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Correlation of the toxicity of organic compounds to tadpoles using the Abraham model

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Abstract

The narcotic and lethal concentrations of organic compounds have been compiled for several tadpole species (*Rana temporaria, Rana pipiens, Rana japonica, Xenopus laevis* and *Rana brevipoda porosa*). The narcotic and lethal concentrations have been correlated using the Abraham solvation parameter model to yield an equation that can be used to predict the narcotic concentrations of additional nonpolar and polar narcotic compounds to *R. temporaria*, and a more general correlation that should be applicable to different species of tadpoles. The more general equation is based on 240 experimental data points. A training set of 123 compounds could be fitted with the Abraham solvation parameters with $R^2 = 0.931$ and S.D. = 0.343 log units. The training equation predicted the test set of 122 values with AE = −0.022 log units, S.D. = 0.300 log units and an average absolute error, AAE, of 0.227 log units. The structural features that are important in narcosis of tadpoles have been examined; it is concluded that hydrogen bond basicity reduces narcotic activity of compounds and that compound size increases narcotic activity. The solvation parameter model enables narcosis of tadpoles to be compared to various other biological processes and to physicochemical processes that might be used as models for narcosis.
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1. Introduction

Environmental risk assessment typically involves finding the maximum concentration of a given chemical compound that could be safely tolerated in the environment and still protect most (preferably all) species/organisms from harmful chemical exposure. The concentration, referred to in the literature as the "no observed effect concentration", NOEC, can be experimentally determined by exposing the individual organism to varying concentrations of the chemical under consideration. Such measurements are both expensive and time-consuming, particularly if a large number of compounds and/or organisms need to be studied. Recognizing that it is impossible to perform experimental measurements on every known chemical and organism, researchers have developed predictive methods as a means to generate desired values in the absence of actual experimental toxicity data. Equations have been reported for estimating the toxicity of organic compounds to selected organisms based on molecular structure considerations (Martin and Young, 2001; Casalegno et al., 2005), molecular descriptors of either theoretical (Netzeva et al., 2005; Ramos

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et al., 1998; Katritzky et al., 2001; Eldred et al., 1999; McCoy and Sykes, 2003; Roy and Ghosh, 2004) and/or experimental origin (Kamlet et al., 1987; Abraham and Rafols, 1995; Gunatilleka and Poole, 1999, 2000), and by extrapolation methods that employ known experimental data for test species that are considered surrogates for species in the ecosystems (Dyer et al., 2006).

To date we (Hoover et al., 2005, in press; Bowen et al., in press) have examined the application of the Abraham solvation parameter model for correlating the toxicity of nonpolar and polar narcotic compounds to select aquatic organisms. Expressed in terms of toxicities, the basic linear free energy (LFER) model takes the following mathematical form:

$$-\log \text{ toxicity} = c + e \cdot E + s \cdot S + a \cdot A + b \cdot B + v \cdot V \quad (1)$$

where the dependent property, −log toxicity, is the negative logarithm of the solute molar concentration corresponding to a specific endpoint. In the case of fish and daphnids, the endpoints are the median lethal and median immobilization molar toxicant concentrations, respectively. For the protozoan *Tetrahymena pyriformis* the endpoint is the concentration for a 50% inhibition of population growth. The independent variables, or descriptors, are solute properties as follows: E and S refer to the excess molar refraction and dipolarity/polarizability of the solute, respectively, A and B denote the overall solute hydrogen-bond acidity and basicity, and V is the McGowan volume of the solute. The equation coefficients (c, e, s, a, b and v) depend on the aquatic organism and toxicity endpoint under consideration.

Eq. (1) has provided a very reasonable mathematical description of the toxic behavior of organic compounds having nonpolar or polar narcosis mechanisms to six species of fish (*Pimephales promelas, Poecilia reticulata, Lepomis macrchirus, Leuciscus idus melanotus, Carassius auratus* and *Oryzias latipes*), to three water fleas (*Daphnia magna, Daphnia pulex* and *Ceriodaphnia dubia*), to five protozoas (*Tetrahymena pyriformis, Spirostomum ambiguum, Entosiphon sulcantum, Uronema parduczi* and *Chilomonas paramecium*) and to one bacterium (*Pseudomonas putida*) (Hoover et al., 2005, in press; Bowen et al., in press). Reported correlations described the observed toxicity data to within approximately ±0.28 log units, which was comparable to the experimental uncertainty associated with many of the observed values. Experimental uncertainties were based on inter-laboratory variations in the observed values, as well as the standard deviations calculated from replicate independent measurements.

In the present communication we extend our toxicity investigations to tadpoles. Abraham and Rafols (1995) have previously correlated the Overton data (1901, 1991) and data from the publication of Lipnick (1989) for tadpole (*Rana temporaria*) narcosis with the Abraham model

$$-\log C_{\text{narc}} = 0.609 + 0.866\ E - 0.347\ S - 0.174\ A - 2.808\ B^{\circ} + 3.054\ V \quad (2)$$

where C_{narc} is the narcotic concentration of the solute (mol dm^{-3}) and B° denotes the solute overall hydrogen-bond basicity, respectively. The alternative hydrogen-bond basicity descriptor, B°, is used for select solutes in water-solvent systems when the "wet" solvent contains appreciable quantities of water. (For notational simplicity we have used the newest descriptor abbreviations.) Eq. (2) had $N=84$, $R^2=0.948$, S.D.$=0.244$, and $F=287$. In Eq. (2), N corresponds to the number of solutes but in later equations where there are duplicate entries N is the total number of data points. R denotes the correlation coefficient, S.D. is the standard deviation and F corresponds to the Fisher F-statistic. Abraham and Rafols (1995) actually compiled a much larger set of data for *R. temporaria* narcosis, and we have used this data set and data on other tadpole species to attempt to obtain a much more general equation for tadpole narcosis.

2. Toxicity data and solute descriptors

Our search of the published chemical literature yielded toxicity data for a total of 130 compounds for *R. temporaria* (Abraham and Rafols, 1995; Overton, 1901, 1991; Lipnick, 1989; Paulov, 1987; Vernon, 1914; Dickenson et al., 1993; Altenburg, 1981) 32 compounds for *Rana pipiens* (Alifimoff et al., 1987, 1989; Raines et al., 1993; Munch, 1972; Kita and Miller, 1982), 47 compounds for *Rana japonica* (Huang et al., 2003a,b; Wang et al., 2001), 11 compounds for *Xenopus laevis* (Curry et al., 1991; Moss et al., 1991), 18 compounds for *Rana brevipoda porosa* (Nishiuchi, 1984), and 7 alcohols (Pringle et al., 1981) for which the tadpole species was not identified. The total number of toxicity values is thus 245. The toxicity endpoint in several of the studies was taken to be the immobilization of the organism, whereas in other studies the authors referred to the data as a lethal concentration. The two endpoints are different; however, we suspect that the molar concentration that first induces the organism's immobilization does not differ too significantly from the lethal molar concentration. Given the nature of biological toxicity data in general and the level of uncertainty that

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