APPENDIX C: DATA MANAGEMENT

C.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.

C.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 two 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 two 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.

C.3 CALCULATING TOTALS

Concentrations for several analyte sums were calculated as follows:

- **Total PCBs** were calculated using only detected concentrations for the PCB congeners. If all results are reported and non-detected then the highest RL was selected as the total PCB concentration and assigned a "U" qualifier to indicate the lack of detected concentrations.

C.4 CALCULATION OF PCB CONGENER TEQ

PCB congener TEQs were calculated using the WHO consensus TEF values (Van den Berg et al. 1998) for mammals presented in Table B-1. 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 C-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

C.5 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.

- 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