APPENDIX D: DATA MANAGEMENT

D.1 LABORATORY REPLICATES

Chemical concentrations obtained from the analysis of laboratory duplicates or replicates (two or more analyses on the same sample) were averaged for a closer representation of the "true" concentration compared to the results of a single analysis. Averaging rules were dependent on whether the individual results were "detects" or "non-detects." If all concentrations were detects for a given parameter, the values were simply averaged arithmetically. If all concentrations were undetected for a given parameter, the minimum detection limit was reported. If the concentrations are a mixture of detects and non-detects, any two or more detected concentrations were averaged arithmetically and any detection limits were ignored. If there was a single detected concentration and one or more non-detects, the detected concentration was reported and the detection limit(s) ignored. The latter two rules were applied regardless of whether the detection limit was higher or lower than the detected concentration.

D.2 SIGNIFICANT FIGURES AND ROUNDING

The laboratory reported results with various numbers of significant figures depending on the instrument, parameter, and the concentration relative to the reporting limit. The reported (or assessed) precision of each observation is explicitly stored in the project database by recording the number of significant figures assigned by the laboratory. Tracking of significant figures becomes important when calculating averages and performing other data summaries.

When a calculation involves addition, such as totaling PCBs or PAHs, the calculation can only be as precise as the least precise number that went into the calculation. Example (assuming 2 significant figures):

> 210 + 19=229, but this would be reported as 230 because the trailing zero in the number 210 is not significant.

When a calculation involves multiplication or division, such as when carbon normalizing, all significant figures are carried through the calculation and then the total result is rounded at the end of the calculation to reflect the value used in the calculation with the fewest significant figures. Example:

> 59.9 x 1.2 = 71.88, to be reported as 72 because there are 2 significant figures in the number 1.2

When rounding, if the number following the last significant figure is less than 5, the digit is left unchanged. If the number following the last significant figure is equal to or greater than 5, the digit is increased by 1.

D.3 CALCULATING TOTALS

Concentrations for several analyte sums were calculated as follows:

- **Total PCBs** were calculated, in accordance with the methods of the Washington State Sediment Management Standards (SMS), using only detected values for seven Aroclor mixtures[1]. For individual samples in which none of the seven Aroclor mixtures were detected, total PCBs were given a value equal to the highest reporting limit of the seven Aroclors and assigned a "U" qualifier indicating the lack of detected concentrations.
- **Total LPAHs, HPAHs, PAHs, and benzofluoranthenes** were also calculated in accordance with the methods of the SMS. Total LPAHs are the sum of detected concentrations for naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, and anthracene. Total HPAHs are the sum of detected concentrations for fluoranthene, pyrene, benzo(a)anthracene, chrysene, total benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene. Total benzofluoranthenes are the sum of the b (i.e., benzo(b)fluoranthene), j, and k isomers. Because the j isomer is rarely quantitated, this sum is typically calculated with only the b and k isomers. For samples in which all individual compounds within any of the three groups described above were undetected, the single highest reporting limit for that sample represents the sum.
- **Total DDTs** were calculated using only detected values for the six DDT isomers: 2,4'-DDD, 4,4'-DDD, 2,4'-DDE, 4,4'-DDE, 4,4'-DDT, and 4,4'-DDT. For individual samples in which none of the isomers were detected, total DDTs were given a value equal to the highest reporting limit of the six isomers and assigned a "U" qualifier, indicating the lack of detected concentrations.
- **Total chlordane** was calculated using only detected values for the following compounds: alpha-chlordane, gamma-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor. For individual samples in which none of these compounds was detected, total chlordane was given a value equal to the highest reporting limit of the five compounds listed above and assigned a "U"qualifier, indicating the lack of detected concentrations.

D.4 CALCULATION OF TOXIC EQUIVALENTS FOR PCB CONGENERS

PCB congener toxic equivalents (TEQs) were calculated using the World Health Organization consensus toxic equivalence factors (TEFs) (Van den Berg et al. 1998) for mammals presented in Table 1. The TEQ is calculated as the sum of each congener concentration multiplied by the corresponding TEF value. When the

[1] Aroclors 1016, 1221, 1232, 1242, 1248, 1254, and 1260

congener concentration was reported as non-detected, then the TEF was multiplied by zero, half the RL, or the full RL, depending on the calculation method specified.

Table D-1. Mammalian TEF values for PCB congeners

PCB Congener Number	TEF Value (unitless)
77	0.0001
81	0.0001
105	0.0001
114	0.0005
118	0.0001
123	0.0001
126	0.1
156	0.0005
157	0.0005
167	0.00001
169	0.01
189	0.0001

D.5 Calculation of Toxic Equivalents for Dioxin/furan Congeners

Dioxin/furan congener TEQs were calculated using the World Health Organization consensus TEF values (Van den Berg et al. 1998) for mammals presented in Table 2. The TEQ is calculated as the sum of each congener concentration multiplied by the corresponding TEF value. When the congener concentration was reported as non-detected, then the TEF was multiplied by zero, half the RL, or the full RL, depending on the calculation method specified.

Table D-2. Mammalian TEF values for dioxin/furan congeners

Dioxin/Furan Congener	TEF Value (unitless)
1,2,3,4,6,7,8-Heptachlorodibenzofuran	0.01
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	0.01
1,2,3,4,7,8,9-Heptachlorodibenzofuran	0.01
1,2,3,4,7,8-Hexachlorodibenzofuran	0.1
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	0.1
1,2,3,6,7,8-Hexachlorodibenzofuran	0.1
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	0.1
1,2,3,7,8,9-Hexachlorodibenzofuran	0.1
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	0.1
1,2,3,7,8-Pentachlorodibenzofuran	0.05
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	1
2,3,4,6,7,8-Hexachlorodibenzofuran	0.1
2,3,4,7,8-Pentachlorodibenzofuran	0.5
2,3,7,8-Tetrachlorodibenzofuran	0.1
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1

DIOXIN/FURAN CONGENER	TEF VALUE (UNITLESS)
Octachlorodibenzofuran	0.0001
Octachlorodibenzo-p-dioxin	0.0001

D.6 MULTIPLE RESULTS FOR THE SAME ANALYTE

The following rules have been used to select a value when multiple results have been reported for a single analyte for a single sample because the analyte is reported by more than one method (e.g., hexachlorobenzene):

- If all results are reported as detected without qualification as an estimated value (i.e., J qualifier), then the highest concentration is selected as a health-protective approach.
- If a mixture of J-qualified and unqualified detected results are reported, then the unqualified detected result is selected.
- If all results are reported as detected with J-qualification, the highest concentration is selected.
- If both non-detected and detected results are reported, then the detected result is selected. If there are multiple detected results and one or more non-detect results, then the highest detected concentration is selected.
- If all results are reported as non-detected, then the lowest reporting limit is selected.