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Bioaccumulation of ionizable organic chemicals in fish – The quest for reliable predictors

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Dietary bioaccumulation in fish is quantified using biomagnification factors (BMFs), which are derived under controlled conditions according to OECD guideline 305-III. To reduce *in vivo* experimental efforts, pre-screening using statistical models for BMF prediction is becoming increasingly popular. While dietary bioaccumulation of neutral chemicals has been successfully associated to lipophilicity descriptors, no suitable predictor has yet been identified for ionizable chemicals.

In this study, we investigated the capability of selected chemical properties (e.g., molar volume, adsorption to albumin, lipophilicity, solubility, topological polar surface area) to predict bioaccumulation of organic electrolytes in fish with specific focus on dietary exposure studies. Measured dietary BMFs were collected from existing literature, and empirical correlations with measured or estimated chemical descriptors were evaluated.

The dataset includes dietary BMFs in whole fish obtained under laboratory-scale conditions closely resembling or directly referring to the OECD 305-III guideline. In total, BMF data were available for 29 ionizable chemicals (of which 10 are perfluorinated chemicals); including 24 acids and 19 permanently ionized chemicals at environmental pH (range 3 to 9). A parallel dataset was compiled with bioconcentration factors (BCFs) of the same chemicals derived in water exposure studies with fish (OECD 305-I guideline).

Bivariate correlation analysis (Pearson and Spearman) revealed that a) logK_{OW} was not a sufficient predictor of BMF, although with significant positive correlation ($R>0.40$), and b) that significant correlation was shown only with log$D$ at pH=3 ($R=0.35$). Furthermore, significant negative correlation was shown between BMF and solubility ($R< -0.60$). These

preliminary results indicate that commonly used predictors for bioaccumulation (e.g., logK_{OW}) are of limited relevance for ionizable chemicals, and other predictors should be identified.

Ongoing research is focusing on the prediction of BCF from quantum-chemistry-based estimations of partitioning coefficients (to membrane lipids, structural proteins and albumin). Estimation of BCFs from BMF for the investigated chemicals will be also performed and verified with existing BCF measurements. Eventually, identified empirical regressions between BMF and chemical descriptors will be validated with *ad hoc* experimental data with radiolabelled test chemicals.

Keywords: Biomagnification; perfluorinated chemicals; correlation analysis; partitioning coefficients

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