6(14)
N6(33) = N6(35) : N6(34) = N6(36) : N6(37) = N6(35) : N6(38) = N6(36)
N6(41) = N6(39) : N6(42) = N6(40)

2490 RETURN

2500 REM Calculate RF values

2520 CLS : PRINT : PRINT
2548 PRINT : PRINT
2549 IF J=N THEN PRINT"* Please be patient ..."
2550 IF QQ = 1 THEN 2570 ELSE IF QQ = 2 THEN 2650 ELSE IF QQ = 3_ THEN 2730 ELSE IF QQ = 4 THEN 2810 ELSE IF QQ=5 THEN 2863_ 2560 ELSE IF QQ = 6 THEN 2864

2570 REM Calculate RF's using standard Q1
2580 FOR I = 1 TO LABEL
2590 RFL(I,J) = LP(I,J)/(L1(I))
2600 NEXT I
2610 FOR I = 1 TO NAT
2620 RFN(I,J) = NP(I,J)/(N1(I))
2630 NEXT I
2640 GOTO 2865

2650 REM Calculate RF's using standard Q2
2660 FOR I = 1 TO LABEL
2670 RFL(I,J) = LP(I,J)/(L2(I))
2680 NEXT I
2690 FOR I = 1 TO NAT
2700 RFN(I,J) = NP(I,J)/(N2(I))
2710 NEXT I
2720 GOTO 2865

2730 REM Calculate RF's using standard Q3
2740 FOR I = 1 TO LABEL
2750 RFL(I,J) = LP(I,J)/(L3(I))
2760 NEXT I
2770 FOR I = 1 TO NAT
2780 RFN(I,J) = NP(I,J)/(N3(I))
2790 NEXT I
2800 GOTO 2865

2810 REM Calculate RF's using standard Q4
2820 FOR I = 1 TO LABEL
2830 RFL(I,J) = LP(I,J)/(L4(I))
2840 NEXT I
2850 FOR I = 1 TO NAT
REM Calculate RF's using standard Q5
FOR I = 1 TO LABEL
   RFL(I,J) = LP(I,J)/(L5(I))
NEXT I
FOR I = 1 TO NAT
   RFN(I,J) = NP(I,J)/(N5(I))
NEXT I
GOTO 2865

REM Calculate RF's using standard Q6
FOR I = 1 TO LABEL
   RFL(I,J) = LP(I,J)/(L6(I))
NEXT I
FOR I = 1 TO NAT
   RFN(I,J) = NP(I,J)/(N6(I))
NEXT I
GOTO 2865

REM tcdf
FOR I = 1 TO 6
   RFLC(I,J) = RFL(2,J)
NEXT I
REM 1234 tcdd
FOR I = 7 TO 8
   RFLC(I,J) = RFL(3,J)
NEXT I
REM 2378 tcdd
FOR I = 9 TO 10
   RFLC(I,J) = RFL(4,J)
NEXT I
REM pcdf
FOR I = 11 TO 20
   RFLC(I,J) = RFL(5,J)
NEXT I
REM pcdd
FOR I = 21 TO 22
   RFLC(I,J) = RFL(6,J)
NEXT I
REM hxcdf
FOR I = 23 TO 32
   RFLC(I,J) = RFL(7,J)
NEXT I
REM hxcdd
FOR I = 33 TO 38
   RFLC(I,J) = RFL(8,J)
NEXT I
REM hpcf
FOR I = 39 TO 42
    RFLC(I,J) = RFL(I,J)
NEXT I

REM hpcf, ocdf, ocdd
RFLC(43,J) = RFL(10,J):
RFLC(44,J) = RFL(10,J):
RFLC(45,J) = RFL(11,J):
RFLC(46,J) = RFL(11,J):
RFLC(47,J) = RFL(12,J):
RFLC(48,J) = RFL(12,J)
NEXT J

REM RRF's (relative to 334) for calculating recoveries
FOR J = 1 TO N
    FOR I = I TO LABEL
        RRF(I,J) = RFL(I,J)/RFL(I,J)
    NEXT I
NEXT J

REM RF's natural ions, natural/label
FOR J = 1 TO N
    FOR I = 1 TO NAT
        IF RFLC(I,J) < 0 THEN RRFN(I,J) = RFN(I,J)/RFLC(I,J) ELSE RRFN(I,J) = 0
    NEXT I
NEXT J

RETURN

REM Subroutine: calculate average RF, RRF, RRT of N iterations,
REM sum squares, if value of N is 3 or greater
REM Average RFL
FOR I = 1 TO LABEL
    SUM = 0
    SUMSQ = 0
    FOR J = 1 TO N
        SUM = SUM + RFL(I,J)
        SUMSQ = SUMSQ + RFL(I,J)^2
    NEXT J
    SUML(I) = SUM
    SUMSQL(I) = SUMSQ
    RFLA(I) = SUML(I)/N
NEXT I

REM Average RFN
FOR I = 1 TO NAT
    SUM = 0
    SUMSQ = 0
    FOR J = 1 TO N
        SUM = SUM + RFN(I,J)
        SUMSQ = SUMSQ + RFN(I,J)^2
    NEXT J
    SUMN(I) = SUM
    SUMSQN(I) = SUMSQ
    RFNA(I) = SUMN(I)/N
NEXT I
REM Average RRFL
FOR I = 1 TO LABEL
  SUM = 0
  SUMSQ = 0
  FOR J = 1 TO N
    SUM = SUM + RRFL(I,J)
  NEXT J
  SUMS@ = SUMSQ + RRFL(I,J)^2
  RRFLA(I) = SUM/RRFL(I,J)^2
NEXT I

REM Average RRFN
FOR I = 1 TO NAT
  SUM = 0
  SUMSQ = 0
  FOR J = 1 TO N
    SUM = SUM + RRFN(I,J)
  NEXT J
  SUMS@ = SUMSQ + RRFN(I,J)^2
  RRFNA(I) = SUMSQ/RRFN(I,J)^2
NEXT I

REM Average LRT
FOR I = 1 TO LABEL
  SUM = 0
  SUMSQ = 0
  FOR J = 1 TO N
    DLRT(I,J) = FNCONVERT(LRT(I,J))
    SUM = SUM + DLRT(I,J)
  NEXT J
  SUMS@ = SUMSQ + DLRT(I,J)^2
  SUMLT(I) = SUM
  SUMSOLT(I) = SUMS@
  DLRTA(I) = SUMLT(I)/N
  LRTA(I) = FNMINSEC(DLRTA(I))
NEXT I

REM Average NRT
FOR I = 1 TO NAT
  SUM = 0
  SUMSQ = 0
  FOR J = 1 TO N
    DNRT(I,J) = FNCONVERT(NRT(I,J))
    SUM = SUM + DNRT(I,J)
  NEXT J
  SUMS@ = SUMSQ + DNRT(I,J)^2
  SUMNT(I) = SUM
  SUMSQNT(I) = SUMS@
  DNRTA(I) = SUM/DNRT(I,J)^2
  NRTA(I) = FNMINSEC(DNRTA(I))
NEXT I
REM Calculate Relative Retention Times (w/respect to REFF)
REM Normalize RRT's w/respect to 2378-TCDD
REFF = DLRTA(4)

FOR I = 1 TO LABEL
  IF REFF>0 AND DLTA(I)>0 THEN RRTL(I)=(DLRTA(I)/REFF) ELSE RRTL(I)=0
NEXT I

FOR I = 1 TO NAT
  IF REFF>0 AND DNRTA(I)>0 THEN RRTN(I)=(DNRTA(I)/REFF) ELSE RRTN(I)=0
NEXT I

RETURN

REM Subroutine: Calculate standard deviations
IF N >= 3 THEN 4010 ELSE 4990

FOR I = 1 TO LABEL
  VRFL(I) = ABS((SUMSQL(I) -(SUML(I)^2/N))/(N-1))
  VLRT(I) = ABS((SUMSLT(I)-(SUMLT(I)^2/N))/(N-1))
NEXT I

FOR I = 1 TO NAT
  VRFN(I) = ABS(SUMSNL(I)-(SUMN(I)^2/N))/(N-1))
  VNRT(I) = ABS(SUMSNT(I)-(SUMNT(I)^2/N))/(N-1))
NEXT I

FOR I = 1 TO LABEL
  IF RFLA(I)>0 THEN RSDRFL(I)=SQR(VRFL(I))/RFLA(1) ELSE RSDRFL(I)=0
  IF LRTA(I)>0 THEN RSDLRT(I)=SQR(VLRT(I))/DLRTA(I) ELSE RSDLRT(I)=0
NEXT I

FOR I = 1 TO NAT
  IF RFNA(I)>0 THEN RSDRFN(I)=SQR(VRFN(I))/RFNA(I) ELSE RSDRFN(I)=0
  IF NRTA(I)>0 THEN RSDNRT(I)=SQR(VNRT(I))/DNRIA(I) ELSE RSDNRT(I)=0
NEXT I

RETURN

REM Subroutine: biosignificant standard, RT and RRT data
ALYTE$(1)= '2378-TCDF'
ALYTE$(2)= '2367-TCDF'
ALYTE$(3)= '3467-TCDF'
ALYTE$(4)= '1234-TCDD'
ALYTE$(5)= '2378-TCDD'
ALYTE$(6)= '13467-PCDF'
ALYTE$(7)= '12378-PCDF'
ALYTE$(8)= '12367-PCDF'
ALYTE$(9)= '23478-PCDF'
ALYTE$(10)= '23467-PCDF'
ALYTE$(11)= '12378-PCDD'
ALYTE$(12)= '12378-HxCDF'
ALYTE$(13)= '123467-PCDF'
ALYTE$(14)= '123678-HxCDF'
ALYTE$(15)= '234678-HxCDF'
ALYTE$(16)= '1234678-HxCDF'
ALYTE$(17)= '1234789-HxCDD'
ALYTE$(18)= '1236789-HpCDF'
ALYTE$(19)= '1234678-HpCDF'
ALYTE$(20)= '1234789-HpCDF'
ALYTE$(21)= '1234678-HpCDD'
ALYTE$(22)= 'OCDF'
ALYTE$(23)= 'OCDD'

REM add new analytes to target list 9-17-86
ALYTE$(13)= "123467-HxCDF'
ALYTE$(16)= "1234789-HxCDF"
REM Natural ions for biosig standard
BION(1)= 306 : BION(2)= 306 : BION(3)= 306 : BION(4)= 322 : BION(5)= 322
BION(11)= 356 : BION(12)= 374 : BION(13)= 374 : BION(14)= 374 : BION(15)= 374
BION(16)= 390 : BION(17)= 390 : BION(18)= 390 : BION(19)= 390 : BION(20)= 408 : BION(21)= 408 : BION(22)= 424
BION(23)= 444 : BION(24)= 460 : BION(25)= 374 : BION(26)= 374

CLS : PRINT : PRINT
PRINT"This portion of RFACTOR calculates RRT's from your "
PRINT"Biosignificant PCDD/PCDF standard": PRINT : PRINT : BEEP
PRINT"Enter your retention time for "
PRINT ALYTES(B) : PRINT
CLS : PRINT : PRINT
PRINT ALYTES(B), BRT(B) : PRINT
INPUT"Is the data correct? Answer 'Y' or 'N'; CORRECTS
IF CORRECTS= 'N' THEN 5110 ELSE 5150

NEIT B
CLS

REM Substitute values from Q for isomers not in biosig standard
BRT(4) = NRTA(8)
REM 1234789-HpCDF not in Q or biosig standards

REM Calculate RRT's
FOR B = 1 TO HALFNAT
IF BRT(B)<0 THEN DBRT(B) = FNCONVERT(BRT(B)) ELSE DBRT(B)=0
NEXT B

FOR B = 1 TO HALFNAT
IF DBRT(S)<0 THEN RRBT(B) = DBRT(B)/DBRT(S) ELSE RRBT(B)=0
NEXT B

RETURN

REM Subroutine: output user input to printer
CLS : PRINT : PRINT
PRINT"Adjust your printer paper, if necessary, for hardcopy"
INPUT"Strike the ENTER key when ready ...", ANY$ : PRINT
CLS : PRINT : PRINT
PRINT"Your input will now be sent to the printer."
FINPS= "## # ******************** #.##"

FOR J = 1 TO N
FOR I = 1 TO LABEL
LPRINT USING FINPS; J, I, LP(I,J), LRT(I,J)
NEXT I
NEXT J
NEXT I
FOR I = 1 TO NAT
    LPRINT USING FINP$; J, I, NP(I,J), NRT(I,J)
NEXT I

PRINT "If it is accurate, enter 'Y'. If it contains mistakes,"
INPUT "enter 'N' " ; INP$
IF INP$ = "N" THEN 200 ELSE 5990
RETURN

REM Subroutine: RT and RRT values from WSU window marker standard
REM not being used in this version
RETURN

REM Subroutine: Disk, printer output for average RF, RRF, PT, SD

CLS: PRINT: PRINT: BEEP
PRINT "Place your disk in drive A or B, for output of RF and RRF."
PRINT "Enter the complete name of your file in quotation marks, ", RSFACS
OPEN RSFACS FOR OUTPUT AS #1
LPRINT 'File I.D. : '; RSFACS
LPRINT 'Output from REACTOR program'
LPRINT 'The number of standards averaged was '; N
LPRINT 'Q Standard Data
####.##.##  #11.##   ###.##  ##.##  #11
LPRINT 'Labeled RF
LPRINT 'Ion RT RSD RRT (Label/334) RSD NO."
FOR I = 1 TO LABEL
    WRITE #1, LION(I), LRTA(I), RFLA(I), RRFLA(I)
LPRINT USING FORMS; LION(I), LRTA(I), RSDLRT(I), RRTL(I), RRFLA(I), RSDRFL(I), I
NEXT I
FOR I = 1 TO 47 : LPRINT : NEIT I
LPRINT * Natural RF
LPRINT * Ion RT RSD RRT (Nat/label) RSD NO."
FOR I = 1 TO NAT
WRITE #1, NION(I), NRTA(I), RFNA(I), RRFNA(I)
LPRINT USING FORMS; NION(I), NRTA(I), RSDNRT(I), RRTN(I), RRFNA(I), RSRDFN(I), I
NEXT I

REM Biosig standard
FOR I = 1 TO 20 : LPRINT : NEIT I
LPRINT"Biosignificant Standard"
FOR I = 1 TO 20
LPRINT USING FORMS: B, BRT(B), RRBT(B), ALYTE(B), PRMS(B), Y(B)-EY(B)
WRITE #1, BION(B), BRT(B), RRBT(B), ALYTE(B)
NEXT B
LPRINT : LPRINT 'regression statistics
LPRINT 'coefficient of determination = ', CR
LPRINT 'coefficient of correlation = ', CC
LPRINT 'standard deviation of the estimate = ', SE
LPRINT 'linear model: Predict decimal RT = ';A;' + ';W;' LIB'
LPRINT : LPRINT
CLOSE #1
RETURN

REM subroutine for RFACTOR program ver. 6.1
'linear regression of library values on user biosig input
'DIM LIB(30), X(30), Y(30), PRMS(30), EY(30)
'dim only when using as stand alone program

DEF FNCONVERT(A)
FNCONVERT = INT(I) + ((I - INT(I))/.6000)
END DEF

DEF FNMINSEC(A)
FNMINSEC = INT(I) + ((I - INT(I))*.6000)
END DEF

REM remove this block after debugging
FOR I = 1 TO 24
READ BRT(I)
NEXT I

CLS : PRINT : PRINT : BEEP
PRINT "SIMPLE LINEAR REGRESSION"
PRINT "independent variable = library RRT values"
PRINT "dependent variable = your flyash or biosignificant standard RT's"
PRINT: PRINT
INPUT "Strike the ENTER key when ready ... ", ANY$ 

60SUB 6002 : REM input library values for correct column
60SUB 6100 : REM simple linear regression of LIB on DBRT

RETURN 264

6002 ' Relative Retention Time libraries
' all times relative to 2378-TCDD
' libraries are self- documenting for easy updates
' last update on Feb 8, 1987, based on old temp programs
' which start at 120 C

CLS : PRINT : PRINT
PRINT "Choose a library from one of three listed below:"
PRINT
PRINT * 1 30 m X .32 mm DB5 *
PRINT * 2 60 m X .32 mm DB5 *
PRINT * 3 60 m X .32 mm SP2330 *
PRINT * 4 Skip regression, exit to next routine

PRINT: PRINT
INPUT "Enter the correct number: ", CHOICE%
IF (CHOICE% = 1) THEN
   GOTO 6010
ELSEIF (CHOICE% = 2) THEN
   PRINT : PRINT "this library has not been built yet, you lose buddy!"
   GOTO 6002
ELSEIF (CHOICE% = 3) THEN
   GOTO 6030
ELSEIF (CHOICE% = 4) THEN
   RETURN 264
ELSE GOTO 6002
END IF

6010 REM library for 30 M x .32 mm DB5 capillary column
'decimal absolute values, NOT relative
'data from my thesis see also UWS memo dated 1/12/87

LIB(01) = 17.38 ' 2378-TCDF
LIB(02) = 17.78 ' 2367-TCDF
LIB(03) = 17.98 ' 3467-TCDF
LIB(04) = 17.93 ' 1234-TCDD
LIB(05) = 18.15 ' 2378-TCDD
LIB(06) = 20.75 ' 13467-PCDF
LIB(07) = 21.73 ' 12378-PCDF
LIB(08) = 21.95 ' 2367-PCDF
LIB(09) = 22.75 ' 23476-PCDF
LIB(10) = 22.92 ' 23467-PCDF
LIB(11) = 23.28 ' 12378-PCDD
LIB(12) = 26.58 ' 123478-HxCDF
LIB(13) = 26.58 ' 123467-HxCDF
LIB(14) = 26.80 ' 123678-HxCDF
LIB(15) = 27.65 ' 234678-HxCDF
LIB(16) = 28.53 ' 123789-HxCDF
LIB(17) = 27.90 ' 123478-HxCDD
LIB(18) = 28.03 ' 123678-HxCDD
LIB(19) = 28.37 ' 123789-HxCDD
LIB(20) = 31.12 ' 1234678-HpCDF
LIB(21) = 33.17 ' 1234789-HpCDF
LIB(22) = 32.72 ' 1234678-HpCDD
LIB(23) = 38.32 ' OCDF
LIB(24) = 38.25 ' OCDD

RETURN

6020 REM library for 60 M x .32 mm DB5 capillary column

LIB(01) = 1 ' 2378-TCDF
LIB(02) = 1 ' 2367-TCDF
LIB(03) = 1 ' 3467-TCDF
LIB(04) = 1 ' 1234-TCDD
LIB(05) = 1 ' 2378-TCDD
LIB(06) = 1 ' 13467-PCDF
LIB(07) = 1 ' 12378-PCDF
LIB(08) = 1 ' 12367-PCDF
LIB(09) = 1 ' 23476-PCDF
LIB(10) = 1 ' 23467-PCDF
LIB(11) = 1 ' 12378-PCDD
LIB(12) = 1 ' 123478-HxCDF
LIB(13) = 1 ' 123467-HxCDF
LIB(14) = 1 ' 123678-HxCDF
LIB(15) = 1 ' 234678-HxCDF
LIB(16) = 1 ' 123789-HxCDF
LIB(17) = 1 ' 123478-HxCDD
LIB(18) = 1 ' 123678-HxCDD
LIB(19) = 1 ' 123789-HxCDD
LIB(20) = 1 ' 1234678-HpCDF
LIB(21) = 1 ' 1234789-HpCDF
LIB(22) = 1 ' 1234678-HpCDD
LIB(23) = 1 ' OCDF
LIB(24) = 1 ' OCDD

RETURN

6030 REM library for 60 M x .32 mm SP2330 capillary column
REM Using linear regression this program will estimate a
 line, Y = A + BX, where X is the independent variable and
 Y is the dependent variable. If more than 30
 observations are used, the dimension statements must
 be changed. Subroutine REGRESSION may be used by other
 programs if data is provided in the arrays X and Y and
 the number of observations is provided in variable IN.

 REM subroutine linear regression calcs

 IN = HALFNAT - 2 'OCDD not included in regression calcs

6190 CLS : PRINT : PRINT *AVAILABLE OPTIONS:*  
PRINT TAB(7) "1- LIST INPUT DATA"  
PRINT TAB(7) "2- MODIFY INPUT DATA"  
PRINT TAB(7) "3- PERFORM REGRESSION ANALYSIS"  
PRINT TAB(7) "4- QUIT"  
INPUT "OPTION" ; IP
6260 IF IP=1 THEN GOSUB 6330
6270 IF IP=2 THEN GOSUB 6450
6280 IF IP=3 THEN GOSUB 6520
6290 IF IP=4 THEN GOSUB 6870
6300 GOTO 6190
6320 REM SUBROUTINE: LIST DATA
6330 PRINT:PRINT "LISTING OF DATA"
   PRINT * "LIB", * "BRT"
   IC=1
   FOR I=1 TO IN
      IF IC>(IC*15) THEN 6400
      IC=IC+1
      PRINT:INPUT "Strike the ENTER key to continue ... ",Y$:PRINT
      PRINT LIB(I), BRT(I)
   NEXT I
   PRINT:
   INPUT'Strike the ENTER key to continue ...", ANY$
6420 RETURN
6440 REM SUBROUTINE: MODIFY DATA
6450 PRINT:INPUT "ENTER NUMBER OF DATA POINT TO BE MODIFIED"; ID
6460 PRINT "NEW VALUES FOR LIB AND BRT FOR POINT"; ID;
6470 INPUT LIB(ID), BRT(ID)
6480 INPUT "ANY MORE DATA POINTS TO BE MODIFIED (Y/N)"; Y$
6490 IF (Y$="Y") THEN GOTO 6450
6500 RETURN
6520 REM SUBROUTINE REGRESSION
   ' Convert to decimal here, to incorporate changes into DBRT array
   FOR I = 1 TO IN
      DBRT(I) = INT(BRT(I)) + (( BRT(I) - (INT(BRT(I))))/.6000)
   NEXT I
   ' enter LIB and DBRT into X and Y arrays
   FOR I = 1 TO IN
      X(I) = LIB(I)
      Y(I) = DBRT(I)
   NEXT I
   ' the following code is modified from Wolfe, P.M., and Koelling, C.P.
   ' (1983) Basic Engineering and Scientific Programs for the IBM PC,
   ' William J. Brady Co., Bowie, Md., chapter 4
6530 SX=0:SY=0:SI2=0:SY2=0:SXY=0
6540 FOR I=1 TO IN
6550 SX=SX+X(I)  'SUM OF X
6560 SY=SY+Y(I)  'SUM OF Y
6570 SI2=ABS(SI2+X(I)^2) 'SUM OF X^2
6580 SY2=ABS(SY2+Y(I)^2) 'SUM OF Y^2
6590 SXY=SXY+X(I)*Y(I) 'SUM OF XY
6600 NEXT I
6610 W=(IN*SXY-SX*SY)/IN:SI2-SX^2
6620 A=(SY-W*SX)/IN  'INTERCEPT OF LINE
6630 REM Coefficient of correlation
6640 SQXY=ABS(SY2-SY^2/IN-W*(SXY-SX*SY/IN))
6660 SSE=ABS(SY2-SY^2/IN-W*(SXY-SX*SY/IN))  'ERROR SUM OF SQUARES
6670 SE=SQR(SSE/IN-2)  'STD DEVIATION OF ESTIMATE
6680 REM SUBROUTINE: PRINT RESULTS
6700 CLS: PRINT "REGRESSION EQUATION:";
6710 PRINT "DBRT(Y)=A; W;"; LIB(X)";
6720 PRINT "COEFFICIENT OF DETERMINATION="; CR
6730 PRINT "COEFFICIENT OF CORRELATION="; CC
6740 PRINT "STANDARD DEVIATION OF THE ESTIMATE="; SE
6750 PRINT "ACTUAL VERSUS ESTIMATED VALUES"
6760 PRINT "X", "Y", "ESTIMATED Y", "ERROR"
6770 IC=1
6780 FOR I=1 TO IN
6790 IF IC>(IC+14) THEN 6820
6800 PRINT:"PRESS ENTER TO CONTINUE";Y$:PRINT
6810 IC=IC+1
6820 EY(I)=A+W*X(I)
6830 PRINT X(I), Y(I), EY(I), Y(I)-EY(I)
6840 NEXT I
6840 REM Convert EY(I) from decimal to minsec format
6850 FOR I=1 TO IN
6860 PRMS(I)=FNMINSEC(EY(I))
6870 NEXT I
6850 PRINT: INPUT "PRESS ENTER TO CONTINUE"; Y$
CLS: PRINT: PRINT
IF(CR <= .990) THEN
  PRINT" Your isomer assignments do not correlate well with"
  PRINT" the standard library for this column."
ELSEIF (CR > .990) THEN
  PRINT" Your isomer assignments correlate well with the "
  PRINT" standard library."
END IF
PRINT: INPUT "Strike the ENTER key to continue ...", ANY$

6860 RETURN

6870 PRINT: PRINT TAB(7) "END OF REGRESSION CALCULATIONS"
       PRINT TAB(7) "YOUR OUTPUT WILL BE SENT TO THE LINE PRINTER"

6880 PRINT: INPUT "Strike the ENTER key to exit the regression routine ...", ANY$

6890 CLS: PRINT: PRINT"Adjust the printer paper for your RFACTOR output"
       PRINT: PRINT
       INPUT"Strike the enter key when ready ...", ANY$
       CLS

RETURN 264
Program DFQUANT Ver. 6.1 1/23/87
Murray Hackett
Toxicology Program
Oregon State University
Corvallis, Oregon 97331
60 meter DB5 version
A program in ten subroutines to quantify
dioxin/furan residues from GC-MS data

10 REM Initialize arrays
105 DIM L3(30), N3(50), L4(30), N4(50), QREC(20), QAREC(30)
110 DIM LP(30), LRT(30), NP(50), NRT(50), LHQ(5), LH8(5), LHS(5)
120 DIM RRFL(30), RRFN(50), CRRTN(30), DSLRT(20), DSNRT(50), RECC(50)
130 DIM SLP(30), SNP(50), SLRT(30), SNRT(50), C(30), RATRANGE(30)
140 DIM REC(30), LION(30), THEORY(30), CD(30), RFL(20), RFN(50)
141 DIM SNLS(30), SNMDL(30), NE(30), HB(30), HS(30), HR(30), QNRT(50)
142 DIM CQA(30), SDS(30), RRT(30), RRT(50), QLION(30), QNION(50)
150 DIM RATS(30), NION(50), BION(30), BRT(30), RRBT(30), ALYTE$(30)
155 REM user functions to convert RT values to decimal format for calculating RRT
156 DEF FNCONVERT(X)
158 FNCONVERT = INT(X) + ((X-INT(X))/0.60)
160 END DEF
162 DEF FNMINSEC(Y)
164 FNMINSEC = INT(Y) + ((Y-INT(Y))*.60)
166 END DEF

174 REM Subroutines
176 CLS : KEY OFF
178 PRINT PRINT PRINT"You are about to be victimized by Murray's DFQUANT Program!"* 
180 PRINT"Be sure and set the Caps Lock Key so only caps will* 
185 PRINT"be entered, otherwise this does not work. " 
190 PRINT : PRINT
195 INPUT"Strike ENTER key when ready ... ", ANYS
210 CONC = 24 : REM Number of Concentrations Reported
212 LABEL = 12 : REM Number of labeled isomers
215 NAT = 48 : REM Number of natural ions
216 REM Error Handling routine not included this version
220 GOSUB 2500 : REM read RF and RRF values from disk file
225 GOSUB 2600 : REM enter raw data from disk file (optional)
230 GOSUB 3000 : REM enter raw data interactively
235 GOSUB 3300 : REM quantitation calculations for isotope dilution method
240 GOSUB 4000 : REM calculate recoveries
250 GOSUB 5000 : REM calculate ion ratios for QA purposes
260 GOSUB 7000 : REM calculate S/N or S/N and MDL
270 GOSUB 8700 : REM calculate RRT's
280 GOSUB 9000 : REM output report form to printer, disk
290 GOSUB 10000 : REM not used in this version
300 GOSUB 11000 : REM output for Phil's data base
400 CLS : PRINT : PRINT : BEEP
410 PRINT"You are now finished with this run of DFQUANT" 
500 END
REM Subroutine to read RF and RRF values from disk file
CLS : PRINT : PRINT
PRINT "Place your diskette with RF'S in drive A or B."
PRINT "Enter the complete name of your file in quotation marks, ", RFAC$
CLS
OPEN RFACS FOR INPUT AS #2
FOR J = 1 TO LABEL
INPUT #2, QLION(J), LRT(J), RFL(J), RRFL(J)
NEXT J
FOR K = 1 TO NAT
INPUT #2, QNION(K), QNRT(K), RFN(K), RRFN(K)
NEXT K
FOR I = 1 TO CONC
INPUT #2, BION(I), BRT(I), RRBT(I), ALYTE$(I)
NEXT I
CLOSE #2
RETURN

REM Subroutine to enter raw data from disk file
PRINT "Quantification of an unknown sample 
PRINT 
PRINT "Do you wish to enter peak area and RT data from disk file" 
PRINT "or interactively from your written notes? " 
INPUT "Enter 'D' for disk or 'I' for interactive: ", UNKNOS
IF UNKNOS = "D" THEN 2670 ELSE IF UNKNOS = "I" THEN RETURN
PRINT 
PRINT "Enter your data base file name, in quotes, including 
INPUT "Drive designator: ", RAWDATS
OPEN RAWDATS FOR INPUT AS 13
INPUT #3, MSIDS, PCIDS, OTHERS
FOR I = 1 TO LABEL
INPUT #3, LION(I), SLRT(I), RRTL(I), RECC(I), QREC(I)
NEXT I
FOR I = 1 TO CONC
INPUT #3, BION(I), NRT(I), CRRTN(I), C(I), CD(I), RATS(I), THEORY(I)
INPUT #3, HS(I), SGNS(I), SMD(I), CD(I), SGDS(I)
NEXT I
REM User input, should not normally be used in data base
FOR I = 1 TO LABEL
INPUT #3, SLP(I), LRT(I)
NEXT I
FOR I = 1 TO NAT
INPUT #3, SNP(I), SNRT(I)
NEXT I
FOR I = 1 TO CONC
INPUT #3, LBH(I), LHS(I), LHQ(I)
NEXT I
CLOSE #3
CLS
RETURN
REM Subroutine: interactive input

IF UNKNOS = "D" THEN 3355 ELSE 3028

CLS

INPUT "enter peak areas for 2378 TCDF, 304 and 306 "; SNP(1), SNP(2)
INPUT "enter RT's for 304, 306 "; SNRT(1), SNRT(2)

CLS

INPUT "enter peak areas for 2367 TCDF, 304 and 306 "; SNP(3), SNP(4)
INPUT "enter RT's for 304, 306 "; SNRT(3), SNRT(4)

CLS

INPUT "enter peak areas for 3467 TCDF, 304 and 306 "; SNP(5), SNP(6)
INPUT "enter RT's for 304, 306 "; SNRT(5), SNRT(6)

CLS

INPUT "enter area for 13C12 2378 TCDF, 318 "; SLP(2)
INPUT "enter RT for 13C12 2378 TCDF "; SLRT(2)

CLS

INPUT "enter peak areas for 1234 TCDD, 320 and 322 "; SNP(7), SNP(8)
INPUT "enter RT's for 320, 322 "; SNRT(7), SNRT(8)

CLS

INPUT "enter peak areas for 2378 TCDD, 320 and 322 "; SNP(9), SNP(10)
INPUT "enter RT's for 320, 322 "; SNRT(9), SNRT(10)

CLS

INPUT "enter peak area for 37CL4 2378 TCDD, 328 "; SLP(4)
INPUT "enter RT for 37CL4 2378 TCDD "; SLRT(4)

CLS

INPUT "enter peak area for 13C6 1234 TCDD, 328 "; SLP(3)
INPUT "enter RT for 13C6 1234 TCDD "; SLRT(3)

CLS

INPUT "enter peak area for 13C12 1234 TCDD, 334 "; SLP(1)
INPUT "enter RT for 13C12 1234 TCDD "; SLRT(1)

CLS

INPUT "enter peak areas for 13467 PCDF, 340 and 342 "; SNP(11), SNP(12)
INPUT "enter RT's for 340, 342 "; SNRT(11), SNRT(12)

CLS

INPUT "enter peak areas for 12378 PCDF, 340 and 342 "; SNP(13), SNP(14)
INPUT "enter RT's for 340, 342 "; SNRT(13), SNRT(14)

CLS

INPUT "enter peak areas for 12367 PCDF, 340 and 342 "; SNP(15), SNP(16)
INPUT "enter RT's for 340, 342 "; SNRT(15), SNRT(16)

CLS

INPUT "enter peak areas for 23478 PCDF, 340 and 342 "; SNP(17), SNP(18)
INPUT "enter RT's for 340, 342 "; SNRT(17), SNRT(18)

CLS

INPUT "enter peak areas for 23467 PCDF, 340 and 342 "; SNP(19), SNP(20)
INPUT "enter RT's for 340, 342 "; SNRT(19), SNRT(20)

CLS

INPUT "enter peak area for 13C12 12378 PCDF, 352 "; SLP(5)
INPUT "enter peak RT for 13C12 12378 PCDF "; SLRT(5)

CLS

INPUT "enter peak areas for 12378 PCDD, 356 and 358 "; SNP(21), SNP(22)
INPUT "enter RT's for 356, 358 "; SNRT(21), SNRT(22)

CLS

INPUT "enter peak area for 13C12 12378 PCDD, 368 "; SLP(6)
INPUT "enter RT for 13C12 12378 PCDD "; SLRT(6)
INPUT "enter peak areas for 123478 HxCDF, 374 and 376 "; SNP(23), SNP(24)
INPUT "enter RT's for 374, 376 "; SNRT(23), SNRT(24)
CLS
INPUT "enter peak areas for 123467 HxCDF, 374 and 376 "; SNP(25), SNP(26)
INPUT "enter RT's for 374, 376 "; SNRT(25), SNRT(26)
CLS
INPUT "enter peak areas for 123678 HxCDF, 374 and 376 "; SNP(27), SNP(28)
INPUT "enter RT's for 374, 376 "; SNRT(27), SNRT(28)
CLS
INPUT "enter peak areas for 234678 HxCDF, 374 and 376 "; SNP(29), SNP(30)
INPUT "enter RT's for 374, 376 "; SNRT(29), SNRT(30)
CLS
INPUT "enter peak areas for 1234678 HxCDD, 390 and 392 "; SNP(33), SNP(34)
INPUT "enter RT's for 390, 392 "; SNRT(33), SNRT(34)
CLS
INPUT "enter peak areas for 123678 HxCDD, 390 and 392 "; SNP(35), SNP(36)
INPUT "enter RT's for 390, 392 "; SNRT(35), SNRT(36)
CLS
INPUT "enter peak areas for 13C12 123478 HxCDF, 386 "; SLP(7)
INPUT "enter RT for 13C12 123678 HxCDF "; SLRT(7)
CLS
INPUT "enter peak areas for 123478 HxCDD, 390 and 392 "; SNP(33), SNP(34)
INPUT "enter RT's for 390, 392 "; SNRT(33), SNRT(34)
CLS
INPUT "enter peak areas for 123678 HxCDD, 390 and 392 "; SNP(35), SNP(36)
INPUT "enter RT's for 390, 392 "; SNRT(35), SNRT(36)
CLS
INPUT "enter peak areas for 13C12 123478 HxCDD, 402 "; SLP(8)
INPUT "enter RT for 13C12 123678 HxCDD "; SLRT(8)
CLS
INPUT "enter peak areas for 1234678 HpCDF, 408 and 410 "; SNP(39),SNP(40)
INPUT "enter RT's for 408, 410 "; SNRT(39), SNRT(40)
CLS
INPUT "enter peak areas for 123478 HpCDF, 408 and 410 "; SNP(39),SNP(40)
INPUT "enter RT's for 408, 410 "; SNRT(39), SNRT(40)
CLS
INPUT "enter peak areas for 1234678 HpCDD, 424, 426 "; SNP(43), SNP(44)
INPUT "enter RT for 424, 426 "; SNRT(43), SNRT(44)
CLS
INPUT "enter peak areas for 13C12 1234678 HpCDD, 436 "; SLP(10)
INPUT "enter RT for 13C12 1234678 HpCDD "; SLRT(10)
CLS
INPUT "enter peak areas for OCDF, 444 and 446 "; SNP(45), SNP(46)
INPUT "enter RT's for 444, 446 "; SNRT(45), SNRT(46)
CLS
INPUT "enter peak area for 13C12 OCDF, 456 "; SLP(11)
INPUT "enter RT for 13C12 OCDF "; SLRT(11)
CLS
INPUT "enter peak areas for OCDD, 458 and 460 "; SNP(47), SNP(48)
INPUT "enter RT's for 458, 460 "; SNRT(47), SNRT(48)
CLS
INPUT "enter peak area for 13C12 OCDD, 472 "; SLP(12)
INPUT "enter RT for 13C12 OCDD "; SLRT(12)

REM output user input in interactive mode to printer
CLS : PRINT : PRINT
PRINT"Adjust your printer paper, if necessary"
INPUT"Strike the ENTER key when ready ... "; ANY$ 

FOR I = 1 TO 2 : LPRINT : NEXT I

INPS = ' 11$$$$$$$$$$$$ Wit
It

LPRINT'USER INPUT'

LPRINT 'Labeled Ion RT Iteration '

FOR I = 1 TO LABEL 
LPRINT USING INN SLP(I), SNRT(I), I 
NEXT I

FOR I = 1 TO 50 : LPRINT : NEXT I

LPRINT'USER INPUT'

LPRINT 'Natural Ion RT Iteration '

FOR I = 1 TO NAT 
LPRINT USING INP$; SNP(I), SNRT(I), I 
NEXT I

FOR I = 1 TO 20 : LPRINT : NEXT I

CLS : PRINT : PRINT
PRINT 'Please inspect the hardcopy of your input to make 
sure it is correct; type 'Y' or 'N': ', CHOICES
IF CHOICES = 'Y' THEN RETURN ELSE 3028

REM Subroutine: quantitation calculations
CLS : PRINT : PRINT : REM enter mass of sample in grams
INPUT "enter sample mass in units of grams: "; MASS

REM constant to correct for sample size 
KC = 20 / MASS 

REM Input constant to adjust for volume of spiking soln 
CLS : PRINT : PRINT 
PRINT "Enter volume of spiking soln added to sample, "; KS

KSP=KS/100

K334 = 100 
REM remove redundant code for next version

REM calculate "wet weight" concentration of analyte in sample 
REM tcdf

IF (SLP(2)<>0 AND RRFN(2)<0) THEN C(1) = SNP(2)*25*KC*KSP/ (SLP(2)*RRFN(2)) ELSE C(1) = 0

IF (SLP(2)<>0 AND RRFN(4)<0) THEN C(2) = SNP(4)*25*KC*KSP/ (SLP(2)*RRFN(4)) ELSE C(2) = 0

IF (SLP(3)<>0 AND RRFN(6)<0) THEN C(3) = SNP(6)*25*KC*KSP/ (SLP(2)*RRFN(6)) ELSE C(3) = 0

REM 1234 tcdd

IF (SLP(3)<>0 AND RRFN(8)<0) THEN C(4) = SNP(8)*29*KKSP/ (SLP(3)*RRFN(8)) ELSE C(4) = 0

REM 2378 tcdd

IF (SLP(4)<>0 AND RRFN(10)<0) THEN C(5) = SNP(10)*25*KC*KSP/ (SLP(2)*RRFN(10)) ELSE C(5) = 0

REM pcdf

IF (SLP(5)<>0 AND RRFN(11)<0) THEN C(6) = SNP(11)*50*KC*KSP/ (SLP(5)*RRFN(11)) ELSE C(6) = 0

IF (SLP(5)<>0 AND RRFN(13)<0) THEN C(7) = SNP(13)*50*KC*KSP/ (SLP(5)*RRFN(13)) ELSE C(7) = 0

IF (SLP(5)<>0 AND RRFN(15)<0) THEN C(8) = SNP(15)*50*KC*KSP/ (SLP(5)*RRFN(15)) ELSE C(8) = 0

IF (SLP(5)<>0 AND RRFN(17)<0) THEN C(9) = SNP(17)*50*KC*KSP/ (SLP(5)*RRFN(17)) ELSE C(9) = 0

IF (SLP(5)<>0 AND RRFN(19)<0) THEN C(10) = SNP(19)*50*KC*KSP/ (SLP(5)*RRFN(19)) ELSE C(10) = 0

REM pcd
122

IF (SLP(6)>0 AND RRFN(21)=0) THEN C(11) = SNP(21)*100*KUKSP/(SLP(6)*RRFN(21)) ELSE C(11) = 0
REM hxcdf

IF (SLP(7)>0 AND RRFN(23)>0) THEN C(12) = SNP(23)*100*KUKSP/(SLP(7)*RRFN(23)) ELSE C(12) = 0

IF (SLP(7)>0 AND RRFN(25)>0) THEN C(13) = SNP(25)*100*KUKSP/(SLP(7)*RRFN(25)) ELSE C(13) = 0

REM hxcdd

IF (SLP(8)>0 AND RRFN(27)>0) THEN C(14) = SNP(27)*100*KUKSP/(SLP(8)*RRFN(27)) ELSE C(14) = 0

IF (SLP(9)>0 AND RRFN(31)>0) THEN C(16) = SNP(31)*100*KUKSP/(SLP(9)*RRFN(31)) ELSE C(16) = 0

REM hpcdf

IF (SLP(10)>0 AND RRFN(33)>0) THEN C(17) = SNP(33)*100*KUKSP/(SLP(10)*RRFN(33)) ELSE C(17) = 0

IF (SLP(11)>0 AND RRFN(35)>0) THEN C(18) = SNP(35)*100*KUKSP/(SLP(11)*RRFN(35)) ELSE C(18) = 0

IF (SLP(12)>0 AND RRFN(37)>0) THEN C(19) = SNP(37)*100*KUKSP/(SLP(12)*RRFN(37)) ELSE C(19) = 0

REM hpcdd

If (SLP(13)>0 AND RRFN(39)>0) THEN C(20) = SNP(39)*100*KUKSP/(SLP(13)*RRFN(39)) ELSE C(20) = 0

REM ocdf

IF (SLP(14)>0 AND RRFN(41)>0) THEN C(21) = SNP(41)*100*KUKSP/(SLP(14)*RRFN(41)) ELSE C(21) = 0

REM ocdd

If (RFN(39)>0) THEN C(20) = SNP(39)*KC*K334/((RFN(39)/RFL(1))*SLP(1)) ELSE C(20) = 0

REM calculate dry weight of tissue or solid

CLS
PRINT
PRINT
PRINT'Enter X lipid (tissue), 100 - % moisture (solids) or *
INPUT 10(water sample): " , KD

KND = KD/100
FOR N = 1 TO CONC
IF (KND > 0 AND C(N)>0) THEN CD(N) = C(N)/KND ELSE CD(N) = 0
NEXT N
CLS
RETURN

REM Subroutine: calculate % recovery for each isomer group

K334 = 100 : REM Constant for 20 ul volume, 100 pg/ul 13C12 TCDD
REM WARNING!!! Change this constant if I.S. is handled differently
FOR I = 2 TO 4
IF (RRFL(I)>0 AND SLP(1)>0) THEN REC(I) = SLP(I)*K334/(RRFL(I)*SLP(1)*KSP*25) ELSE REC(I) = 0
NEXT I
FOR I = 5 TO 6
IF (RRFL(I)>0 AND SLP(1)>0) THEN REC(I) = SLP(I)*K334/(RRFL(I)*SLP(1)*KSP*50) ELSE REC(I) = 0
NEXT I
FOR I = 7 TO 10
IF (RRFL(I)>0 AND SLP(1)>0) THEN REC(I) = SLP(I)*K334/(RRFL(I)*SLP(I)*KSP*100) ELSE REC(I) = 0
NEXT I
FOR I = 11 TO 12
IF (RRFL(I)>0 AND SLP(1)>0) THEN REC(I) = SLP(I)*K334/(RRFL(I)*SLP(I)*KSP*200) ELSE REC(I) = 0
NEXT I
REM output to video for %recovery subroutine
PRINT
PRINT
PRINT 'Congener', 'X Recovery'
FOR I = 2 TO LABEL
PRINT I, REC(I)$100
NEXT I
RETURN

FOR L = 1 TO CONC
FOR J = 1 TO (2*L)-1 STEP 2
FOR K = 2 TO (J+1) STEP 2
IF (SNP(K) = 0) THEN RATS(L) = 0 ELSE RATS(L) = SNP(J)$1/SNP(K)
NEXT K
NEXT J
NEXT L
REM set flag to mark if ratios fall within allowable ranges
FOR M = 1 TO 5 : REM tetras
IF (RATS(M) < .655 OR RATS(M) > .865) THEN RATRANGE(M) = 0 ELSE RATRANGE(M) = 1
NEXT M
FOR M = 6 TO 11 : REM pentas
IF (RATS(M) < 1.35 OR RATS(M) > 1.70) THEN RATRANGE(M) = 0 ELSE RATRANGE(M) = 1
NEXT M
FOR M = 12 TO 19 : REM hexas
IF (RATS(M) < 1.03 OR RATS(M) > 1.43) THEN RATRANGE(M) = 0 ELSE RATRANGE(M) = 1
NEXT M
FOR M = 20 TO 22 : REM heptas
IF (RATS(M) < .865 OR RATS(M) > 1.22) THEN RATRANGE(M) = 0 ELSE RATRANGE(M) = 1
NEXT M
REM ocdf and ocd2 ratranges
IF (RATS(23) < 1.28 OR RATS(23) > 1.78) THEN RATRANGE(23) = 0 ELSE RATRANGE(23) = 1
IF (RATS(24) < .675 OR RATS(24) > 1.13) THEN RATRANGE(24) = 0 ELSE RATRANGE(24) = 1
CLS
RETURN

REM Subroutine calculates detection limits, S/N
CLS : PRINT : PRINT
PRINT 'Choose the lowest concentration Q series standard
in your set which can be used to generate MDL's
NQ(1) = 1 : NQ(2) = 1 : NQ(3) = 1 : NQ(4) = 2.5
NQ(5) = 1 : NQ(6) = 2 : NQ(7) = 2 : NQ(8) = 2
NQ(9) = 2 : NQ(10) = 2 : NQ(11) = 2
NQ(12) = 4 : NQ(13) = 4 : NQ(14) = 4 : NQ(15) = 4
NQ(16) = 4 : NQ(17) = 4 : NQ(18) = 4 : NQ(19) = 4
NQ(20) = 4 : NQ(21) = 4 : NQ(22) = 4 : NQ(23) = 8 : NQ(24) = 8
GOTO 7700
REM Values for variable NQ, standard Q2
NQ(1) = 5 : NQ(2) = 5 : NQ(3) = 5 : NQ(4) = 2.5
NQ(5) = 5 : NQ(6) = 10 : NQ(7) = 10 : NQ(8) = 10
7700 RETURN
7215  NQ(9) = 10 : NQ(10) = 10 : NQ(11) = 10
7220  NQ(12) = 20 : NQ(13) = 20 : NQ(14) = 20 : NQ(15) = 20
7225  NQ(16) = 20 : NQ(17) = 20 : NQ(18) = 20 : NQ(19) = 20
7230  NQ(20) = 20 : NQ(21) = 20 : NQ(22) = 20 : NQ(23) = 40 : NQ(24) = 40
7235  GOTO 7700
7300  REM Values for variable NQ, standard Q3
7305  NQ(1) = 12.5 : NQ(2) = 12.5 : NQ(3) = 12.5 : NQ(4) = 2.5
7310  NQ(5) = 25 : NQ(6) = 25 : NQ(7) = 25 : NQ(8) = 25
7315  NQ(9) = 25 : NQ(10) = 25 : NQ(11) = 25
7320  NQ(12) = 50 : NQ(13) = 50 : NQ(14) = 50 : NQ(15) = 50
7325  NQ(16) = 50 : NQ(17) = 50 : NQ(18) = 50 : NQ(19) = 50
7330  NQ(20) = 50 : NQ(21) = 50 : NQ(22) = 50 : NQ(23) = 100 : NQ(24) = 100
7335  GOTO 7700
7400  REM Values for variable NQ, standard Q4
7405  NQ(1) = 25 : NQ(2) = 25 : NQ(3) = 25 : NQ(4) = 5
7410  NQ(5) = 25 : NQ(6) = 50 : NQ(7) = 50 : NQ(8) = 50
7415  NQ(9) = 50 : NQ(10) = 50 : NQ(11) = 50
7420  NQ(12) = 100 : NQ(13) = 100 : NQ(14) = 100 : NQ(15) = 100
7425  NQ(16) = 100 : NQ(17) = 100 : NQ(18) = 100 : NQ(19) = 100
7430  NQ(20) = 100 : NQ(21) = 100 : NQ(22) = 100 : NQ(23) = 200 : NQ(24) = 200
7500  REM Stick Q5 here, should it be added in the future
7600  REM Stick Q6 here
7700  REM Covert REC(i), i = 11, to QAREC(i), i = 24 isomers
7705  FOR I = 1 TO 3 : QAREC(I) = REC(2) : NEXT I : QAREC(4) = REC(3) : QAREC(5) = REC(4)
7710  FOR I = 6 TO 10 : QAREC(I) = REC(5) : NEXT I : QAREC(11) = REC(6)
7715  FOR I = 12 TO 16 : QAREC(I) = REC(7) : NEXT I
7720  FOR I = 17 TO 19 : QAREC(I) = REC(8) : NEXT I : QAREC(20) = REC(9) : QAREC(21) = REC(9)
7725  QAREC(22) = REC(10) : QAREC(23) = REC(11) : QAREC(24) = REC(12)
8000  REM
8020  CLS : PRINT : PRINT
8030  PRINT "This portion of the program generates S/N and MDL data"
8040  PRINT "for your sample" : PRINT : PRINT
8050  REM Enter data from disk or interactively
8060  PRINT : PRINT
8070  PRINT "Do you wish to enter peak height data from disk files or interactively?"
8080  PRINT "from disk files or interactively?"
8090  PRINT
8100  INPUT "Enter 'D' for disk or 'I' for interactive: ", UNKNO$
8110  CLS
8120  IF UNKNO$ = "D" THEN 8495 ELSE 8270
8270  CLS : PRINT : PRINT
8280  REM interactive input
8290  PRINT "Enter your peak height data for the lowest Q series standard"
8300  PRINT "in your set": PRINT : PRINT
8302  INPUT "Strike ENTER key when ready ... ", ANY$
8304  CLS : PRINT : PRINT
8306  INPUT "Enter your peak height for 13C12 1234-TCDD, 334 ion: ", LHQ(1)
8308  CLS : PRINT : PRINT
8310  FOR I = 1 TO CONC
8312  PRINT "Enter your peak height for "; ALYTE$(I); PRINT" ion ";
PRINT BION(I)
8314 INPUT ", HQ(I)
8316 CLS : PRINT : PRINT
8317 NEXT I
8318 PRINT "334", "13C12 TCDD", LHQ(I)
8320 FOR I = 1 TO CONC
8322 PRINT BION(I), ALYTES(I), HQ(I)
8324 NEXT I
8328 INPUT "Is your data correct? Type 'Y' or 'N': ", CHECKS
8330 IF CHECKS = "Y" THEN 8370 ELSE 8270
8335 CLS : PRINT : PRINT
8337 PRINT "Enter your peak height data for the noise windows in your sample:
8338 INPUT "Strike ENTER key when ready ... ", ANY$.
8339 CLS : PRINT : PRINT
8340 INPUT "Enter your peak height for 13C12-234-TCDD, 334 ion:
8341 CLS : PRINT : PRINT
8342 FOR I = 1 TO CONC
8343 PRINT "Enter your peak height for "; ALYTES(I); "ion "; PRINT BION(I)
8344 INPUT HB(I)
8345 CLS : PRINT : PRINT
8346 NEXT I
8348 REM default noise to two counts (8230 only), no democracy here!
8349 FOR I = 1 TO CONC
8350 IF( HB(I) > 0 AND HB(I) < 2 ) THEN
8351 HB(I) = 2
8352 END IF
8353 NEXT I
8355 CLS
8356 PRINT "334", "13C12 TCDD", LHB(1)
8358 FOR I = 1 TO CONC
8360 PRINT BION(I), ALYTES(I), HB(I)
8361 NEXT I
8365 INPUT "Is your data correct? Type 'Y' or 'N': ", CHECKS
8366 IF CHECKS = "Y" THEN 8456 ELSE 8370
8401 CLS
8402 PRINT "334", "13C12 TCDD", LHB(1)
8404 FOR I = 1 TO CONC
8406 PRINT BION(I), ALYTES(I), HB(I)
8408 NEXT I
8413 INPUT "Is your data correct? Type 'Y' or 'N': ", CHECKS
8414 IF CHECKS = "Y" THEN 8456 ELSE 8370
8450 CLS : PRINT : PRINT
8451 PRINT "Enter your peak height data for sample peak heights: 
8452 INPUT "Strike ENTER key when ready ... ", ANY$
8454 CLS : PRINT : PRINT
8456 INPUT "Enter your peak height for 13C12-234-TCDD, 334 ion: ", LHS(I)
8458 CLS : PRINT : PRINT
8460 FOR I = 1 TO CONC
8462 PRINT "Enter your peak height for "; ALYTES(I); "ion "; PRINT BION(I)
8464 INPUT HS(I)
8466 CLS : PRINT : PRINT
8468 NEXT I
8470 FOR I = 1 TO CONC
8472 PRINT "Enter your peak height for "; ALYTES(I); "ion "; PRINT BION(I)
8474 INPUT HS(I)
8476 CLS : PRINT : PRINT
8478 NEXT I
8480 CLS
REM default sample to two counts (B230 only)
FOR I = 1 TO CONC
  IF (HS(I)<0 AND HS(I)<2) THEN
    HS(I) = 2
  END IF
NEXT I

PRINT * 334*, "13C12 TCDD", LHS(I)
FOR I = 1 TO CONC
  PRINT BION(I), ALYTES(I), HS(I)
END I

REM Output peak heights entered for S/N and MDL calcs
CLS
FOR Z = 1 TO CONC:
  PRINT HEZ, HB(Z), HS(Z):
NEXT Z
LION(1) = 334: IS = 0

LPRINT USER INPUT

CLS: PRINT: PRINT: BEEP

LPRINT * Ion Peak Height Peak Height Peak Height *
LPRINT * Noise Sample Standard Iteration *
LPRINT USING INPMDL$: LION(1), LHB(1), LHS(1), LHB(1), IS
FOR N = 1 TO CONC
  LPRINT USING INPMDL$: BION(N), HB(N), HS(N), HQ(N), N
END I

CLS
PRINT:
PRINT:
BEEP

REM Calculate S/N for positives, S/N and MDL for negatives
KMDL = 20: REM Constant assumes 20 ul final volume in microvial
FOR M = 1 TO CONC: REM logic is not easy to follow
IF (HB(M)<0) THEN 8570 ELSE 8590
SGNS(M) = (HS(M)/LHS(1))/(HB(M)/LHB(1))
  REM note assumption I.S. same conc in both
  IF (SGNS(M) < 2.5 OR RATRANGE(M) = 0) THEN
    SGDS(M) = 0
  ELSEIF (SGNS(M)>= 2.5 AND RATRANGE(M) = 1) THEN
    SGDS(M) = 1
  END IF
  IF (SGDS(M) = 0) THEN S6NS(M) = 0
  IF (SGNS(M) = 0) THEN 8590 ELSE 8610
END M

IF (HS(M)<0) THEN 8590 ELSE 8590
SNMMDL(M) = (HO(M)/LH(M)) /((HS(M)/LHS(1)))-2.5) ELSE SNMDL(M)=0

REM mdl for negatives
IF (GAREC(M)<0 AND SNMDL(M)<0) THEN CQA(M) = MDL/(GAREC(M)*MASS# SNMDL(M)) ELSE CQA(M) = 0
IF (CQA(M)<.195 AND CQA(M)>0) THEN CQA(M) = .2 ELSE 8610
NEXT M
PRINT"Did you recover sufficient natural 1234-TCDD for purposes"
PRINT"of calculating an MDL for 2378-TCDD using the 'surrogate" 
PRINT"analyte approach? Type 'Y' or 'N': ", SURR$: PRINT
PRINT
PRINT"If you answer 'N' then the MDL will default to the method " 
PRINT"used for all other PCDD's and PCDF's" : PRINT
INPUT"Strike ENTER key when ready ... ", ANY$  
END IF
IF (RATRANGE(4)=0) THEN
CLS : PRINT
PRINT
PRINT"You have a bad ion ratio for natural 1234-TCDD." 
PRINT"Or, you failed to enter both ions when prompted" 
PRINT"for peak areas for 1234-TCDD. The surrogate analyte " 
PRINT"approach cannot be used under these circumstances." 
PRINT : PRINT
INPUT"Strike the ENTER key when ready... ", ANY$  
GOTO 8630
END IF
SGNS(5) = (HS(5)/LHS(1)) / (HB(5)/LHB(1)) : REM note assumption that I.S. same conc in both
IF (SGNS(5) < 2.5 OR RATRANGE(5) = 0) THEN SGDS(5) = 0
IF (SGDS(5) = 0) THEN SGNS(5) = 0
IF (SGNS(5) = 0) THEN SNMDL(5) = HS(5)+2.5 ELSE SNMDL(5) = 0
IF (SGNS(5) = 0) THEN CQA(5) = (SNMDL(5)/HS(4)) * (RFN(8)/RFN(10)) # 5.0 ELSE CQA(5) = 0
REM Adjust reported concentrations based on SGDS indicator variable
FOR I = 1 TO CONC
IF (C(I) < .195 OR SGDS(I)=0) THEN
C(I) = 0
CD(I) = 0
END IF  
NEXT I
REM Adjust S/N for negatives, redundancy necessary if data base used for input
FOR I = 1 TO CONC
IF(SGDS(I)=1) THEN
SNMDL(I) = 0
CQA(I) = 0
END IF  
NEXT I
REM concentrations should remain unchanged if data passes QA
RETURN
REM Subroutine: calculate RRT's for sample
CLS : PRINT : PRINT : BEEP
FOR I = 1 TO LABEL
DSLRT(I) = FNCONVERT(SLRT(I))
NEXT I
FOR I = 1 TO NAT
8714  DSNRT(I) = FNCONVERT(SNRT(I))
8716  NEIT I
8720  SREFF = DSLRT(4) : REM for DB5 normalize to 2378-tcdd
8730  FOR I = 1 TO LABEL
8735    IF SREFF>0 THEN RRTL(I)= (DSLRT(I)/SREFF) ELSE RRTL(I)=0
8740  NEIT I
8745  FOR I = 1 TO NAT
8750    IF SREFF>0 THEN RRTN(I)= (DSNRT(I)/SREFF) ELSE RRTN(I)=0
8755  NEIT I
8790  RETURN

9000  REM Subroutines: prepare final report for sample; output to printer, screen
9002  REM QA recovery minimums
9004  OREC(2)= 50 : OREC(3)= 50 : OREC(4)= 50 : OREC(5)= 35 : OREC(6)= 35
9006  OREC(7)= 35 : OREC(8)= 35 : OREC(9)= 35 : OREC(10)=35: OREC(11)= 25
9008  OREC(12)= 25
9010  REM Convert REC(i) to % for output
9012  FOR I = 2 TO LABEL
9014    RECC(I) = REC(I):100
9019  NEXT I
9019  REM List of labeled ions used for quant and recovery
9020  LION(1) = 334 : LION(2) = 318 : LION(3) = 328 : LION(4) = 328
9030  LION(5) = 352 : LION(6) = 368 : LION(7) = 386 : LION(8) = 402
9040  LION(9) = 420 : LION(10) = 436 : LION(11) = 456 : LION(12) = 472
9050  REM Theoretical ion ratios to match those calculated from sample
9060  THEORY(1) = .76 : THEORY(2) = .76 : THEORY(3) = .76 : THEORY(4) = .76
9062  THEORY(5) = .76 : THEORY(6) = 1.53 : THEORY(7) = 1.53
9064  THEORY(8) = 1.53 : THEORY(9) = 1.53 : THEORY(10) = 1.53
9066  THEORY(11) = 1.53
9070  FOR I = 12 TO 19
9072    THEORY(I) = 1.23 : NEIT I
9074  THEORY(20) = 1.02 : THEORY(21) = 1.02
9076  REM Translate from n=48 to n=24 retention times for output
9077  M = 0
9078  FOR I = 2 TO NAT STEP 2
9080    NRT(M) = SNRT(I)
9082  NEXT I
9082  NEXT I
9090  PRINT
9100  INPUT "enter mass spec run number: ", MSID$  
9110  INPUT "enter prep chemist I.D. number: ", PCIDS$  
9120  INPUT "enter other I.D.: ", OTHERS$  
9130  CLS : KEY OFF
9140  PRINT ; PRINT ; PRINT
9150  PRINT "Mass Spec Run Number: "; MSID$  
9160  PRINT "Preparation Chemistry I.D. number: "; PCIDS$  
9170  PRINT "Other Sample Identification: "; OTHERS$  
9180  PRINT
9190  FORMS=' ##  ### MI* #1i.#1: ### t## 
9200  PRINT "Labeled Sample minimum QA 
9210  PRINT "Ion RT RRT % Recovery % Recovery 
9220  PRINT "-- ------ ----- ----- --------- --------- 
9230  REM
FOR M = 2 TO LABEL
PRINT USING FORMS; M, LION(M), SLRT(M), RRTL(M), RECC(M), GREC(M)
NEXT M
REM Report quantitation
PRINT : PRINT
FIIS= "重大..."
PRINT* Major pg/gram pg/gram Ratio Ratio
PRINT* N ion RT RRT wet dry Observed Theory
PRINT* -- ----- ----- -------- -------- -------- -------
FOR M = 1 TO CONC
PRINT USING FIIS; M, BION(M), NRT(M), CRRTN(M), C(M), CD(M), RATS(M), THEORY(M)
NEXT M
FOR I = 1 TO 6 : LPRINT : NEXT I
LPRINT * Labeled Sample minimum QA *
LPRINT * N ion RT RRT % Recovery % Recovery *
LPRINT * -- ----- ----- -------- -------- -------- -------
FOR M = 2 TO LABEL
LPRINT USING FORMS; M, LION(M), SLRT(M), RRTL(M), RECC(M), GREC(M)
NEXT M
REM Report for S/N data
FOR I = 1 TO 20 : LPRINT : NEXT I
REM Space output to two sheets
REM Output to printer
PRINT : PRINT
PRINT* If necessary, rearrange your printer paper for DFQUANT'S output. *
INPUT* Strike the ENTER key when ready for output ... ", ANY$";
LPRINT "Mass Spec Run Number: "; MSIDS
LPRINT "Preparation Chemistry I.D. number: "; PCIDS
LPRINT "Other Sample Identification: "; OTHERS
LPRINT LPRINT
LPRINT 'Mass Spec Run Number: '; MSIDS
LPRINT 'Preparation Chemistry I.D. number: '; PCIDS
LPRINT 'Other Sample Identification: '; OTHERS
LPRINT LPRINT
LPRINT 'Major Sample minimum QA *
LPRINT 'N Ion RT RRT X Recovery X Recovery *
LPRINT '-------- ------- -------- ------- -------
FOR M = 2 TO LABEL
LPRINT USING FORMS; M, LION(M), SLRT(M), RRTL(M), RECC(M), QREC(M)
NEXT M
REM Quantitation Report
FOR I = 1 TO 6 : LPRINT : NEXT I
LPRINT* Major pg/gram pg/gram Ratio Ratio *
LPRINT* N ion RT RRT wet dry Observed Theoretical *
LPRINT* -- ----- ----- -------- -------- -------- -------
FOR M = 1 TO CONC
LPRINT USING FIIS; M, BION(M), NRT(M), CRRTN(M), C(M), CD(M), RATS(M), THEORY(M)
NEXT M
REM Report for S/N data
FOR I = 1 TO 20 : LPRINT : NEXT I
REM Space output to two sheets
REM Output to disk file is optional
CLS : PRINT : PRINT
PRINT "Do you desire output to a disk file for your report form?
PRINT
INPUT "Enter 'Y' or 'N': ", DOUT$}
IF DOUT$ = "Y" THEN 9750 ELSE 9995
CLS : PRINT : PRINT
PRINT "Enter the complete name of your output file in quotation marks, including the drive: ", DOUT$
OPEN DOUT$ FOR OUTPUT AS #4
PRINT #4, : PRINT #4,
PRINT #4, "Mass Spec Run Number: "; MSID$
PRINT #4, "Preparation Chemistry I.D. number: "; PCID$
PRINT #4, "Other Sample Identification: "; OTHER$
PRINT #4, "Labeled X Minimum QA"
PRINT #4, "N Ion RT RRT Recovery % Recovery"
FOR M = 2 TO LABEL
PRINT #4, USING FORMS; M, LION(M), SLRT(M), RRTL(M), RECC(M), QREC(M)
NEXT M
REM Report quantitation
PRINT #4, "Major pg/gram pg/gram Ratio Ratio"
PRINT #4, "N ion RT RRT wet dry Observed Theoretical"
FOR M = 1 TO CONC
PRINT #4, USING FIIS; M, BION(M), NRT(M), CRRTN(M), C(M), CD(M), RATS(M), THEORY(M)
NEXT M
REM Report for S/N data
FOR I = 1 TO 25 : PRINT #4, : NEXT I : REM Space hardcopy over two pages
PRINT #4, "Major Peak Positives Not Detectable"
PRINT #4, "N ion RT RRT Height S/N S/N at MDL"
PRINT #4, "-- ----- ----- ------ ------ ------ ------ ------"
FOR M = 1 TO CONC
PRINT #4, USING F25; M, BION(M), NRT(M), CRRTN(M), HS(M), SGNS(M), SNMDL(M), CGA(M)
NEXT M
PRINT #4, : PRINT #4,
CLOSE #4
RETURN

REM Subroutine reserved for future expansion, debugging output
RETURN

REM Subroutine: Output to sequential file to be read into Phil's data base
CLS : PRINT : PRINT
PRINT "Please enter the name of your file for Phil's data base,"
INPUT "in quotes, including the drive designator: ", PHIL$
OPEN PHIL$ FOR OUTPUT AS #5
WRITE #5, MSID$, PCID$, OTHER$
FOR I = 1 TO LABEL
WRITE #5, LION(I), SLRT(I), RRTL(I), RECC(I), QREC(I)
NEXT I
RETURN
11090 FOR I = 1 TO CONC
11100   WRITE #5, BION(I), NRT(I), CRRTN(I), C(I), CD(I), RATS(I), THEORY(I)
11105   WRITE #5, HS(I), SGMS(I), SNMDL(I), COA(I), SGDS(I)
11110 NEXT I
11120 REM User input, should not normally be used in data base
11130 FOR I = 1 TO LABEL
11140   WRITE #5, SLP(I), SLRT(I)
11150 NEXT I
11160 FOR I = 1 TO NAT
11170   WRITE #5, SNP(I), SNRT(I)
11180 NEXT I
11190 WRITE #5, LHB(I), LHS(I), LHG(I)
11200 FOR I = 1 TO CONC
11210   WRITE #5, HB(I), HS(I), H0(I)
11220 NEXT I
11230 CLOSE #5
11500 CLS
11700 RETURN
EXAMPLE OF DFQUANT OUTPUT

Mass Spec Run Number: MAT86800
Preparation Chemistry I.D. number: B071086MH
Other Sample Identification: ADIPOSE-REPLICATE

<table>
<thead>
<tr>
<th>N</th>
<th>Labeled Ion</th>
<th>RT</th>
<th>RRT</th>
<th>% Recovery</th>
<th>% Recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>318</td>
<td>18.05</td>
<td>0.96</td>
<td>74</td>
<td>50</td>
</tr>
<tr>
<td>3</td>
<td>328</td>
<td>18.53</td>
<td>1.00</td>
<td>74</td>
<td>50</td>
</tr>
<tr>
<td>4</td>
<td>328</td>
<td>22.30</td>
<td>1.19</td>
<td>61</td>
<td>35</td>
</tr>
<tr>
<td>5</td>
<td>368</td>
<td>24.04</td>
<td>1.27</td>
<td>82</td>
<td>35</td>
</tr>
<tr>
<td>6</td>
<td>386</td>
<td>27.27</td>
<td>1.45</td>
<td>59</td>
<td>35</td>
</tr>
<tr>
<td>7</td>
<td>402</td>
<td>28.52</td>
<td>1.53</td>
<td>73</td>
<td>35</td>
</tr>
<tr>
<td>8</td>
<td>420</td>
<td>31.57</td>
<td>1.69</td>
<td>55</td>
<td>35</td>
</tr>
<tr>
<td>9</td>
<td>436</td>
<td>33.31</td>
<td>1.77</td>
<td>55</td>
<td>35</td>
</tr>
<tr>
<td>10</td>
<td>456</td>
<td>37.56</td>
<td>2.01</td>
<td>39</td>
<td>25</td>
</tr>
<tr>
<td>11</td>
<td>472</td>
<td>37.54</td>
<td>2.01</td>
<td>39</td>
<td>25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>N</th>
<th>Major Ion</th>
<th>RT</th>
<th>RRT</th>
<th>pg/gram wet</th>
<th>pg/gram dry</th>
<th>Ratio Observed</th>
<th>Ratio Theoretical</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>306</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>0.76</td>
</tr>
<tr>
<td>2</td>
<td>306</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>0.76</td>
</tr>
<tr>
<td>3</td>
<td>306</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>0.76</td>
</tr>
<tr>
<td>4</td>
<td>322</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>0.76</td>
</tr>
<tr>
<td>5</td>
<td>322</td>
<td>18.53</td>
<td>1.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>0.76</td>
</tr>
<tr>
<td>6</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.53</td>
</tr>
<tr>
<td>7</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.53</td>
</tr>
<tr>
<td>8</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.53</td>
</tr>
<tr>
<td>9</td>
<td>340</td>
<td>23.33</td>
<td>1.25</td>
<td>40.3</td>
<td>53.0</td>
<td>1.56</td>
<td>1.53</td>
</tr>
<tr>
<td>10</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.53</td>
</tr>
<tr>
<td>11</td>
<td>356</td>
<td>24.03</td>
<td>1.27</td>
<td>22.8</td>
<td>29.9</td>
<td>1.36</td>
<td>1.53</td>
</tr>
<tr>
<td>12</td>
<td>374</td>
<td>27.28</td>
<td>1.45</td>
<td>96.9</td>
<td>127.5</td>
<td>1.21</td>
<td>1.23</td>
</tr>
<tr>
<td>13</td>
<td>374</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.23</td>
</tr>
<tr>
<td>14</td>
<td>374</td>
<td>27.37</td>
<td>1.46</td>
<td>56.7</td>
<td>74.6</td>
<td>1.22</td>
<td>1.23</td>
</tr>
<tr>
<td>15</td>
<td>374</td>
<td>28.27</td>
<td>1.51</td>
<td>17.7</td>
<td>23.3</td>
<td>1.19</td>
<td>1.23</td>
</tr>
<tr>
<td>16</td>
<td>374</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.23</td>
</tr>
<tr>
<td>17</td>
<td>390</td>
<td>28.52</td>
<td>1.53</td>
<td>0.0</td>
<td>0.0</td>
<td>1.21</td>
<td>1.23</td>
</tr>
<tr>
<td>18</td>
<td>390</td>
<td>28.52</td>
<td>1.53</td>
<td>2173.4</td>
<td>2859.8</td>
<td>1.21</td>
<td>1.23</td>
</tr>
<tr>
<td>19</td>
<td>390</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.23</td>
</tr>
<tr>
<td>20</td>
<td>408</td>
<td>31.57</td>
<td>1.69</td>
<td>422.7</td>
<td>556.1</td>
<td>0.96</td>
<td>1.02</td>
</tr>
<tr>
<td>21</td>
<td>408</td>
<td>0.00</td>
<td>0.00</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.02</td>
</tr>
<tr>
<td>22</td>
<td>424</td>
<td>33.31</td>
<td>1.77</td>
<td>2225.6</td>
<td>2928.5</td>
<td>1.02</td>
<td>1.02</td>
</tr>
<tr>
<td>23</td>
<td>444</td>
<td>37.56</td>
<td>2.01</td>
<td>31.1</td>
<td>40.9</td>
<td>1.55</td>
<td>1.53</td>
</tr>
<tr>
<td>24</td>
<td>460</td>
<td>37.54</td>
<td>2.01</td>
<td>12625.6</td>
<td>16612.6</td>
<td>0.92</td>
<td>0.88</td>
</tr>
<tr>
<td>N</td>
<td>Major Ion</td>
<td>RT</td>
<td>RRT</td>
<td>Peak Height</td>
<td>Positives S/N</td>
<td>Not Detectable S/N at MDL</td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>----------</td>
<td>----</td>
<td>-----</td>
<td>-------------</td>
<td>-------------</td>
<td>--------------------------</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>306</td>
<td>0.00</td>
<td>0.00</td>
<td>8</td>
<td>0.0</td>
<td>1.3</td>
<td>2.1</td>
</tr>
<tr>
<td>2</td>
<td>306</td>
<td>0.00</td>
<td>0.00</td>
<td>8</td>
<td>0.0</td>
<td>1.3</td>
<td>2.1</td>
</tr>
<tr>
<td>3</td>
<td>306</td>
<td>0.00</td>
<td>0.00</td>
<td>8</td>
<td>0.0</td>
<td>1.3</td>
<td>2.1</td>
</tr>
<tr>
<td>4</td>
<td>322</td>
<td>0.00</td>
<td>0.00</td>
<td>4</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>322</td>
<td>18.52</td>
<td>1.00</td>
<td>19</td>
<td>0.0</td>
<td>0.4</td>
<td>6.8</td>
</tr>
<tr>
<td>6</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>2.7</td>
<td>2.4</td>
</tr>
<tr>
<td>7</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>2.7</td>
<td>2.4</td>
</tr>
<tr>
<td>8</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>2.7</td>
<td>2.4</td>
</tr>
<tr>
<td>9</td>
<td>340</td>
<td>23.33</td>
<td>1.25</td>
<td>169</td>
<td>33.8</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>340</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>2.7</td>
<td>2.4</td>
</tr>
<tr>
<td>11</td>
<td>356</td>
<td>24.03</td>
<td>1.27</td>
<td>82</td>
<td>20.5</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>12</td>
<td>374</td>
<td>27.28</td>
<td>1.45</td>
<td>536</td>
<td>107.2</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>13</td>
<td>374</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>4.8</td>
<td>2.7</td>
</tr>
<tr>
<td>14</td>
<td>374</td>
<td>27.37</td>
<td>1.46</td>
<td>254</td>
<td>50.8</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>374</td>
<td>28.27</td>
<td>1.51</td>
<td>93</td>
<td>18.6</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>16</td>
<td>374</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>4.8</td>
<td>2.7</td>
</tr>
<tr>
<td>17</td>
<td>390</td>
<td>28.52</td>
<td>1.53</td>
<td>7486</td>
<td>1497.2</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>18</td>
<td>390</td>
<td>28.52</td>
<td>1.53</td>
<td>7486</td>
<td>1497.2</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>19</td>
<td>390</td>
<td>0.00</td>
<td>0.00</td>
<td>5</td>
<td>0.0</td>
<td>4.1</td>
<td>2.7</td>
</tr>
<tr>
<td>20</td>
<td>408</td>
<td>31.57</td>
<td>1.69</td>
<td>1263</td>
<td>157.9</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>21</td>
<td>408</td>
<td>0.00</td>
<td>0.00</td>
<td>10</td>
<td>0.0</td>
<td>2.1</td>
<td>6.8</td>
</tr>
<tr>
<td>22</td>
<td>424</td>
<td>33.31</td>
<td>1.77</td>
<td>5311</td>
<td>663.9</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>23</td>
<td>444</td>
<td>37.56</td>
<td>2.01</td>
<td>60</td>
<td>10.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>24</td>
<td>460</td>
<td>37.54</td>
<td>2.01</td>
<td>30000</td>
<td>5000.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Program QAD

Murray Hackett

Toxicology Program

Oregon State University

Corvallis, Oregon 97331

'Quick And Dirty' output pending Phil's database

10-3-86

REM

DIM BION(30), C(30), CD(30), CQA(30), LION(12), SLRT(12), RRTL(12), RECC(12), QREC(12)
DIM ALYTES(30), NRT(30), CRRTN(30), RATS(30), THEORY(30), HS(30), SGNS(30)
DIM SNMDL(30), S6DS(30)

ALYTE$(1) = "2378-TCDF" : ALYTE$(2) = "2378-TCDF" : ALYTE$(3) = "3467-TCDF"
ALYTE$(4) = "1234-TCDD" : ALYTE$(5) = "2378-TCDD" : ALYTE$(6) = "13467-PCDF"
ALYTE$(7) = "12378-PCDF" : ALYTE$(8) = "23478-PCDF" : ALYTE$(9) = "123467-PCDF"
ALYTE$(10) = "123789-PCDF" : ALYTE$(11) = "123467-HxCDF" : ALYTE$(12) = "123478-HxCDF"
ALYTE$(13) = "123467-HxCDD" : ALYTE$(14) = "1234678-HxCDF" : ALYTE$(15) = "1234678-HxCDD"
ALYTE$(16) = "1234678-HxCDF" : ALYTE$(17) = "1234678-HxCDD" : ALYTE$(18) = "123478-HxCDD"
ALYTE$(19) = "1234678-HpCDF" : ALYTE$(20) = "1234678-HpCDD" : ALYTE$(21) = "1234678-HxCDF"
ALYTE$(22) = "1234678-HxCDD" : ALYTE$(23) = "0CDF" : ALYTE$(24) = "OCDF"

CLS : PRINT : PRINT

PRINT "Welcome to the program QAD" : PRINT : PRINT

PRINT "Enter your database file number in quotes, including:

INPUT "your drive designator: ", DRIVE$

CLS : PRINT : PRINT

PRINT "Enter the results from any previous 2378-TCDD analysis"
INPUT "in units of ppt, wet weight, or nd, P2NA, etc.: ", OLDS

GOSUB 10
GOSUB 100

PRINT : PRINT "The program is finished with your data" END

10 REM Subroutine: data file input
OPEN DRIVE$ FOR INPUT AS #1
INPUT #1, MSID$, PCID$, OTHER$

20 FOR I = 1 TO 12
    INPUT #1, LION(I), SLRT(I), RRTL(I), RECC(I), QREC(I)
30 NEXT I

40 FOR I = 1 TO 24
    INPUT #1, BION(I), WRT(I), CRRTN(I), C(I), CD(I), RATS(I), THEORY(I)
    INPUT #1, HS(I), SGNS(I), SNMDL(I), CQA(I), S6DS(I)
REM Subroutine: output

LPRINT : LPRINT
LPRINT*SCC NUMBER: "; OTHER$
LPRINT*SAMPLE PREP: "; PCID$
LPRINT*MASS SPEC I.D.: "; MSID$
LPRINT
LPRINT*PREVIOUS TCDD ANALYSIS: "; OLD$
LPRINT
LPRINT*Isomers pg/gram wet MDL *
FORMS="\ 
\ 8888888.0 88888.0 *
LPRINT*--------- ---------- ---- *

FOR I = 1 TO 24
  LPRINT USING FORMS; ALYTE(I), C(I), CQA(I)
NEXT I

FOR I = 1 TO 32
  LPRINT
NEXT I

RETURN
<table>
<thead>
<tr>
<th>Isomers</th>
<th>pg/gram wet</th>
<th>MDL</th>
</tr>
</thead>
<tbody>
<tr>
<td>2378-TCDF</td>
<td>0.0</td>
<td>2.1</td>
</tr>
<tr>
<td>2367-TCDF</td>
<td>0.0</td>
<td>2.1</td>
</tr>
<tr>
<td>3467-TCDF</td>
<td>0.0</td>
<td>2.1</td>
</tr>
<tr>
<td>1234-TCDD</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2378-TCDD</td>
<td>0.0</td>
<td>6.8</td>
</tr>
<tr>
<td>13467-PCDF</td>
<td>0.0</td>
<td>2.4</td>
</tr>
<tr>
<td>12378-PCDF</td>
<td>0.0</td>
<td>2.4</td>
</tr>
<tr>
<td>12367-PCDF</td>
<td>0.0</td>
<td>2.4</td>
</tr>
<tr>
<td>23478-PCDF</td>
<td>40.3</td>
<td>0.0</td>
</tr>
<tr>
<td>23467-PCDF</td>
<td>0.0</td>
<td>2.4</td>
</tr>
<tr>
<td>12378-PCDD</td>
<td>22.8</td>
<td>0.0</td>
</tr>
<tr>
<td>123478-HxCDF</td>
<td>96.9</td>
<td>0.0</td>
</tr>
<tr>
<td>123467-HxCDF</td>
<td>0.0</td>
<td>2.7</td>
</tr>
<tr>
<td>123678-HxCDF</td>
<td>56.7</td>
<td>0.0</td>
</tr>
<tr>
<td>234678-HxCDF</td>
<td>17.7</td>
<td>0.0</td>
</tr>
<tr>
<td>123789-HxCDF</td>
<td>0.0</td>
<td>2.7</td>
</tr>
<tr>
<td>123478-HxCDD</td>
<td>0.0</td>
<td>2.7</td>
</tr>
<tr>
<td>123678-HxCDD</td>
<td>2173.4</td>
<td>0.0</td>
</tr>
<tr>
<td>123789-HxCDD</td>
<td>0.0</td>
<td>2.7</td>
</tr>
<tr>
<td>1234678-HpCDF</td>
<td>422.7</td>
<td>0.0</td>
</tr>
<tr>
<td>1234789-HpCDF</td>
<td>0.0</td>
<td>6.8</td>
</tr>
<tr>
<td>1234678-HpCDD</td>
<td>2225.6</td>
<td>0.0</td>
</tr>
<tr>
<td>OCDF</td>
<td>31.1</td>
<td>0.0</td>
</tr>
<tr>
<td>OCDD</td>
<td>12625.6</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Example of program output for QAD