



Standard Practice for Using Octanol-Water Partition Coefficient to Estimate Median Lethal Concentrations for Fish Due to Narcosis¹

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1. Scope

1.1 This practice covers a procedure for estimating the fathead minnow (*Pimephales promelas*) 96-h LC50 of non-reactive (that is, covalently bonded without unsaturated residues) and nonelectrolytic (that is, require vigorous reagents to facilitate substitution, addition, replacement reactions and are non-ionic, non-dissociating in aqueous solutions) organic chemicals acting solely by narcosis, also referred to as Meyer-Overton toxicity relationship.²

1.2 This procedure is accurate for organic chemicals that are toxic due to narcosis and are non-reactive and non-electrolytic. Examples of appropriate chemicals are: alcohols, ketones, ethers, simple halogenated aliphatics, aromatics, and aliphatic substituted aromatics. It is not appropriate for chemicals whose structures include a potential toxiphore (that structural component of a chemical molecule that has been identified to show mammalian toxicity, for example CN is known to be responsible for inactivation of enzymes, NO₂ for decoupling of oxidative phosphorylation, both leading to mammalian toxicity). Examples of inappropriate chemicals are: carbamates, organophosphates, phenols, beta-gamma unsaturated alcohols, electrophiles, and quaternary ammonium salts.

2. Referenced Documents

2.1 ASTM Standards:

E 729 Guide for Conducting Acute Toxicity Tests on Test Materials with Fishes, Macroinvertebrates, and Amphibians³

E 943 Terminology Relating to Biological Effects and Environmental Fate³

¹ This practice is under the jurisdiction of ASTM Committee E47 on Biological Effects and Environmental Fate and is the direct responsibility of Subcommittee E47.01 on Aquatic Assessment and Toxicology.

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² Lipnick, Robert L., "Validation and Extension of Fish Toxicity QSARs and Interspecies Comparisons for Certain Classes of Organic Chemicals," *QSAR in Toxicology and Xenobiochemistry*, Elsevier, 1985.

³ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For Annual Book of ASTM Standards volume information, refer to the standard's Document Summary page on the ASTM website.

E 1023 Guide for Assessing the Hazard of a Material to Aquatic Organisms and Their Uses³

E 1147 Test Method for Partition Coefficient (N-Octanol/Water) Estimation by Liquid Chromatography³

3. Terminology

3.1 Definitions:

3.1.1 *narcosis*—a reversible state of stupor, unconsciousness, or arrested activity produced by the influence of chemicals on critical sites within membranes or by disrupting the normal functioning of certain proteins by means of nonspecific binding of organic chemical(s) to hydrophobic sites. Death results if exposure is not terminated after a length of time which varies with concentration.

3.1.2 *octanol-water partition coefficient* (K_{ow})—referred to as *P* in some literature.

3.1.3 *toxiphore*—a chemical structure substituent group that when present gives rise to an adverse effect in exposed organisms.

3.2 For definitions of other terms used in this standard, refer to Guide E 729, Terminology E 943, and Guide E 1023.

4. Summary of Practice

4.1 The hydrophobicity of a non-reactive and non-electrolytic organic chemical as quantified by log of the octanol-water partition coefficient is substituted into an experimentally derived equation and an approximate 96-h log LC50 for fathead minnow is calculated. This value is a maximum value. The actual LC50 could be lower, but should not be higher.

5. Significance and Use

5.1 This procedure can be used to limit the need for screening tests prior to performing a test for estimating the LC50 of a non-reactive and non-electrolytic chemical to the fathead minnow. By eliminating the screening test, fewer fish need be tested. The time used for preparing and performing the screening test can also be saved. The value obtained in this procedure can be used as the preliminary estimate of the LC50 in a full-scale test.