



PORTLAND HARBOR RI/FS

**ROUND 3B SEDIMENT  
DATA REPORT**

**APPENDIX F**

**SUMMATION RULES AND SCRA DATABASE,  
EXCEL FLAT FILE FORMAT**

**(FOUND ON ACCOMPANYING CD)**

**DRAFT**

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**Prepared for**  
The Lower Willamette Group

**Prepared by**  
Integral Consulting Inc.

## 1.0 CALCULATED TOTALS

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Calculated totals were created for analytes evaluated on the basis of summed concentrations. The calculated totals include: total PCB Aroclors, total PCB congeners, total PAH, total low-molecular-weight PAH (LPAH), total high-molecular-weight PAH (HPAH), total DDD, total DDE, total DDT, total DDx, total chlordanes, total endosulfans, total xylenes, total benzene + toluene + ethylbenzene + xylene (BTEX), total fines, TPH, and total PCDD/Fs. All totals were either T or A qualified to indicate that the values were manipulated values (i.e., summed or selected). The A qualifier was used when all of the individual analytes necessary for the total were not available (i.e., a partial sum).

### 1.1 GENERAL SUMMATION RULES

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Calculated totals are the sum of all detected concentrations. If all of the analytes were not detected, then the highest reporting detection limit was the selected value for the calculated total, and a U qualifier was added to indicate the lack of detected values.

### 1.2 CALCULATED TOTALS

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Total PCBs were calculated two ways: as total PCB Aroclors and as total PCB congeners. Total PCB Aroclors represented the sum of Aroclors. Total PCB congeners represented the sum of the individual congeners.

Total LPAHs were calculated with the concentrations for 2-methylnaphthalene, acenaphthene, acenaphthylene, anthracene, fluorene, naphthalene, and phenanthrene. Total HPAHs were calculated with the concentrations for fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene. Total PAHs were calculated with the concentrations of the individual LPAHs and HPAHs.

Total DDx were calculated with the concentrations of the six DDx compounds: 2,4'-DDD; 4,4'-DDD; 2,4'-DDE; 4,4' DDE; 2,4'-DDT; and 4,4'-DDT. Total DDD were calculated with 2,4'-DDD and 4,4'-DDD; total DDE were calculated with 2,4'-DDE and 4,4'-DDE; and total DDT were calculated with 2,4'-DDT and 4,4'-DDT.

Total chlordanes were calculated as the sum of the following compounds: cis-chlordane, trans-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor.

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Total endosulfans were calculated as the sum of alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

Total xylenes were calculated as the sum of m,p-xylene and o-xylene.

BTEX were calculated as the sum of benzene, toluene, ethylbenzene, and xylenes.

Total fines were calculated as the sum of all silt and clay grain-size fractions passing U.S. standard sieve #230 (0.0625-mm openings).

Total petroleum hydrocarbons were calculated as the sum of diesel-range hydrocarbons, residual-range hydrocarbons, and gasoline-range hydrocarbons.

Total PCDD/Fs were calculated as the sum of dioxin and furan homologs: tetrachlorodibenzo-p-dioxins, pentachlorodibenzo-p-dioxins, hexachlorodibenzo-p-dioxins, heptachlorodibenzo-p-dioxins, octachlorodibenzo-p-dioxin, tetrachlorodibenzofurans, pentachlorodibenzofurans, hexachlorodibenzofurans, heptachlorodibenzofurans, and octachlorodibenzofuran.

### **1.3 CALCULATION OF TOXICITY EQUIVALENTS**

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#### **1.3.1 Calculation of PCB Congener TEQs**

PCB congener toxic equivalents (TEQs) were calculated using the 2005 World Health Organization (WHO) consensus toxic equivalency factor (TEF) values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each congener concentration (or detection limit for non-detects) multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied times the TEF value.

#### **1.3.2 Calculation of Dioxin and Furan TEQs**

Dioxin and furan TEQs were calculated using the 2005 WHO consensus TEF values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each congener concentration (or detection limit for non-detects) multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied time the TEF value.

### **1.4 SIGNIFICANT FIGURES**

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The laboratories provided results in electronic text files. The text values were maintained in the database so that the number of significant figures provided by the

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labs would not be lost by either the addition or removal of trailing zeros. For example, if the lab file contained 1.0, then that text string would be maintained to avoid conversion to either 1.00 or 1. In some cases, the lab reported value appeared to have only one significant figure (1, for example). But a minimum of two significant figures was assumed for all results, which was consistent with the standard reporting requirements of analytical laboratories.

During calculations, such as averaging replicates or summing for totals, all significant figures were carried through the calculation. The final result was then rounded to the smallest number of significant figures found in the values used in the calculation. For example:  $7010 + 105 + 20.8 = 7135.8$ , and with three significant figures equals 7140.

## **2.0 REFERENCES**

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Van den Berg, M. L.S. Birnbaum, M. Denison, M. De Vito, W. Farland, M. Freeley, H. Fiedler, H. Hakansson, A. Hanberg, L. Haws, M. Rose, S. Safe, D. Schrenk, C. Tohyama, A. Tritscher, J. Tuomisto, M. Tysklind, N. Walker, and R.E. Peterson. 2006. The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds. *Toxicological Sciences* 93(2), 223-241.