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

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Polychlorinated dibenzo-p-dioxins (PCDD's) and dibenzofurans (PCDF's) are environmental pollutants associated 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

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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) $$C_n = \frac{A_n\ C_l}{A_l\ \ RRF}$$

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 labled ion
RRF = Rn/Rl, relative response
R = absolute response of ion, ADC counts/pg

2) $$\%REC = \frac{C_{l\ measured}\ (100)}{C_{l\ spiked}}$$

Where: $$C_{l\ measured} = \frac{A_l\ C_{334}}{A_{334}\ \ RF}$$
C_{334} = concentration of I.S. B
A_{334} = area of I.S. B
$RF = R_l/R_{334}$

The internal standard method used was superior to methods based on external calibration curves in that losses occuring 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 Missisippi 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 chhlorophenates (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.

V. CONTROL SITE, BEAVERCREEK, OREGON

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 1 Descriptions of Tissue Samples

OSU no.	% lipid	Description, including date collected
1	NR‡	adipose, stillborn foal, Arabian horse farm 3-29-85
3	NA	whole blood, stillborn foal, Arabians horse farm, 3-29-85
4	NR‡	liver, stillborn foal, Arabian horse farm, 3-29-85
5	NR‡	placenta, stillborn foal, Arabian horse farm, 3-29-85
6	NR‡	spleen, stillborn foal, Arabian horse farm, 3-29-85
7	NR‡	thymus, stillborn foal, Arabian horse farm, 3-29-85
9	NR‡	liver, "Caraa" (Arabian mare), Arabian horse farm, collected at necropsy, OSU Vet. Med., 5-23-83
420	NR	heart(composite of muscle/adipose), bull, farm near sawmill site 2, 5-13-85
421	NR	liver, bull, 5-13-85
422	NR	muscle, bull, 5-13-85
501	3	liver, "grey mare control", received from Dr. Hultgren OSU Vet. Med., 9-10-86
502	88	adipose, "grey mare control", received from Dr. Hultgren OSU Vet. Med., 9-10-86
504	2	liver, "13 yr old mare control", received from Dr. Hultgren OSU Vet. Med., 9-10-86
505	91	adipose, "13 yr old mare control", received from Dr. Hultgren, OSU Vet. Med., 9-10-86
506	77	adipose, "Coyns Fortune"(stallion), Arabian horse farm, collected at necropsy, OSU Vet. Med., October 1985
508	9	brain, "Coyns Fortune", collected at necropsy, OSU Vet. Med., October 1985
509	4	liver, "Coyns Fortune", collected at necropsy, OSU Vet. Med., October 1985
510	5	kidney, "Coyns Fortune", collected at necropsy, OSU Vet. Med., October 1985

NR‡ not recorded due to insufficient sample, sample lost or damaged
NA not applicable

Table 2

Descriptions of Soil/Sediment/Other Samples

OSU no.	% Moisture	Description
EH#1	58	Eagle Harbor, WA sediment, received from EPA Region 10, April 1985
EH#2	67	Eagle Harbor, WA sediment, received from EPA Region 10, April 1985
EH05-6	54	Eagle Harbor, WA sediment, received from EPA Newport, OR Environmental Res. Lab., 8-28-85
EH2	37	Eagle Harbor, WA sediment, received from EPA Newport, OR Environmental Res. Lab., dated 8-9-85, received 9-24-85
Reichold	NA	crystalline technical grade pentachlorophenol "4-9-162", gift from Reichold Chemical Co., Tacoma WA
Aldrich	NA	crystalline technical grade pentachlorophenol, lot no. CC022487, gift of Dr. Nancy Kerkvliet, OSU Vet. Med. School
11	NA	diptank sludge from mill, Site 2, collected by DEQ in 1984
12	44	soil collected from drainage ditch between road and lumber yard, see Figure 2, 2-12-85, Site 2
33	NA	wood chips, from "Caraa's" stall, Columbia Labs no. 8604, Arabian horse farm, 6-84
53	19	surface soil collected from underneath easternmost stall in barn, Arabian horse farm, 5-10-85
55	56	surface soil collected from drainage ditch between Road and lumber yard, see Figure 2, 5-10-85, Site 2
80	25	surface soil collected from drainage ditch between Road and lumber yard, see Figure 2, 5-10-85, Site 2
92	28	surface soil collected from drainage ditch between Road and and lumber yard, see Figure 2, 5-10-85, Site 2

(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, 2ft 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, 6-13-85, 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, "G4 core top", received from OSU 8-28-85
405	35	Beaver Creek control sample, "G4 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

NR‡ 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

n	isomer	sample, units are microgram/gram of t-PCP (Reichold*)	(Aldrich**)
1	2378-TCDF	nd(0.10)	nd(0.10)
2	2367-TCDF	nd(0.07)	nd(0.15)
3	3467-TCDF	nd(0.07)	nd(0.15)
4	1234-TCDD	NR	NR
5	2378-TCDD	nd(0.05)	nd(0.08)
6	13467-PCDF	nd(0.01)	nd(0.14)
7	12378-PCDF	1.10	1.61
8	12367-PCDF	nd(0.07)	nd(0.14)
9	23478-PCDF	0.30	0.48
10	23467-PCDF	0.47	0.63
11	12378-PCDD	nd(0.11)	nd(0.15)
12	123478-HxCDF	1.43	nd(0.80)
13	123467-HxCDF	nd(0.04)	nd(0.04)
14	123678-HxCDF	0.55	nd(0.51)
15	234678-HxCDF	0.32	0.62
16	123789-HxCDF	0.62	0.19
17	123478-HxCDD	nd(0.07)	nd(0.10)
18	123678-HxCDD	8.30	12.68
19	123789-HxCDD	0.51	0.22
20	1234678-HpCDF	8.92	39.50
21	1234789-HpCDF	nd(0.67)	0.47
22	1234678-HpCDD	83.1	157
23	OCDF	4.97	210
24	OCDD	1500	1100

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. CC022487, 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

Congener Group	sample, units are microgram/gram of t-PCP (Reichold)	(Aldrich)	(from reference (14))
TCDF‡‡‡	nd(0.10)	5.42	NR
PCDF	6.05	3.20	nd(2.0)
HxCDF	18.0	52.5	57
HpCDF	24.3	158	130
OCDF	4.97	210	90
TCDD‡‡‡	nd(0.06)	nd(0.083)	NR
PCDD	nd(0.11)	nd(0.15)	nd(1.0)
HxCDD	21.0	29.2	15.0
HpCDD	138	221	410
OCDD	1500	1100	1500

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

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

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

	Sample, units are pg/gram dryweight			
Congener Group	(EH#1‡)	(EH#2‡)	(EH-05-6)	(EH2‡‡)
TCDF‡‡‡	nd(2)	nd(3)	nd(2)	10
PCDF	nd(6)	nd(64)	nd(8)	35
HxCDF	207	750	56	60
HpCDF	980	1980	910	175
OCDF	980	1440	350	250
TCDD‡‡‡	nd(8)	nd(12)	nd(4)	nd(2)
PCDD	nd(6)	nd(75)	nd(4)	12
HxCDD	67	660	17	45
HpCDD	4400	7200	1800	1100
OCDD	37000	42000	6050	4500

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‡

n	isomer	Sample, units are pg/gram dry weight (12)#	(55)	(202)	(207)	(208)
1	2378-TCDF	nd(51)	nd(32)	nd(23)	nd(0.5)	nd(0.4)
2	2367-TCDF	nd(1.6)	2.0	nd(1.6)	nd(0.5)	nd(0.4)
3	3467-TCDF	nd(1.6)	nd(2.3)	nd(0.2)	nd(0.5)	nd(0.4)
4	1234-TCDD	NR	NR	NR	NR	NR
5	2378-TCDD	nd(12)	nd(11)	nd(11)	nd(1.1)	nd(0.6)
6	13467-PCDF	nd(1.2)	nd(0.2)	nd(0.2)	nd(0.6)	nd(0.5)
7	12378-PCDF	123	73	21	nd(0.6)	nd(1.2)
8	12367-PCDF	nd(50)	nd(0.2)	nd(0.2)	nd(0.6)	nd(0.5)
9	23478-PCDF	163	40	23	nd(0.6)	nd(1.7)
10	23467-PCDF	nd(1.2)	58	28	nd(6.5)	nd(2.4)
11	12378-PCDD	nd(151)	56	90	nd(1.6)	nd(4.0)
12	123478-HxCDF	116	49	nd(0.3)	nd(1.2)	nd(2.1)
13	123467-HxCDF	nd(0.9)	nd(0.3)	nd(0.3)	nd(1.2)	nd(2.1)
14	123678-HxCDF	157	122	29	nd(1.2)	nd(2.1)
15	234678-HxCDF	126	45	3.8	nd(1.2)	nd(2.1)
16	123789-HxCDF	nd(0.9)	nd(5.9)	nd(1.5)	nd(1.2)	nd(2.1)
17	123478-HxCDD	nd(2.1)	nd(1.3)	nd(200)	nd(4.9)	nd(6.5)
18	123678-HxCDD	3250	1400	531	8.1	17
19	123789-HxCDD	678	461	197	nd(3.0)	nd(6.5)
20	1234678-HpCDF	1810	731	437	nd(237)	NR
21	1234789-HpCDF	2580	22	11	nd(32)	NR
22	1234678-HpCDD	20600	5190	4940	479	NR
23	OCDF	569	324	131	50	NR
24	OCDD	68100	20200	19200	7650	NR

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 7, continued)

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

n	isomer	Sample, units are pg/gram dry weight (92)‡‡	(209)	(211)	(214)	(217)	(220)
1	2378-TCDF	nd(50)	nd(2.0)	nd(5.1)	nd(8.0)	nd(0.5)	nd(0.6)
2	2367-TCDF	nd(4.8)	nd(0.4)	nd(1.0)	nd(1.2)	nd(0.5)	nd(0.4)
3	3467-TCDF	nd(2.6)	nd(0.4)	nd(2.0)	nd(0.9)	nd(0.5)	nd(0.5)
4	1234-TCDD	NR	NR	NR	NR	NR	NR
5	2378-TCDD	nd(0.5)	nd(0.6)	nd(2.4)	nd(4.9)	nd(1.1)	nd(0.7)
6	13467-PCDF	nd(1.0)	nd(0.4)	nd(0.9)	nd(0.7)	nd(0.3)	nd(0.2)
7	12378-PCDF	nd(68)	nd(2.1)	nd(5.7)	nd(13)	nd(0.6)	nd(0.7)
8	12367-PCDF	nd(1.0)	nd(0.4)	nd(0.9)	nd(0.7)	nd(0.3)	nd(0.2)
9	23478-PCDF	42	1.3	nd(10)	11	nd(0.3)	nd(0.9)
10	23467-PCDF	61	2.8	nd(13)	16	nd(0.3)	nd(1.3)
11	12378-PCDD	110	nd(4.2)	nd(9.6)	22	nd(1.1)	nd(1.6)
12	123478-HxCDF	47	2.5	nd(6.0)	18	nd(1.0)	nd(1.8)
13	123467-HxCDF	nd(1.6)	nd(0.7)	nd(1.3)	nd(0.9)	nd(0.5)	nd(0.3)
14	123678-HxCDF	74	2.6	nd(2.0)	nd(1.3)	nd(0.5)	nd(1.3)
15	234678-HxCDF	61	2.7	5.0	15	nd(0.5)	nd(0.8)
16	123789-HxCDF	20	nd(3.0)	nd(3.3)	5.8	nd(0.5)	nd(0.3)
17	123478-HxCDD	nd(9.2)	nd(6.6)	nd(5.9)	nd(49)	nd(3.7)	nd(4.1)
18	123678-HxCDD	1090	34	57	233	nd(25)	6.1
19	123789-HxCDD	253	5.7	8.9	52	nd(3.1)	nd(2.7)
20	1234678-HpCDF	803	87	163	207	98	21
21	1234789-HpCDF	17	nd(5.2)	nd(10)	nd(7.2)	nd(27)	nd(4.2)
22	1234678-HpCDD	8770	548	860	2560	716	136
23	OCDF	253	55	83	66	NR‡	NR‡
24	OCDD	29900	6240	5500	13400	NR‡	NR‡

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

(Table 7, continued)

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

n	isomer	Sample, units are pg/gram dry weight (218)	(219)	(221)	(222)	(223)	(80)**
1	2378-TCDF	50	nd(1.5)	nd(12.5)	120	nd(0.7)	20
2	2367-TCDF	1.5	nd(0.7)	nd(1.2)	16	nd(0.7)	nd(6.9)
3	3467-TCDF	1.2	nd(0.7)	0.5	17	nd(1.1)	nd(3.7)
4	1234-TCDD	NR	NR	NR	NR	NR	NR
5	2378-TCDD	3.0	nd(1.7)	nd(0.5)	2.0	nd(1.5)	0.5
6	13467-PCDF	nd(2.0)	nd(1.2)	nd(0.3)	nd(1.8)	nd(1.2)	nd(1.6)
7	12378-PCDF	159	nd(1.2)	nd(26)	252	nd(1.2)	37
8	12367-PCDF	nd(2.0)	nd(1.2)	nd(0.3)	nd(1.8)	nd(1.2)	nd(1.6)
9	23478-PCDF	179	nd(1.2)	11	127	nd(1.2)	37
10	23467-PCDF	308	nd(1.2)	17	524	nd(1.2)	53
11	12378-PCDD	441	nd(3.5)	27	250	nd(4.9)	152
12	123478-HxCDF	223	nd(1.9)	15	293	nd(1.6)	33
13	123467-HxCDF	nd(3.1)	nd(1.9)	nd(0.6)	nd(2.9)	nd(1.6)	nd(2.4
14	123678-HxCDF	314	nd(1.9)	24	315	nd(1.6)	78
15	234678-HxCDF	323	nd(1.9)	17	320	nd(1.6)	53
16	123789-HxCDF	115	nd(1.9)	nd(12)	143	nd(1.6)	12
17	123478-HxCDD	nd(546)	nd(4.2)	nd(2.9)	612	nd(6.1)	76
18	123678-HxCDD	4800	nd(21)	284	5100	nd(23)	830
19	123789-HxCDD	1140	nd(4.2)	54	908	nd(12)	326
20	1234678-HpCDF	3690	10	348	7170	22	844
21	1234789-HpCDF	57	nd(4.1)	nd(3.6)	221	nd(3.4)	20
22	1234678-HpCDD	46100	70	3180	77000	159	9440
23	OCDF	893	nd(11)	nd(142)	2000	nd(30)	296
24	OCDD	218000	600	13400	650000#	1200	51800

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

(Table 7, continued)

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

n	isomer	Sample, units are pg/gram dry weight (203)	(204)	(205)	(210)
1	2378-TCDF	nd(1.0)	5.5	28	nd(0.8)
2	2367-TCDF	nd(0.2)	2.3	nd(3.6)	nd(0.2)
3	3467-TCDF	nd(0.2)	nd(0.9)	nd(2.4)	nd(0.5)
4	1234-TCDD	NR	NR	NR	NR
5	2378-TCDD	nd(0.5)	3.0	7.2	nd(2.4)
6	13467-PCDF	nd(0.2)	nd(4.0)	nd(5.0)	nd(0.7)
7	12378-PCDF	nd(0.5)	nd(13)	57	nd(0.7)
8	12367-PCDF	nd(0.2)	nd(0.2)	nd(5.0)	nd(0.7)
9	23478-PCDF	nd(0.3)	10	74	nd(0.7)
10	23467-PCDF	nd(0.2)	22	105	1.1
11	12378-PCDD	nd(2.0)	25	120	nd(1.8)
12	123478-HxCDF	1.3	15	92	nd(2.2)
13	123467-HxCDF	nd(0.2)	nd(0.3)	65	nd(0.4)
14	123678-HxCDF	nd(2.3)	19	92	3.0
15	234678-HxCDF	0.9	16	86	1.8
16	123789-HxCDF	nd(0.4)	4.9	40	nd(0.8)
17	123478-HxCDD	nd(0.9)	nd(1.3)	100	nd(1.0)
18	123678-HxCDD	10	250	2340	28
19	123789-HxCDD	4.3	72	371	nd(8.0)
20	1234678-HpCDF	25	300	1500	36
21	1234789-HpCDF	nd(0.9)	10	43	nd(1.4)
22	1234678-HpCDD	183	1900	7000	437
23	OCDF	32	232	649	32
24	OCDD	5820	14000	72000*	2500

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

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

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

n	isomer	Sample, units are dimensionless* (11)
1	2378-TCDF	0.51
2	2367-TCDF	0.087
3	3467-TCDF	nd(0.0010)
4	1234-TCDD	NR
5	2378-TCDD	0.0033
6	13467-PCDF	NR
7	12378-PCDF	0.20
8	12367-PCDF	nd(0.0050)
9	23478-PCDF	0.28
10	23467-PCDF	0.080
11	12378-PCDD	0.22
12	123478-HxCDF	nd(0.008)
13	123467-HxCDF	nd(0.008)
14	123678-HxCDF	nd(0.008)
15	234678-HxCDF	11
16	123789-HxCDF	1.3
17	123478-HxCDD	nd(0.01)
18	123678-HxCDD	19
19	123789-HxCDD	3.2
20	1234678-HpCDF	3.9
21	1234789-HpCDF	2.5
22	1234678-HpCDD	770
23	OCDF	100
24	OCDD	10000

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

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

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

n	isomer	sample, units are pg/gram dry weight (401)	(402)	(402)	(403)	(404)	(405)
1	2378-TCDF	nd(0.8)	nd(0.8)	nd(12)	nd(1.5)	nd(0.7)	nd(2.3
2	2367-TCDF	nd(0.6)	nd(0.8)	nd(1.4)	nd(0.9)	0.4	0.7
3	3467-TCDF	nd(0.3)	nd(0.8)	nd(0.3)	nd(0.6)	nd(0.2)	nd(0.9)
4	1234-TCDD	NR	NR	NR	NR	NR	NR
5	2378-TCDD	nd(0.3)	nd(0.5)	nd(0.5)	nd(0.5)	nd(1.6)	nd(0.7)
6	13467-PCDF	nd(0.2)	nd(0.3)	nd(0.3)	nd(0.2)	nd(0.2)	nd(0.3)
7	12378-PCDF	nd(0.5)	nd(1.3)	0.9	nd(1.1)	nd(1.5)	nd(0.7)
8	12367-PCDF	nd(0.2)	nd(0.3)	nd(0.3)	nd(0.2)	nd(0.2)	nd(0.3)
9	23478-PCDF	nd(1.4)	nd(2.0)	nd(0.3)	nd(1.9)	nd(1.2)	nd(1.3)
10	23467-PCDF	nd(0.9)	1.6	nd(6.2)	nd(2.8)	nd(1.3)	nd(0.7)
11	12378-PCDD	nd(1.1)	nd(3.3)	nd(1.5)	nd(1.2)	0.8	nd(1.6)
12	123478-HxCDF	nd(1.9)	2.7	3.6	nd(0.3)	nd(0.4)	nd(0.7)
13	123467-HxCDF	nd(0.4)	nd(0.6)	nd(0.4)	nd(4.1)	1.6	nd(0.7)
14	123678-HxCDF	nd(0.6)	nd(2.9)	2.6	nd(2.3)	nd(3.6)	nd(0.5)
15	234678-HxCDF	nd(0.6)	nd(3.2)	nd(3.7)	nd(1.4)	3.5	nd(0.5)
16	123789-HxCDF	nd(0.4)	nd(2.9)	nd(2.3)	nd(1.5)	nd(2.4)	nd(0.5)
17	123478-HxCDD	nd(1.4)	1.3	1.7	nd(0.4)	nd(2.1)	nd(1.4)
18	123678-HxCDD	nd(4.7)	10	14	4.3	18	nd(7.6)
19	123789-HxCDD	nd(1.8)	4.2	6.5	2.4	nd(9.2)	nd(1.4)
20	1234678-HpCDF	3.6	32	49	15	64	nd(9.5)
21	1234789-HpCDF	nd(1.2)	1.2	nd(5.0)	nd(0.4)	nd(3.1)	nd(1.0)
22	1234678-HpCDD	19	151	218	62	683	nd(46)
23	OCDF	nd(18)	71	66	32	54	nd(16)
24	OCDD	296	1290	1630	536	18000	595

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

* samples recieved 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 ‡

n	isomer	sample, units are pg/gram wet weight of homogenized tissue (501)	(502)	(502)	(504)	(505)
1	2378-TCDF	nd(0.4)	nd(1.3)	nd(0.5)	nd(0.2)	nd(0.6)
2	2367-TCDF	nd(0.4)	nd(1.3)	nd(0.5)	nd(0.2)	nd(0.6)
3	3467-TCDF	nd(0.4)	nd(1.3)	nd(0.5)	nd(0.2)	nd(0.6)
4	1234-TCDD	NR	NR	NR	NR	NR
5	2378-TCDD	nd(1.0)	nd(1.3)	nd(1.1)	nd(1.1)	nd(1.6)
6	13467-PCDF	nd(0.7)	nd(0.7)	nd(1.6)	nd(0.4)	nd(1.3)
7	12378-PCDF	nd(0.7)	nd(0.7)	nd(1.6)	nd(0.4)	nd(1.3)
8	12367-PCDF	nd(0.7)	nd(0.7)	nd(1.6)	nd(0.4)	nd(1.3)
9	23478-PCDF	nd(0.7)	nd(0.7)	nd(1.6)	nd(0.4)	nd(1.3)
10	23467-PCDF	nd(0.7)	nd(0.7)	nd(1.6)	nd(0.4)	nd(1.3)
11	12378-PCDD	nd(2.6)	nd(6.1)	nd(5.8)	nd(1.8)	nd(5.5)
12	123478-HxCDF	nd(2.2)	nd(2.3)	nd(6.1)	nd(1.7)	nd(2.4)
13	123467-HxCDF	nd(2.2)	nd(2.3)	nd(6.1)	nd(1.7)	nd(2.4)
14	123678-HxCDF	nd(2.2)	nd(2.3)	nd(6.1)	nd(1.7)	nd(2.4)
15	234678-HxCDF	nd(2.2)	nd(2.3)	nd(6.1)	nd(1.7)	nd(2.4)
16	123789-HxCDF	nd(2.2)	nd(2.3)	nd(6.1)	nd(1.7)	nd(2.4)
17	123478-HxCDD	nd(7.5)	nd(5.1)	nd(3.9)	nd(4.6)	nd(4.6)
18	123678-HxCDD	nd(7.5)	33	42	nd(4.6)	nd(38)
19	123789-HxCDD	nd(7.5)	nd(5.1)	nd(3.9)	nd(4.6)	nd(4.6)
20	1234678-HpCDF	nd(2.2)	24	24	3.6	6.2
21	1234789-HpCDF	nd(2.2)	nd(4.3)	nd(4.4)	nd(1.2)	nd(2.0)
22	1234678-HpCDD	50	243	228	32	67
23	OCDF	nd(4.1)	nd(8.4)	nd(10)	nd(3.4)	nd(4.9)
24	OCDD	140	1890	604	211	152

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 11

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Tissues Collected From "Coyns Fortune", Arabian horse farm‡

n	isomer	Sample, units are pg/gram wet weight of homogenized tissue (506)	(506)	(508)	(509)	(510)
1	2378-TCDF	nd(2.1)	nd(1.0)	nd(0.4)	nd(1.0)	nd(0.4)
2	2367-TCDF	nd(2.1)	nd(1.0)	nd(0.4)	nd(1.0)	nd(0.4)
3	3467-TCDF	nd(2.1)	nd(1.0)	nd(0.4)	nd(1.0)	nd(0.4)
4	1234-TCDD	NR	NR	NR	NR	NR
5	2378-TCDD	nd(6.8)	nd(4.2)	nd(1.7)	nd(1.4)	nd(1.1)
6	13467-PCDF	nd(2.4)	nd(2.6)	nd(0.7)	nd(2.6)	nd(1.5)
7	12378-PCDF	nd(2.4)	nd(2.6)	nd(0.7)	nd(2.6)	nd(1.5)
8	12367-PCDF	nd(2.4)	nd(2.6)	nd(0.7)	nd(2.6)	nd(1.5)
9	23478-PCDF	40	34	nd(0.7)	58	nd(1.5)
10	23467-PCDF	nd(2.4)	nd(2.6)	nd(0.7)	nd(2.6)	nd(1.5)
11	12378-PCDD	23	24	nd(2.1)	nd(44)	nd(2.3)
12	123478-HxCDF	97	101	nd(2.5)	117	nd(7.1)
13	123467-HxCDF	nd(2.7)	nd(3.3)	nd(2.5)	nd(3.7)	nd(7.1)
14	123678-HxCDF	57	59	nd(2.5)	84	nd(7.1)
15	234678-HxCDF	18	17	nd(2.5)	99	nd(7.1)
16	123789-HxCDF	nd(2.7)	nd(3.3)	nd(2.5)	nd(3.7)	nd(7.1)
17	123478-HxCDD	nd(2.7)	nd(4.3)	nd(7.1)	nd(3.8)	nd(2.8)
18	123678-HxCDD	2173	2426	nd(7.1)	1516	38
19	123789-HxCDD	nd(2.7)	nd(4.3)	nd(7.1)	nd(3.8)	nd(2.8)
20	1234678-HpCDF	422	502	nd(6.1)	805	8
21	1234789-HpCDF	nd(6.8)	nd(12)	nd(6.1)	nd(10)	nd(1.4)
22	1234678-HpCDD	2230	2370	nd(12)	3570	29
23	OCDF	31	36	nd(4.7)	33	nd(7.6)
24	OCDD	12600	12800	nd(68)	15000	161

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*

n	isomer	sample, units are nanogram/gram of wood chips, wet weight as received (33)
1	2378-TCDF	nd(0.007)
2	2367-TCDF	0.066
3	3467-TCDF	nd(0.007)
4	1234-TCDD	NR
5	2378-TCDD	nd(0.019)
6	13467-PCDF	nd(0.008)
7	12378-PCDF	1.450
8	12367-PCDF	nd(0.008)
9	23478-PCDF	1.000
10	23467-PCDF	1.600
11	12378-PCDD	21.80
12	123478-HxCDF	4.020
13	123467-HxCDF	nd(0.020)
14	123678-HxCDF	2.780
15	234678-HxCDF	2.330
16	123789-HxCDF	nd(0.023)
17	123478-HxCDD	nd(0.021)
18	123678-HxCDD	30.90
19	123789-HxCDD	3.530
20	1234678-HpCDF	43.90
21	1234789-HpCDF	2.550
22	1234678-HpCDD	1170
23	OCDF	714
24	OCDD	28000

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 ‡‡

n	isomer	sample, units are pg/gram wet weight of tissue (3)	(4)	(420)
1	2378-TCDF	nd(0.2)	nd(0.5)	nd(0.4)
2	2367-TCDF	nd(0.2)	nd(0.5)	nd(0.4)
3	3467-TCDF	nd(0.2)	nd(0.5)	nd(0.4)
4	1234-TCDD	NR	NR	NR
5	2378-TCDD	nd(0.2)	nd(0.6)	nd(0.5)
6	13467-PCDF	nd(0.2)	nd(1.4)	nd(0.4)
7	12378-PCDF	nd(0.2)	nd(1.4)	nd(0.4)
8	12367-PCDF	nd(0.2)	nd(1.4)	nd(0.4)
9	23478-PCDF	nd(0.2)	nd(1.4)	1.8
10	23467-PCDF	nd(0.2)	nd(1.4)	nd(0.4)
11	12378-PCDD	nd(0.6)	nd(6.2)	nd(13)
12	123478-HxCDF	nd(0.8)	nd(1.8)	2.0
13	123467-HxCDF	nd(0.8)	nd(1.8)	nd(0.6)
14	123678-HxCDF	nd(0.8)	nd(1.8)	1.1
15	234678-HxCDF	nd(0.8)	nd(1.8)	nd(0.6)
16	123789-HxCDF	nd(0.8)	nd(1.8)	nd(0.6)
17	123478-HxCDD	nd(1.5)	nd(3.3)	nd(0.9)
18	123678-HxCDD	nd(1.5)	18	15
19	123789-HxCDD	nd(1.5)	nd(3.3)	nd(0.9)
20	1234678-HpCDF	nd(1.1)	nd(12.6)	nd(6.7)
21	1234789-HpCDF	nd(1.1)	nd(2.2)	nd(0.8)
22	1234678-HpCDD	3.4	24	21
23	OCDF	2.8	nd(5.1)	nd(1.3)
24	OCDD	19	180	50

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 14

Summary Table of Results, Biosignificant Isomers of PCDD, PCDF found in Soil Collected From Arabian horse farm*

n	isomer	Sample, units are pg/gram dry weight (53)
1	2378-TCDF	nd(0.4)
2	2367-TCDF	nd(0.4)
3	3467-TCDF	nd(0.2)
4	1234-TCDD	NR
5	2378-TCDD	nd(0.4)
6	13467-PCDF	nd(0.3)
7	12378-PCDF	nd(0.4)
8	12367-PCDF	nd(0.3)
9	23478-PCDF	nd(0.8)
10	23467-PCDF	nd(0.7)
11	12378-PCDD	nd(0.6)
12	123478-HxCDF	nd(1.0)
13	123467-HxCDF	nd(0.4)
14	123678-HxCDF	nd(0.8)
15	234678-HxCDF	nd(0.6)
16	123789-HxCDF	nd(0.6)
17	123478-HxCDD	nd(0.7)
18	123678-HxCDD	4.4
19	123789-HxCDD	nd(0.7)
20	1234678-HpCDF	6.0
21	1234789-HpCDF	nd(1.1)
22	1234678-HpCDD	46
23	OCDF	nd(27)
24	OCDD	309

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 farm*

Congener Group	sample, units are pg/gram wet weight (1)	(4)	(5)	(7)	(6)
TCDF***	nd(0.5)	nd(6.0)	nd(1.0)	nd(2.0)	nd(2.0
PCDF	nd(2.0)	nd(0.5)	nd(2.0)	nd(1.0)	nd(3.0)
HxCDF	nd(10)	nd(10)	nd(4.0)	nd(100)	nd(17)
HpCDF	NR	NR	NR	NR	NR
OCDF	NR	NR	NR	NR	NR
TCDD***	nd(0.5)	nd(7.0)	nd(1.0)	nd(1.0)	nd(9.0)
PCDD	nd(54)	nd(13)	nd(7.0)	nd(3.0)	nd(3.0)
HxCDD	110	20	nd(12)	50	110
HpCDD	110	20	48	62	280
OCDD	360	150	490	230	3000

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‡‡

Congener Group	sample, units are pg/gram wet weight (9)	(421)	(422)
TCDF‡‡‡	nd(3.6)	nd(3.0)	nd(3.9)
PCDF	nd(3.0)	nd(3.0)	nd(3.0)
HxCDF	nd(50)	nd(15)	nd(93)
HpCDF	200	nd(40)	nd(40)
OCDF	NR	NR	NR
TCDD‡‡‡	nd(18)	nd(30)	nd(5)
PCDD	nd(2.0)	nd(17)	nd(18)
HxCDD	2000	nd(50)	nd(35)
HpCDD	1900	50	nd(20)
OCDD	19000	1700	142

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, 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 17

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

	Units are pg/gram wet weight of tissue					
isomer	(REP1)	(REP2)	(REP3)	(REP4)	(REP5)	(BLANK)
2378-TCDF	15	14	13	13	14	nd(0.5)
1234-TCDD‡	200	160	160	200	142	170
2378-TCDD	59	56	56	59	47	nd(0.5)
12378-PCDF	1.1	1.1	1.2	1.0	1.5	nd(0.2)
12378-PCDD	4	3	3	4	3	nd(1)
123678-HxCDD	9	7	7	8	6	nd(2)
1234678-HpCDD	12	11	12	12	12	nd(2)
OCDD‡‡	26	17	16	17	24	5

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

isomer	Units are pg/gram wet weight of sediment (REP1)	(REP2)	(REP3)	(REP4)	(REP5)	(REP6)
2378-TCDF	nd(2.1)	nd(0.8)	nd(0.7)	nd(1.9)	nd(0.7)	nd(1.1)
1234-TCDD	NR	NR	NR	NR	NR	NR
2378-TCDD	4.5	4.2	5.3	4.5	5.3	4.1
12378-PCDF	nd(0.6)	nd(0.6)	nd(0.5)	nd(0.7)	nd(0.9)	nd(1.3)
12378-PCDD	nd(2.1)	nd(1.9)	nd(1.9)	nd(2.2)	nd(3.0)	nd(4.3)
123678-HxCDD	nd(1.9)	nd(1.4)	nd(1.4)	nd(1.7)	nd(2.7)	nd(2.9)
1234678-HpCDD‡‡	21	23	25	35	20	29
OCDD‡‡	129	143	149	267	127	179

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

Statisical Summmary of Fish Replicate Data
(from Table 17)

isomer	(n)	(mean)	(%RSD)
2378-TCDF	5	14.2	3.2
1234-TCDD	5	172	13
2378-TCDD	5	55	9.0
12378-PCDF	5	1.2	16
12378-PCDD	5	3.4	16
123678-HxCDD	5	7.4	15
1234678-HpCDD	5	12	3.8
OCDD	5	15	31

Table 20

Statisical Summmary of Sediment Replicate Data
(from Table 18)

isomer	(n)	(mean)	(%RSD)
2378-TCDF	6	nd(1.2)	52
1234-TCDD	6	NR	NR
2378-TCDD	6	4.7	11
12378-PCDF	6	nd(0.7)	30
12378-PCDD	6	nd(2.6)	37
123678-HxCDD	6	nd(2.0)	33
1234678-HpCDD	6	25	22
OCDD	6	166	32

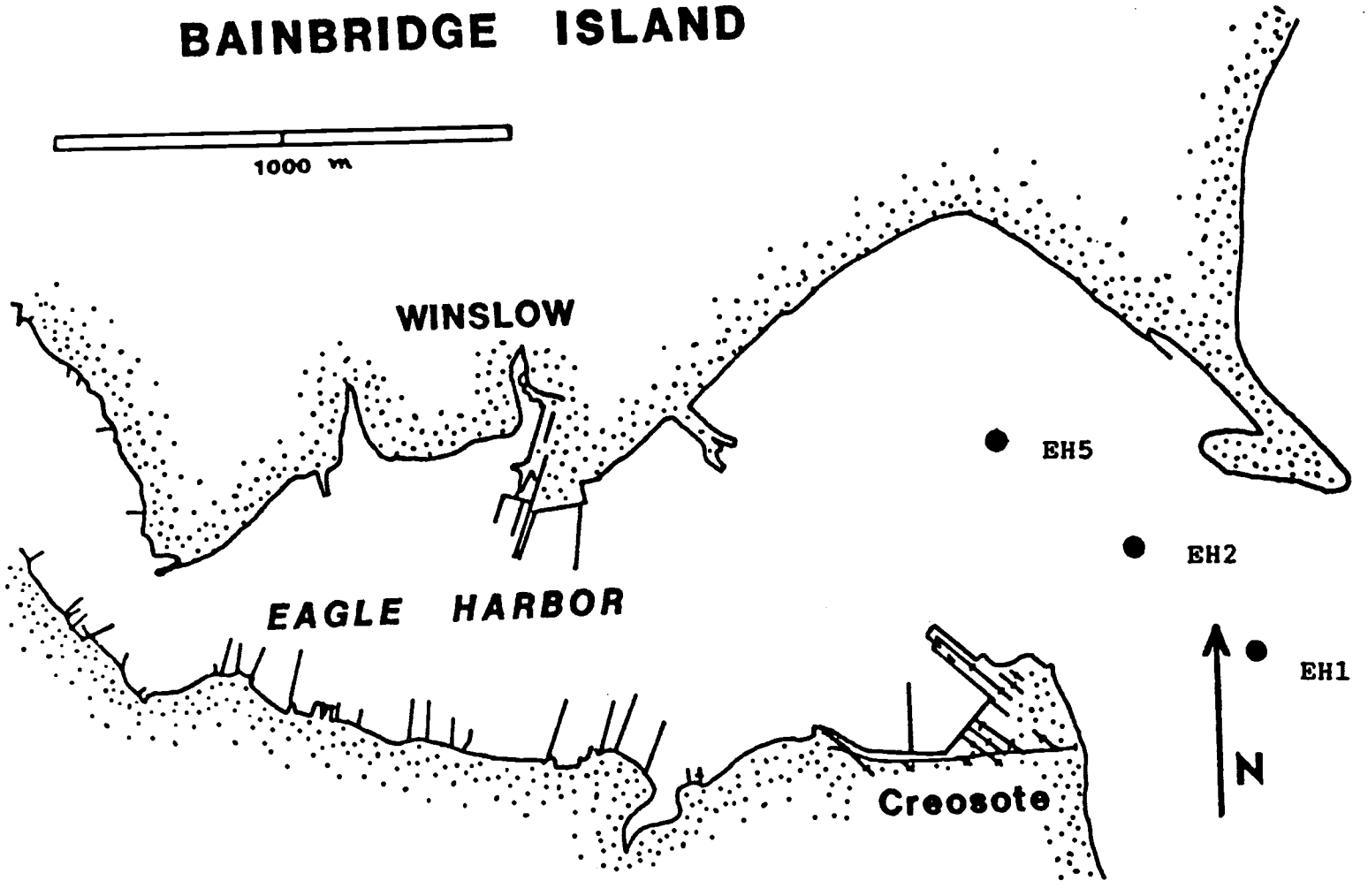

Figure 1: Sampling Locations for Eagle Harbor Site (taken, with permission, from Swartz et al., Toxicity of sediment from Eagle Harbor, Washington to the Infaunal Amphipod, Rhepoxynius Abronius, Environ. Sci. Technol., in press)

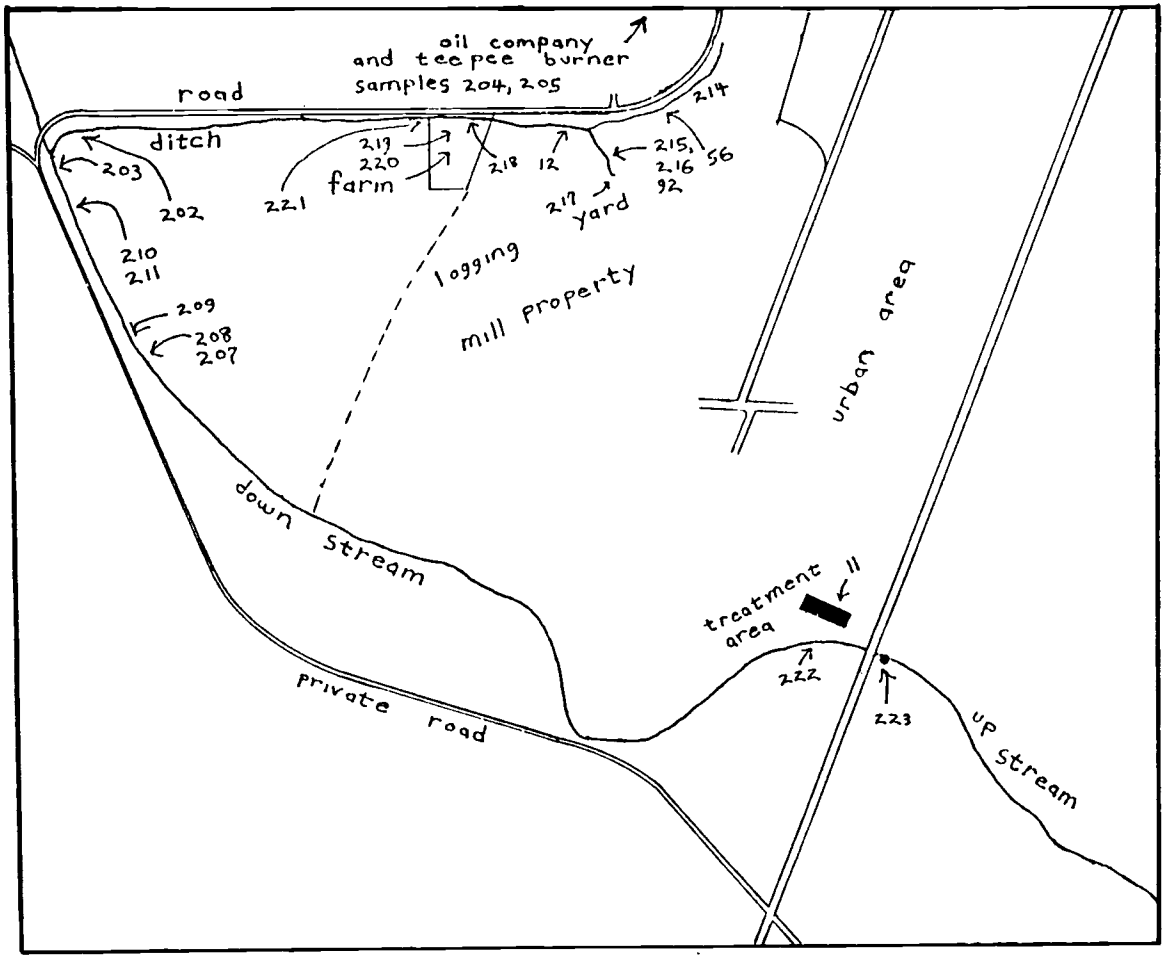

Figure 2: Sketch of Sampling Locations, Site 2 (scale is approximately 1 inch = 725 feet)

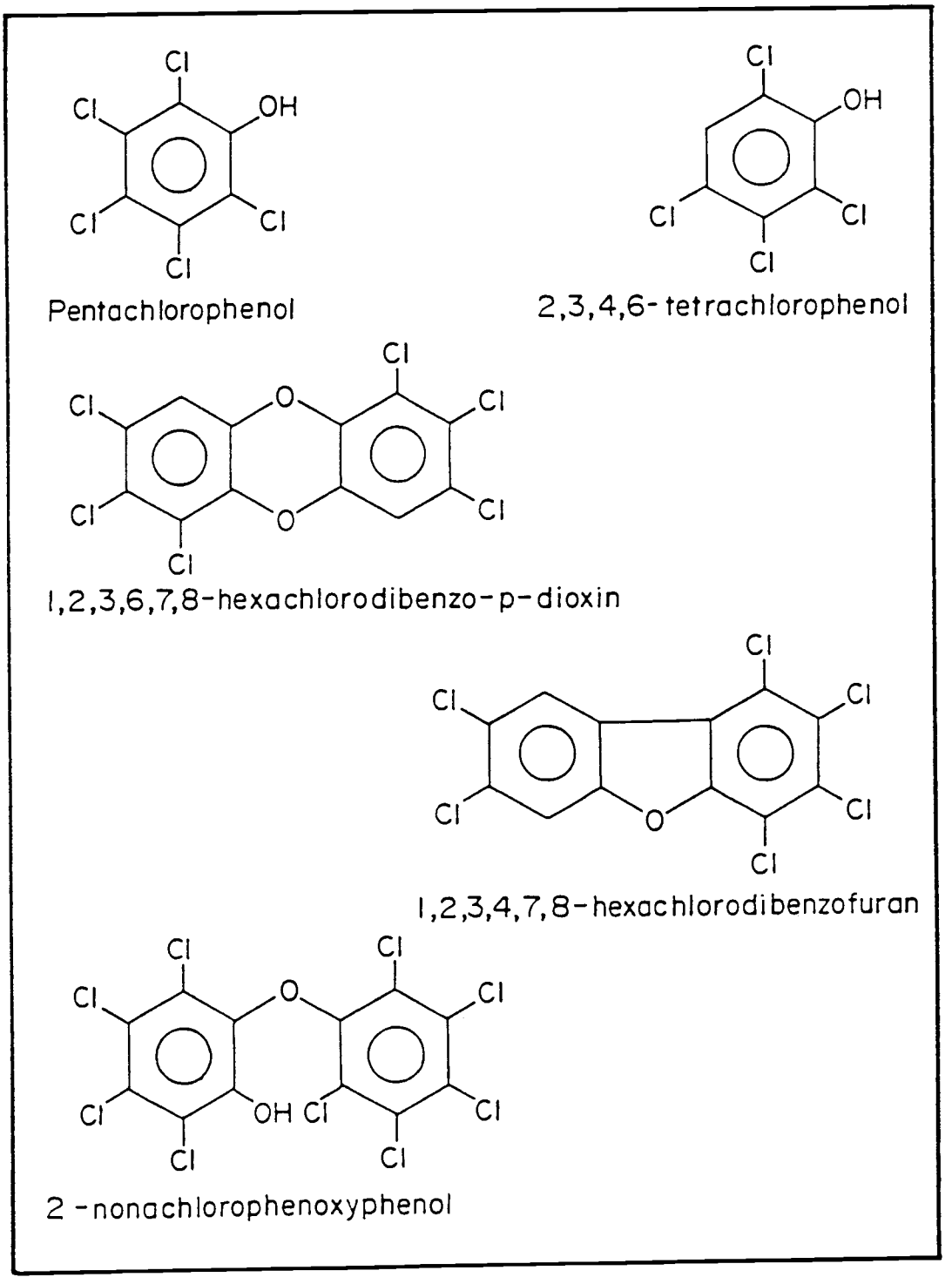

Figure 3

Chemical Structures of Some Compounds Found in t-PCP

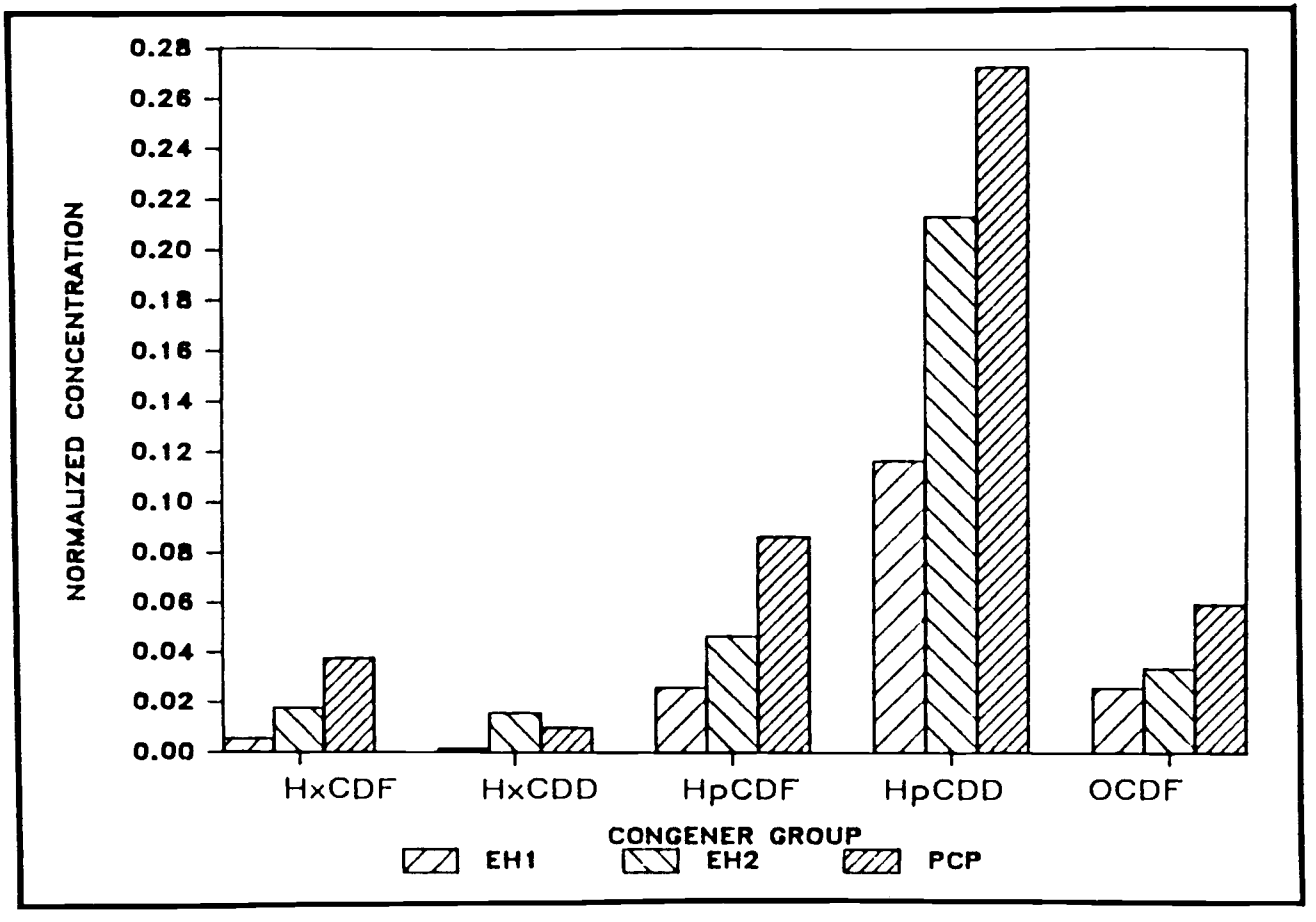

Figure 4

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

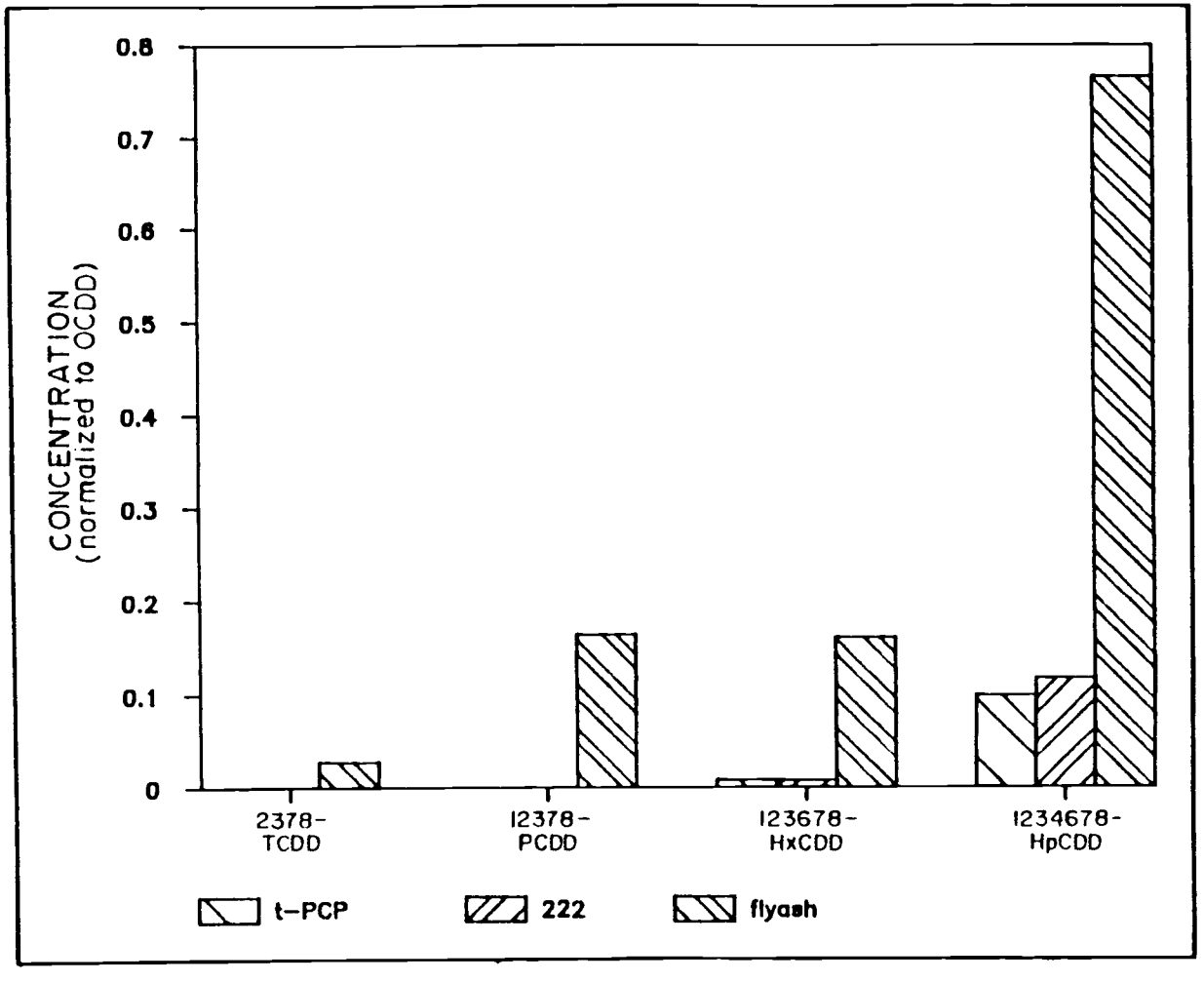

Figure 5: Sample 222 Compared to Concentrations of Four Selected PCDD's Found in t-PCP and Flyash (the values for t-PCP were calculated by averaging the two samples shown in Table 3)

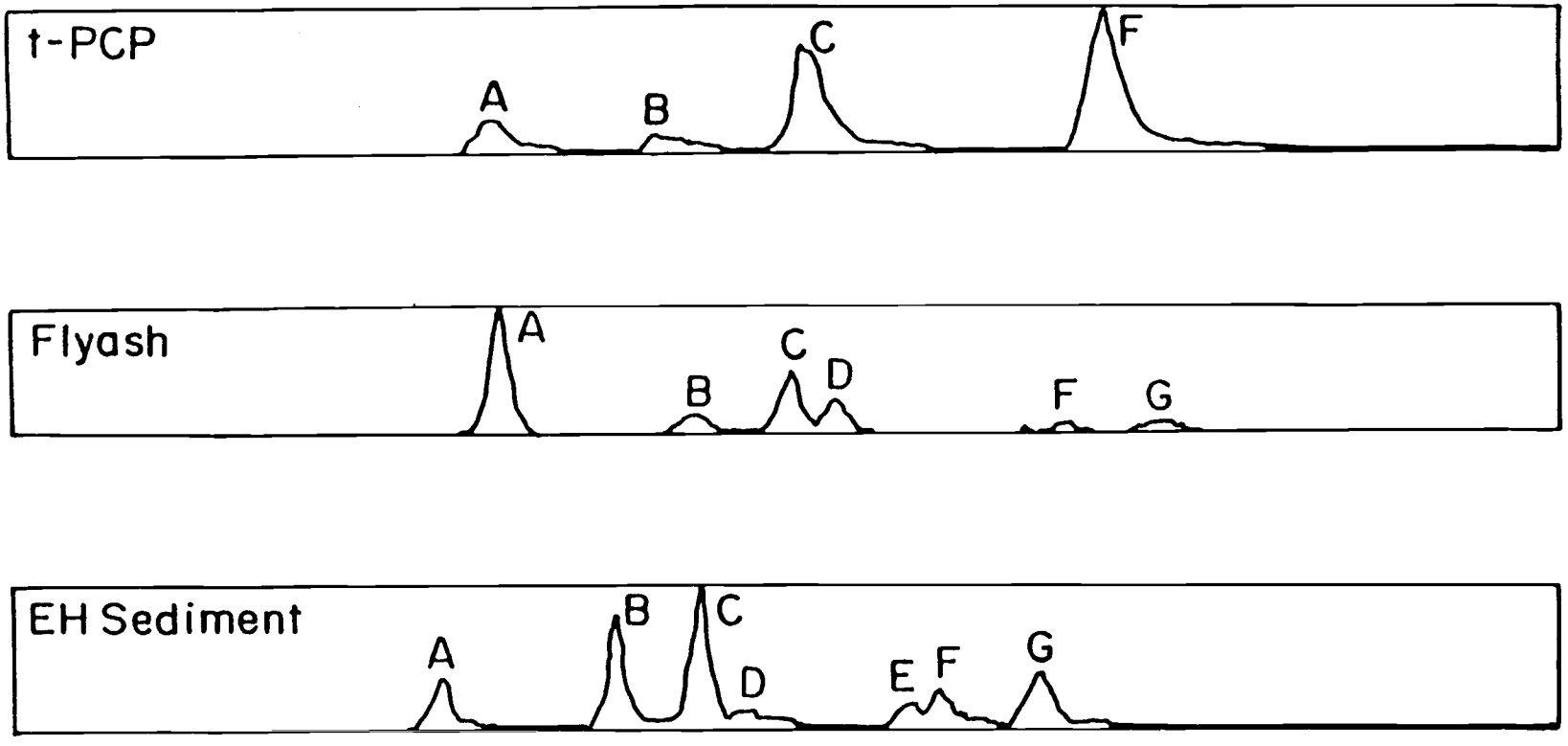

Figure 6

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

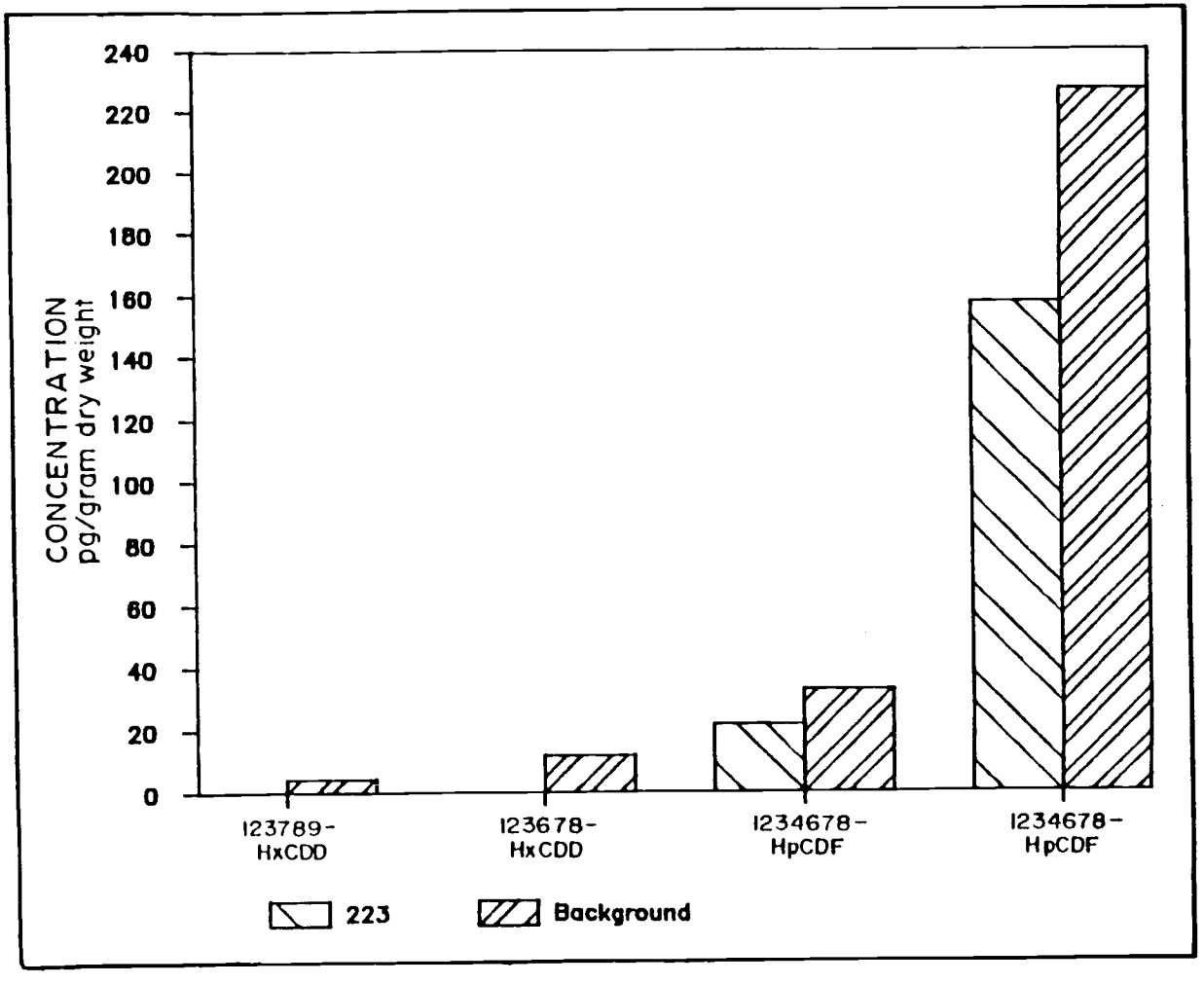

Figure 7: Mean Values for Positives for Four Selected Isomers of PCDD/PCDF Shown in Table 9 Compared with Those Found in Sample 223 (Table 9 values were used as background control values)

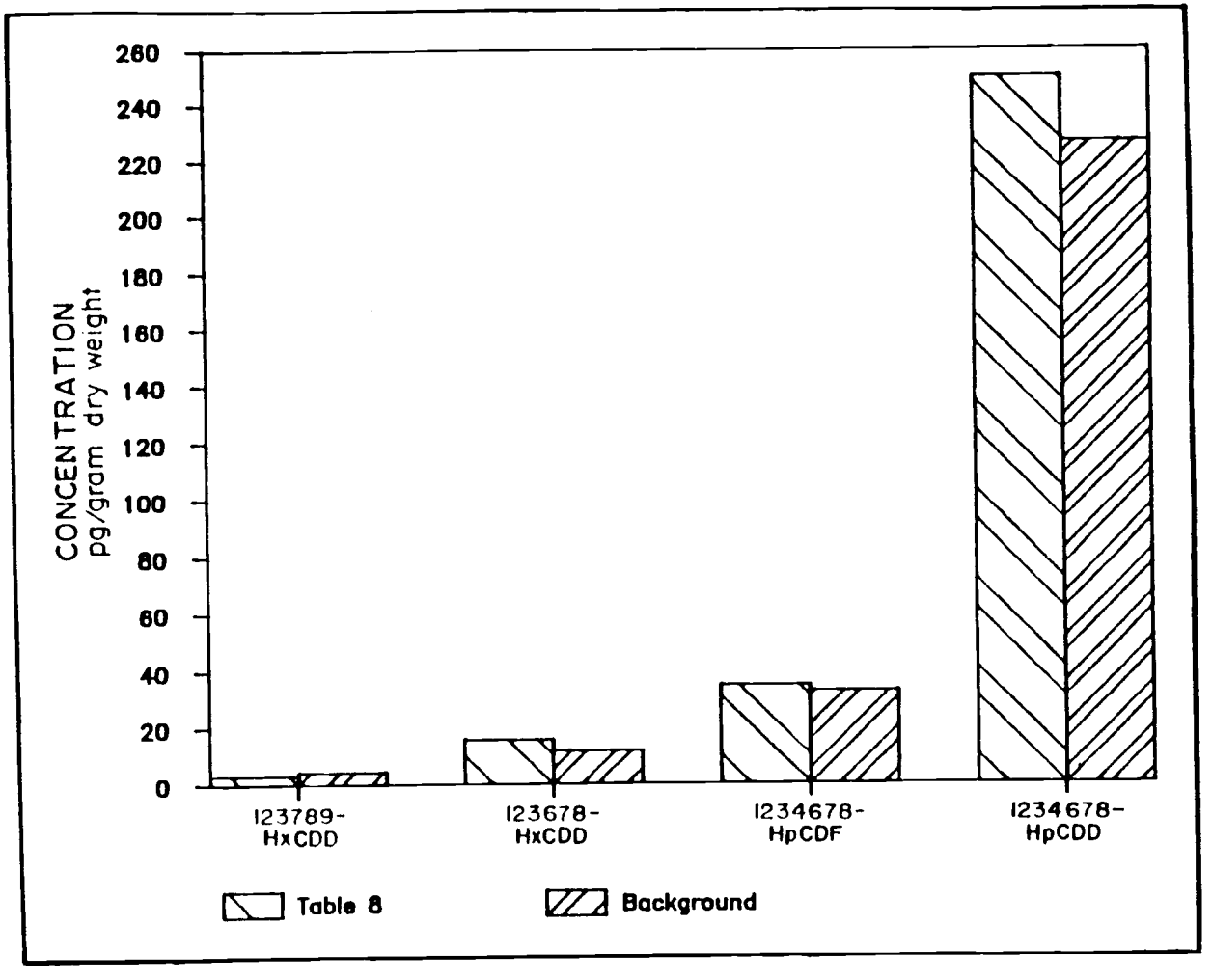

Figure 8: Mean Values for Positives in Table 9 Compared with Table 8 for Four Selected Isomers of PCDD/PCDF (Table 9 values were used as background control values)

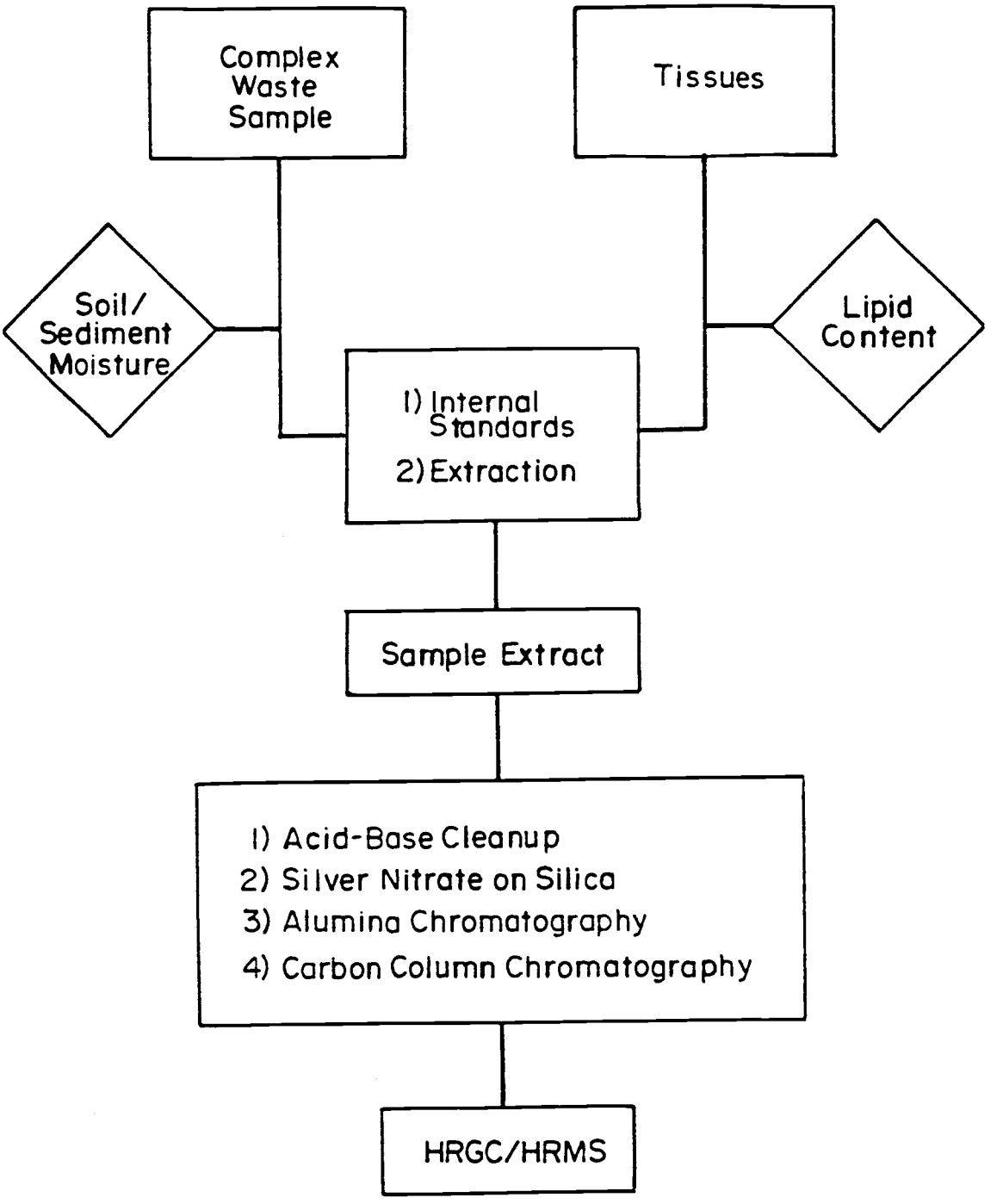

Figure 9

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

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APPENDICES

APPENDIX A

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

compound(s)	TEF
2,3,7,8-TCDD	1.00
1,2,3,7,8-PCDD	0.20
1,2,3,6,7,8-HxCDD	0.04
1,2,3,7,8,9-HxCDD	0.04
1,2,3,4,7,8-HxCDD	0.04
1,2,3,4,6,7,8-HpCDD	0.001
other TCDD**	0.01
other PCDD**	0.002
other HxCDD**	0.0004
other HpCDD**	0.00001
OCDD	0.0
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, isooctane, 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 Tennesee

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 sililica 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 convieniently 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 isooctane. 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 isooctane.

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 Na_2SO_4.

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 disgarded 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 colunm 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). All

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 disgarded. This fraction contained PCB's and polychlorinated napthalenes. The alumina column was then placed such that it drained directly into a resevoir 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 resevoir was washed three times with 0.5 mls 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 disgarded. 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.

APPENDIX C

Sample Cleanup Methods for Biological Tissues

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 mortal 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 mls 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 isooctane. 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

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

Internal Standard B Concentrations

Compound	Solution pg/ul	Sample* ppt
13C12-1,2,3,4-TCDD	2000	100

* 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:

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

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 paramters 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 paramters 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

	Ion Ratio* (+/- error)	Method Efficiency	Accuracy at 10 pg/g (+/-)	Precision at 10 pg/g (+/-)	S/N minimum
TCDD	.76+.10	>50%	+50%	+50%	2.5
PCDD	1.53+.15	>35%	+50%	+50%	2.5
HxCDD	1.23+.15	>35%	+100%	+100%	2.5
HpCDD	1.02+.15	>35%	+100%	+100%	2.5
OCDD	.88+.20	>25%	+200%	+100%	2.5
TCDF	.76+.10	>50%	+50%	+50%	2.5
PCDF	1.53+.15	>35%	+50%	+50%	2.5
HxCDF	1.23+.15	>35%	+100%	+100	2.5
HpCDF	1.02+.15	>35%	+500%	+500	2.5
OCDF	1.53+.20	>25%	+500%	+500	2.5

* 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. RFACTOR 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 RFACTOR, 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 programing environment.

Examples of program output are included.

The linear regression routine used in RFACTOR is based on that published by Wolfe and Koelling (15).

```
   REM         Program RFACTOR version 6.1 2/8/1987
   REM         Murray Hackett
   REM         Toxicology Program
   REM         Oregon State University
   REM         Corvallis, Oregon  97331

60 REM         DB5 Version
70 REM         A program to calculate RF and RRF values
80 REM         from Q series standards, means and SD's
90 REM         Also RT and RRT values for Biosig standard, WSU window markers

92 REM         Convert from min:sec to decimal, decimal to min: sec


93     DEF FNCONVERT(X)
94           FNCONVERT = INT(X) + ((X - INT(X))/.6000)
95     END DEF

96     DEF FNMINSEC(Y)
97           FNMINSEC = INT(Y) +  ((Y - INT(Y))* .6000)
98     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 RFLA(20), RFNA(50), RRFLA(20), RRFNA(50)
       DIM NRTA(50), LRTA(20), SUMNT(50), SUMLT(20), SUML(20)
       DIM SUMN(50), SUMRL(20), SUMRN(50)
       DIM RSDNRT(50), RSDLRT(50), RSDRFN(50), RSDRFL(20), RRTL(20)
       DIM SUMSQN(50), SUMSQRN(50), SUMSQNT(50), RRTN(50)
       DIM SUMSQL(20), SUMSQRL(20), SUMSQLT(20)
       DIM  VRFL(20), VRRL(20), VLRT(20)
       DIM  VRFN(50), VRRN(50), VNRT(50)
       DIM ALYTE$(30), BION(30),  RRBT(30), LION(20), NION(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)


175    REM  User must enter raw peak area and RT data interactively
180    REM  calculate RF and RRF values from Q series standards

190    CLS   :  PRINT : PRINT : KEY OFF
191    PRINT"Be sure and set the Caps Lock Key so that only"
192    PRINT"caps will be printed, otherwise things will not work!"
193    PRINT  :  PRINT
194    INPUT"Strike ENTER key when ready ... ", ANY$
195    CLS : PRINT : PRINT
200    INPUT"How many Q series standards do you wish to average "; N
212    CLS
```

```
215   LABEL = 12     : REM Number of labeled ions, loop counter
220     NAT = 48     : REM Number of natural ions, loop counter
222   HALFNAT = 24   : REM Number of natural analytes

225   REM subroutines
230    GOSUB 1080 : REM Enter picograms/ul for Q Standards
240    GOSUB 280  : REM  enter data, calculate RF and RRF values
250    GOSUB 3000 : REM  average RF, RRF, RRT data for n standards
255    GOSUB 4000 : REM  Standard Deviations, Q standards
260    GOSUB 5000 : REM  Biosignificant standard
261    GOSUB 5500 : REM  output user data to printer, check accuracy
262    GOSUB 5995 : REM  WSU Window standard
263    GOSUB 6000 : REM linear regression routine for isomer identification
264    GOSUB 7000 : REM  Output to printer, disk


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


270    END


280   REM  Subroutine: enter peak areas and RT's for Q Standards
290   FOR J = 1 TO N
300   REM
310   PRINT"Are you ready to enter data for Q Standard?    "
315   PRINT :  PRINT
320   INPUT"Strike ENTER key when ready ... ", ANY$
330   CLS : PRINT : PRINT
332   PRINT"Which Q Standard is being used for this iteration? "
335   INPUT"Enter '1', '2', '3' '4', '5', or '6'  ",  QQ
338   CLS
340   INPUT "enter peak areas for 2378 TCDF, 304 and 306 "; NP(1,J), NP(2,J)
350   INPUT "enter RT's for 304, 306 "; NRT(1,J), NRT(2,J)
360   CLS
370   INPUT "enter peak area for 13C12 2378 TCDF, 318 "; LP(2,J)
380   INPUT "enter RT for 13C12 2378 TCDF "; LRT(2,J)
390   CLS
400   INPUT "enter peak areas for 1234 TCDD, 320 and 322 "; NP(7,J), NP(8,J)
410   INPUT "enter RT's for 320, 322 "; NRT(7,J), NRT(8,J)
420   CLS
430   INPUT "enter peak areas for 2378 TCDD, 320 and 322 "; NP(9,J), NP(10,J)
440   INPUT "enter RT's for 320, 322 "; NRT(9,J), NRT(10,J)
450   CLS
460   INPUT "enter peak area for 37CL4 2378 TCDD, 327.8847 "; LP(4,J)
470   INPUT "enter RT for 37CL4 2378 TCDD "; LRT(4,J)
480   CLS
490   INPUT "enter peak area for 13C6 1234 TCDD, 327.9137 "; LP(3,J)
500   INPUT "enter RT for 13C6 1234 TCDD  "; LRT(3,J)
510   CLS
520   INPUT "enter peak area for 13C12 1234 TCDD, 334 "; LP(1,J)
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530  INPUT "enter RT for 13C12 1234 TCDD "; LRT(1,J)
540  CLS
550  INPUT "enter peak areas for 12378 PCDF, 340 and 342 "; NP(13,J), NP(14,J)
560  INPUT "enter RT's for 340, 342 "; NRT(13,J), NRT(14,J)
570  CLS
580  INPUT "enter peak area for 13C12 12378 PCDF, 352 "; LP(5,J)
590  INPUT "enter peak RT for 13C12 12378 PCDF "; LRT(5,J)
600  CLS
610  INPUT "enter peak areas for 12378 PCDD, 356 and 358 "; NP(21,J), NP(22,J)
620  INPUT "enter RT's for 356, 358 "; NRT(21,J), NRT(22,J)
630  CLS
640  INPUT "enter peak area for 13C12 12378 PCDD, 368 "; LP(6,J)
650  INPUT "enter RT for 13C12 12378 PCDD "; LRT(6,J)
660  CLS
670  INPUT"enter peak areas for 123478 HxCDF,374 and 376 ";NP(23,J),NP(24,J)
680  INPUT "enter RT's for 374, 376 "; NRT(23,J), NRT(24,J)
690  CLS
700  INPUT "enter peak area for 13C12 123478 HxCDF, 386 "; LP(7,J)
710  INPUT "enter RT for 13C12 123478 HxCDF "; LRT(7,J)
720  CLS
730  INPUT "enter peak areas for 123678 HxCDD, 390 and 392 "; NP(35,J), NP(36,J)
740  INPUT "enter RT's for 390, 392 "; NRT(35,J), NRT(36,J)
750  CLS
760  INPUT "enter peak area for 13C12 123678 HxCDD, 402 "; LP(8,J)
770  INPUT "enter RT for 13C12 123678 HxCDD "; LRT(8,J)
780  CLS
790  INPUT"enter peak areas for 1234678 HpCDF, 408 and 410 ";NP(39,J),NP(40,J)
800  INPUT "enter RT's for 408, 410 "; NRT(39,J), NRT(40,J)
810  CLS
820  INPUT "enter peak area for 13C12 1234678 HpCDF, 420 "; LP(9,J)
830  INPUT "enter RT for 13C12 1234678 HpCDF "; LRT(9,J)
840  CLS
850  INPUT "enter peak areas for 1234678 HpCDD, 424, 426 "; NP(43,J), NP(44,J)
860  INPUT "enter RT for 424, 426 "; NRT(43,J), NRT(44,J)
870  CLS
880  INPUT "enter peak area for 13C12 1234678 HpCDD, 436 "; LP(10,J)
890  INPUT "enter RT for 13C12 1234678 HpCDD "; LRT(10,J)
900  CLS
910  INPUT "enter peak areas for OCDF, 444 and 446 "; NP(45,J), NP(46,J)
920  INPUT "enter RT's for 444, 446 "; NRT(45,J), NRT(46,J)
930  CLS
940  INPUT "enter peak area for 13C12 OCDF, 456 "; LP(11,J)
950  INPUT "enter RT for 13C12 OCDF "; LRT(11,J)
960  CLS
970  INPUT "enter peak areas for OCDD, 458 and 460 "; NP(47,J), NP(48,J)
980  INPUT "enter RT's for 458, 460 "; NRT(47,J), NRT(48,J)
990  CLS
1000 INPUT "enter peak area for 13C12 OCDD, 472 "; LP(12,J)
1010 INPUT "enter RT for 13C12 OCDD "; LRT(12,J)

1015 CLS : REM add natural ions for biosig compounds not in Q standards
1020 NP(3,J) = NP(1,J)  : NP(5,J) = NP(1,J)  : NP(4,J) = NP(2,J)  : NP(6,J)= NP(2,J)
1025 NP(11,J)= NP(13,J) : NP(15,J)= NP(13,J) : NP(17,J)= NP(13,J) : NP(19,J)= NP(13,J)
1030 NP(12,J)= NP(14,J) : NP(16,J)= NP(14,J) : NP(18,J)= NP(14,J) : NP(20,J)= NP(14,J)
1035 NP(25,J)= NP(23,J) : NP(27,J)= NP(23,J) : NP(26,J)= NP(24,J) : NP(28,J)= NP(24,J)
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1040  NP(29,J)= NP(23,J) : NP(31,J)= NP(23,J) : NP(30,J)= NP(24,J) : NP(32,J)= NP(24,J)
1045  NP(33,J)= NP(35,J) : NP(34,J)= NP(36,J) : NP(37,J)= NP(35,J) : NP(38,J)= NP(36,J)
1050  NP(41,J)= NP(39,J) : NP(42,J)= NP(40,J)

1070   GOTO 2500

1072   REM  pg/ul for each Q standard, Q1-Q6
1074   REM  Subroutine:  Enter concentrations for Q standards
1075   REM  Standard Q3
1080   L3(1) = 100  : REM pg 13C12 1234 TCDD ion 334
1090   L3(3) = 12.5 : REM pg 13C6  1234 TCDD ion 328
1100   L3(4) = 12.5 : REM pg 37CL4 2378 TCDD ion 328
1110   L3(2) = 12.5 : REM pg 13C12 2378 TCDF ion 318
1120   L3(5) = 25   : REM pg 13C12 12378 PCDF  ion 352
1130   L3(6) = 25   : REM pg 13C12 12378 PCDD  ion 368
1140   L3(7) = 50   : REM pg 13C12 123478 HxCDF  ion 386
1150   L3(8) = 50   : REM pg 13C12 123678 HxCDD  ion 402
1160   L3(9) = 50   : REM pg 13C12 1234678 HpCDF   ion 420
1170   L3(10) = 50   : REM pg 13C12 1234678 HpCDD   ion 436
1180   L3(11) = 100  : REM pg 13C12 12346789 OCDF     ion 456
1190   L3(12) = 100  : REM pg 13C12 12346789 OCDD     ion 472

1210   N3(1)  = 12.5 : REM pg nat   2378 TCDF ion 304
1220   N3(2)  = 12.5 : REM pg nat   2378 TCDF ion 306
1230   N3(7)  =  2.5 : REM pg nat   1234 TCDD ion 320
1240   N3(8)  =  2.5 : REM pg nat   1234 TCDD ion 322
1250   N3(9)  = 12.5 : REM pg nat   2378 TCDD ion 320
1260   N3(10)  = 12.5 : REM pg nat   2378 TCDD ion 322
1270   N3(13)  = 25   : REM pg nat   12378 PCDF  ion 340
1280   N3(14)  = 25   : REM pg nat   12378 PCDF  ion 342
1290   N3(21)  = 25   : REM pg nat   12378 PCDD ion 356
1300   N3(22) = 25   : REM pg nat   12378 PCDD ion 358
1310   N3(23) = 50   : REM pg nat   123478 HxCDF  ion 374
1320   N3(24) = 50   : REM pg nat   123478 HxCDF  ion 376
1330   N3(35) = 50   : REM pg nat   123678 HxCDD  ion 390
1340   N3(36) = 50   : REM pg nat   123678 HxCDD  ion 392
1350   N3(39) = 50   : REM pg nat   1234678 HpCDF   ion 408
1360   N3(40) = 50   : REM pg nat   1234678 HpCDF   ion 410
1370   N3(43) = 50   : REM pg nat   1234678 HpCDD   ion 424
1380   N3(44) = 50   : REM pg nat   1234678 HpCDD   ion 426
1390   N3(47) = 100  : REM pg nat   12346789 OCDD     ion 458
1400   N3(48) = 100  : REM pg nat   12346789 OCDD     ion 460
1410   N3(45) = 100  : REM pg nat   12346789 OCDF     ion 444
1420   N3(46) = 100  : REM pg nat   12346789 OCDF     ion 446

1425   REM add natural ions for biosig compounds not in Q3 standard
1426  N3(3)= N3(1) : N3(5)= N3(1) : N3(4)= N3(2) : N3(6)= N3(2)
1427  N3(11)= N3(13) : N3(15)= N3(13) : N3(17)= N3(13) : N3(19)= N3(13)
1428  N3(12)= N3(14) : N3(16)= N3(14) : N3(18)= N3(14) : N3(20)= N3(14)
1429  N3(25)= N3(23) : N3(27)= N3(23) : N3(26)= N3(24) : N3(28)= N3(24)
1430  N3(29)= N3(23) : N3(30)= N3(24) : N3(31)= N3(23) : N3(32)= N3(24)
1435  N3(33)= N3(35) : N3(34)= N3(36) : N3(37)= N3(35) : N3(38)= N3(36)
1437  N3(41)= N3(39) : N3(42)= N3(40)

1440   L4(1) =  100  : REM pg 13C12 1234 TCDD ion 334
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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 HpCDF   ion 420
1530  L4(10) = 100  : REM pg 13C12 1234678 HpCDD   ion 436
1540  L4(11) = 200  : REM pg 13C12 12346789 OCDF     ion 456
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   1234678 HpCDF   ion 408
1710  N4(40) = 100  : REM pg nat   1234678 HpCDF   ion 410
1720  N4(43) = 100  : REM pg nat   1234678 HpCDD   ion 424
1730  N4(44) = 100  : REM pg nat   1234678 HpCDD   ion 426
1740  N4(47) = 200  : REM pg nat   12346789 OCDD      ion 458
1750  N4(48) = 200  : REM pg nat   12346789 OCDD      ion 460
1760  N4(45) = 200  : REM pg nat   12346789 OCDF      ion 442
1770  N4(46) = 200  : REM pg nat   12346789 OCDF      ion 446

1771  CLS : REM add natural ions for biosig compounds not in Q4 standard
1772  N4(3)= N4(1) : N4(5)= N4(1) : N4(4)= N4(2) : N4(6)= N4(2)
1773  N4(11)= N4(13) : N4(15)= N4(13) : N4(17)= N4(13) : N4(19)= N4(13)
1774  N4(12)= N4(14) : N4(16)= N4(14) : N4(18)= N4(14) : N4(20)= N4(14)
1775  N4(25)= N4(23) : N4(27)= N4(23) : N4(26)= N4(24) : N4(28)= N4(24)
1776  N4(29)= N4(23) : N4(30)= N4(24) : N4(31)= N4(23) : N4(32)= N4(24)
1777  N4(33)= N4(35) : N4(34)= N4(36) : N4(37)= N4(35) : N4(38)= N4(36)
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(3) = 12.5 : REM pg 13C6  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 HpCDF   ion 420
1880   L2(10) = 50   : REM pg 13C12 1234678 HpCDD   ion 436
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1890  L2(11) = 100  : REM pg 13C12 12346789 OCDF     ion 456
1900  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 PCDF  ion 342
1990  N2(21) =   10 : REM pg nat   12378 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(35) =  20  : REM pg nat   123678 HxCDD  ion 390
2040  N2(36) =  20  : REM pg nat   123678 HxCDD  ion 392
2050  N2(39) =  20  : REM pg nat   1234678 HpCDF   ion 408
2060  N2(40) =  20  : REM pg nat   1234678 HpCDF   ion 410
2070  N2(43) =  20  : REM pg nat   1234678 HpCDD   ion 424
2080  N2(44) =  20  : REM pg nat   1234678 HpCDD   ion 426
2090  N2(47) =  40  : REM pg nat   12346789 OCDD      ion 458
2100  N2(48) =  40  : REM pg nat   12346789 OCDD      ion 460
2110  N2(45) =  40  : REM pg nat   12346789 OCDF      ion 444
2120  N2(46) =  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)
2123  N2(11)= N2(13) : N2(15)= N2(13) : N2(17)= N2(13) : N2(19)= N2(13)
2124  N2(12)= N2(14) : N2(16)= N2(14) : N2(18)= N2(14) : N2(20)= N2(14)
2125  N2(25)= N2(23) : N2(27)= N2(23) : N2(26)= N2(24) : N2(28)= N2(24)
2126  N2(29)= N2(23) : N2(30)= N2(24) : N2(31)= N2(23) : N2(32)= N2(24)
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 1234678 HpCDF   ion 420
2230   L1(10) = 50   : REM pg 13C12 1234678 HpCDD   ion 436
2240   L1(11) = 100  : REM pg 13C12 12346789 OCDF     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
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2330  N1(13) =  2   : REM pg nat   12378 PCDF  ion 340
2340  N1(14) =  2   : REM pg nat   12378 PCDF  ion 342
2350  N1(21) =  2   : REM pg nat   12378 PCDD ion 356
2360  N1(22) = 2   : REM pg nat   12378 PCDD ion 358
2370  N1(23) = 4   : REM pg nat   123478 HxCDF  ion 374
2380  N1(24) = 4   : REM pg nat   123478 HxCDF  ion 376
2390  N1(35) = 4   : REM pg nat   123678 HxCDD  ion 390
2400  N1(36) = 4   : REM pg nat   123678 HxCDD  ion 392
2410  N1(39) = 4   : REM pg nat   1234678 HpCDF   ion 408
2420  N1(40) = 4   : REM pg nat   1234678 HpCDF   ion 410
2430  N1(43) = 4   : REM pg nat   1234678 HpCDD   ion 424
2440  N1(44) = 4   : REM pg nat   1234678 HpCDD   ion 426
2450  N1(47) = 8   : REM pg nat   12346789 OCDD     ion 458
2460  N1(48) = 8   : REM pg nat   12346789 OCDD     ion 460
2470  N1(45) = 8   : REM pg nat   12346789 OCDF     ion 444
2480  N1(46) = 8   : REM pg nat   12346789 OCDF     ion 446

2481  CLS : REM add natural ions for biosig compounds not in Q1 standard
2482  N1(3)= N1(1) : N1(5)= N1(1) : N1(4)= N1(2) : N1(6)= N1(2)
2483  N1(11)= N1(13) : N1(15)= N1(13) : N1(17)= N1(13) : N1(19)= N1(13)
2484  N1(12)= N1(14) : N1(16)= N1(14) : N1(18)= N1(14) : N1(20)= N1(14)
2485  N1(25)= N1(23) : N1(27)= N1(23) : N1(26)= N1(24) : N1(28)= N1(24)
2486  N1(29)= N1(23) : N1(30)= N1(24) : N1(31)= N1(23) : N1(32)= N1(24)
2487  N1(33)= N1(35) : N1(34)= N1(36) : N1(37)= N1(35) : N1(38)= N1(36)
2488  N1(41)= N1(39) : N1(42)= N1(40)

2489   REM  Q5

      L5(1) =  100  : REM pg 13C12 1234 TCDD ion 334
      L5(3) =   25  : REM pg 13C6  1234 TCDD ion 328
      L5(4) =   25  : REM pg 37CL4 2378 TCDD ion 328
      L5(2) =   25  : REM pg 13C12 2378 TCDF ion 318
      L5(5) =   50  : REM pg 13C12 12378 PCDF  ion 352
      L5(6) =   50  : REM pg 13C12 12378 PCDD  ion 368
      L5(7) =  100  : REM pg 13C12 123478 HxCDF  ion 386
      L5(8) =  100  : REM pg 13C12 123678 HxCDD  ion 402
      L5(9) =  100  : REM pg 13C12 1234678 HpCDF   ion 420
      L5(10) = 100  : REM pg 13C12 1234678 HpCDD   ion 436
      L5(11) = 200  : REM pg 13C12 12346789 OCDF     ion 456
      L5(12) = 200  : REM pg 13C12 12346789 OCDD     ion 472

      N5(1) =  50  : REM pg nat   2378 TCDF ion 304
      N5(2) =  50  : REM pg nat   2378 TCDF ion 306
      N5(7) =   5  : REM pg nat   1234 TCDD ion 320
      N5(8) =   5  : REM pg nat   1234 TCDD ion 322
      N5(9) =  50  : REM pg nat   2378 TCDD ion 320
      N5(10) = 50  : REM pg nat   2378 TCDD ion 322
      N5(13) = 100 : REM pg nat   12378 PCDF  ion 338
      N5(14) = 100 : REM pg nat   12378 PCDF  ion 342
      N5(21) = 100 : REM pg nat   12378 PCDD ion 356
      N5(22) = 100 : REM pg nat   12378 PCDD ion 358
      N5(23) = 200 : REM pg nat   123478 HxCDF  ion 374
      N5(24) = 200  : REM pg nat   123478 HxCDF  ion 376
      N5(35) = 200  : REM pg nat   123678 HxCDD  ion 390
      N5(36) = 200  : REM pg nat   123678 HxCDD  ion 392
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N5(39) = 200  : REM pg nat   1234678 HpCDF   ion 408
N5(40) = 200  : REM pg nat   1234678 HpCDF   ion 410
N5(43) = 200  : REM pg nat   1234678 HpCDD   ion 424
N5(44) = 200  : REM pg nat   1234678 HpCDD   ion 426
N5(47) = 400  : REM pg nat   12346789 OCDD     ion 458
N5(48) = 400  : REM pg nat   12346789 OCDD     ion 460
N5(45) = 400  : REM pg nat   12346789 OCDF     ion 442
N5(46) = 400  : REM pg nat   12346789 OCDF     ion 446

CLS : REM add natural ions for biosig compounds not in Q5 standard
N5(3)= N5(1) : N5(5)= N5(1) : N5(4)= N5(2) : N5(6)= N5(2)
N5(11)= N5(13) : N5(15)= N5(13) : N5(17)= N5(13) : N5(19)= N5(13)
N5(12)= N5(14) : N5(16)= N5(14) : N5(18)= N5(14) : N5(20)= N5(14)
N5(25)= N5(23) : N5(27)= N5(23) : N5(26)= N5(24) : N5(28)= N5(24)
N5(29)= N5(23) : N5(30)= N5(24) : N5(31)= N5(23) : N5(32)= N5(24)
N5(33)= N5(35) : N5(34)= N5(36) : N5(37)= N5(35) : N5(38)= N5(36)
N5(41)= N5(39) : N5(42)= N5(40)

REM  Q6

L6(1) =  100  : REM pg 13C12 1234 TCDD ion 334
L6(3) =   25  : REM pg 13C6  1234 TCDD ion 328
L6(4) =   25  : REM pg 37CL4 2378 TCDD ion 328
L6(2) =   25  : REM pg 13C12 2378 TCDF ion 318
L6(5) =   50  : REM pg 13C12 12378 PCDF  ion 352
L6(6) =   50  : REM pg 13C12 12378 PCDD  ion 368
L6(7) =  100  : REM pg 13C12 123478 HxCDF  ion 386
L6(8) =  100  : REM pg 13C12 123678 HxCDD  ion 402
L6(9) =  100  : REM pg 13C12 1234678 HpCDF   ion 420
L6(10) = 100  : REM pg 13C12 1234678 HpCDD   ion 436
L6(11) = 200  : REM pg 13C12 12346789 OCDF     ion 456
L6(12) = 200  : REM pg 13C12 12346789 OCDD     ion 472
N6(1) =  100  : REM pg nat   2378 TCDF ion 304
N6(2) =  100  : REM pg nat   2378 TCDF ion 306
N6(7) =    5  : REM pg nat   1234 TCDD ion 320
N6(8) =    5  : REM pg nat   1234 TCDD ion 322
N6(9) =  100  : REM pg nat   2378 TCDD ion 320
N6(10) = 100  : REM pg nat   2378 TCDD ion 322
N6(13) = 200  : REM pg nat   12378 PCDF  ion 338
N6(14) = 200  : REM pg nat   12378 PCDF  ion 342
N6(21) = 200  : REM pg nat   12378 PCDD ion 356
N6(22) = 200  : REM pg nat   12378 PCDD ion 358
N6(23) = 400  : REM pg nat   123478 HxCDF  ion 374
N6(24) = 400  : REM pg nat   123478 HxCDF  ion 376
N6(35) = 400  : REM pg nat   123678 HxCDD  ion 390
N6(36) = 400  : REM pg nat   123678 HxCDD  ion 392
N6(39) = 400  : REM pg nat   1234678 HpCDF   ion 408
N6(40) = 400  : REM pg nat   1234678 HpCDF   ion 410
N6(43) = 400  : REM pg nat   1234678 HpCDD   ion 424
N6(44) = 400  : REM pg nat   1234678 HpCDD   ion 426
N6(47) = 800  : REM pg nat   12346789 OCDD     ion 458
N6(48) = 800  : REM pg nat   12346789 OCDD     ion 460
N6(45) = 800  : REM pg nat   12346789 OCDF     ion 442
N6(46) = 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(11)= N6(13) : N6(15)= N6(13) : N6(17)= N6(13) : N6(19)= N6(13)
      N6(12)= N6(14) : N6(16)= N6(14) : N6(18)= N6(14) : N6(20)= N6(14)
      N6(25)= N6(23) : N6(27)= N6(23) : N6(26)= N6(24) : N6(28)= N6(24)
      N6(29)= N6(23) : N6(30)= N6(24) : N6(31)= N6(23) : N6(32)= N6(24)
      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
```

```
2860          RFN(I,J) = NP(I,J)/(N4(I))
2862       NEXT I
           GOTO 2865

2863       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

2864       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

           REM tcdf
2865       FOR I = 1 TO 6
              RFLC(I,J) = RFL(2,J)
           NEXT I

           REM 1234 tcdd
2866       FOR I = 7 TO 8
              RFLC(I,J) = RFL(3,J)
           NEXT I

           REM 2378 tcdd
2868       FOR I = 9 TO 10
              RFLC(I,J) = RFL(4,J)
           NEXT I

           REM pcdf
2870       FOR I = 11 TO 20
              RFLC(I,J) = RFL(5,J)
           NEXT I

           REM pcdd
2872       FOR I = 21 TO 22
              RFLC(I,J) = RFL(6,J)
           NEXT I

           REM hxcdf
2874       FOR I = 23 TO 32
              RFLC(I,J) = RFL(7,J)
           NEXT I

           REM hxcdd
2876       FOR I = 33 TO 38
              RFLC(I,J) = RFL(8,J)
           NEXT I
```

```
        REM hpcdf
2878    FOR I = 39 TO 42
           RFLC(I,J)= RFL(9,J)
        NEXT I
2880
        REM hpcdd, 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)
2888  NEXT J

2890  REM RRF's (relative to 334) for calculating recoveries
2900  FOR J = 1 TO N
2910     FOR I = 1 TO LABEL
2920        RRFL(I,J) = RFL(I,J)/RFL(1,J)
2930     NEXT I
2940  NEXT J

2950  REM  RF's natural ions, natural/label
2960  FOR J = 1 TO N
2970     FOR I = 1 TO NAT
2980      IF RFLC(I,J)<>0 THEN RRFN(I,J) = RFN(I,J)/RFLC(I,J) ELSE RRFN(I,J)=0
2981     NEXT I
2982  NEXT J

2995  RETURN


3000  REM   Subroutine: calculate average RF, RRF, RRT of N iterations,
3010  REM   sum squares, if value of N is 3 or greater
3040  REM   Average RFL
3050  FOR   I = 1 TO LABEL
3060        SUM  = 0
3062        SUMSQ = 0
3070        FOR J = 1 TO N
3080            SUM  = SUM  + RFL(I,J)
3082        SUMSQ = SUMSQ + RFL(I,J)^2
3090        NEXT J
3100        SUML(I) = SUM
3105        SUMSQL(I)  = SUMSQ
3110        RFLA(I) = SUML(I)/N
3120  NEXT I

3130  REM   Average RFN
3140  FOR   I = 1 TO  NAT
3145        SUM = 0
3150        SUMSQ = 0
3160        FOR J = 1 TO N
3170            SUM = SUM + RFN(I,J)
3175        SUMSQ = SUMSQ + RFN(I,J)^2
3180        NEXT J
3190        SUMN(I) = SUM
3195        SUMSQN(I) = SUMSQ
3200        RFNA(I) = SUMN(I)/N
3210  NEXT I
```

```
3220  REM   Average RRFL
3230  FOR   I = 1 TO LABEL
3240        SUM  = 0
3245        SUMSQ = 0
3250        FOR J = 1 TO N
3260            SUM  = SUM  + RRFL(I,J)
3265        SUMSQ = SUMSQ + RRFL(I,J)^2
3270        NEXT J
3280        SUMRL(I) = SUM
3285        SUMSQRL(I) = SUMSQ
3290        RRFLA(I) = SUMRL(I)/N
3300  NEXT I

3310  REM   Average RRFN
3320  FOR   I = 1 TO  NAT
3330        SUM = 0
3335        SUMSQ = 0
3340        FOR J = 1 TO N
3350            SUM = SUM + RRFN(I,J)
3355            SUMSQ = SUMSQ + RRFN(I,J)^2
3360        NEXT J
3370        SUMRN(I) = SUM
3375        SUMSQRN(I) = SUMSQ
3380        RRFNA(I) = SUMRN(I)/N
3390  NEXT I

3400  REM   Average LRT
3410  FOR   I = 1 TO  LABEL
3420        SUM = 0
3425        SUMSQ = 0
3430        FOR J = 1 TO N
3435            DLRT(I,J) = FNCONVERT(LRT(I,J))
3440            SUM = SUM + DLRT(I,J)
3445            SUMSQ = SUMSQ + DLRT(I,J)^2
3450        NEXT J
3460        SUMLT(I) = SUM
3465        SUMSQLT(I) = SUMSQ
3470        DLRTA(I) = SUMLT(I)/N
3475        LRTA(I) = FNMINSEC(DLRTA(I))
3480  NEXT I

3490  REM   Average NRT
3500  FOR   I = 1 TO  NAT
3510        SUM = 0
3515        SUMSQ = 0
3520        FOR J = 1 TO N
3522            DNRT(I,J) = FNCONVERT(NRT(I,J))
3530            SUM = SUM + DNRT(I,J)
3535            SUMSQ = SUMSQ + DNRT(I,J)^2
3540        NEXT J
3550        SUMNT(I) = SUM
3555        SUMSQNT(I) = SUMSQ
3560        DNRTA(I) = SUMNT(I)/N
3565        NRTA(I) = FNMINSEC(DNRTA(I))
```

```
3570   NEXT I

3575   REM Calculate Relative Retention Times (w/respect to REFF)
3580   REM Normalize RRT's w/respect to 2378-TCDD
3585   REFF = DLRTA(4)

3595   REM
3600   FOR I = 1 TO LABEL
3605     IF REFF>0 AND DLRTA(I)>0 THEN RRTL(I)=(DLRTA(I)/REFF) ELSE RRTL(I)=0
3610   NEXT I

3615   FOR I = 1 TO NAT
3620     IF REFF>0 AND DNRTA(I)>0 THEN RRTN(I)=(DNRTA(I)/REFF) ELSE RRTN(I)=0
3625   NEXT I

3990   RETURN


4000   REM  Subroutine: Calculate standard deviations
4005   IF N  >= 3 THEN 4010 ELSE 4990

4010   FOR I = 1 TO LABEL
4015      VRFL(I) = ABS((SUMSQL(I) -(SUML(I)^2/N))/(N-1))
4025      VLRT(I) = ABS((SUMSQLT(I)-(SUMLT(I)^2/N))/(N-1))
4030   NEXT I

4035   FOR I = 1 TO NAT
4040      VRFN(I) = ABS((SUMSQN(I)-(SUMN(I)^2/N))/(N-1))
4050      VNRT(I) = ABS((SUMSQNT(I)-(SUMNT(I)^2/N))/(N-1))
4055   NEXT I

4060   FOR I = 1 TO LABEL
4065     IF RFLA(I)>0 THEN RSDRFL(I)=SQR(VRFL(I))/RFLA(I) ELSE RSDRFL(I)=0
4075     IF LRTA(I)>0 THEN RSDLRT(I)=SQR(VLRT(I))/DLRTA(I) ELSE RSDLRT(I)=0
4080   NEXT I

4082   FOR I = 1 TO NAT
4085     IF RFNA(I)>0 THEN RSDRFN(I)=SQR(VRFN(I))/RFNA(I) ELSE RSDRFN(I)=0
4095     IF NRTA(I)>0 THEN RSDNRT(I)=SQR(VNRT(I))/DNRTA(I) ELSE RSDNRT(I)=0
4100   NEXT I

4990   RETURN


5000   REM Subroutine: biosignificant standard, RT and RRT data
5010   ALYTE$(1)= "2378-TCDF" : ALYTE$(2)= "2367-TCDF" : ALYTE$(3)= "3467-TCDF"
5015   ALYTE$(4)= "1234-TCDD" : ALYTE$(5)= "2378-TCDD" : ALYTE$(6)= "13467-PCDF"
5020   ALYTE$(7)= "12378-PCDF" : ALYTE$(8)= "12367-PCDF" : ALYTE$(9)= "23478-PCDF"
5025   ALYTE$(10)= "23467-PCDF" : ALYTE$(11)= "12378-PCDD" : ALYTE$(12)= "123478-HxCDF"
5030   ALYTE$(14)= "123678-HxCDF" : ALYTE$(15)= "234678-HxCDF" : ALYTE$(17)= "123478-HxCDD"
5035   ALYTE$(18)= "123678-HxCDD" : ALYTE$(19)= "123789-HxCDD" : ALYTE$(20)= "1234678-HpCDF"
5040   ALYTE$(21)= "1234789-HpCDF" : ALYTE$(22)= "1234678-HpCDD"
5045   ALYTE$(23)= "OCDF"  :  ALYTE$(24)= "OCDD"
5047   REM add new analytes to target list 9-17-86
5048   ALYTE$(13)= "123467-HxCDF" : ALYTE$(16)= "123789-HxCDF"
```

```
5050   REM Natural ions for biosig standard
5055   BION(1)= 306 : BION(2)= 306 : BION(3)= 306 : BION(4)= 322 : BION(5)= 322
5060   BION(6)= 340 : BION(7)= 340 : BION(8)= 340 : BION(9)= 340 : BION(10)= 340
5065   BION(11)= 356 : BION(12)= 374 : BION(13)= 374 : BION(14)= 374 : BION(17)= 390
5070   BION(18)= 390 : BION(19)= 390 : BION(20)= 408 : BION(21)= 408 : BION(22)= 424
5075   BION(23)= 444 : BION(24)= 460 : BION(15)= 374 : BION(16)= 374

5080   CLS : PRINT : PRINT
5085   PRINT"This portion of RFACTOR calculates RRT's from your "
5088   PRINT"Biosignificant PCDD/PCDF standard" : PRINT : PRINT : BEEP
5090   INPUT"Strike ENTER key when ready ...", ANY$
5092   REM
5095   HALFNAT = 24

5100   FOR B = 1 TO HALFNAT
5110         CLS  :  PRINT  :  PRINT
5120         PRINT "Enter your retention time for "
5130         PRINT ALYTE$(B) : PRINT
5140         INPUT" "; BRT(B)
             CLS : PRINT : PRINT
             PRINT ALYTE$(B), BRT(B) : PRINT
             INPUT"Is the data correct? Answer 'Y' or 'N'"; CORRECT$
             IF CORRECT$= "N" THEN 5110 ELSE 5150
5150   NEXT B
5153   CLS

5155   REM  Substitute values from Q for isomers not in biosig standard
5157   BRT(4) = NRTA(8) : REM 1234789-HpCDF not in Q or biosig standards

5160   REM Calculate RRT's
5170   FOR B = 1 TO HALFNAT
5180          IF BRT(B)<>0 THEN DBRT(B) = FNCONVERT(BRT(B)) ELSE DBRT(B)=0
5190   NEXT B

5200   FOR B = 1 TO HALFNAT
5210          IF DBRT(5)<>0 THEN RRBT(B) = DBRT(B)/DBRT(5) ELSE RRBT(B)=0
5220   NEXT B

5300   RETURN


5500   REM Subroutine:  output user input to printer
5510   CLS : PRINT : PRINT
       PRINT"Adjust your printer paper, if necessary, for hardcopy"
       INPUT"Strike the ENTER key when ready ...", ANY$
       CLS : PRINT : PRINT

5520   PRINT"Your input will now be sent to the printer."
5540   FINP$=" ##    ##     ############     ##.##      "

5545   FOR J = 1 TO N
5550   FOR I = 1 TO LABEL
           LPRINT USING FINP$; J, I, LP(I,J), LRT(I,J)
5560   NEXT I
```

```
5580  FOR I = 1 TO NAT
          LPRINT USING FINP$; J, I, NP(I,J), NRT(I,J)
5590  NEXT I

5592  LPRINT : LPRINT : LPRINT : LPRINT : LPRINT

5595  NEXT J

5600  PRINT"If it is accurate, enter 'Y'. If it contains mistakes,"
5610  INPUT"enter 'N' "; INP$
5620  IF INP$ = "N" THEN 200 ELSE 5990

5990  RETURN


5995  REM  Subroutine: RT and RRT values from WSU window marker standard
      REM not being used in this version
      RETURN

7000  REM Subroutine: Disk, printer output for average RF, RRF, RT, SD
7002  LION(1)= 334 : LION(2)= 318 : LION(3)= 328 : LION(4)= 328 : LION(5)= 352
7004  LION(6)= 368 : LION(7)= 386 : LION(8)= 402 : LION(9)= 420 : LION(10)= 436
7006  LION(11)= 456 : LION(12)= 472
7010  NION(1)= 304 : NION(2)= 306 : NION(3)= 304 : NION(4)= 306 : NION(5)=304 : NION(6)=306
7012  NION(7)= 320 : NION(8)= 322 : NION(9)= 320 : NION(10)= 322 : NION(11)=340 : NION(12)= 342
7013  NION(13)= 340 : NION(14)= 342 : NION(15)= 340 : NION(16)= 342 : NION(17)= 340 : NION(18)= 342
7014  NION(19)= 340 : NION(20)= 342 : NION(21)= 356 : NION(22)= 358 : NION(23)= 374 : NION(24)= 376
7015  NION(25)= 374 : NION(26)= 376 : NION(27)= 374 : NION(28)= 376 : NION(33)= 390 : NION(34)= 392
7016  NION(35)= 390 : NION(36)= 392 : NION(37)= 390 : NION(38)= 392 : NION(39)= 408 : NION(40)= 410
7017  NION(41)= 408 : NION(42)= 410 : NION(43)= 424 : NION(44)= 426 : NION(45)= 444 : NION(46)= 446
7018  NION(47)= 458 : NION(48)= 460 : NION(29)= 374 : NION(30)= 376 : NION(31)= 374 : NION(32)= 376

7019  CLS  :   PRINT  :  PRINT : BEEP
7020  PRINT "Place your disk in drive A or B, for output of RF and RRF."
7030  PRINT "Enter the complete name of your file in quotation marks, "
7040  INPUT "including the drive designator: ", RSFAC$
7050  REM
7060  OPEN RSFAC$ FOR OUTPUT AS #1
7061  LPRINT"File I.D. :  "; RSFAC$
7062  LPRINT"Output from RFACTOR program"
7063  LPRINT"The number of standards averaged was "; N
7064  LPRINT"@ Standard Data "
7065  FORM$="     ###   ##.## #.###  ##.##        ###.##       ##.##    ## "
7068  LPRINT" Labeled                             RF                        "
7069  LPRINT"     Ion      RT   RSD    RRT        (Label/334)    RSD    NO."

7070  FOR I = 1 TO LABEL
7080      WRITE #1, LION(I), LRTA(I), RFLA(I),  RRFLA(I)
7090      LPRINT USING FORM$; LION(I), LRTA(I), RSDLRT(I), RRTL(I), RRFLA(I), RSDRFL(I), I
7100  NEXT I
7102  FOR I = 1 TO 47 : LPRINT : NEXT I
7105  LPRINT" Natural                             RF                        "
7106  LPRINT"     Ion      RT   RSD    RRT        (Nat/label)    RSD    NO."
```

```
7110   FOR I = 1 TO NAT
7120     WRITE #1, NION(I), NRTA(I), RFNA(I),  RRFNA(I)
7130     LPRINT USING FORM$; NION(I), NRTA(I), RSDNRT(I), RRTN(I), RRFNA(I), RSDRFN(I), I
7140   NEXT I

7150   REM  Biosig standard
7155   FOR I = 1 TO 20 : LPRINT : NEXT I
7160   LPRINT"Biosignificant Standard"
7170   LPRINT " Iteration                                          (min.sec)     (RT-PRT)  "
7180   LPRINT "     No.      RT          RRT   Compound           Predicted RT   Error    "
7190   FORMB$="     ###   ##.##      ####.##   \               \  ##.##      #####.#######"
7210   FOR B = 1 TO HALFNAT
7220      LPRINT USING FORMB$; B, BRT(B), RRBT(B), ALYTE$(B), PRMS(B),  Y(B)-EY(B)
7230      WRITE #1, BION(B), BRT(B), RRBT(B), ALYTE$(B)
7240   NEXT B
7250   LPRINT : LPRINT  'regression statistics

       LPRINT "      coefficient of determination  =  ", CR
       LPRINT "        coefficient of correlation  =  ", CC
       LPRINT "standard deviation of the estimate  =  ", SE
       LPRINT
       LPRINT "linear model: Predict decimal RT = ";A;"  +  ";W;" LIB"
       LPRINT : LPRINT

7260   CLOSE #1

7270   RETURN


6000 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

     '       DATA



     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$


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


      RETURN 264


6002       '  Relative Retention Time librarys
           '  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 buit yet, you lose buddy!"  'GOTO 6020
          INPUT"Strike the ENTER key to return to the last menu", ANY$
          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            '  12367-PCDF
    LIB(09)  =  22.75            '  23478-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                '  23478-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
```

```
      ' from Doug Kuehl, east coast flyash paper Feb 86
      ' old temp program

     LIB(01)   =  23.450            '  2378-TCDF
     LIB(02)   =  24.400            '  2367-TCDF
     LIB(03)   =  25.900            '  3467-TCDF
     LIB(04)   =  19.650            '  1234-TCDD
     LIB(05)   =  19.380            '  2378-TCDD
     LIB(06)   =  22.650            '  13467-PCDF
     LIB(07)   =  24.400            '  12378-PCDF
     LIB(08)   =  25.267            '  12367-PCDF
     LIB(09)   =  32.733            '  23478-PCDF
     LIB(10)   =  34.067            '  23467-PCDF
     LIB(11)   =  26.100            '  12378-PCDD
     LIB(12)   =  31.800            '  123478-HxCDF
     LIB(13)   =  33.017            '  123467-HxCDF
     LIB(14)   =  32.167            '  123678-HxCDF
     LIB(15)   =  46.267            '  234678-HxCDF
     LIB(16)   =  42.217            '  123789-HxCDF
     LIB(17)   =  34.933            '  123478-HxCDD
     LIB(18)   =  35.356            '  123678-HxCDD
     LIB(19)   =  38.183            '  123789-HxCDD
     LIB(20)   =  42.483            '  1234678-HpCDF
     LIB(21)   =  56.217            '  1234789-HpCDF
     LIB(22)   =  51.950            '  1234678-HpCDD
     LIB(23)   =  74.700            '  OCDF
     LIB(24)   =  76.333            '  OCDD

     RETURN



6100   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        'OCTAS 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


6250 IF(IP<1) OR (IP>4) THEN 6190
```

```
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 I<> (IC*15) THEN 6400
              IC=IC+1
              PRINT:INPUT "Strike the ENTER key to continue ... ",Y$:PRINT
6400          PRINT LIB(I), BRT(I)
6410 NEXT I
     PRINT : INPUT"Strike the ENTER key to continue ...", ANY$

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:SX2=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    SX2= ABS(  SX2+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 X*Y
6600 NEXT I
6610 W=(IN*SXY-SX*SY)/(IN*SX2-SX^2)     'SLOPE OF LINE
6620 A=(SY-W*SX)/IN                     'INTERCEPT OF LINE
6630 REM Coefficient of correlation



6640 SQXY = (SQR((SX2-(SX^2)/IN)*(SY2-(SY^2)/IN)))
     IF(SQXY <= 0) THEN
        CC = 0
        CR = 0
        ELSEIF(SQXY >0) THEN
        CC=(SXY-SX*SY/IN)/ SQXY             'COEFFICIENT OF DETERMINATION
        CR = CC^2
     END IF

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


6690 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:PRINT "ACTUAL VERSUS ESTIMATED VALUES"
6760 PRINT "X", "Y", "ESTIMATED Y", "ERROR"
6770 IC=1
6780 FOR I=1 TO IN
6790     IF I<>(IC*14) THEN 6820
6800     PRINT:INPUT "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

     REM  Convert EY(i) from decimal to minsec format
     FOR I = 1 TO IN
           PRMS(I) = FNMINSEC(EY(I))
     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."
        PRINT : PRINT
        PRINT" CHECK YOUR ISOMER ASSIGNMENTS AND/OR THE QUALITY OF "
        PRINT" YOUR CHROMATOGRAPHY, assuming you entered the RT data correctly."
     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 : PRINT"Adjust the printer paper for your RFACTOR output"
       PRINT : PRINT
       INPUT"Strike the enter key when ready ...", ANY$
       CLS


      RETURN 264
```

```
10 REM          Program DFQUANT Ver. 6.1 1/23/87
20 REM          Murray Hackett
30 REM          Toxicology Program
40 REM          Oregon State University
50 REM          Corvallis, Oregon  97331
60 REM          60 meter DB5 version
70 REM          A program in ten subroutines to quantify
80 REM          dioxin/furan residues from GC-MS data

100    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), LHB(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 SGNS(30), SNMDL(30), NQ(30), HB(30), HS(30), HQ(30), QNRT(50)
142    DIM CQA(30), SGDS(30), RRTL(30), RRTN(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))/.60)
160    END DEF
162    DEF FNMINSEC(Y)
164        FNMINSEC = INT(Y) + ((Y-INT(Y))*.60)
168    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 ...  ", ANY$
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 3385 : 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
```

```
2500    REM Subroutine to read RF and RRF values from disk file
2505    CLS  :  PRINT :  PRINT
2510    PRINT "Place your diskette with RF'S in drive A or B."
2515    PRINT "Enter the complete name of your file in quotation marks, "
2520    INPUT "including the drive designator:  ", RFAC$
2522    CLS
2525    OPEN  RFAC$  FOR INPUT AS #2
2530    FOR J = 1 TO LABEL
2535        INPUT #2, QLION(J), LRT(J), RFL(J), RRFL(J)
2540    NEXT J
2545    FOR K = 1 TO NAT
2550        INPUT #2, QNION(K), QNRT(K), RFN(K), RRFN(K)
2560    NEXT K
2566    FOR I = 1 TO CONC
2567        INPUT #2, BION(I), BRT(I), RRBT(I), ALYTE$(I)
2568    NEXT I
2565    CLOSE #2
2570    RETURN


2600    REM Subroutine to enter raw data from disk file
2610    PRINT "Quantification of an unknown sample "
2620    PRINT : PRINT
2630    PRINT "Do you wish to enter peak area and RT data from disk file"
2640    PRINT "or interactively from your written notes? "
2650    INPUT "enter 'D'for disk or 'I' for interactive:  ", UNKNO$
2660    IF UNKNO$ = "D" THEN 2670 ELSE IF UNKNO$ = "I" THEN RETURN
2670    PRINT : PRINT
2680    PRINT"Enter your data base file name, in quotes, including"
2690    INPUT"the drive designator:  ", RAWDAT$
2695    OPEN RAWDAT$ FOR INPUT AS #3
2700        INPUT #3, MSID$, PCID$, OTHER$
2705        FOR I = 1 TO LABEL
                INPUT #3, LION(I), SLRT(I), RRTL(I), RECC(I), QREC(I)
2710        NEXT I
2715        FOR I = 1 TO CONC
2720            INPUT #3, BION(I), NRT(I), CRRTN(I), C(I), CD(I), RATS(I), THEORY(I)
2725            INPUT #3, HS(I), SGNS(I), SNMDL(I), CQA(I), SGDS(I)
2730        NEXT I
2735    REM  User input, should not normally be used in data base
2740        FOR I = 1 TO LABEL
2745            INPUT #3, SLP(I), LRT(I)
2750        NEXT I
2755        FOR I = 1 TO NAT
2760            INPUT #3,  SNP(I), SNRT(I)
2765        NEXT I
2770        INPUT #3,  LHB(1), LHS(1), LHQ(1)
2775        FOR I = 1 TO CONC
2780            INPUT #3,  HB(I), HS(I), HQ(I)
2790        NEXT I
2795        CLOSE #3
2800    CLS
2939    RETURN
```

```
3000  REM Subroutine:  interactive input
3010  IF UNKNO$ = "D" THEN 3355  ELSE  3028
3028  CLS
3030  INPUT "enter peak areas for 2378 TCDF, 304 and 306 "; SNP(1), SNP(2)
3032  INPUT "enter RT's for 304, 306 "; SNRT(1), SNRT(2)
3034  CLS
3036  INPUT "enter peak areas for 2367 TCDF, 304 and 306 "; SNP(3), SNP(4)
3038  INPUT "enter RT's for 304, 306 "; SNRT(3), SNRT(4)
3040  CLS
3042  INPUT "enter peak areas for 3467 TCDF, 304 and 306 "; SNP(5), SNP(6)
3044  INPUT "enter RT's for 304, 306 "; SNRT(5), SNRT(6)
3046  CLS
3048  INPUT "enter peak area for 13C12 2378 TCDF, 318 "; SLP(2)
3050  INPUT "enter RT for 13C12 2378 TCDF "; SLRT(2)
3055  CLS
3060  INPUT "enter peak areas for 1234 TCDD, 320 and 322 "; SNP(7), SNP(8)
3065  INPUT "enter RT's for 320, 322 "; SNRT(7), SNRT(8)
3070  CLS
3075  INPUT "enter peak areas for 2378 TCDD, 320 and 322 "; SNP(9), SNP(10)
3080  INPUT "enter RT's for 320, 322 "; SNRT(9), SNRT(10)
3085  CLS
3090  INPUT "enter peak area for 37CL4 2378 TCDD, 328 "; SLP(4)
3095  INPUT "enter RT for 37CL4 2378 TCDD "; SLRT(4)
3100  CLS
3105  INPUT "enter peak area for 13C6 1234 TCDD, 328 "; SLP(3)
3115  INPUT "enter RT for 13C6 1234 TCDD  "; SLRT(3)
3120  CLS
3125  INPUT "enter peak area for 13C12 1234 TCDD, 334 "; SLP(1)
3130  INPUT "enter RT for 13C12 1234 TCDD  "; SLRT(1)
3135  CLS
3138  INPUT "enter peak areas for 13467 PCDF, 340 and 342 "; SNP(11), SNP(12)
3140  INPUT "enter RT's for 340, 342 "; SNRT(11), SNRT(12)
3142  CLS
3144  INPUT "enter peak areas for 12378 PCDF, 340 and 342 "; SNP(13), SNP(14)
3146  INPUT "enter RT's for 340, 342 "; SNRT(13), SNRT(14)
3148  CLS
3150  INPUT "enter peak areas for 12367 PCDF, 340 and 342 "; SNP(15), SNP(16)
3152  INPUT "enter RT's for 340, 342 "; SNRT(15), SNRT(16)
3154  CLS
3156  INPUT "enter peak areas for 23478 PCDF, 340 and 342 "; SNP(17), SNP(18)
3158  INPUT "enter RT's for 340, 342 "; SNRT(17), SNRT(18)
3160  CLS
3162  INPUT "enter peak areas for 23467 PCDF, 340 and 342 "; SNP(19), SNP(20)
3164  INPUT "enter RT's for 340, 342 "; SNRT(19), SNRT(20)
3166  CLS
3168  INPUT "enter peak area for 13C12 12378 PCDF, 352 "; SLP(5)
3170  INPUT "enter peak RT for 13C12 12378 PCDF "; SLRT(5)
3172  CLS
3174  INPUT "enter peak areas for 12378 PCDD, 356 and 358 "; SNP(21), SNP(22)
3176  INPUT "enter RT's for 356, 358 "; SNRT(21), SNRT(22)
3178  CLS
3180  INPUT "enter peak area for 13C12 12378 PCDD, 368 "; SLP(6)
3182  INPUT "enter RT for 13C12 12378 PCDD "; SLRT(6)
3184  CLS
```

```
3186  INPUT "enter peak areas for 123478 HxCDF, 374 and 376 "; SNP(23), SNP(24)
3188  INPUT "enter RT's for 374, 376 "; SNRT(23), SNRT(24)
3189  CLS
3190  INPUT "enter peak areas for 123467 HxCDF, 374 and 376 "; SNP(25), SNP(26)
3191  INPUT "enter RT's for 374, 376 "; SNRT(25), SNRT(26)
3192  CLS
3193  INPUT "enter peak areas for 123678 HxCDF, 374 and 376 "; SNP(27), SNP(28)
3194  INPUT "enter RT's for 374, 376 "; SNRT(27), SNRT(28)
3196  CLS
3197  INPUT "enter peak areas for 234678 HxCDF, 374 and 376 "; SNP(29), SNP(30)
3198  INPUT "enter RT's for 374, 376 "; SNRT(29), SNRT(30)
3199  CLS
3200  INPUT "enter peak areas for 123789 HxCDF, 374 and 376 "; SNP(31), SNP(32)
3201  INPUT "enter RT's for 374, 376 "; SNRT(31), SNRT(32)
3202  CLS
3204  INPUT "enter peak area for 13C12 123478 HxCDF, 386 "; SLP(7)
3206  INPUT "enter RT for 13C12 123678 HxCDF "; SLRT(7)
3208  CLS
3210  INPUT "enter peak areas for 123478 HxCDD, 390 and 392 "; SNP(33), SNP(34)
3212  INPUT "enter RT's for 390, 392 "; SNRT(33), SNRT(34)
3214  CLS
3216  INPUT "enter peak areas for 123678 HxCDD, 390 and 392 "; SNP(35), SNP(36)
3218  INPUT "enter RT's for 390, 392 "; SNRT(35), SNRT(36)
3220  CLS
3222  INPUT "enter peak areas for 123789 HxCDD, 390 and 392 "; SNP(37), SNP(38)
3224  INPUT "enter RT's for 390, 392 "; SNRT(37), SNRT(38)
3226  CLS
3228  INPUT "enter peak area for 13C12 123678 HxCDD, 402 "; SLP(8)
3230  INPUT "enter RT for 13C12 123678 HxCDD "; SLRT(8)
3232  CLS
3234  INPUT "enter peak areas for 1234678 HpCDF, 408 and 410 "; SNP(39),SNP(40)
3238  INPUT "enter RT's for 408, 410 "; SNRT(39), SNRT(40)
3240  CLS
3242  INPUT "enter peak areas for 1234789 HpCDF, 408 and 410 "; SNP(41),SNP(42)
3246  INPUT "enter RT's for 408, 410 "; SNRT(41), SNRT(42)
3248  CLS  : REM  This isomer is not in any biosig or Q standard
3260  INPUT "enter peak area for 13C12 1234678 HpCDF, 420  "; SLP(9)
3265  INPUT "enter RT for 13C12 1234678 HpCDF "; SLRT(9)
3270  CLS
3275  INPUT "enter peak areas for 1234678 HpCDD, 424, 426 "; SNP(43), SNP(44)
3280  INPUT "enter RT for 424, 426 "; SNRT(43), SNRT(44)
3285  CLS
3290  INPUT "enter peak area for 13C12 1234678 HpCDD, 436 "; SLP(10)
3295  INPUT "enter RT for 13C12 1234678 HpCDD "; SLRT(10)
3300  CLS
3305  INPUT "enter peak areas for OCDF, 444 and 446 "; SNP(45), SNP(46)
3310  INPUT "enter RT's for 444, 446 "; SNRT(45), SNRT(46)
3312  CLS
3315  INPUT "enter peak area for 13C12 OCDF, 456 "; SLP(11)
3320  INPUT "enter RT for 13C12 OCDF "; SLRT(11)
3325  CLS
3330  INPUT "enter peak areas for OCDD, 458 and 460 "; SNP(47), SNP(48)
3335  INPUT "enter RT's for 458, 460 "; SNRT(47), SNRT(48)
3340  CLS
3345  INPUT "enter peak area for 13C12 OCDD, 472 "; SLP(12)
```

```
3350   INPUT "enter RT for 13C12 OCDD "; SLRT(12)

3355 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$

3357 FOR I = 1 TO 2 : LPRINT : NEXT I
3360 INP$ = " ###############   ##.##    ##           "
3361 LPRINT"USER INPUT"
3362 LPRINT "   Labeled  Ion   RT       Iteration     "
3364 FOR I = 1 TO LABEL
3366    LPRINT USING INP$; SLP(I), SLRT(I), I
3368 NEXT I
3370 FOR I = 1 TO 50 : LPRINT : NEXT I
3371 LPRINT"USER INPUT"
3372 LPRINT "   Natural Ion    RT       Iteration     "
3374 FOR I = 1 TO NAT
3376    LPRINT USING INP$; SNP(I), SNRT(I), I
3377 NEXT I
     FOR I = 1 TO 20 : LPRINT : NEXT I

3378 CLS : PRINT : PRINT
3379 PRINT"Please inspect the hardcopy of your input to make "
3380 INPUT"sure it is correct; type 'Y' or 'N':   ", CHOICE$
3381 IF CHOICE$ = "Y" THEN  RETURN ELSE 3028


3385   REM Subroutine:  quantitation calculations
3386   CLS :  PRINT : PRINT :  REM   enter mass of sample in grams
3387   INPUT "enter sample mass in units of grams:  ", MASS
3389   REM  constant to correct for sample size
3390   KC = 20/MASS
3392   REM   Input constant to adjust for volume of spiking soln
3394   CLS  :  PRINT  :  PRINT
3395   PRINT "Enter volume of spiking soln added to sample,   "
3396   INPUT "'100', '200', '300' or '400'microliters:  ", KS
3397   KSP=KS/100
3398   K334 = 100  :  REM remove redundant code for next version
3400   REM  calculate "wet weight" concentration of analyte in sample
       REM tcdf
3410  IF (SLP(2)<>0 AND RRFN(2)<>0) THEN  C(1) = SNP(2)*25*KC*KSP/ (SLP(2)*RRFN(2)) ELSE C(1) = 0
3412  IF (SLP(2)<>0 AND RRFN(4)<>0) THEN  C(2) = SNP(4)*25*KC*KSP/ (SLP(2)*RRFN(4)) ELSE C(2) = 0
3414  IF (SLP(2)<>0 AND RRFN(6)<>0) THEN  C(3) = SNP(6)*25*KC*KSP/ (SLP(2)*RRFN(6)) ELSE C(3) = 0
     REM 1234 tcdd
3416  IF (SLP(3) <> 0 AND RRFN(8) <> 0) THEN C(4) = SNP(8)*25*KC*KSP/ (SLP(3)*RRFN(8)) ELSE C(4) = 0
     REM 2378 tcdd
3418  IF (SLP(4) <>0 AND RRFN(10)<>0) THEN C(5) = SNP(10)*25*KC*KSP/ (SLP(4)* RRFN(10)) ELSE C(5) = 0
     REM pcdf
3420  IF (SLP(5)<>0 AND RRFN(11)<>0) THEN  C(6) = SNP(11)*50*KC*KSP/ (SLP(5)*RRFN(11)) ELSE C(6) = 0
3422  IF (SLP(5)<>0 AND RRFN(13)<>0) THEN  C(7) = SNP(13)*50*KC*KSP/ (SLP(5)*RRFN(13)) ELSE C(7) = 0
3424  IF (SLP(5)<>0 AND RRFN(15)<>0) THEN  C(8) = SNP(15)*50*KC*KSP/ (SLP(5)*RRFN(15)) ELSE C(8) = 0
3426  IF (SLP(5)<>0 AND RRFN(17)<>0) THEN  C(9) = SNP(17)*50*KC*KSP/ (SLP(5)*RRFN(17)) ELSE C(9) = 0
3428  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 pcdd
```

```
3430  IF (SLP(6)<>0 AND RRFN(21)<>0) THEN C(11) = SNP(21)*50*KC*KSP/ (SLP(6)*RRFN(21)) ELSE C(11) = 0
      REM hxcdf
3432  IF (SLP(7)<>0 AND RRFN(23)<>0) THEN  C(12) = SNP(23)*100*KC*KSP/  (SLP(7)*RRFN(23)) ELSE C(12) = 0
3434  IF (SLP(7)<>0 AND RRFN(25)<>0) THEN  C(13) = SNP(25)*100*KC*KSP/  (SLP(7)*RRFN(25)) ELSE C(13) = 0
3436  IF (SLP(7)<>0 AND RRFN(27)<>0) THEN  C(14) = SNP(27)*100*KC*KSP/  (SLP(7)*RRFN(27)) ELSE C(14) = 0
3437  IF (SLP(7)<>0 AND RRFN(29)<>0) THEN  C(15) = SNP(29)*100*KC*KSP/  (SLP(7)*RRFN(29)) ELSE C(15) = 0
3438  IF (SLP(7)<>0 AND RRFN(31)<>0) THEN  C(16) = SNP(31)*100*KC*KSP/  (SLP(7)*RRFN(31)) ELSE C(16) = 0

      REM hxcdd
3439  IF (SLP(8)<>0 AND RRFN(33)<>0) THEN C(17) =  SNP(33)*100*KC*KSP/ (SLP(8)*RRFN(33)) ELSE C(17) = 0
3440  IF (SLP(8)<>0 AND RRFN(35)<>0) THEN C(18) =  SNP(35)*100*KC*KSP/ (SLP(8)*RRFN(35)) ELSE C(18) = 0
3442  IF (SLP(8)<>0 AND RRFN(37)<>0) THEN C(19) =  SNP(37)*100*KC*KSP/ (SLP(8)*RRFN(37)) ELSE C(19) = 0
      REM  hpcdf
3444       IF (SLP(9)<>0 AND RRFN(39)<>0) THEN C(20) = SNP(39)*100*KC* KSP /(SLP(9)*RRFN(39)) ELSE C(20) = 0
3446       IF (SLP(9)<>0 AND RRFN(41)<>0) THEN C(21) = SNP(41)*100*KC* KSP /(SLP(9)*RRFN(41)) ELSE C(21) = 0
3448  REM IF (RFN(39)<>0) THEN C(20) = SNP(39)*KC*K334/((RFN(39)/RFL(1))*SLP(1))  ELSE C(20) = 0
3450  REM IF (RFN(41)<>0) THEN C(21) = SNP(41)*KC*K334/((RFN(41)/RFL(1))*SLP(1))  ELSE C(21) = 0
      REM hpcdd
3452  IF (SLP(10)<>0 AND RRFN(43)<>0) THEN C(22)= SNP(43)*100*KC*KSP/  (SLP(10)*RRFN(43)) ELSE C(22) = 0
      REM  ocdf
3454  IF (SLP(11)<>0 AND RRFN(45)<>0) THEN C(23)= SNP(45)*200*KC*KSP/(SLP(11)*RRFN(45)) ELSE C(23) = 0
3458  REM IF (RFN(45)<>0) THEN  C(23)= SNP(45)*KC*K334/((RFN(45)/RFL(1))*SLP(1))  ELSE C(23) = 0
REM   ocdd
3460  IF (SLP(12)<>0 AND RRFN(48)<>0) THEN C(24)= SNP(48)*200*KC*KSP/  (SLP(12)*RRFN(48)) ELSE C(24) = 0
3600   REM calculate dry weight of tissue or solid
3605   CLS   :    PRINT  :  PRINT
3610   PRINT"Enter % lipid (tissue), 100 - % moisture (solids) or    "
3615   INPUT"0   (water sample):  ", KD
3620   KKD = KD/100
3625   FOR N = 1 TO CONC
3630     IF (KKD>0 AND C(N)>0) THEN CD(N)= C(N)/KKD ELSE CD(N)=0
3635   NEXT N
3640   CLS
3800   RETURN


4000   REM  Subroutine:  calculate % recovery for each isomer group
4005   K334 = 100 : REM Constant for 20 ul volume, 100 pg/ul 13C12 TCDD
4006   REM WARNING!!! Change this constant if I.S. is handled differently
4010   FOR I = 2 TO 4
4015      IF (RRFL(I)<>0 AND SLP(1)<>0) THEN REC(I) = SLP(I)*K334/(RRFL(I) *SLP(1)*KSP*25) ELSE REC(I) = 0
4020   NEXT I
4025   FOR I = 5 TO 6
4030      IF (RRFL(I)<>0 AND SLP(1)<>0) THEN REC(I) = SLP(I)*K334/(RRFL(I) *SLP(1)*KSP*50) ELSE REC(I) = 0
4035   NEXT I
4040   FOR I = 7 TO 10
4045      IF (RRFL(I)<>0 AND SLP(1)<>0) THEN REC(I) = SLP(I)*K334/(RRFL(I) *SLP(1)*KSP*100) ELSE REC(I) = 0
4050   NEXT I
4055   FOR I = 11 TO 12
4060      IF (RRFL(I)<>0 AND SLP(1)<>0) THEN REC(I) = SLP(I)*K334/(RRFL(I) *SLP(1)*KSP*200) ELSE REC(I) = 0
4065   NEXT I
4070   REM   output to video for %recovery subroutine
4075   PRINT
4080   PRINT
4085   PRINT "Congener", "% Recovery "
```

```
4090   FOR I = 2  TO LABEL
4095      PRINT I, REC(I)*100
4100   NEXT I
4105   RETURN


5000   REM  Subroutine for calculating ion ratios for QA
5200   REM  Ratios for unknown sample
5205   FOR L = 1 TO CONC
5210   FOR J = 1 TO (2*L)-1 STEP 2
5215   FOR K = 2 TO (J+1) STEP 2
5225      IF (SNP(K) = 0) THEN RATS(L) = 0 ELSE RATS(L) = SNP(J)*1/SNP(K)
5230   NEXT K
5235   NEXT J
5240   NEXT L
5250   REM  set flag to mark if ratios fall within allowable ranges
5260   FOR M = 1 TO 5  : REM tetras
         IF (RATS(M) < .655 OR RATS(M) >.865) THEN RATRANGE(M) = 0 ELSE RATRANGE(M) = 1
5270   NEXT M
5280   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
5290   NEXT M
5300   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
5310   NEXT M
5320   FOR M = 20 TO 22 : REM heptas
         IF (RATS(M) < .865 OR RATS(M) >1.22) THEN RATRANGE(M) = 0 ELSE RATRANGE(M) = 1
5330   NEXT M
5335    REM  ocdf and ocdd ratranges
5340    IF (RATS(23) < 1.28 OR RATS(23) > 1.78) THEN RATRANGE(23) = 0 ELSE RATRANGE(23) = 1
5350    IF (RATS(24) < .675 OR RATS(24) > 1.13) THEN RATRANGE(24) = 0 ELSE RATRANGE(24) = 1
5490   CLS
5500   RETURN


7000    REM  Subroutine calculates detection limits, S/N
7100    REM  pg/ul values for Q series standards
7110    CLS   :   PRINT  :  PRINT
7120    PRINT "Choose the lowest concentration Q series standard "
7130    PRINT "in your set which can be used to generate MDL's   "
7135    KQA334 = 100 : REM pg/ul 13C12 1234-TCDD in Q series standards
7140    INPUT "Enter '1', '2', '3', or '4':  ", QQ
7150    IF QQ = 1 THEN 7160 ELSE IF QQ = 2 THEN 7200 ELSE IF QQ = 3 THEN_
        7300 ELSE IF QQ = 4 THEN 7400
7160    REM  Values for variable NQ, standard Q1, assume same value for missing biosigs as Q
7165    NQ(1) = 1      : NQ(2) = 1     : NQ(3) = 1     : NQ(4) = 2.5
7170    NQ(5) = 1      : NQ(6) = 2     : NQ(7) = 2     : NQ(8) = 2
7175    NQ(9) = 2       : NQ(10)= 2      : NQ(11)= 2
7180    NQ(12) = 4      : NQ(13) = 4     : NQ(14) = 4     : NQ(15) = 4
7185    NQ(16) = 4      : NQ(17) = 4     : NQ(18) = 4     : NQ(19) = 4
7190    NQ(20) = 4      : NQ(21)= 4      : NQ(22) = 4     : NQ(23) = 8    :  NQ(24) = 8
7195    GOTO  7700
7200    REM  Values for variable NQ, standard Q2
7205    NQ(1) = 5      : NQ(2) = 5     : NQ(3) = 5      : NQ(4) = 2.5
7210    NQ(5) = 5      : NQ(6) = 10    : NQ(7) = 10     : NQ(8) = 10
```

```
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) = 12.5      : 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 "
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(1)
8320   FOR I = 1 TO CONC
8322      PRINT  BION(I), ALYTE$(I), HQ(I)
8324   NEXT I
8328   INPUT"Is your data correct? Type 'Y' or 'N':  ", CHECK$
8330   IF CHECK$ = "Y" THEN 8370 ELSE 8270
8370   CLS : PRINT : PRINT
8380   PRINT"Enter your peak height data for the noise windows in your sample:  "
8382   INPUT "Strike ENTER key when ready ... ", ANY$
8384   CLS : PRINT : PRINT
8386   INPUT "Enter your peak height for 13C12 1234-TCDD, 334 ion:  ", LHB(1)
8388   CLS : PRINT : PRINT

8390   FOR I = 1 TO CONC
8392     PRINT"Enter your peak height for "; ALYTE$(I);
         PRINT" ion ";
         PRINT BION(I)
8394     INPUT HB(I)
8396     CLS : PRINT : PRINT
8398   NEXT I

8399   REM  default noise to two counts (8230 only), no democracy here!
       FOR I = 1 TO CONC
           IF( HB(I)<>0 AND HB(I)<2 ) THEN
           HB(I) = 2
           END IF
8400   NEXT I

8401   CLS
8402   PRINT" 334", "13C12 TCDD",  LHB(1)
8404   FOR I = 1 TO CONC
8408      PRINT  BION(I), ALYTE$(I), HB(I)
8410   NEXT I
8412   INPUT"Is your data correct? Type 'Y' or 'N':  ", CHECK$
8414   IF CHECK$ = "Y" THEN 8456 ELSE 8370

8456   CLS : PRINT : PRINT
8460   PRINT"Enter your peak height data for sample peak heights:   "
8462   INPUT "Strike ENTER key when ready ... ", ANY$
8464   CLS : PRINT : PRINT
8466   INPUT "Enter your peak height for 13C12 1234-TCDD, 334 ion:  ", LHS(1)
8468   CLS : PRINT : PRINT
8470   FOR I = 1 TO CONC
8472     PRINT"Enter your peak height for "; ALYTE$(I);
         PRINT" ion ";
         PRINT BION(I)
8474     INPUT HS(I)
8476     CLS : PRINT : PRINT
8478   NEXT I
8480   CLS
```

```
8481    REM  default sample to two counts (8250 only)
        FOR I = 1 TO CONC
            IF( HS(I)<>0 AND HS(I)<2 ) THEN
            HS(I) = 2
            END IF
8482    NEXT I

8483    PRINT" 334", "13C12 TCDD",  LHS(I)
8484    FOR I = 1 TO CONC
8486       PRINT  BION(I), ALYTE$(I), HS(I)
8488    NEXT I
8490    INPUT"Is your data correct? Type 'Y' or 'N':  ", CHECK$
8492    IF CHECK$ = "Y" THEN 8495 ELSE 8456

8495    REM Output peak heights entered for S/N and MDL calcs
        CLS
        FOR Z = 1 TO CONC   : PRINT HQ(Z), HB(Z), HS(Z) : NEXT Z

8497    LION(1) = 334 : IS = 0
8498    INPMDL$ = "  ###     ########      ########      ########    ##        "
        LPRINT"USER INPUT"
8500    LPRINT    "  Ion  Peak Height   Peak Height   Peak Height             "
8502    LPRINT    "             Noise        Sample      Standard    Iteration "
8504    LPRINT USING INPMDL$; LION(1), LHB(1), LHS(1), LHQ(1), IS
8506    FOR N = 1 TO CONC
8508       LPRINT USING INPMDL$; BION(N), HB(N), HS(N),  HQ(N), N
8510    NEXT N
8512    FOR I = 1 TO 34 : LPRINT : NEXT I

8515    CLS : PRINT : PRINT : BEEP
8520    INPUT"Is your data correct? Type 'Y' or 'N':  ", CHECK$
8530    IF CHECK$ = "Y" THEN 8540 ELSE 8000

8540    REM  Calculate S/N for positives, S/N and MDL for negatives
8545    KMDL = 20 : REM  Constant assumes 20 ul  final volume in microvial
8550    FOR M = 1 TO CONC : REM logic is not easy to follow
8560        IF (HB(M)<>0) THEN 8570 ELSE 8590
8570        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 SGNS(M) = 0

            IF (SGNS(M) = 0) THEN 8590 ELSE 8610

8590        IF (HS(M)<>0) THEN SNMDL(M) =  (HQ(M)/ LHQ(1)) /((HS(M)/LHS(1))*2.5) ELSE SNMDL(M)=0

8595        REM mdl for negatives
8600        IF (QAREC(M)<>0 AND SNMDL(M)<>0) THEN CQA(M)= NQ(M)*KMDL/(QAREC(M)*MASS* SNMDL(M)) ELSE CQA(M) = 0
8605        IF (CQA(M)<.195 AND CQA(M)>0) THEN CQA(M)=.2 ELSE 8610
8610    NEXT M
```

```
8612    CLS : PRINT : PRINT : BEEP :  REM S/N, MDL calcs for 2378-TCDD
8614    PRINT"Did you recover sufficient natural 1234-TCDD for purposes"
8616    PRINT"of calculating an MDL for 2378-TCDD using the 'surrogate "
8618    INPUT"analyte approach? Type 'Y' or 'N':  ", SURR$ : PRINT
8619    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$
8620    IF SURR$ = "Y" THEN 8621 ELSE 8630


8621    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"The program will use the default method instead."
            PRINT : PRINT
            INPUT"Strike the ENTER key when ready...", ANY$
            GOTO 8630
        END IF

8622    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

8630        REM Adjust reported concentrations based on SGDS indicator variable
8632        FOR I = 1 TO CONC
                IF (C(I) < .195 OR SGDS(I)=0)  THEN
                C(I) = 0
                CD(I) = 0
                END IF
8640        NEXT I

8650        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
8660        NEXT I

8690        REM concentrations should remain unchanged if data passes QA
8699    RETURN


8700    REM Subroutine: calculate RRT's for sample
8705    CLS : PRINT : PRINT : BEEP
8708    FOR I = 1 TO LABEL
8709            DSLRT(I) = FNCONVERT(SLRT(I))
8710    NEXT I
8712    FOR I = 1 TO NAT
```

```
8714            DSNRT(I) = FNCONVERT(SNRT(I))
8716    NEXT I
8728    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    NEXT I
8745    FOR I = 1 TO NAT
8750      IF SREFF>0 THEN RRTN(I)= (DSNRT(I)/SREFF) ELSE RRTN(I)=0
8755    NEXT I
8990    RETURN


9000  REM  Subroutine:  prepare final report for sample; output to printer, screen
9002  REM  QA recovery minimums
9004  QREC(2)= 50 : QREC(3)= 50 : QREC(4)= 50 : QREC(5)= 35 : QREC(6)= 35
9006  QREC(7)= 35 : QREC(8)= 35 : QREC(9)= 35 : QREC(10)=35: QREC(11)= 25
9008  QREC(12)= 25
9010  REM  Convert REC(i) to % for output
9012  FOR I = 2 TO LABEL
          RECC(I) = REC(I)*100
      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 : THEORY(I) = 1.23 : NEXT I
9072  THEORY(20) = 1.02 : THEORY(21) = 1.02
9074  THEORY(22) = 1.02 : THEORY(23) = 1.53 : THEORY(24) = .88
9076  REM Translate from n=48 to n=24 retention times for output
9077  M = 0
9078  FOR I = 2 TO NAT STEP 2
          M = I/2
9080      NRT(M) = SNRT(I)
9081      CRRTN(M) = RRTN(I)
9082  NEXT I
9099  PRINT
9100  INPUT "enter mass spec run number:  ", MSID$
9110  INPUT "enter prep chemist I.D. number:  ", PCID$
9120  INPUT "enter other I.D.:  ", OTHER$
9130  CLS  :  KEY OFF
9140  PRINT  :   PRINT  :   PRINT
9150  PRINT "Mass Spec Run Number: "; MSID$
9160  PRINT "Preparation Chemistry I.D. number: "; PCID$
9170  PRINT "Other Sample Identification: "; OTHER$
9180  PRINT
9190  FORM$=" ##       ###  ##.##  ##.##    ###         ###           "
9200  PRINT "      Labeled                  Sample      minimum  QA    "
9210  PRINT "  N       Ion     RT    RRT    % Recovery   % Recovery    "
9220  PRINT " --   -------  -----  -----    ----------  -----------    "
9230  REM
```

```
9240  FOR M = 2 TO LABEL
9250     PRINT USING FORM$; M, LION(M),SLRT(M),RRTL(M), RECC(M), QREC(M)
9260  NEXT M
9270  REM  Report quantitation
9280  PRINT : PRINT
9290  FII$=" ##     ###  ##.##  ##.## ########.# ########.#      #.##  #.##  "
9300  PRINT"      Major                 pg/gram    pg/gram     Ratio  Ratio "
9310  PRINT"  N     ion     RT    RRT        wet        dry  Observed  Theory"
9320  PRINT" --   -----  -----  -----   --------   --------  --------  ------"
9325  FOR M = 1 TO CONC
9330   PRINT USING FII$; M, BION(M),NRT(M),CRRTN(M),C(M), CD(M), RATS(M), THEORY(M)
9335  NEXT M
9340  PRINT
9350  REM  Report for S/N data
9360  F2$ ="  ##    ###  ##.##  ##.##  ######    ######.# #####.#   ######.# "
9370   PRINT"      Major                  Peak   Positives     Not Detectable "
9375   PRINT"   N    ion     RT    RRT  Height         S/N     S/N    at  MDL "
9380   PRINT"  --  -----  -----  ----- -------    --------  ------    ------- "
9385  FOR M = 1 TO CONC
9390   PRINT USING F2$; M, BION(M),NRT(M),CRRTN(M),HS(M),SGNS(M),SNMDL(M),CQA(M)
9392  NEXT M

9393  REM   Output to printer
      PRINT : PRINT
9394  PRINT"If necessary, rearrange your printer paper for DFQUANT'S output. "
9396  INPUT"Strike the ENTER key when ready for output ... ", ANY$
9450  LPRINT "Mass Spec Run Number: "; MSID$
9460  LPRINT "Preparation Chemistry I.D. number: "; PCID$
9470  LPRINT "Other Sample Identification: "; OTHER$
9480  LPRINT
9510  LPRINT "      Labeled                  Sample      minimum  QA    "
9520  LPRINT "  N       Ion     RT    RRT    % Recovery   % Recovery    "
9530  LPRINT " --   -------  -----  -------- ----------  -----------    "
9540  FOR M = 2 TO LABEL
9550     LPRINT USING FORM$; M, LION(M), SLRT(M), RRTL(M), RECC(M), QREC(M)
9560  NEXT M
9570  REM   Quantitation Report
9580  FOR I = 1 TO 6 : LPRINT : NEXT I
9600 LPRINT"      Major                 pg/gram    pg/gram     Ratio  Ratio      "
9610 LPRINT"  N     ion     RT    RRT        wet        dry  Observed  Theoretical"
9620 LPRINT" --   -----  -----  -----   --------   --------  --------  --------   "
9625  FOR M = 1 TO CONC
9630  LPRINT USING FII$; M, BION(M),NRT(M),CRRTN(M),C(M), CD(M), RATS(M), THEORY(M)
9635  NEXT M
9640  REM  Report for S/N data
9645  FOR I = 1 TO 20 : LPRINT : NEXT I : REM  Space output to two sheets
9655  LPRINT"      Major                  Peak   Positives     Not Detectable     "
9660  LPRINT"   N    ion     RT    RRT  Height         S/N     S/N    at  MDL     "
9665  LPRINT"  --  -----  -----  ----- -------    --------  ------    -------     "
9670  FOR M = 1 TO CONC
9675    LPRINT USING F2$;M, BION(M),NRT(M),CRRTN(M),HS(M),SGNS(M),SNMDL(M),CQA(M)
9680  NEXT M
9685  LPRINT : LPRINT

9700  REM   Output to disk file is optional
```

```
9710  CLS  :  PRINT  :  PRINT
9720  PRINT"Do you desire output to a disk file for your report form"
9725  BEEP
9730  INPUT"Enter 'Y' or 'N':  ", DOUT$
9740  IF DOUT$ = "Y" THEN 9750 ELSE 9995
9750  CLS  :  PRINT  :  PRINT
9760  PRINT"Enter the complete name of your output file in quotation
9770  INPUT"marks, including the drive:  ", DFQT$
9780  OPEN DFQT$ FOR OUTPUT AS #4
9790  PRINT #4, :   PRINT #4,
9791  PRINT #4, "Mass Spec Run Number: "; MSID$
9792  PRINT #4, "Preparation Chemistry I.D. number: "; PCID$
9793  PRINT #4, "Other Sample Identification: "; OTHER$
9794  PRINT #4,
9800  PRINT #4, "      Labeled                %          Minimum QA       "
9810  PRINT #4, "  N       Ion    RT    RRT    Recovery   % Recovery       "
9820  PRINT #4, " --     ----- -----  -------- ---------  ----------       "
9840  FOR M = 2 TO LABEL
9850  PRINT #4, USING FORM$; M, LION(M),SLRT(M),RRTL(M), RECC(M), QREC(M)
9860  NEXT M
9870  REM  Report quantitation
9880  PRINT #4,
9900  PRINT #4,"      Major                 pg/gram    pg/gram     Ratio  Ratio      "
9905  PRINT #4,"  N     ion     RT    RRT        wet        dry  Observed  Theoretical"
9910  PRINT #4," --   -----  -----  -----   --------   --------  --------  --------   "
9915  FOR M = 1 TO CONC
9920  PRINT #4, USING FII$; M, BION(M),NRT(M),CRRTN(M),C(M), CD(M), RATS(M), THEORY(M)
9925  NEXT M
9930  PRINT #4,
9940  REM  Report for S/N data
9945  FOR I = 1 TO 25 : PRINT #4, : NEXT I : REM  Space hardcopy over two pages
9955   PRINT #4, "      Major                  Peak   Positives     Not Detectable "
9960   PRINT #4, "   N    ion     RT    RRT  Height         S/N     S/N    at  MDL "
9965   PRINT #4, "  --  -----  -----  ----- -------    --------  ------    ------- "
9970  FOR M = 1 TO CONC
9975  PRINT #4, USING F2$; M, BION(M),NRT(M),CRRTN(M),HS(M),SGNS(M),SNMDL(M),CQA(M)
9980  NEXT M
9985  PRINT #4,  :    PRINT #4,
9990  CLOSE #4
9995  RETURN


10000 REM Subroutine reserved for future expansion, debugging output
10990 RETURN

11000 REM Subroutine:  Output to sequential file to be read into
11010 REM              Phil's data base
11020 CLS : PRINT : PRINT
11030 PRINT"Please enter the name of your file for Phil's data base,"
11040 INPUT"in quotes, including the drive designator:  ", PHIL$
11050 OPEN PHIL$ FOR OUTPUT AS #5
11060 WRITE #5, MSID$, PCID$, OTHER$
11065 FOR I = 1 TO LABEL
11070       WRITE #5, LION(I), SLRT(I), RRTL(I), RECC(I), QREC(I)
11080 NEXT I
```

```
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), SGNS(I), SNMDL(I), CQA(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(1), LHS(1), LHQ(1)
11200 FOR I = 1 TO CONC
11210       WRITE #5, HB(I), HS(I), HQ(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

N	Labeled Ion	RT	RRT	% Recovery	Minimum QA % Recovery
2	318	18.05	0.96	74	50
3	328	0.00	0.00	0	50
4	328	18.53	1.00	74	50
5	352	22.30	1.19	61	35
6	368	24.04	1.27	82	35
7	386	27.27	1.45	59	35
8	402	28.52	1.53	73	35
9	420	31.57	1.69	55	35
10	436	33.31	1.77	55	35
11	456	37.56	2.01	39	25
12	472	37.54	2.01	39	25

N	Major Ion	RT	RRT	pg/gram wet	pg/gram dry	Ratio Observed	Ratio Theoretical
1	306	0.00	0.00	0.0	0.0	0.00	0.76
2	306	0.00	0.00	0.0	0.0	0.00	0.76
3	306	0.00	0.00	0.0	0.0	0.00	0.76
4	322	0.00	0.00	0.0	0.0	0.00	0.76
5	322	18.52	1.00	0.0	0.0	0.65	0.76
6	340	0.00	0.00	0.0	0.0	0.00	1.53
7	340	0.00	0.00	0.0	0.0	0.00	1.53
8	340	0.00	0.00	0.0	0.0	0.00	1.53
9	340	23.33	1.25	40.3	53.0	1.56	1.53
10	340	0.00	0.00	0.0	0.0	0.00	1.53
11	356	24.03	1.27	22.8	29.9	1.36	1.53
12	374	27.28	1.45	96.9	127.5	1.21	1.23
13	374	0.00	0.00	0.0	0.0	0.00	1.23
14	374	27.37	1.46	56.7	74.6	1.22	1.23
15	374	28.27	1.51	17.7	23.3	1.19	1.23
16	374	0.00	0.00	0.0	0.0	0.00	1.23
17	390	28.52	1.53	0.0	0.0	1.21	1.23
18	390	28.52	1.53	2173.4	2859.8	1.21	1.23
19	390	0.00	0.00	0.0	0.0	0.00	1.23
20	408	31.57	1.69	422.7	556.1	0.96	1.02
21	408	0.00	0.00	0.0	0.0	0.00	1.02
22	424	33.31	1.77	2225.6	2928.5	1.02	1.02
23	444	37.56	2.01	31.1	40.9	1.55	1.53
24	460	37.54	2.01	12625.6	16612.6	0.92	0.88

EXAMPLE OF DFQUANT OUTPUT (CONTINUED)

N	Major Ion	RT	RRT	Peak Height	Positives S/N	Not Detectable S/N	at MDL
1	306	0.00	0.00	8	0.0	1.3	2.1
2	306	0.00	0.00	8	0.0	1.3	2.1
3	306	0.00	0.00	8	0.0	1.3	2.1
4	322	0.00	0.00	4	0.0	0.0	0.0
5	322	18.52	1.00	19	0.0	0.4	6.8
6	340	0.00	0.00	5	0.0	2.7	2.4
7	340	0.00	0.00	5	0.0	2.7	2.4
8	340	0.00	0.00	5	0.0	2.7	2.4
9	340	23.33	1.25	169	33.8	0.0	0.0
10	340	0.00	0.00	5	0.0	2.7	2.4
11	356	24.03	1.27	82	20.5	0.0	0.0
12	374	27.28	1.45	536	107.2	0.0	0.0
13	374	0.00	0.00	5	0.0	4.8	2.7
14	374	27.37	1.46	254	50.8	0.0	0.0
15	374	28.27	1.51	93	18.6	0.0	0.0
16	374	0.00	0.00	5	0.0	4.8	2.7
17	390	28.52	1.53	5	0.0	4.1	2.7
18	390	28.52	1.53	7486	1497.2	0.0	0.0
19	390	0.00	0.00	5	0.0	4.1	2.7
20	408	31.57	1.69	1263	157.9	0.0	0.0
21	408	0.00	0.00	10	0.0	2.1	6.8
22	424	33.31	1.77	5311	663.9	0.0	0.0
23	444	37.56	2.01	60	10.0	0.0	0.0
24	460	37.54	2.01	30000	5000.0	0.0	0.0

```
      REM  Program QAD
      REM  Murray Hackett
      REM  Toxicology Program
      REM  Oregon State University
      REM  Corvallis, Oregon  97331

      REM  'Quick And Dirty' output pending Phil's data base
      REM   10-3-86

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


      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)="123478-HxCDF"
      ALYTE$(13)="123467-HxCDF" : ALYTE$(14)="123678-HxCDF" : ALYTE$(15)="234678-HxCDF"
      ALYTE$(16)="123789-HxCDF" : ALYTE$(17)="123478-HxCDD" : ALYTE$(18)="123678-HxCDD"
      ALYTE$(19)="123789-HxCDD" : ALYTE$(20)="1234678-HpCDF": ALYTE$(21)="1234789-HPCDF"
      ALYTE$(22)="1234678-HpCDD": ALYTE$(23)="OCDF"         : ALYTE$(24)="OCDD"


      CLS : PRINT : PRINT

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

      PRINT"Enter your data base 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.:  ", OLD$

      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), NRT(I), CRRTN(I), C(I), CD(I), RATS(I), THEORY(I)
          INPUT #1, HS(I), SGNS(I), SNMDL(I), CQA(I), SGDS(I)
```

```
70      RETURN


100     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           "
        FORM$="\                  \  #########.#        ####.#          "
        LPRINT"-------------        -----------         -----           "

110     FOR I = 1 TO 24
           LPRINT USING FORM$; ALYTE$(I), C(I),  CRA(I)
120     NEXT I

        FOR I = 1 TO 32
           LPRINT
        NEXT I


130     RETURN
```

SCC NUMBER: ADIPOSE--REPLICATE--COYS FORTUNE
SAMPLE PREP: B071086MH
MASS SPEC I.D.: MAT86800

PREVIOUS TCDD ANALYSIS: TEST

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

Example of program output for QAD