# [SC8] A Tiered Approach for Screening Chemicals for Biomagnification Potential in Humans

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Bioaccumulation is a process in which the chemical concentration in an organism exceeds the concentration in the respiratory medium, the diet or both and is an integral aspect of hazard and risk assessment [1]. It is influenced by a combination of physical-chemical properties (e.g. partition coefficients (Kow and Koa)) and biological factors related to organism (e.g. biotransformation rate constants (kB)). Here we present a tiered approach for screening the bioaccumulation potential of organic chemicals in air-breathing organisms. Biomagnification Factor (BMF) derived from a typical human diet as calculated by the Risk Assessment IDentification And Ranking (RAIDAR) model [2] is the metric for assessing bioaccumulation potential of approximately 13,000 chemicals. Input parameters Kow, Koa, biopartitioning coefficients, and biotransformation Half-Lives (HLB) are calculated by different QSAR models based on fragments (e.g. EPISUITE) [3,4], molecular descriptors [5] and poly-parameters Linear Free Energy Relationships (ppLFER) [6]. Great attention is given to the Applicability Domain to define the structural boundaries of each model; in particular, where possible, we set up an automated method to define the EPISUITE models' Applicability Domain based on molar mass, fragments count and response range. This is fundamental to provide reliable predictions and get more accurate BMF estimates. Tiers that do not consider biotransformation estimate a high percentage of chemicals with BMF > 1 (over 93%). In the last Tier, the introduction of the HLB has a high impact on the screening results, reducing the BMF estimate to < 1 for most of the compounds (about 90%). This shows how models based only on partition coefficients are not sufficient to describe and address the bioaccumulation and biomagnification processes, and can lead to overly conservative estimates ("false-positives"). Moreover the study highlights the key role of biotransformation in bioaccumulation assessment for air-breathing organisms and highlights the need for reliable data on biotransformation to effectively categorize chemicals for hazard.

Bibliography:

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