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Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Sediment-Associated Biota: 1997 Revision

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Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Sediment-Associated Biota: 1997 Revision

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PREFACE

The purpose of this report, *Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Sediment-Associated Biota: 1997 Revision* (ES/ER/TM-95/R4), is to present sediment benchmark data and discuss their use as benchmarks for determining the level of toxicological effects on sediment-associated biota and to briefly describe three categories of approaches to the development of sediment quality benchmarks. This work was performed under Work Breakdown Structure 1.4.12.2.3.04.05.04 (Activity Data Sheet 8304, "Technical Integration—Risk Assessment"). Publication of this document meets a milestone for the Environmental Restoration Risk Assessment Program. This report is an update of two prior reports (Jones et al. 1997; Jones et al. 1996; and Hull and Suter 1994). It contains new benchmarks for freshwater sediments, equilibrium partitioning benchmarks corrected to two significant figures, and all of the freshwater and estuarine benchmarks included in the previous version.

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ABBREVIATIONS

AET apparent effects threshold

ARCS Assessment and Remediation of Contaminated Sediment

ASTM American Society for Testing and Materials

AVS acid volatile sulfide

CERCLA Comprehensive Environmental Response, Compensation, and Liability Act

DOC dissolved organic carbon DOE U.S. Department of Energy

EPA U.S. Environmental Protection Agency

EqP equilibrium partitioning
ERA ecological risk assessment
ER-L Effects Range-Low
ER-M Effects Range-Median
ET Ecotox Threshold

FDEP Florida Department of Environmental Protection

 f_{oc} fraction organic carbon

K_{oc} organic carbon/water partition coefficient

 $egin{array}{lll} K_{ow} & octanol/water partition coefficient \\ K_{p} & sediment/water partition coefficient \\ NAWOC & National Ambient Water Quality Criteria \\ \end{array}$

NEC high No Effect Concentration

NOAA National Oceanic and Atmospheric Administration

OC organic carbon

OECD Organization for Economic Cooperation and Development

Ontario MOE Ontario Ministry of the Environment ORNL Oak Ridge National Laboratory

ORR Oak Ridge Reservation

OSWER Office of Solid Waste and Emergency Response

PAHs polycyclic aromatic hydrocarbons
PCBs polychlorinated biphenyls
PEC probable effect concentration
PEL Probable Effects Level
PQL Practical Quantitation Limit
SEC sediment effect concentration

SEC sediment effect concentration
SEM simultaneously extracted metal
SLC screening level concentration
SQB sediment quality benchmark
SQC sediment quality criteria

SSLC species screening level concentration

TEC threshold effect concentration TEL Threshold Effects Level

TIE toxicity identification evaluation

TOC total organic carbon
WQB water quality benchmark
WQC water quality criteria

EXECUTIVE SUMMARY

A hazardous waste site may contain hundreds of chemicals; therefore, it is important to screen contaminants of potential concern for the ecological risk assessment. Often this screening is done as part of a screening assessment, the purpose of which is to evaluate the available data, identify data gaps, and screen contaminants of potential concern. Screening may be accomplished by using a set of toxicological benchmarks. These benchmarks are helpful in determining whether contaminants warrant further assessment or are at a level that requires no further attention. If a chemical concentration or the reported detection limit exceeds a proposed lower benchmark, further analysis is needed to determine the hazards posed by that chemical. If, however, the chemical concentration falls below the lower benchmark value, the chemical may be eliminated from further study.

The use of multiple benchmarks is recommended for screening chemicals of concern in sediments. Integrative benchmarks developed for the National Oceanic and Atmospheric Administration and the Florida Department of Environmental Protection are included for inorganic and organic chemicals. Equilibrium partitioning benchmarks are included for screening nonionic organic chemicals. Freshwater sediment effect concentrations developed as part of the U.S. Environmental Protection Agency's (EPA's) Assessment and Remediation of Contaminated Sediment Project are included for inorganic and organic chemicals (EPA 1996). Field survey benchmarks developed for the Ontario Ministry of the Environment are included for inorganic and organic chemicals. In addition, EPA-proposed sediment quality criteria are included along with screening values from EPA Region IV and Ecotox Threshold values from the EPA Office of Solid Waste and Emergency Response. Pore water analysis is recommended for ionic organic compounds; comparisons are then made against water quality benchmarks.

This report is an update of three prior reports (Jones et al. 1997; Jones et al. 1996; and Hull and Suter 1994). It contains new benchmarks for freshwater sediments, equilibrium partitioning benchmarks corrected to two significant figures, and all of the freshwater and estuarine benchmarks included in the previous version.

1. INTRODUCTION

A hazardous waste site may contain hundreds of chemicals; therefore, it is important to screen contaminants of potential concern for the ecological risk assessment (ERA). Often this screening is done as part of a screening assessment, the purpose of which is to evaluate the available data, identify data gaps, and screen contaminants of potential concern (Suter 1995). Screening may be accomplished by using a set of toxicological benchmarks. These benchmarks are helpful in determining whether contaminants warrant further assessment or are at a level that requires no further attention. If a chemical concentration or the reported detection limit exceeds a lower benchmark, further analysis is needed to determine the hazards posed by that chemical. If, however, the chemical concentration falls below the lower benchmark value, the chemical may be eliminated from further study. Concentrations exceeding an upper screening benchmark indicate that the chemical in question is clearly of concern and that remedial actions are likely to be needed.

The use of multiple benchmarks also indicates the likelihood and nature of effects. For example, exceedance of only one conservatively estimated benchmark may provide weak evidence of real effects, whereas exceedance of multiple benchmarks of varying conservatism may provide strong evidence of real effects. Likewise, if a nonionic organic chemical only exceeds benchmarks that are not normalized to site-specific organic carbon content, then organisms that ingest sediment may be more exposed than those that do not. These inferences can be used to refine future sampling and remediation efforts.

In recent years, protecting sediment quality has been viewed as a logical and necessary extension of water quality protection (Adams et al. 1992). The U.S. Environmental Protection Agency (EPA) is authorized to develop and implement sediment quality criteria (SQC) under Section 304(a) of the Clean Water Act (EPA 1989a). EPA released five SQC documents in 1993 (EPA 1993a–e). In addition, EPA Region IV (1995) and the Office of Solid Waste and Emergency Response (OSWER) (1996) released sediment screening values in 1995. Until EPA's task is complete, efforts will continue around the United States and abroad (EPA 1996; MacDonald 1993; Persaud et al. 1993) to develop SQC and benchmark values for the assessment of sediment quality at hazardous waste sites.

Sediment quality benchmarks (SQBs) are necessary, in addition to water quality benchmarks (WQBs), because (1) various toxic contaminants found in only trace amounts in the water column accumulate in sediments to elevated levels; (2) sediments serve as both a reservoir and a source of contaminants to the water column; (3) sediments integrate contaminant concentrations over time, whereas water column contaminant concentrations are much more variable and dynamic; (4) sediment contaminants in addition to water column contaminants affect benthic and other sediment-associated organisms; and (5) sediments are an integral part of the aquatic environment, providing habitat, feeding, and rearing areas for many aquatic organisms (Chapman 1989).

To make decisions as to whether a chemical or biological measurement of sediment quality indicates impairment, site-specific data may be compared with benchmarks that indicate whether sediment quality is acceptable. Existing criteria and standards are considered a type of benchmark. The purpose of this report is to present sediment benchmark data and discuss their use as benchmarks for determining the level of toxicological effects on sediment-associated biota.

It is important to note that these benchmarks do not represent remediation goals. Remediation goals must consider adverse effects on habitat and remobilization of contaminants caused by removal or remediation of sediments.

The benchmarks in this report are to be used at the U.S. Department of Energy's (DOE's) Oak Ridge Reservation (ORR) and at the Portsmouth and Paducah gaseous diffusion plants as screening values only to show the nature and extent of contamination and identify the need for additional site-specific investigation (e.g., biological and chemical testing).

Sediment benchmarks also can be used for baseline ERAs, which are required under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) at Superfund sites. These assessments evaluate the risks to the environment posed by the hazardous waste site. Sediment benchmarks must not be used as the sole measure of sediment toxicity. Field studies and toxicity tests will be the primary indicators of toxicity of sediments; benchmarks may be used to determine which chemicals present in the sediment are most likely causing the toxicity. This integrative approach allows a more accurate evaluation of adverse ecological impact, which is necessary in a baseline risk assessment.

This report is an update of three prior reports (Jones et al. 1997; Jones et al. 1996; and Hull and Suter 1994). It contains new benchmarks for freshwater sediments, equilibrium partitioning benchmarks corrected to two significant figures, and all of the freshwater and estuarine benchmarks included in the previous version.

2. REVIEW OF POSSIBLE APPROACHES TO BENCHMARK DEVELOPMENT

Three distinct categories of approaches can be used in the development of SQBs. These approaches are based on analytical chemistry, toxicity test results, and field survey data. A fourth integrative approach incorporates all three types of data. Regardless of the method, a numeric benchmark results.

The scientific and regulatory communities are still debating the best methods to be used to develop sediment quality guidelines. This diversity of opinion is demonstrated by the wide variety of methods being studied and by the fact that the state of Washington has implemented sediment quality standards based on the apparent effects threshold (AET) approach, whereas the equilibrium partitioning (EqP) approach is favored by the EPA Office of Water (EPA 1996). Additionally, the Organization for Economic Cooperation and Development (OECD) recommended three methods for deriving sediment quality objectives: the EqP approach, the measurement of interstitial water, and spiked sediment toxicity tests (OECD 1992). Several of the possible approaches to developing SQBs have been reviewed (Adams et al. 1992; MacDonald et al. 1992; MacDonald 1994; Chapman 1989) and are briefly described in the following sections.

2.1 ANALYTICAL CHEMISTRY APPROACHES

2.1.1 Direct Measurement of Interstitial Water

The direct measurement of interstitial water approach compares the concentrations of contaminants in sediment interstitial (pore) waters with the EPA water quality criteria (WQC) (EPA 1993f) and other WQBs. WQBs of varying conservatism have been developed at Oak Ridge National Laboratory (ORNL) (Suter and Tsao 1996) because many chemicals do not have national ambient WQC. Maughan (1993) suggests that the analysis of sediment pore water is a more appropriate method for screening than using bulk sediment chemistry. He cites the advantages of the flexibility and acceptance of pore water testing.

It can be argued that benthic organisms are exposed to contaminants via other exposure routes, such as dermal absorption and ingestion of sediment particles. An analysis of the feeding habits of freshwater benthic species concluded that these species were not sediment ingesters, except for the oligochaetes (aquatic earthworms) and some chironomids that are both filter feeders and occasional sediment ingesters (Adams 1987). In contrast to this, marine burrowing species frequently ingest sediment (Adams 1987). For the clam *Macoma nasuta*, uptake of highly lipophilic pollutants occurred primarily by ingestion of solids (63–84%), followed by ventilation of interstitial water across the gills (11–12%) (Boese et al. 1990). This may be because *Macoma nasuta* predominantly ventilates overlying water, not interstitial water.

Such discrimination between overlying and interstitial water also may be important for tube dwellers (e.g., chironomids, hexagenia) that pump overlying water through their burrows (Landrum and Robbins 1990). Maughan (1993) argues that if the organism is in equilibrium with the pore water, then the concentration in the pore water would reflect the sum of all exposure routes. Therefore, an organism that has accumulated contaminants, through feeding, at a higher concentration than the equilibrium with pore water would reestablish the equilibrium by losing contaminants to the pore water (Maughan 1993). However, factors may influence whether the organism can establish an equilibrium with the pore water. For example, diffusion within the interstitial water may limit transfer of desorbed compounds to the organism (Landrum and Robbins 1990).

2.1.2 Estimation of Interstitial Water Concentrations: Sediment/Water EqP Approach

2.1.2.1 Nonionic organics

This approach calculates a bulk sediment chemical concentration benchmark. The calculation uses the WQBs together with correction factors for the effects of organic carbon (OC) (EPA 1993f). By using this method, a SQB is calculated as follows (EPA 1993f): If the WQB (micrograms per liter) is a water quality benchmark for the chemical of interest (Suter and Tsao 1996), then the SQB (micrograms per kilogram sediment) is computed by using the partition coefficient K_p (liters per kilogram sediment) between sediment and water:

$$SQB = K_n \times WQB .$$

The partitioning of nonionic chemicals between particles and water depends on the partition coefficient K_{oc} for the particles' OC and the mass fraction of OC (f \dot{k} kilograms OC per kilogram sediment) of the particles:

$$K_p = f_{oc} \times K_{oc}$$
.

Where the K_{oc} is unavailable, it is estimated by the octanol-water partition coefficient K_{ow} of the chemical for sediments by using the following equation (Di Toro 1985):

$$\log_{10}(K_{oc}) = 0.00028 + 0.983 \log_{10}(K_{ow})$$
.

Therefore,

$$SQB = f_{oc} \times K_{oc} \times WQB$$
.

The EqP approach requires four major assumptions: (1) partitioning of the organic chemical between OC and interstitial water is stable at equilibrium; (2) the sensitivities of benthic species and species tested to derive WQBs, predominantly water column species, are similar; (3) the levels of protection afforded by WQBs are appropriate for benthic organisms; and (4) exposures are similar regardless of feeding type or habitat (EPA 1993a).

EqP can be used only if $f_{\rm oc} > 0.2\%$. At $f_{\rm oc} < 0.2\%$, the factors controlling second-order effects on partitioning (e.g., particle size, sorption to nonorganic mineral fractions) become relatively more important (EPA 1993f).

For both the direct measurement and EqP approaches for estimating pore water effects concentrations, it is assumed that the WQBs, when applied to the interstitial water of sediments, would protect infaunal organisms. EPA (1993f) has concluded that the sensitivities of benthic species are sufficiently similar to those of water column species to tentatively permit the use of WQBs for the derivation of SQBs.

The EqP approach is favored by the EPA over the direct measuring of pore water approach (EPA 1993f). The free chemical concentration in pore water can be estimated directly from the OC normalized sediment concentration, and the estimate is independent of the dissolved organic carbon (DOC) concentration. Using the pore water chemical concentration to estimate the free pore water chemical concentration requires that the DOC concentration and the DOC partition coefficient be known; this is because the proportion of a chemical in pore water that is complexed to DOC can be substantial. However, it is the free, uncomplexed component that is bioavailable and that is in equilibrium with the OC normalized sediment concentration. Therefore, for highly hydrophobic chemicals and where there is significant DOC complexing, the solid-phase chemical concentration gives a more direct estimate of the bioavailable pore water contaminant concentration than do the pore water concentrations (EPA 1993f).

2.1.2.2 Metals

EqP approach. Significant complexities are associated with inorganic chemicals when using the EqP approach. Uptake (and therefore effects) of sediment-associated contaminants is largely a function of bioavailability. Bioavailability is strongly influenced by a complex suite of physical, chemical, and biological factors in the sediments. Trace metals can be adsorbed at particle surfaces, bound to carbonates, occluded in iron and/or manganese oxyhydroxides, bound to organic matter, bound to sulphide, bound to a matrix, or dissolved in the interstitial water. The complexity of trace metal bioavailability associated with these phases hinders the prediction of effects (Campbell and Tessier 1991).

Acid volatile sulfide method. Acid volatile sulfide (AVS) is a reactive pool of solid-phase sulfide that is available to bind metals and render that portion unavailable and nontoxic to biota (Di Toro et al.

1992). The AVS is extracted from sediment using hydrochloric acid. The metal concentration that is simultaneously extracted is termed the simultaneously extracted metal (SEM). For [SEM]/[AVS] <1, no acute toxicity (mortality >50%) has been observed in any sediment for any benthic test organism. For [SEM]/[AVS] >1, less sensitive organisms can tolerate increased metal activity. However, the mortality of sensitive species (e.g., amphipods) increases in the range of 1.5 to 2.5 μ mol of SEM/ μ mol of AVS (Di Toro et al. 1992). For this reason, the AVS method is used only to predict when a sediment in not acutely toxic.

The AVS approach requires the measurement of all toxic SEMs that are present in amounts that would contribute significantly to the SEM sum. Failure to do so could lead to an incorrect conclusion of lack of acute toxicity (Di Toro et al. 1992). Use of the AVS method would be invalid if the sediment AVS content is very low. This would occur in fully oxidized sediments (Adams et al. 1992). In addition, only five metals (Cd, Cu, Pb, Ni, and Zn) currently can be evaluated using AVS (EPA 1994), and the AVS method has not been adapted for chronic toxicity.

2.2 SEDIMENT TOXICITY TEST APPROACHES

2.2.1 Bulk Sediment Toxicity Tests

Organisms are exposed to either contaminated field-collected sediments or background sediments spiked in the laboratory with known amounts of single chemicals or mixtures. Mortality or sublethal effects are observed, and dose-response relationships are determined (Chapman 1989; Long and Morgan 1991). A major advantage to this approach is that it follows the methods used to develop WQC; therefore, the procedure and rationale are technically acceptable and legally defensible (Chapman 1989). The use of sediment toxicity tests has become firmly entrenched in many dredged material permitting and benthic survey programs (Burton and Scott 1992).

2.2.2 Pore Water Toxicity Tests

Sediment pore water can be used in standardized toxicity tests, and toxicity identification evaluation (TIE) procedures can be used to characterize, identify, and then confirm the toxic components of a complex aqueous solution. However, TIE procedures may be difficult and costly (Maughan 1993). Currently, no universally accepted method for extracting pore water from sediment exists. In addition, pore water is difficult to extract from sediment without potentially altering the toxicity of the pore water (Maughan 1993).

2.3 FIELD SURVEY APPROACHES

2.3.1 Screening Level Concentration Approach

The screening level concentration (SLC) approach estimates the highest concentration of a particular contaminant in sediment that can be tolerated by approximately 95% of benthic infauna (Neff et al. 1988). The SLC is derived from synoptic data on sediment chemical concentrations and benthic invertebrate distributions. First, the species screening level concentration (SSLC) is calculated by plotting the frequency distribution of the contaminant concentrations over all sites (at least 10) where the species is present. The 90th percentile of this distribution is taken as the SSLC for that species. Next, a large number of SSLCs are plotted as a frequency distribution to determine the contaminant

concentration above which 95% of the SSLCs occur. This final concentration is the SLC (Neff et al. 1988).

The SLC approach has several advantages: it can be used with any chemical contaminant, it can be developed using existing databases and methodologies, and it does not require *a priori* assumptions concerning mechanisms of interaction between organisms and toxic contaminants (Chapman 1989). Disadvantages include the following: a large amount of field data is required, a precise level of infaunal taxonomic identification is required, calculation of SLCs is affected by the range and distribution of contaminant concentrations and species, selection criteria for species have not been established, and no mechanism has been established to separate single contaminant effects from the effects of all contaminants combined (Chapman 1989).

2.3.2 Apparent Effects Threshold Approach

The AET approach uses data from matched sediment chemistry and biological effects measures. Biological effects could be assessed by either benthic community survey or sediment toxicity tests. An AET concentration is the sediment concentration of a selected chemical above which statistically significant biological effects always occur (EPA 1989b). This concentration is alternatively identified as the high No Effect Concentration (NEC) (EPA 1996).

The major strengths of the approach are that (1) combined chemical effects can be considered (EPA 1989b); (2) there are no constraints on the type of contaminant or biological effects that can be used; (3) contaminants that are most likely associated with observed biological effects are identified on a site-specific basis; and (4) because observed biological effects always occur above the AET, the approach provides values based on noncontradictory evidence of biological impacts (Chapman 1989). Disadvantages to this approach include the following: (1) it is site-specific (EPA 1989b), (2) it may be underprotective because biological effects are observed at chemical concentrations well below AET values, (3) it requires a large database for chemical variables and at least one biological indicator, and (4) combined contaminant effects cannot be separated from single contaminant effects (Chapman 1989).

2.4 INTEGRATIVE APPROACHES

2.4.1 National Oceanic and Atmospheric Administration Approach

Because the EqP approach is impractical for inorganics, other benchmark values were needed. The National Oceanic and Atmospheric Administration (NOAA) annually collects and chemically analyzes sediment samples from sites located in coastal marine and estuarine environments throughout the United States. These data were used to evaluate three basic approaches to the establishment of effects-based criteria: the EqP approach, the spiked-sediment toxicity test approach, and various methods of evaluating synoptically collected biological and chemical data in field surveys (Long and Morgan 1991). Chemical concentrations observed or predicted by these methods to be associated with biological effects were ranked, and the lower 10th percentile [Effects Range–Low (ER-L)] and median [Effects Range–Median (ER-M)] concentrations were identified.

The ER-L and ER-M values were recalculated by Long et al. (1995) after omitting a small amount of freshwater data included in the Long and Morgan (1991) calculations and adding more recent data.

2.4.2 Florida Department of Environmental Protection Approach

The Florida Department of Environmental Protection (FDEP) approach (MacDonald 1994) is similar to the NOAA approach. The updated and revised data set used by Long et al. (1995) also was used by MacDonald (1994) to calculate Threshold Effects Levels (TELs) and Probable Effects Levels (PELs); these data are presented by MacDonald et al. (1994). However, unlike the ER-Ls and ER-Ms, the TELs and PELs also incorporate chemical concentrations observed or predicted to be associated with no adverse biological effects (no effects data). Specifically, the TEL is the geometric mean of the 15th percentile in the effects data set and the 50th percentile in the no effects data set. The PEL is the geometric mean of the 50th percentile in the effects data set and the 85th percentile in the no effects data set. Therefore, the TEL represents the upper limit of the range of sediment contaminant concentrations dominated by no effects data. The PEL represents the lower limit of the range of contaminant concentrations that are usually or always associated with adverse biological effects (MacDonald 1994).

2.5 BACKGROUND CONCENTRATIONS

Comparison of site contaminant levels with background levels is a simple screening method. The assumption is that concentrations that are not higher than background are not hazardous. Appropriate background samples must be obtained for waste site samples. The American Society for Testing and Materials (ASTM) is currently developing guidelines for selection of sediment and soil background sampling locations (ASTM Sect. E47.13.01, Task E).

This approach has two major disadvantages: it has no biological effects basis, and it cannot be used for synthetic organic compounds, which should not be present in background sediments. Therefore, it is not appropriate to use this approach as the only screening method. However, it is appropriate to use the background concentrations to screen the other sediment benchmarks, such that sediment benchmarks that are within the range of background concentrations are not used to identify chemicals of potential ecological concern.

3. RECOMMENDED SEDIMENT BENCHMARKS

The following section presents the recommended sediment benchmarks for use at DOE's ORR and at the Portsmouth and Paducah gaseous diffusion plants. The rationale, interpretation, and general considerations for using these benchmarks in screening sediment chemical data are also briefly discussed. Chemical-specific considerations are presented in Chap. 4.

This revision includes a new set of toxicity test-based benchmarks for freshwater sediments (EPA 1996) and previously presented benchmarks for marine and estuarine sediments (e.g., FDEP TELs and PELs, NOAA ER-Ls and ER-Ms, Washington state AET, EPA screening values). The freshwater benchmarks are recommended for use at the aforementioned DOE sites. The marine benchmarks are retained and recommended for use because the parties to the Federal Facility Agreement have not yet sanctioned the use of the freshwater benchmarks and because freshwater benchmarks are not available for all chemicals. The use of multiple benchmarks of varying conservatism is recommended to provide a robust evaluation of the chemical data. That is, a suite of benchmarks reduces the chances of missing a chemical of potential ecological concern and increases the interpretive value of the chemical data set.

It is strongly recommended that the suite of benchmarks, or the rules for selecting a subset of benchmarks, be explicitly included in the Data Quality Objectives process to get early and informed regulator agreement for their use in a given project.

3.1 MARINE AND ESTUARINE SEDIMENTS

3.1.1 Integrative Benchmarks

EPA Region IV (1995) has recommended the NOAA and FDEP values as potential lower screening values, and EPA OSWER (1996) has recommended the NOAA values as potential ecotoxicological threshold values. The NOAA and FDEP values also are supported by ORNL as SQBs when bulk sediment chemical concentrations are available.

The data compiled by MacDonald et al. (1994) are from marine and estuarine locations only. The use of the NOAA and FDEP values for freshwater is appropriate in the absence of reliable freshwater sediment benchmarks. Klapow and Lewis (1979) investigated the question of whether or not it was legitimate to combine freshwater and marine aqueous toxicity data to develop marine water quality benchmarks. A statistical test of medians was applied to freshwater and marine acute toxicity data for nine metals (As, Cd, Cr, Cu, Pb, Hg, Ni, Ag, and Zn) and nonchlorinated phenolic compounds. In only one case (Cd) was there a statistically significant difference in the median response of marine and freshwater organisms. The NOAA and FDEP values were developed from data from several investigations throughout the United States, and these studies used different approaches to evaluate sediment quality (e.g., toxicity tests, EqP, AET). It is assumed that the use of numerous data and the calculation of percentiles help eliminate the influence of a single (possibly outlier) data point, thereby making the sediment quality values more credible (Long and Morgan 1991).

The NOAA values may be used to help identify sites with the potential to cause adverse biological effects. These are not NOAA criteria or standards and are not intended for use in regulatory decisions or any other similar applications (Long and Morgan 1991). The available NOAA and FDEP values are presented in Table 1.

3.1.2 Apparent Effects Thresholds

The AET is the sediment chemical concentration above which statistically significant biological effects always occur (EPA 1989b). Therefore, they may be underprotective because biological effects are observed at chemical concentrations well below AET values (Chapman 1989). AET values for several ionic and polar organic chemicals are retained in this revision because of the significant complexities associated with using the EqP approach.

Organic compounds that are polar or ionic include methyl and thiocarbamates, triazines, amines and analines, and organic acid pesticides (aliphatic and aromatic acids and esters, phenoxy compounds, and ureas). Unlike nonpolar and nonionic organic contaminants, both polar and ionic organic compounds may adsorb onto sediments by a variety of mechanisms, including hydrophobic interaction, nonspecific ion association, ion exchange, ion-dipole interactions, hydrogen bonding, and complex formation by surface metals (Shea 1988). It is possible that a multiple-term model might account for polar organic partitioning between sediment and aqueous phases but such a model does not exist (Shea 1988).

Table 1. Summary of selected integrative sediment quality benchmarks for marine and estuarine sediments a

	NOA	$\mathbf{A}\mathbf{A}^{b}$	FDI	E P ^c
Chemical	ER-L	ER-M	TEL	PEL
Antimony	2^d	25^d		
Arsenic	8.2	70	7.24	41.6
Cadmium	1.2	9.6	0.68	4.21
Chromium	81	370	52.3	160
Copper	34	270	18.7	108
Lead	46.7	218	30.2	112
Mercury	0.15	0.71	0.13	0.7
Nickel	20.9	51.6	15.9	42.8
Silver	1.0	3.7	0.73	1.77
Zinc	150	410	124	271
(Organics (µg/kg	g dry weight)		
Acenaphthene	16	500	6.71	88.9
Acenaphthylene	44	640	5.87	128
Anthracene	85.3	1100	46.9	245
Benz(a)anthracene	261	1600	74.8	693
Benzo(a)pyrene	430	1600	88.8	763
ВНС				
BHC, alpha-				
BHC, beta-				
Bis(2-ethylhexyl)phthalate			182	2647
Chlordane	0.5^{d}	6^d	2.26	4.79
Chrysene	384	2800	108	846
DDD, o,p'-+ p,p'-	2^d	20^d		
DDD, p,p'-			1.22	7.81
DDE, p,p'-	2.2	27	2.07	374
DDT, o,p'-+p,p'-	1^d	7^d	_,,	
DDT, p,p'-	•	,	1.19	4.77
DDT, Total ^e	1.58	46.1	3.89	51.7
Dibenzo(a,h)anthracene	63.4	260	6.22	135
Dieldrin	0.02^{d}	8^d	0.72	4.3
	0.02^{d}		0.72	4.3
Endrin		45 ^d	112	1.40.4
Fluoranthene	600	5100	113	1494
Fluorene	19	540	21.2	144
Lindane (gamma-BHC)			0.32	0.99
2-Methyl naphthalene	70	670	20.2	201
Naphthalene	160	2100	34.6	391

10 **Table 1 (continued)**

	NO	$\mathbf{A}\mathbf{A}^b$	FD	\mathbf{EP}^c
Chemical	ER-L	ER-M	TEL	PEL
PAH, Total LMW ^f	552	3160	312	1442
PAH, Total HMW ^f	1700	9600	655	6676
PAH, Total ^f	4022	44792	1684	16770
PCB, Total	22.7	180	21.6	189
Phenanthrene	240	1500	86.7	544
Pyrene	665	2600	153	1398

[&]quot;Benchmark values are presented herein with the same number of significant digits used in the source document.

^fLMW = low molecular weight and is the sum of the concentrations of acenaphthene, acenaphthylene, anthracene, fluorene, 2-methylnaphthalene, naphthalene, and phenanthrene; HMW = high molecular weight and is the sum of the concentrations of benz(a)anthracene, benzo(a)pyrene, chrysene, dibenzo(a,h)anthracene, fluoranthene, and pyrene; Total is the sum of the concentrations of the aforementioned low and high molecular weight PAHs.

The behavior of ionic organic pollutants has not been extensively studied. As with the nonionic organic chemicals, OC appears to be a critical factor in the partitioning behavior in sediments (Jafvert 1990). The critical micelle concentration (Di Toro et al. 1990) and pH (Jafvert 1990) also appear to be dominating factors.

The state of Washington has developed sediment quality standards for some polar and ionic organic compounds (Table 2). AET are site-specific and should be used cautiously. Because little information is available for ionic organics, these contaminants should not be eliminated in a screening risk assessment. Preliminary comparisons can be made to the Washington state sediment quality standards to give an indication of the magnitude of the contamination. In addition, EqP SQBs for two of the polar chemicals (2-methylphenol and phenol) are presented in Table 3.

WQBs do exist for several of these chemicals (Suter and Tsao 1996). If pore water concentrations of these chemicals are available, they should be screened against those benchmarks; this was the methodology followed in the Phase I Screening ERA for the Clinch River (Cook et al. 1992).

^bNOAA = National Oceanic and Atmospheric Administration; ER-L = Effects Range–Low; ER-M = Effects Range–Median; except where noted, effects levels are the updated and revised values from Long et al. (1995).

^{&#}x27;FDEP = Florida Department of Environmental Protection; TEL = threshold effects level; PEL = probable effects level; source document is MacDonald (1994).

^dSource document is Long and Morgan (1991).

[&]quot;Total DDT is the sum of the concentrations of the o,p'- and p,p'- isomers of DDD, DDE, and DDT.

Table 2. Washington state sediment quality standards for ionizable organic compounds (micrograms per kilogram dry weight)

Compound	Washington state sediment quality standard
Benzoic acid	650
Benzyl alcohol	57
Pentachlorophenol	360
Phenol	420
2-Methyl phenol	63
4-Methyl phenol	670
2,4-Dimethyl phenol	29

Source: Ginn and Pastorak 1992

3.2 FRESHWATER SEDIMENTS

3.2.1 EqP Benchmarks

The EPA has chosen the EqP approach for developing SQC for nonionic organics (EPA 1993f). This is also a methodology that ORNL supports for developing SQBs when bulk sediment concentrations and WQBs are available.

The EqP approach requires a WQB, a K_{oc} value, and a measured or assumed site-specific total organic carbon (TOC) value. Because many chemicals do not have National Ambient Water Quality Criteria (NAWQC), sets of WQBs of varying conservatism have been developed at ORNL (Suter and Tsao 1996); consult this publication, or its most recent revision, for a complete discussion of the aquatic benchmarks and their uses. Secondary chronic values are intended to be conservative predictors of effects. If concentrations exceed benchmarks that used the NAWQC, the chemicals must be contaminants of concern because the NAWQC are applicable or relevant and appropriate requirements. Concentrations that exceed Lowest Chronic Value benchmarks indicate a risk of real effects. Table 3 lists available log K_{ow} values for selected nonionic organic contaminants, sources of these values, calculated log K_{ow} values, and estimated SQBs corresponding to the conventional aqueous benchmarks; these SQBs are normalized assuming 1% TOC.

For polar organic chemicals, adsorption mechanisms other than hydrophobicity may significantly increase the fraction of the chemical sorbed to the sediment particles (EPA 1993f). Therefore, the K_{oc} -based model is likely to overestimate the free, and therefore bioavailable, chemical concentration. SQBs for selected polar nonionic organic chemicals are included in Table 3 as conservative benchmarks and are denoted appropriately.

The bulk sediment contaminant concentrations measured at a site can be compared directly to the SQBs presented in Table 3. It is recommended, however, that these benchmarks be adjusted by multiplying the SBQ by the site-specific percent TOC. For example, the SQC for acenaphthene is 1300 μ g/kg assuming 1% TOC and 13,000 μ g/kg assuming 10% TOC (EPA 1993a). However, the

Table 3. Summary of EqP-derived sediment quality benchmarks for nonionic organic chemicals corresponding to conventional aqueous benchmarks a

					Lowest chronic value		
Chemical	Log Kow ^b	Log Koc	NAWQC chronic	Secondary chronic value	Fish	Daphnids	Nondaphnid invertebrates
Acenaphthene	3.92	3.85	1300^{c}		5300	470,000	16,000
Acetone ^d	-0.24	-0.24		8.7	3000	9.1	
Anthracene	4.55	4.47		220	27	<620	
Benzene	2.13	2.09		160		>120,000	
Benzidine d	1.66	1.63		1.7	57		
Benzo(a)anthracene	5.70	5.60		110		2600	
Benzo(a)pyrene	6.11	6.01		140		3000	
Benzyl alcohol ^d	1.11	1.09		1.1	73		
BHC (lindane)	3.73	3.67	3.7		680	670	150
BHC (other)	3.80^e	3.74		120		5200	
Biphenyl	3.96 ^f	3.89		1100			
Bis(2-ethylhexyl)phthalate	7.60^{g}	7.47		890,000			
4-Bromophenyl phenyl ether	5.00	4.92		1200			
Butylbenzyl phthalate	4.84	4.76		11,000			
2-Butanone ^d	0.29^{g}	0.29		270	5400	27,000	
Carbon disulfide	2.00	1.97		0.85	8800	230	
Carbon tetrachloride	2.73	2.68		47	9500	27,000	
Chlordane	6.32	6.21	2800		26,000	260,000	18,000
Chlorobenzene	2.86	2.81		410	7800	97,000	
Chloroform	1.92	1.89		22	960	3500	
p,p'-DDD	6.10	6.00		110	17,000		

						Lowest chronic va	lue
Chemical	${\bf Log}\;{\bf Kow}^b$	Log Koc	NAWQC chronic	Secondary chronic value	Fish	Daphnids	Nondaphnid invertebrates
DDT	6.53	6.42		340^{bf}	19,000	420	
Decane	5.01^{g}	4.93		41,000		6,600,000	
Di-n-butyl phthalate	4.61	4.53		11,000	240,000	240,000	
Diazinon	3.70 ^f	3.64		1.9			
Dibenzofuran	4.12^{g}	4.05		420		110,000	
1,2-Dichlorobenzene	3.43	3.37		330			
1,3-Dichlorobenzene	3.43^{f}	3.37		1700			
1,4-Dichlorobenzene	3.42	3.36		340			
1,1-Dichloroethane	1.79	1.76		27	8400		
1,2-Dichloroethane	1.47	1.45		250	12,000	4200	
1,1-Dichloroethene	2.13	2.09		31	>3500	5900	
1,2-Dichloroethene	1.86^e	1.83		400	6400		
1,3-Dichloropropene	2.00	1.97		0.051	220	740	
Dieldrin	5.37	5.28	110^{c}				
Diethyl phthalate	2.50	2.46		600			
Endosulfan, all isomers	4.10	4.03		5.5			
Endrin	5.06	4.97	42^c				
Ethyl benzene	3.14	3.09		89	>5400	160,000	
Fluoranthene	5.12	5.03	6200^{c}		32,000	16,000	
Fluorene	4.21	4.14		540			
Heptachlor	6.10^{g}	6.00		68	12,000	31,000	
Hexachloroethane	4.00	3.93		1000			

Table 3 (continued)

Table 3 (continued)

					Lowest chronic value		
Chemical	Log Kow ^b	Log Koc	NAWQC chronic	Secondary chronic value	Fish	Daphnids	Nondaphnid invertebrates
Hexane	3.90^{g}	3.83		40	4,500,000		
2-Hexanone ^d	1.38^{g}	1.36		22	7400		
Methoxychlor	5.08	4.99		19			
1-Methylnaphthalene	3.87^g	3.80		130	34,000		
4-Methyl-2-pentanone ^d	1.31^{g}	1.29		33	15,000		
2-Methylphenol ^d	1.99	1.96		12	440	1200	
Methylene chloride	1.25	1.23		370	18,000	7200	
Naphthalene	3.36	3.30		240	12,000	23,000	
2-Octanone ^d	2.37^{g}	2.33		18			
PCBs Aroclor® 1221	4.70^h	4.62		120	25,000		
Aroclor® 1232	5.10^{h}	5.01		600	130,000		
Aroclor® 1242	5.60^{h}	5.51		170	29,000		16,000
Aroclor® 1248	6.20^{h}	6.09		1000			
Aroclor® 1254	6.50^{h}	6.39		810		71,000	
Aroclor® 1260	6.80^{h}	6.68		4,500,000	<63,000		
Pentachlorobenzene	5.26	5.17		700			
1-Pentanol ^d	1.51^{g}	1.48		34	9300		
Phenanthrene	4.55	4.47	1800^{c}			59,000	
Phenol	1.48	1.46	31		<57	570	
2-Propanol ^d	0.05	0.05		0.084	6.6		
1,1,2,2 Tetrachloroethane	2.39	2.35		1400	5400	22,000	

Table 3 (continued)

					Lowest chronic value		
Chemical	Log Kow ^b	Log Koc	Log Koc NAWQC chronic	Secondary chronic value	Fish	Daphnids	Nondaphnid invertebrates
Tetrachloroethene	2.67	2.62		410	3500	3200	
Toluene	2.75	2.70		50	6400	130,000	
Tribromomethane	2.35^{f}	2.31		650			
1,2,4-Trichlorobenzene	4.01	3.94		9600			
1,1,1-Trichloroethane	2.48	2.44		30	9600		
1,1,2-Trichloroethane	2.05	2.02		1200	9700	19,000	
Trichloroethene	2.71	2.66		220	51,000	33,000	
Vinyl acetate	0.73	0.72		0.84	42		
Xylene	3.13^e	3.08		160	740,000		
<i>m</i> -Xylene	3.20	3.15		25			

[&]quot;Conventional aqueous benchmarks are presented in Suter and Tsao (1996). EqP = equilibrium partioning. All sediment benchmarks are in $\mu g/kg$ and are estimated to two significant figures assuming 1% TOC. Estimated sediment quality benchmarks greater than 10% (100,000,000 $\mu g/kg$) are not included because such concentrations are assumed to be exceedingly unlikely under natural conditions [applies to bis(2-ethylhexyl)phthalate and di-n-octylphthalate].

^bLog Kow values are from EPA (1995a), except where noted otherwise.

^cDenotes proposed EPA sediment quality criteria.

^dDenotes polar nonionic organic compounds, for which the EqP model is likely to provide a conservative estimate of exposure.

^{&#}x27;Most conservative (i.e., lowest) recommended value for reported configurations. BHC (other) is lowest of alpha-, beta-, and delta-BHC, only.

^fSource is EPA (1995b).

⁸Source is search of Syracuse Research Corporation, Environmental Sciences Center's on-line Experimental Log P Database conducted on June 7, 1996.

^hSource is ATSDR (1989).

EqP methodology, and therefore these benchmarks, is not appropriate for sediments with less than 0.2% TOC (EPA 1993f).

3.2.2 Sediment Effect Concentrations

The National Biological Service produced a set of sediment benchmarks for the EPA Great Lakes National Program Office as part of the Assessment and Remediation of Contaminated Sediment (ARCS) Project (EPA 1996). Sediment effect concentrations (SECs) were calculated using laboratory data on the toxicity of contaminants associated with up to 62 sediment samples collected predominantly from freshwater sites. The exception was six samples from Mobile Bay, Alabama, and five samples from Galveston Bay, Texas, which were used, with 10% salinity in the overlying water, in one of the three tests. The test organisms and the measured endpoints were (1) reduction in survival, growth, or sexual maturation of the amphipod Hyalella azteca and (2) reduction in survival or growth of the midge Chironomus riparius. SECs were calculated for 14-day C. riparius tests, 14-day H. azteca tests, and 28-day *H. azteca* tests. Three of the methods previously discussed were used to calculate SECs for each of these tests: the NOAA method for ER-Ls and ER-Ms, the FDEP method for TELs and PELs, and the AET method for NECs. Therefore, up to 15 SECs were calculated for each contaminant (e.g., 5 SECs for each of 3 tests). Each SEC was evaluated for its ability to correctly classify samples in the database as toxic or nontoxic (EPA 1996). Table A.1 in the Appendix presents the key results of this process, including the percentage of nontoxic samples incorrectly classified as toxic (% False Positive), the percentage of toxic samples incorrectly classified as nontoxic (% False Negative), and the overall percentage of samples correctly classified as toxic or nontoxic (% Total Correct). We selected a subset of the SECs for each chemical on the basis of these results.

ER-Ls and ER-Ms are generally as reliable as paired TELs and PELs (EPA 1996). Therefore, one of the three ERLs and three TELs for each chemical was selected as the representative threshold effect concentration (TEC). Similarly, a representative probable effect concentration (PEC) was selected for each chemical from the three ERMs and three PELs. A representative high No Effect Concentration also was selected for each chemical from the three NECs. The NECs are generally higher than the other benchmarks and tend to decrease the percentage of false positives, but increase the percentage of false negatives, relative to the other SECs (EPA 1996). Table 4 presents the representative benchmarks, which were selected by screening each SEC against a set of minimum requirements and then ranking the SECs relative to each other based on their reliability and conservatism.

The first requirement for all representative benchmarks is that the % Total Correct had to be greater than 50%. This is an intuitively obvious minimum criterion, which can be thought of as requiring a benchmark to improve the odds of correct sample classification over that of a toss of a fair coin. A second criterion is necessary because the first requirement ignores the fact that two SECs can have the same % Total Correct value, but different % False Positive and % False Negative values. For TECs, the second minimum requirement is that the % False Negatives must be less than 25%. For PECs and NECs, the second minimum requirement is that the % False Positives must be less than 25%. The differences in the second minimum requirements reflect the differences in the intended use and interpretation of these benchmarks. TECs are intended to be relatively conservative screening values, below which effects are rarely expected to occur. As such, it is important to limit the likelihood of incorrectly excluding a site and chemical from further consideration. PECs and NECs are intended to discriminate chemicals that may contribute to toxicity from those that probably contribute to toxicity (i.e., effects are more likely than not). Thus, it is important to limit the chances of incorrectly identifying a chemical as being of concern.

 ${\bf Table~4.~Summary~of~selected~toxicity~test-~and~screening~level~concentration-based~sediment~quality~benchmarks~for~freshwater~sediments^a}$

_		\mathbf{ARCS}^b		Ontario MO)E ^c
Chemical	TEC	PEC	NEC	Low	Severe
	1	norganics (mg/kg dry w	eight)		
Aluminum		58030	73160		
Arsenic	12.1	57	92.9	6	33
Cadmium	0.592	11.7	41.1	0.6	10
Chromium	56	159	312	26	110
Copper	28	77.7	54.8	16	110
Iron				2%	4%
Lead	34.2	396	68.7	31	250
Manganese	1673	1081	819	460	1110
Mercury				0.2	2
Nickel	39.6	38.5	37.9	16	75
Zinc	159	1532	541	120	820
		Organics (µg/kg dry we	eight)		
Aldrin				2	80
Anthracene	31.62	547.72	1700	220	3700
Benz(a)anthracene	260	4200	3500	320	14,800
Benzo(a)pyrene	350	393.7	440	370	14,400
Benzo(k)fluoranthene				240	13,400
Benzo(b,k)fluoranthene	27.2		4000		
Benzo(g,h,i)perylene	290	6300	3800	170	3200
ВНС				3	120
BHC, alpha-				6	100
BHC, beta-				5	210
Chlordane				7	60
Chrysene	500	5200	4000	340	4600
DDD, p,p'-	300	3200	1000	8	60
DDE, p,p'-				5	190
DDT, o,p'- + p,p'-				8	710
DDT, $O, p - + p, p - 1$ DDT, Total ^d				7	120
		29.2	970		
Dibenzo(a,h)anthracene		28.2	870	60	1300
Dieldrin				2	910
Endrin				3	1300
Fluoranthene	64.23	834.27	7500	750	10,200
Fluorene	34.64	651.92	1800	190	1600
HCB				20	240
Heptachlor epoxide				5^e	50 ^f
Indeno(1,2,3-c,d)pyrene	78	836.66	3800	200	3200
Lindane (gamma-BHC)				$3^{e,g}$	$10^{f,g}$
Mirex				7	1300
Naphthalene	32.75	687.39	290		
PAH, Total LMW	786	3369	3040		
PAH, Total HMW	2900	4353.82	51000		
PAH, Total	3553	13660	84600	4000	100,000
PCB, Total	31.62	244.66	194	70^g	5300g

18 **Table 4 (continued)**

	ARCS^b			Ontario MOE ^c		
Chemical	TEC	PEC	NEC	Low	Severe	
PCB, 1016				$7^{e,g}$	530 ^{f,g}	
PCB, 1248				$30^{e,g}$	1500 ^{f,g}	
PCB, 1254				$60^{e,g}$	340 ^{f,g}	
PCB, 1260				$5^{e,g}$	$240^{f,g}$	
Phenanthrene				560	9500	
Pyrene	570	3225	6100	490	8500	

^aBenchmark values are generally presented herein with the same number of significant digits used in the source document. ^bARCS = Assessment and Remediation of Contaminated Sediments Program; TEC = Threshold Effect Concentration, PEC = Probable Effect Concentration; and NEC = high No Effect Concentration from EPA (1996).

Ontario MOE = Ontario Ministry of the Environment; Low = lowest effect level and is the 5th percentile of the screening level concentration, except where noted otherwise; Severe = severe effect level and is the 95th percentile of the screening level concentration, except where noted otherwise; source document is Persaud et al. (1993); values for organic chemicals were normalized assuming 1% total organic carbon.

^dTotal DDT is the sum of the concentrations of the o,p'- and p,p'- isomers of DDD, DDE, and DDT.

For these same reasons, the ranking process emphasized maximizing the % Total Correct for all benchmarks, minimizing the % False Negatives for TECs, and minimizing the % False Positives for PECs and NECs. A score was calculated for each benchmark that met the minimum requirements for recommendation. The score for a TEC was the % Total Correct minus the % False Negatives (i.e., Score = %TC - %FN). The score for a PEC or NEC was the % Total Correct minus the % False Positives(i.e., Score = %TC - %FP). The maximum possible score for any SEC was 100. That is, 100% Total Correct and 0% False Negatives or False Positives. The SEC with the highest score was selected as the representative benchmark. In the event of a tie score, the SEC with the highest % Total Correct was selected. If the % Total Correct values also were the same, then the most conservative SEC was selected (i.e., the one with the lowest concentration).

3.2.3 SLC Benchmarks

The Ontario Ministry of the Environment (Ontario MOE) has prepared provincial sediment quality guidelines using the SLC approach. These values are based on Ontario sediments and benthic species from a wide range of geographical areas within the province (Persaud et al. 1993). The lowest effect level (Low) is the level at which actual ecotoxic effects become apparent. The severe effect level (Severe) represents contaminant levels that could potentially eliminate most of the benthic organisms (Persaud et al. 1993). These "Low" and "Severe" effect values are potential SQBs and are presented in Table 4.

Although SLC-derived values are based on biological effects and are suitable for all classes of chemicals and most types of sediment, the endpoint used to derive them (species absence) is considered insensitive (MacDonald 1994). Therefore, the SLC values may not be adequately protective. A qualitative comparison of the SLC values to the NOAA and FDEP values in Table 5 suggests that the Low values may be moderately underprotective for most organics. Of the 10 Low values, 9 are approximately 2 to 10 times higher than the ER-L or TEL. However, the Low values for metals are remarkably similar to the ER-L or TEL values. Most of the Severe values for metals appear to be reasonably comparable to the ER-M or PEL, but many of the Severe values for organics are 10 to 100 times higher than the ER-M or PEL.

^e10th percentile of the screening level concentration.

^f90th percentile of the screening level concentration.

^gDenotes tentative guideline.

One advantage to the use of the Ontario MOE values for organic chemicals is that they are normalized to 1% TOC. Therefore, these SQBs can be adjusted for site-specific OC content similarly to the adjustment made for EqP SQBs.

3.3 EPA SCREENING VALUES

3.3.1 Ecotox Thresholds

EPA's OSWER has published Ecotox Thresholds (ETs) intended to be used for screening contaminants at CERCLA sites (OSWER 1996). These values are available for 8 metals and 41 organics in sediments and are presented in Table 5; their derivation is briefly explained herein.

The preferred method for determining sediment ETs is to use the proposed SQC values (EPA 1993a–e), which are derived using the EqP method. Superfund has elected to use the lower limit of the 95% confidence interval as the ET, rather than the central tendency value, to maintain an appropriate level of conservatism for screening purposes (OSWER 1996). The SQC ETs in Table 5 are normalized to 1% TOC.

SQBs are used when SQCs are not available. The SQB is calculated in the same manner as the SQC except that a Tier II Secondary Chronic Value is used. Four of these are from the Great Lakes Water Quality Initiative (EPA 1992), 12 are from Suter and Mabrey (1994), and 17 were calculated by OSWER (1996). Three chemicals with OSWER-derived Secondary Chronic Values (endosulfan, methoxyclor, and malathion) had NAWQCs, but the criteria were judged to be old and unreliable. Tier II values were not derived if no daphnia acute values were available. The SQB ETs in Table 5 are normalized to 1% TOC.

The ER-L value is used if neither an SQC nor an SQB was available. OSWER noted that there is relatively low correlation between the incidence of effects and the ER-Ls for mercury, nickel, total PCBs, and DDT (Long et al. 1995) and that the ETs for these four chemicals should be used cautiously.

3.3.2 Region IV Screening Values

EPA Region IV has published ecological screening values for sediments (Region IV 1995); they are presented in Table 5. The selected effect level is the lower of the ER-L (Long et al. 1995) and TEL (MacDonald 1994). The ER-L for antimony is from Long and Morgan (1990). When the Contract Laboratory Program's Practical Quantitation Limit (PQL) is above the effect level, the screening value defaults to the PQL. However, if concentrations below the PQL are reported, they should be compared with the effect level.

Table 5. EPA Region IV and OSWER sediment screening values a

Chemical	Region IV ^b		OSWER ^c	
	Value	\mathbf{Type}^d	Value	Type ^e
	Inorganics (mg/kg	dry weight)		
Antimony	12	PQL		
Arsenic	7.24	TEL	8.2	ER-L
Cadmium	1	PQL	1.2	ER-L
Chromium	52.3	TEL	81	ER-L
Copper	18.7	TEL	34	ER-L
Lead	30.2	TEL	47	ER-L
Mercury	0.13	TEL	0.15	ER-L
Nickel	15.9	ER-L	21	ER-L
Silver	2	PQL		
Zinc	124	TEL	150	ER-L
	Organics (µg/kg d	ry weight)		
Acenaphthene	330	PQL	620	SQC
Acenaphthylene	330	PQL		
Anthracene	330	PQL		
Benzene			57	SQB
Benzo(a)anthracene	330	PQL		
Benzo(a)pyrene	330	PQL	430	ER-L
Biphenyl			1100	SQB
Bis(2-ethylhexyl)phthalate	182	TEL		
4-Bromophenyl phenyl ether			1300	SQB
Butylbenzyl phthalate			11,000	SQB
Chlordane	1.7	PQL		-
Chlorobenzene			820	SQB
Chrysene	330	PQL		
DDD	3.3	PQL		
DDD, p,p'-	3.3	PQL		
DDE	3.3	PQL		
DDT	3.3	PQL		
DDT, p,p'-	3.3	PQL		
DDT, Total ^f	3.3	PQL	1.6	ER-L
Diazinon			1.9	SQB
Dibenzofuran			2000	SQB

Table 5 (continued)

Chemical	Region IV ^b		OSWER ^c	
	Value	\mathbf{Type}^d	Value	Type ^e
Dibenzo(a,h)anthracene	330	PQL		
1,2-Dichlorobenzene			340	SQB
1,3-Dichlorobenzene			1700	SQB
1,4-Dichlorobenzene			350	SQB
Dieldrin	3.3	PQL	52	SQC
Diethyl phthalate			630	SQB
Di-n-butylphthalate			11,000	SQB
Endosulfan, mixed isomers			5.4	SQB
Endosulfan, alpha-			2.9	SQB
Endosulfan, beta-			14	SQB
Endrin	3.3	PQL	20	SQC
Ethylbenzene			3600	SQB
Fluoranthene	330	PQL	2900	SQC
Fluorene	330	PQL		
Hexachloroethane			1000	SQB
Lindane (gamma HCH)	3.3	PQL	3.7	SQB
Malathion			0.67	SQB
Methoxychlor			19	SQB
2-Methyl naphthalene	330	PQL		
Naphthalene	330	PQL	480	SQB
PAHs, Total LMW ^g	330	PQL		
PAHs, Total HMW ^g	655	TEL		
PAHs, Total ^g	1684	TEL	4000	ER-L
PCBs, Total	33	PQL	23	ER-L
Phenanthrene	330	PQL	850	SQC
Pyrene	330	PQL	660	ER-L
1,1,2,2-Tetrachloroethane			940	SQB
Tetrachloroethylene			530	SQB
Tetrachloromethane			1200	SQB
Toluene			670	SQB
Toxaphene			28	SQB
Tribromomethane			650	SQB

22 **Table 5 (continued)**

	Regio	Region IV b		OSWER ^c	
Chemical	Value	\mathbf{Type}^d	Value	\mathbf{Type}^e	
1,2,4-Trichlorobenzene			9200	SQB	
1,1,1-Trichloroethane			170	SQB	
Trichloroethylene			1600	SQB	
—Xylene			25	SQB	

^aScreening values are presented herein with the same number of significant digits used in the EPA source documents.

^fTotal DDT is the sum of the concentrations of the o,p'- and p,p'- isomers of DDD, DDE, and DDT.

LMW = low molecular weight and is the sum of the concentrations of acenaphthene, acenaphthylene, anthracene, fluorene, 2-methylnaphthalene, naphthalene, and phenanthrene; HMW = high molecular weight and is the sum of the concentrations of benz(a)anthracene, benzo(a)pyrene, chrysene, dibenzo(a,h)anthracene, fluoranthene, and pyrene; Total is the sum of the concentrations of the aforementioned low and high molecular weight PAHs.

3.4 BACKGROUND CONCENTRATIONS

Background sediment concentrations should be used as a check for the metals benchmarks. This is because some of these benchmarks are quite conservative, and because the measured concentrations in ambient sediment may include forms that are not bioavailable, benchmark concentrations may be lower than background sediment concentrations. If the background concentrations are valid and represent an uncontaminated state and if the exposure site does not contain forms of the chemicals that are more bioavailable or toxic than the forms at background sites, then screening benchmarks lower than the background concentration should not be used.

4. BENCHMARK USE IN BASELINE ECOLOGICAL RISK ASSESSMENTS

To evaluate ecological effects of contaminated sediments for a baseline ERA, it is recommended that sediment be collected for toxicity testing and the benthic macroinvertebrate community be surveyed. This is important because chemical concentrations are not accurate predictors of biological and ecological effects. This is because the percentage of the chemical that is bioavailable may range from 0 to 100% (Burton and Scott 1992). Benchmarks may be used to determine which chemicals present in the sediment are most likely causing the toxicity. Use of a weight-of-evidence approach enables a more accurate evaluation of adverse ecological impact.

^bReg IV = EPA Region IV ecological screening values for sediments (Region IV 1995) and is either the selected sediment effects value or the PQL, whichever is greater. The selected effects value is the lower of the ER-L and TEL.

OSWER = EPA Office of Solid Waste and Emergency Response Ecotox Thresholds (ET). Only the most preferred ET, as defined in OSWER (1996), is presented.

^dER-L = effects range-low and, except where noted otherwise, is from Long et al. (1995); TEL = threshold effects level and is from MacDonald (1994); PQL = Contract Laboratory Program's practical quantification limit.

^{*}ER-L = is the same as for Reg IV values; SQC = the lower limit of the 95 percent confidence interval of the proposed EPA sediment quality criteria, assuming one percent total organic carbon; SQB = the EPA sediment quality benchmark based EPA Tier II Chronic value (Region IV 1996), assuming one percent total organic carbon.

5. CHEMICAL-SPECIFIC CONSIDERATIONS

Chapters 2 and 3 address the general considerations associated with using sediment benchmarks to evaluate the various chemical types (e.g., metals, nonionic organics, polar organics, ionic organics). The following text addresses chemical-specific information that should be considered when using these benchmarks, with a focus on the reliability of a benchmark for a given chemical. The chemical-specific considerations associated with WQBs used in the EqP SQBs are discussed in Suter and Tsao (1996). MacDonald (1994) and Long et al. (1995) discussed the degree of reliability associated with the FDEP and NOAA values for each chemical. However, a chemical-by-chemical evaluation of the Ontario MOE values was not available (Persaud et al. 1993). A chemical-by-chemical evaluation of the ARCS values is not presented here because the measures of reliability for each chemical and SEC combination were incorporated into the process of selecting a representative benchmark (Chap. 3). These benchmarks can be further evaluated by critically reviewing the information presented in Table A.1.

Reliability of the NOAA and FDEP values is a function of the agreement between the predicted and observed incidence of effects (Long et al. 1995; MacDonald 1994). Reliability of the TEL is low if >25% of the concentrations below the TEL were associated with effects (i.e., the number of "hits" below the TEL divided by the total number of concentrations below the TEL is >0.25). On the basis of this criterion, a TEL with low reliability may be underprotective and caution should be used when attempting to exclude that chemical as a chemical of potential ecological concern. Reliability of the PEL is low if <50% of the concentrations above the PEL were associated with effects. Therefore, a PEL with low reliability may overpredict the potential for real effects; this is primarily of concern when the SQBs are used in baseline assessments to help predict the magnitude of effects and help determine causality of observed effects.

The designations by Long et al. (1995) (relatively high reliability and lower reliability) were somewhat different than the designations by MacDonald (1994) (low, moderate, and high). The designation of low reliability also is used herein for the ER-Ls and ER-Ms, because SQBs of low reliability are of particular concern. Reliability is considered low if the incidence of effects is >25% at concentrations below the ER-L. Reliability of the ER-M is considered low if the incidence of effects is <50% at concentrations above the ER-M. Other factors (e.g., concordance of effects) also were considered by MacDonald (1994) and Long et al. (1995) to determine the overall reliability of the FDEP and NOAA values, respectively. These determinations also are presented in the following text, where appropriate.

5.1 METALS

Antimony—Data are available from only two geographic regions (Puget Sound/Commencement Bay and San Francisco Bay); therefore, the degree of confidence in the NOAA values is moderate (Long and Morgan 1991). No criteria are available for comparison from FDEP or Ontario MOE.

Arsenic—Confidence in the TEL and ER-L is high and relatively high, respectively. Confidence in the ER-M is somewhat lower, and confidence in the PEL is Low. Therefore, the TEL and ER-L appear to be reliable indicators of the threshold for effects, and the ER-M appears to be the better indicator of the level above which real effects are likely.

Cadmium—A relatively large amount of data exists for cadmium, including spiked-sediment toxicity tests and EqP-based assessments (MacDonald et al. 1994). Klapow and Lewis (1979) calculated a statistically significant difference in the medians of acute aqueous toxicity data from saltwater and freshwater organisms. This supports the findings of Eisler (1985) (as referenced in Long and Morgan 1991), who found resistance to cadmium higher among marine than freshwater species. However, the degree of confidence in the lower and upper NOAA and FDEP values is high, and these values are considered to be reliable predictors of effects.

Chromium—There are some inconsistencies in the data available for chromium, possibly because of lack of speciation information. All data were reported as total chromium, whereas the hexavalent form is more toxic than the trivalent form. There also are no supporting data from single-chemical spiked-sediment toxicity tests or from the EqP approach (MacDonald et al. 1994). Overall confidence in the FDEP values, and the PEL in particular, is moderate. Although the overall confidence in the NOAA values is relatively high, Long et al. (1995) cautioned that the incidence of effects may be unduly exaggerated by data from multiple tests performed in only two studies. On the basis of the available evaluations, the TEL and ER-L appear to be reliable predictors of the threshold for effects.

Copper—Considerable data exist for copper in sediments, and a relatively high degree of overall confidence exists for the NOAA values. Overall confidence in the FDEP values, and the PEL in particular, is moderate only. However, the TEL is considered to be a highly reliable predictor of the threshold for effects.

Iron—The only available benchmarks are the Ontario MOE Low and Severe effect levels. Although the reliability of these data was not addressed (Persaud et al. 1993), the Ontario MOE guidelines were derived for freshwater sediments. Therefore, these values appear to warrant a moderate degree of confidence.

Lead—Considerable data exist for lead in sediments, and a relatively high degree of overall confidence exists for the NOAA values. Overall confidence in the FDEP values, and the PEL in particular, is moderate only. However, the TEL is considered to be a reliable predictor of the threshold for effects. This is consistent with expected reliability of the ER-L and ER-M values. Although a relatively large amount of data exist for lead, there were no spiked-sediment toxicity test data to confirm the toxic concentrations (MacDonald et al. 1994).

Manganese—The only available benchmarks are the Ontario MOE Low and Severe effect levels. Although the reliability of these data was not addressed (Persaud et al. 1993), the Ontario MOE guidelines were derived for freshwater sediments. Therefore, these values appear to warrant a moderate degree of confidence.

Mercury—Considerable data exist for mercury, though only total mercury concentrations were reported in the data set (MacDonald et al. 1994). Confidence in the TEL and ER-L is high and relatively high, respectively. Therefore, the lower screening values should be at least conservative predictors of the threshold for effects. The PEL and ER-M may significantly overpredict the likelihood of real effects, given that confidence in these values is Low. In addition, the overall confidence in the FDEP values is low.

Nickel—Toxicity of nickel is greatly influenced by water hardness and salinity (Long and Morgan 1991). Data were from marine and estuarine field studies only, and no spiked-sediment toxicity tests or EqP approaches were used (MacDonald et al. 1994). Confidence in the TEL and ER-L is high and relatively high, respectively. Therefore, the lower screening values should be at least conservative

predictors of the threshold for effects. The PEL and ER-M may significantly overpredict the likelihood of real effects, given that confidence in these values is Low.

Silver—A moderate amount of data is available for silver in sediments, although data exist from spiked-sediment toxicity tests or from EqP approaches (MacDonald et al. 1994). The FDEP and NOAA values hold moderate and relatively high overall confidence, respectively. These data suggest that the ER-L and TEL are likely to be reliable predictors of the threshold for effects. The ER-M is likely to be a better predictor of real effects because confidence in the PEL is Low.

Zinc—Considerable data exist for zinc in sediments, including spiked-sediment toxicity tests and EqP-based assessments (MacDonald et al. 1994). Overall confidence in the FDEP values, and the PEL in particular, is moderate only. However, the TEL is considered to be a reliable predictor of the threshold for effects. This is consistent with expected reliability of the NOAA values.

5.2 ORGANICS

Polycyclic aromatic hydrocarbons (PAHs)—The reliability of the individual TELs and PELs ranged from moderate to high, as did overall reliability of the FDEP values. The TELs and PELs may be somewhat overprotective for four PAHs [i.e., acenaphthene, acenaphthylene, fluorene, benz(a)anthracene, dibenzo(a,h)anthracene, and total high molecular weight polyaromatic hydrocarbons] for which the overall FDEP or ER-M values are considered moderately reliable. The TELs for fluorene and dibenzo(a,h)anthracene are considered to be only moderately reliable predictors of the threshold for effects. The TELs and PELs should be reasonably reliable predictors of the likelihood of effects for the remaining PAHs. Reliability of the ER-Ls for anthracene and fluorene is low, while reliability of the ER-M for dibenzo(a,h)anthracene is relatively low. The reliability of the ER-Ls and ER-Ms for the remaining PAHs is relatively high.

Total polychlorinated biphenyls (PCBs)—The overall reliability of the FDEP values was low, and the reliability of the TEL and PEL was only moderate. Reliability of the ER-M is considered to be relatively low. Concordance of the concentrations and effects was not high for either the NOAA or FDEP values. This may be the result of insufficiently detailed chemical information. That is, the mixture of PCB congeners may have varied considerably among sites and studies, but this information was unavailable or not included in the NOAA and FDEP analyses. Caution should be used when screening PCBs with these benchmarks.

Pesticides—The overall reliability of the FDEP values was low for chlordane, total DDT, and lindane and moderate for dieldrin and the p,p' isomers of DDD, DDE, and DDT. The TEL for total DDT is considered to have low reliability and is likely to be a poor predictor of the threshold for effects. The PELs for chlordane, p,p'-DDD, and lindane are considered to have low reliability and are likely to overpredict the likelihood of real effects. This is also somewhat true of the PELs for the other four pesticides. NOAA values are available for only two pesticides, p,p'-DDE and total DDT, for which poor concordance of effects and concentrations was observed. This may be caused by the inclusion of relatively low EqP values, which were not based on toxicity to benthic organisms (Long et al. 1995). Therefore, the NOAA values may tend to overpredict the likelihood of effects.

Bis(2-ethylhexyl)phthalate—The overall reliability of the FDEP values was high, as was the reliability of the TEL and PEL. These values are expected to be reliable predictors of the likelihood of effects. NOAA values are not available for bis(2-ethylhexyl)phthalate.

6. UNCERTAINTIES/LIMITATIONS

The EqP methodology has several uncertainties. It relies on an empirical model to compute the pore water concentration from the solid phase measurements. Therefore, an uncertainty is associated with the use of the model. In addition, uncertainty exists with respect to the K_{ow} associated with the specific chemical because it is an experimentally determined quantity (EPA 1989a). Various types of organic matter present in sediments can have significantly different binding capacities for organic contaminants; the affinity depends in large part on the source and nature of the carbon. For example, organics associated with sediments contaminated with petroleum hydrocarbons would tend to be much less toxic than those associated with sediments whose OC is natural OC (Lee and Jones-Lee 1993).

The assumption that benthic organisms have similar sensitivities to water column species has a level of uncertainty (EPA 1993f). This may be of particular concern for tube-dwelling amphipods. The tubes tend to isolate them from the interstitial water, causing speculation that their exposure is at the sediment/water interface. Additionally, the amphipod tubes are matrices of organics and inorganics; the tube walls could sorb appreciable amounts of organic contaminants, which could alter the availability of sediment-associated contaminants to those organisms (Lee and Jones-Lee 1993).

The EqP approach is known not to work for all nonpolar organics. It is well known that many pesticides that are sorbed onto soils and sediments are in the form of "bound" pesticide residues that do not participate in equilibrium reactions with water (Lee and Jones-Lee 1993).

The aquatic benchmarks [EPA WQC for the protection of aquatic life and the aquatic benchmarks developed by Suter and Tsao (1996)] for PCBs and several polynuclear aromatic hydrocarbons are class criteria based on the cumulative concentration of all members of the class. In the derivation of sediment benchmarks using the EqP approach and the aquatic benchmarks, it is necessary to apply the class level to each member of the class individually because each has a unique K_{oc} (Lake et al. 1990). In environments where one class member comprises the majority of the sediment burden of the class, this approach should be adequate. However, if numerous class constituents are significantly enriched, a safe threshold for the class as a whole may be exceeded even though no individual constituent violates its predicted safe level (based on the aquatic benchmark) (Pavlou 1987).

The Washington state AET, NOAA, and FDEP values have several limitations. Primarily, all or most of the data used in their derivation were based on marine and estuarine systems. These values are being applied to freshwater systems at the ORR and the Portsmouth and Paducah gaseous diffusion plants. Differences include physico-chemical characteristics of the system as well as possible differences in sensitivity of biota. Washington state, NOAA, and FDEP values are for single chemicals, although sediments containing chemical mixtures were used for their derivation. The Ontario MOE values were derived to be applicable to sediment types throughout the province of Ontario. The differences between Ontario and East Tennessee, Ohio, and Kentucky sediments and biota introduce a level of uncertainty.

The uncertainties associated with the ARCS values are similar to those for the NOAA and FDEP values. That is, the SECs also were derived using sediment samples containing chemical mixtures. Although those sediments were predominantly from freshwater systems, 11 of the 62 possible samples used in one of the three tests (28-d *H. azteca*) were from marine systems. However, the overlying water was only 10% saline. The freshwater sediments also were from areas other than East Tennessee, including the Great Lakes, Illinois, Minnesota, Montana, and Texas.

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APPENDIX SUMMARY OF ALL SEDIMENT EFFECT CONCENTRATIONS THAT MEET THE MINIMUM REQUIREMENTS FOR RECOMMENDATION

	for recommendation ^a											
Chemical	BMK Type ^b	\mathbf{Test}^c	\mathbf{SEC}^d	Conc.	Total Correct (%) ^e	False Positives (%) ^f	False Negatives (%)g	Score ^h	Selected BMK ⁱ			
	-71-			rganics (mg/k		(,,,)	(,,,)					
Aluminum	PEC	HA28	ERM	58030	8) 64	16	20	48	X			
Aluminum	PEC	HA28	PEL	59572.012	52	16	32	36				
Aluminum	NEC	HA28	NEC	73160	52	4	44	48	X			
Arsenic	TEC	HA14	ERL	12.1	69	25	6	63	X			
Arsenic	TEC	HA14	TEL	11.24478	66	28	6	60	**			
Arsenic	TEC	HA28	TEL	10.79768	62	27	12	50				
Arsenic	TEC	CR14	ERL	32	60	31	10	50				
Arsenic	TEC	HA28	ERL	13.1	63	21	15	48				
Arsenic	TEC	CR14	TEL	21.76235	55	36	10	45				
Arsenic	PEC	CR14	ERM	57	71	10	19	61	X			
Arsenic	PEC	CR14	PEL	54.02222	69	12	19	57				
Arsenic	PEC	HA28	PEL	48.38512	63	6	31	57				
Arsenic	PEC	HA28	ERM	49.6	63	6	31	57				
Arsenic	PEC	HA14	ERM	33	66	13	22	53				
Arsenic	PEC	HA14	PEL	39.46644	63	13	25	50				
Arsenic	NEC	HA14	NEC	92.9	59	3	38	56	X			
Arsenic	NEC	HA28	NEC	102	54	2	44	52				
Cadmium	TEC	HA14	TEL	0.59161	81	19	0	81	X			
Cadmium	TEC	HA14	ERL	0.7	81	19	0	81				
Cadmium	TEC	CR14	ERL	9.1	86	2	12	74				
Cadmium	TEC	CR14	TEL	2.89344	69	21	10	59				
Cadmium	TEC	HA28	TEL	0.58327	66	26	8	58				
Cadmium	TEC	HA28	ERL	0.7	66	26	8	58				
Cadmium	PEC	CR14	ERM	11.7	81	2	17	79	X			
Cadmium	PEC	HA14	PEL	3.2249	78	3	19	75				
Cadmium	PEC	CR14	PEL	6.62382	81	7	12	74				
Cadmium	PEC	HA14	ERM	5.2	75	3	22	72				
Cadmium	PEC	HA28	PEL	3.24654	74	5	21	69				
Cadmium	PEC	HA28	ERM	3.875	71	5	24	66				
Cadmium	NEC	CR14	NEC	41.1	74	2	24	72	X			
Cadmium	NEC	HA14	NEC	8	72	3	25	69				
Cadmium	NEC	HA28	NEC	8	71	2	27	69				
Chromium	TEC	HA14	ERL	56	81	13	6	75	X			
Chromium	TEC	HA14	TEL	47.91659	66	28	6	60				
Chromium	TEC	CR14	ERL	39.3	62	36	2	60				
Chromium	TEC	CR14	TEL	39.79686	60	36	5	55				
Chromium	TEC	HA28	TEL	36.28636	60	26	15	45				
Chromium	TEC	HA28	ERL	38.5	60	26	15	45				
Chromium	PEC	CR14	PEL	159.4051	86	2	12	84	X			
Chromium	PEC	CR14	ERM	363	83	0	17	83				
Chromium	PEC	HA14	PEL	130.9217	81	0	19	81				
Chromium	PEC	HA14	ERM	293	78	0	22	78				
Chromium	PEC	HA28	PEL	119.365	73	0	27	73				
Chromium	PEC	HA28	ERM	274	73	0	27	73				

A-4
Table A.1 (continued)

	BMK		an ad		Total Correct		False Negatives	a h	Selected
Chemical	Type ^b	Test ^c	SEC ^d	Conc.	(%) ^e	(%) ^f	(%) ^g	Score ^h	BMK^i
Chromium	NEC	CR14	NEC	312	83	2	14	81	X
Chromium	NEC	HA14	NEC	95	81	3	16	78	
Chromium	NEC	HA28	NEC	95	73	2	26	71	
Copper	TEC	HA14	TEL	28.0125	84	13	3	81	X
Copper	TEC	HA14	ERL	41.3	81	13	6	75	
Copper	TEC	HA28	ERL	41.3	73	15	12	61	
Copper	TEC	HA28	TEL	28.0125	71	19	10	61	
Copper	TEC	CR14	TEL	67.4535	64	26	10	54	
Copper	TEC	CR14	ERL	96.5	64	26	10	54	
Copper	PEC	HA14	PEL	77.71197	81	0	19	81	X
Copper	PEC	HA14	ERM	122.25	78	0	22	78	
Copper	PEC	HA28	PEL	101.2304	71	8	21	63	
Copper	PEC	HA28	ERM	187	69	6	25	63	
Copper	PEC	CR14	ERM	206.5	62	21	17	41	
Copper	PEC	CR14	PEL	291.3271	60	19	21	41	
Copper	NEC	HA14	NEC	54.8	81	3	16	78	X
Copper	NEC	HA28	NEC	583	56	2	42	54	
Manganese	TEC	CR14	ERL	1673	82	8	11	71	X
Manganese	TEC	HA14	ERL	726	83	4	13	70	
Manganese	TEC	CR14	TEL	1079.077	79	11	11	68	
Manganese	TEC	HA14	TEL	614.7219	67	25	8	59	
Manganese	TEC	HA28	ERL	726	68	11	20	48	
Manganese	TEC	HA28	TEL	631.3272	59	25	16	43	
Manganese	PEC	HA14	PEL	1080.689	75	0	25	75	X
Manganese	PEC	CR14	PEL	1538.382	82	8	11	74	
Manganese	PEC	CR14	ERM	2410	79	5	16	74	
Manganese	PEC	HA14	ERM	1678	71	0	29	71	
Manganese	PEC	HA28	PEL	1184.756	61	5	34	56	
Manganese	PEC	HA28	ERM	1673	59	5	36	54	
Manganese	NEC	HA14	NEC	819	71	4	25	67	X
Nickel	TEC	HA14	ERL	39.6	94	0	6	88	X
Nickel	TEC	CR14	ERL	40	93	2	5	88	
Nickel	TEC	HA14	TEL	27.71714	81	16	3	78	
Nickel	TEC	CR14	TEL	26.60827	76	19	5	71	
Nickel	TEC	HA28	ERL	23.8	68	13	19	49	
Nickel	TEC	HA28	TEL	19.5141	65	18	18	47	
Nickel	PEC	HA14	PEL	38.49675	94	0	6	94	X
Nickel	PEC	CR14	PEL	38.68139	90	5	5	85	
Nickel	PEC	CR14	ERM	47.5	83	2	14	81	
Nickel	PEC	HA14	ERM	47.5	78	0	22	78	
Nickel	PEC	HA28	ERM	44.7	73	0	27	73	
Nickel	PEC	HA28	PEL	32.82179	74	5	21	69	
Nickel	NEC	HA14	NEC	37.9	91	3	6	88	x
Nickel	NEC	CR14	NEC	57.9	79	2	19	77	Λ
Nickel	NEC	HA28	NEC	43	73	2	26	71	
Lead	TEC	на28 НА14	TEL	34.17455	73 84	13	3	81	77

A-5
Table A.1 (continued)

	BMK				Total Correct		False Negatives		Selected
Chemical	\mathbf{Type}^{b}	Test ^c	\mathbf{SEC}^d	Conc.	(%) ^e	(%) ^f	(%) ^g	Score ^h	BMK^i
Lead	TEC	CR14	ERL	99	83	7	10	73	
Lead	TEC	HA14	ERL	51	78	13	9	69	
Lead	TEC	CR14	TEL	69.64912	74	21	5	69	
Lead	TEC	HA28	ERL	55	74	15	11	63	
Lead	TEC	HA28	TEL	37.22902	71	21	8	63	
Lead	PEC	CR14	ERM	396	81	2	17	79	X
Lead	PEC	HA14	PEL	117.4947	78	0	22	78	
Lead	PEC	HA14	ERM	251	78	0	22	78	
Lead	PEC	CR14	PEL	191.803	81	5	14	76	
Lead	PEC	HA28	PEL	81.74344	77	6	16	71	
Lead	PEC	HA28	ERM	98.7	74	3	23	71	
Lead	NEC	HA14	NEC	68.7	84	3	13	81	X
Lead	NEC	CR14	NEC	679	76	2	21	74	
Lead	NEC	HA28	NEC	127	71	2	27	69	
Zinc	TEC	HA14	ERL	159	81	16	3	78	X
Zinc	TEC	HA14	TEL	94.15015	78	22	0	78	
Zinc	TEC	HA28	TEL	98.09154	63	31	6	57	
Zinc	TEC	HA28	ERL	113	63	29	8	55	
Zinc	TEC	CR14	ERL	381	64	26	10	54	
Zinc	TEC	CR14	TEL	280.8327	57	36	7	50	
Zinc	PEC	CR14	PEL	1532.482	83	2	14	81	X
Zinc	PEC	CR14	ERM	2750	81	2	17	79	
Zinc	PEC	HA14	PEL	384.043	75	3	22	72	
Zinc	PEC	HA14	ERM	422	75	3	22	72	
Zinc	PEC	HA28	PEL	543.9917	74	6	19	68	
Zinc	PEC	HA28	ERM	547	74	6	19	68	
Zinc	NEC	HA14	NEC	541	72	3	25	69	X
Zinc	NEC	HA28	NEC	1300	69	2	29	67	
				rganics (ug/kg					
Naphthalene	TEC	CA14	TEL .	32.75	78	22	0	78	X
Naphthalene	TEC	CR14	ERL	55	79	19	2	77	
Naphthalene	TEC	CR14	TEL	34.39	76	24	0	76	
Naphthalene	TEC	CA14	ERL	55	78	19	3	75	
Naphthalene	TEC	HA28	TEL	14.65	56	37	6	50	
Naphthalene	TEC	HA28	ERL	13	55	40	5	50	
Naphthalene	PEC	CA14	PEL	687.39	81	2	17	79	X
Naphthalene	PEC	CR14	ERM	1890	81	2	17	79 79	Λ
Naphthalene	PEC	CA14	ERM	325	78	0	22	79 78	
Naphthalene		CR14	PEL	285.04	75	3	22	78 72	
Naphthalene	PEC		PEL		63	13		50	
-	PEC	HA28	PEL ERM	139.64			24 24		
Naphthalene	PEC	HA28		97.5	61 75	15		46 72	
Naphthalene	NEC	CA14	NEC	290	75	3	22	72	X
Naphthalene	NEC	HA28	NEC	1400	68	2	31	66 75	
Fluorene	TEC	HA14	TEL	34.64	75 7.5	25	0	75 72	X
Fluorene	TEC	HA14	ERL	50	75	22	3	72	
Fluorene	TEC	CR14	TEL	29.66	74	24	2	72	

A-6
Table A.1 (continued)

Chemical	BMK Type ^b	\mathbf{Test}^c	\mathbf{SEC}^d	Conc.	Total Correct (%) ^e	False Positives (%) ^f	False Negatives (%) ^g	Score ^h	Selected BMK ⁱ
Fluorene	TEC	CR14	ERL	88	74	19	7	67	DIVIN
Fluorene	PEC	CR14	PEL	651.92	83	2	14	81	X
Fluorene	PEC	HA14	PEL	385.68	81	0	19	81	Λ
Fluorene	PEC	CR14	ERM	1700	81	2	17	79	
Fluorene	PEC	HA14	ERM	595	78	0	22	78	
Fluorene	PEC	HA28	ERM	140	61	13	26	48	
Fluorene	PEC	HA28	PEL	149.67	60	13	27	47	
Fluorene	NEC	CR14	NEC	1800	79	2	19	77	X
Fluorene	NEC	HA14	NEC	290	78	3	19	75	••
Fluorene	NEC	HA28	NEC	3000	63	2	35	61	
Phenanthrene	TEC	CR14	ERL	350	81	17	2	79	X
Phenanthrene	TEC	HA14	ERL	390	81	16	3	78	••
Phenanthrene	TEC	HA14	TEL	197.48	75	25	0	75	
Phenanthrene	TEC	CR14	TEL	95.39	71	26	2	69	
Phenanthrene	TEC	HA28	TEL	18.73	68	27	5	63	
Phenanthrene	TEC	HA28	ERL	27	65	27	8	57	
Phenanthrene	PEC	CR14	PEL	1142.37	83	2	14	81	X
Phenanthrene	PEC	HA14	ERM	1100	81	0	19	81	A
Phenanthrene	PEC	CR14	ERM	2250	81	2	17	79	
Phenanthrene	PEC	HA14	PEL	777.82	78	3	19	75	
Phenanthrene	PEC	HA28	ERM	345	66	13	21	53	
Phenanthrene	PEC	HA28	PEL	409.05	63	13	24	50	
Phenanthrene	NEC	CR14	NEC	6100	79	2	19	77	X
Phenanthrene	NEC	HA14	NEC	1000	78	3	19	75	A
Phenanthrene	NEC	HA28	NEC	20000	61	2	37	59	
Anthracene	TEC	HA14	TEL	31.62	78	22	0	78	X
Anthracene	TEC	HA14	ERL	100	78	19	3	75	
Anthracene	TEC	CR14	TEL	37.42	74	24	2	72	
Anthracene	TEC	CR14	ERL	140	74	19	7	67	
Anthracene	PEC	CR14	PEL	547.72	83	2	14	81	X
Anthracene	PEC	CR14	ERM	1250	81	2	17	79	Α
Anthracene	PEC	HA14	PEL	409.27	78	0	22	78	
Anthracene	PEC	HA14	ERM	670	78	0	22	78	
Anthracene	PEC	HA28	PEL	167.33	63	11	26	52	
Anthracene	PEC	HA28	ERM	140	61	15	24	46	
Anthracene	NEC	CR14	NEC	1700	79	2	19	77	X
Anthracene	NEC	HA14	NEC	290	75	3	22	72	21
Anthracene	NEC	HA28	NEC	2000	65	2	34	63	
Fluoranthene	TEC	CR14	TEL	64.23	69	31	0	69	X
Fluoranthene	TEC	HA14	TEL	144.22	69	28	3	66	4
Fluoranthene	TEC	HA14	ERL	160	69	28	3	66	
Fluoranthene	TEC	CR14	ERL	110	67	31	2	65	
Fluoranthene	TEC	HA28	TEL	31.46	56	32	11	45	
Fluoranthene	TEC	HA28	ERL	33	56	32	11	45	
Fluoranthene	PEC	HA14	PEL	834.27	84	3	13	81	X
Fluoranthene	PEC	CR14	PEL	1484.59	83	2	13	81	Λ

A-7 **Table A.1 (continued)**

	BMK		an ad		Total Correct		False Negatives	a h	Selected
Chemical	Type ^b	Test ^c	\mathbf{SEC}^d	Conc.	(%) ^e	(%) ^f	(%) ^g	Score ^h	\mathbf{BMK}^i
Fluoranthene	PEC	CR14	ERM	2900	81	2	17	79	
Fluoranthene	PEC	HA14	ERM	1200	78	3	19	75	
Fluoranthene	PEC	HA28	PEL	318.59	56	19	24	37	
Fluoranthene	PEC	HA28	ERM	175	55	23	23	32	
Fluoranthene	NEC	CR14	NEC	7500	79	2	19	77	X
Fluoranthene	NEC	HA14	NEC	1200	78	3	19	75	
Fluoranthene	NEC	HA28	NEC	10000	63	2	35	61	
Pyrene	TEC	HA14	ERL	570	81	16	3	78	X
Pyrene	TEC	HA14	TEL	231.47	72	25	3	69	
Pyrene	TEC	CR14	ERL	120	69	29	2	67	
Pyrene	TEC	CR14	TEL	67.53	67	31	2	65	
Pyrene	TEC	HA28	ERL	40	60	32	8	52	
Pyrene	TEC	HA28	TEL	44.27	55	32	13	42	
Pyrene	PEC	CR14	ERM	3225	81	2	17	79	X
Pyrene	PEC	CR14	PEL	1684.64	81	5	14	76	
Pyrene	PEC	HA14	ERM	1100	78	3	19	75	
Pyrene	PEC	HA14	PEL	908.3	78	6	16	72	
Pyrene	PEC	HA28	PEL	493.2	63	16	21	47	
Pyrene	PEC	HA28	ERM	347.5	61	18	21	43	
Pyrene	NEC	CR14	NEC	6100	79	2	19	77	X
Pyrene	NEC	HA14	NEC	1800	75	3	22	72	
Pyrene	NEC	HA28	NEC	9000	65	2	34	63	
Benz(a)anthracene	TEC	HA14	ERL	260	88	9	3	85	X
Benz(a)anthracene	TEC	CR14	ERL	300	81	12	7	74	
Benz(a)anthracene	TEC	HA14	TEL	103.25	72	25	3	69	
Benz(a)anthracene	TEC	CR14	TEL	75.5	67	29	5	62	
Benz(a)anthracene	TEC	HA28	TEL	15.72	56	34	10	46	
Benz(a)anthracene	TEC	HA28	ERL	19	55	34	11	44	
Benz(a)anthracene	PEC	CR14	ERM	4200	83	0	17	83	X
Benz(a)anthracene	PEC	CR14	PEL	1194.99	81	2	17	79	
Benz(a)anthracene	PEC	HA14	ERM	490	78	3	19	75	
Benz(a)anthracene	PEC	HA14	PEL	363.73	78	6	16	72	
Benz(a)anthracene	PEC	HA28	PEL	284.6	68	10	23	58	
Benz(a)anthracene	PEC	HA28	ERM	300	68	10	23	58	
Benz(a)anthracene	NEC	CR14	NEC	3500	81	2	17	79	X
Benz(a)anthracene	NEC	HA14	NEC	690	72	3	25	69	
Benz(a)anthracene	NEC	HA28	NEC	3000	68	2	31	66	
Chrysene	TEC	CR14	ERL	500	88	5	7	81	X
Chrysene	TEC	HA14	ERL	330	84	13	3	81	
Chrysene	TEC	CR14	TEL	122.47	71	24	5	66	
Chrysene	TEC	HA14	TEL	135.94	69	28	3	66	
Chrysene	TEC	HA28	TEL	26.83	52	35	13	39	
Chrysene	TEC	HA28	ERL	30	52	34	15	37	
Chrysene	PEC	CR14	ERM	5200	83	0	17	83	x
Chrysene	PEC	HA14	ERM	690	81	0	19	81	
Chrysene	PEC	CR14	PEL	1512.61	81	2	17	79	

A-8 **Table A.1 (continued)**

Chemical	BMK Type ^b	\mathbf{Test}^c	\mathbf{SEC}^d	Conc.	Total Correct (%) ^e	False Positives (%) ^f	False Negatives (%) ^g	Score ^h	Selected BMK ⁱ
Chrysene	PEC	HA14	PEL	551	81	3	16	78	DIVIL
Chrysene	PEC	HA28	ERM	500	73	3	24	70	
Chrysene	PEC	HA28	PEL	406.2	68	10	23	58	
Chrysene	NEC	CR14	NEC	4000	81	2	17	79	X
Chrysene	NEC	HA14	NEC	600	81	3	16	78	
Chrysene	NEC	HA28	NEC	3000	68	2	31	66	
Benzo(a)pyrene	TEC	HA14	ERL	350	88	3	9	79	X
Benzo(a)pyrene	TEC	HA14	TEL	119.79	75	22	3	72	
Benzo(a)pyrene	TEC	CR14	ERL	210	74	21	5	69	
Benzo(a)pyrene	TEC	CR14	TEL	51.23	69	26	5	64	
Benzo(a)pyrene	TEC	HA28	ERL	84	60	21	19	41	
Benzo(a)pyrene	TEC	HA28	TEL	32.4	53	29	18	35	
Benzo(a)pyrene	PEC	HA14	PEL	393.7	84	3	13	81	X
Benzo(a)pyrene	PEC	CR14	ERM	8500	81	0	19	81	
Benzo(a)pyrene	PEC	CR14	PEL	1724.82	81	2	17	79	
Benzo(a)pyrene	PEC	HA14	ERM	620	78	0	22	78	
Benzo(a)pyrene	PEC	HA28	ERM	465	71	2	27	69	
Benzo(a)pyrene	PEC	HA28	PEL	319.84	71	5	24	66	
Benzo(a)pyrene	NEC	HA14	NEC	440	84	3	13	81	X
Benzo(a)pyrene	NEC	CR14	NEC	5800	81	2	17	79	
Benzo(a)pyrene	NEC	HA28	NEC	1000	68	2	31	66	
Indeno (1,2,3-c,d)pyrene		HA14	ERL	78	69	28	3	66	X
Indeno (1,2,3-c,d)pyrene		CR14	TEL	17.32	67	31	2	65	
Indeno (1,2,3-c,d)pyrene		CR14	ERL	30	67	31	2	65	
Indeno (1,2,3-c,d)pyrene		HA14	TEL	86.53	66	28	6	60	
Indeno (1,2,3-c,d)pyrene		HA28	ERL	30	56	32	12	44	
Indeno (1,2,3-c,d)pyrene		HA28	TEL	17.32	54	33	12	42	
Indeno (1,2,3-c,d)pyrene		CR14	PEL	836.66	81	2	17	79	X
Indeno (1,2,3-c,d)pyrene		CR14	ERM	2800	81	2	17	79	
Indeno (1,2,3-c,d)pyrene		HA14	PEL	326.5	78	0	22	78	
Indeno (1,2,3-c,d)pyrene		HA14	ERM	410	78	0	22	78	
Indeno (1,2,3-c,d)pyrene		HA28	PEL	239.79	67	11	23	56	
Indeno (1,2,3-c,d)pyrene		HA28	ERM	250	67	11	23	56	
Indeno (1,2,3-c,d)pyrene	NEC	CR14	NEC	3800	81	2	17	79	X
Indeno (1,2,3-c,d)pyrene	NEC	HA14	NEC	290	75	6	19	69	
Indeno (1,2,3-c,d)pyrene	NEC	HA28	NEC	770	70	2	28	68	
Benzo(g,h,i)perylene	TEC	CR14	ERL	290	83	7	10	73	X
Benzo(g,h,i)perylene	TEC	CR14	TEL	74.23	71	24	5	66	
Benzo(g,h,i)perylene	TEC	HA14	TEL	89.49	69	28	3	66	
Benzo(g,h,i)perylene	TEC	HA14	ERL	91	69	28	3	66	
Benzo(g,h,i)perylene	TEC	HA28	ERL	13	52	37	11	41	
Benzo(g,h,i)perylene	TEC	HA28	TEL	15.51	52	35	13	39	
Benzo(g,h,i)perylene	PEC	CR14	ERM	6300	83	0	17	83	X
Benzo(g,h,i)perylene	PEC	CR14	PEL	1279.84	81	2	17	79	
Benzo(g,h,i)perylene	PEC	HA14	PEL	349.14	78	0	22	78	
Benzo(g,h,i)perylene	PEC	HA14	ERM	460	78	0	22	78	

A-9 **Table A.1 (continued)**

	BMK	TP 46	gr od	G	Total Correct		False Negatives	a h	Selected
Chemical	Type ^b	Test	SEC ^d	Conc.	(%) ^e	(%) ^f	(%) ^g	Score ^h	BMK^i
Benzo(g,h,i)perylene	PEC	HA28	ERM	275	73	3	24	70	
Benzo(g,h,i)perylene	PEC	HA28	PEL	251.5	71	6	23	65	
Benzo(g,h,i)perylene	NEC	CR14	NEC	3800	81	2	17	79	X
Benzo(g,h,i)perylene	NEC	HA14	NEC	310	75	3	22	72	
Benzo(g,h,i)perylene	NEC	HA28	NEC	1200	68	2	31	66	
Benzo(b,k)fluoranthene	TEC	HA28	TEL	27.2	53	30	16	37	X
Benzo(b,k)fluoranthene	TEC	HA28	ERL	37	53	30	16	37	
Benzo(b,k)fluoranthene	PEC	HA28	PEL	157.64	56	19	26	37	
Benzo(b,k)fluoranthene	NEC	HA28	NEC	4000	67	2	30	65	X
Dibenz(a,h)anthracene	PEC	HA28	PEL	28.2	56	16	28	40	X
Dibenz(a,h)anthracene	PEC	HA28	ERM	15	56	21	23	35	
Dibenz(a,h)anthracene	NEC	HA28	NEC	870	67	2	30	65	X
PAH Total (others)	TEC	HA14	ERL	3553	78	19	3	75	X
PAH Total (others)	TEC	CR14	ERL	1297	74	24	2	72	
PAH Total (others)	TEC	HA14	TEL	1589.4	69	28	3	66	
PAH Total (others)	TEC	CR14	TEL	588.47	67	31	2	65	
PAH Total (others)	TEC	HA28	ERL	240	56	35	8	48	
PAH Total (others)	TEC	HA28	TEL	264.05	55	34	11	44	
PAH Total (others)	PEC	CR14	PEL	13660.65	81	2	17	79	X
PAH Total (others)	PEC	CR14	ERM	33819	81	2	17	79	
PAH Total (others)	PEC	HA14	PEL	6736.42	81	3	16	78	
PAH Total (others)	PEC	HA14	ERM	8498	78	3	19	75	
PAH Total (others)	PEC	HA28	PEL	3368.09	61	16	23	45	
PAH Total (others)	PEC	HA28	ERM	2226.5	58	21	21	37	
PAH Total (others)	NEC	CR14	NEC	84600	79	2	19	77	X
PAH Total (others)	NEC	HA14	NEC	9240	75	3	22	72	
PAH Total (others)	NEC	HA28	NEC	62220	66	2	32	64	
PAH Low	TEC	HA14	ERL	786	78	19	3	75	X
PAH Low	TEC	HA14	TEL	387.46	75	25	0	75	
PAH Low	TEC	CR14	ERL	653	76	21	2	74	
PAH Low	TEC	CR14	TEL	231.4	74	24	2	72	
PAH Low	TEC	HA28	TEL	76.42	63	29	8	55	
PAH Low	TEC	HA28	ERL	80	63	29	8	55	
PAH Low	PEC	HA14	ERM	3369	81	0	19	81	X
PAH Low	PEC	CR14	PEL	4140.86	81	2	17	79	
PAH Low	PEC	CR14	ERM	7204.5	81	2	17	79	
PAH Low	PEC	HA14	PEL	2919.52	78	3	19	75	
PAH Low	PEC	HA28	PEL	1176.59	61	13	26	48	
PAH Low	PEC	HA28	ERM	653	63	16	21	47	
PAH Low	NEC	HA14	NEC	3040	78	3	19	75	X
PAH Low	NEC	CR14	NEC	33600	76	2	21	74	Λ
PAH Low	NEC	HA28	NEC	29380	65	2	34	63	
PAH High	TEC	HA14	ERL	2900	84	13	3	81	X
PAH High	TEC	HA14	TEL	1228.01	69	28	3	66	Λ
PAH High	TEC	CR14	TEL	309.81	67	31	2	65	
PAH High	TEC	CR14 CR14	ERL	309.81 486	67 67	31	2	65	

A-10 Table A.1 (continued)

Chemical	BMK Type ^b	\mathbf{Test}^c	\mathbf{SEC}^d	Conc.	Total Correct (%) ^e	False Positives (%) ^f	False Negatives (%) ^g	Score ^h	Selected BMK ⁱ
PAH High	TEC	HA28	ERL	170	55	37	8	47	
PAH High	TEC	HA28	TEL	192.95	52	35	13	39	
PAH High	PEC	HA14	PEL	4353.82	84	3	13	81	X
PAH High	PEC	CR14	PEL	10122.54	81	2	17	79	
PAH High	PEC	CR14	ERM	26614.5	81	2	17	79	
PAH High	PEC	HA14	ERM	5650	78	3	19	75	
PAH High	PEC	HA28	PEL	2338.4	60	19	21	41	
PAH High	PEC	HA28	ERM	1747	58	21	21	37	
PAH High	NEC	CR14	NEC	51000	79	2	19	77	X
PAH High	NEC	HA14	NEC	6200	75	3	22	72	
PAH High	NEC	HA28	NEC	32840	68	2	31	66	
PCB Total	TEC	HA28	TEL	31.62	69	14	17	52	X
PCB Total	TEC	HA28	ERL	50	69	14	17	52	
PCB Total	PEC	HA28	PEL	244.66	76	0	24	76	X
PCB Total	PEC	HA28	ERM	730	76	0	24	76	
PCB Total	NEC	HA28	NEC	194	72	3	24	69	X

Source: U.S. Environmental Protection Agency 1996. Calculation and Evaluation of Sediment Effect Concentrations for the Amphipod <u>Hyalella azteca</u> and the Midge <u>Chironomus riparius</u>, EPA 905-R96-008, Great Lakes National Program Office, Chicago, Ill.

"All SECs must have % Total Correct values > 50%, TECs must have % False Negative values < 25%, and PECs and NEC must have % False Positive values <25%.

^bBMK Type = Benchmark Type; TEC = Threshold Effect Concentration (i.e., ERLs and TELs); PEC = Probable Effect Concentration (i.e., ERMs and PELs); and NEC = high No Effect Concentration.

°CR14 = Chironomus riparius 14-day test, HA14 = Hyalella azteca 14-day test, and HA28 = Hyalella azteca 28-day test.

^dERL = Effects Range Low, ERM = Effects Range Median, TEL = Threshold Effects Level, and PEL = Probable Effects Level.

^e% Total Correct = the percentage of samples correctly identified as toxic or non-toxic

^f% False Positives = the percentage of samples incorrectly identified as toxic.

^g% False Negatives = the percentage of samples incorrectly identified as non-toxic.

^hThe score for TEC benchmarks = % Total Correct (-) % False Negatives. The score for PEC and NEC benchmarks = % Total Correct (-) % False Positives.

[&]quot;x" indicates the SEC selected as the representative benchmark for that chemical and benchmark type. Selection criteria, in order of priority, are 1) highest score, 2) highest % Total Correct, and 3) lowest concentration.