

The Bioaccumulation Assessment Tool: An Organizational Framework for Bioaccumulation Assessment

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Introduction

- Various regulatory programs require Bioaccumulation “B” assessment, e.g., REACH, with designations of Bioaccumulative (B), very B (vB), not (B/vB)
- Various metrics for Bioaccumulation assessment exist, e.g., K_{OW} , lab BCF, lab BMF, half-life, field BMF, field BAF, field TMF
- Various quantitative criteria and quantitative and qualitative thresholds for the various Bioaccumulation metrics exist, e.g., REACH Annex XIII
- There are no defined implementation strategies to integrate various Lines of Evidence (LOE) in a transparent, Quantitative Weight of Evidence (QWOE) Approach
- A general approach for “B” assessment is proposed in **Figure 1**

Objectives

- Develop a user-friendly, organizational framework and computational tool in the form of an Excel/VBA spreadsheet for integrating various Lines of Evidence (LOE) to aid “B” assessment
- Provide the capacity for transparency and consistency in “B” assessment
- As necessary, guide integrated (tiered) testing strategies (**ITS**; i.e., enabling generation of additional LOE) to address uncertainty in “B” assessment, e.g., **Fig. 1**

Methods

- A conceptual overview of the Bioaccumulation Assessment Tool (BAT) is shown in **Figure 2** for aquatic bioaccumulation assessment and **Figure 3** for terrestrial bioaccumulation assessment
- The BAT brings together measured and modelled data, e.g., chemical properties, in vivo data (BCFs, BMFs, half-lives, absorption efficiency), in vitro data (intrinsic hepatic clearance rate) and in silico data (BCF-QSARs, biotransformation rate), which are treated as Lines of Evidence (LOE)
- Multiple LOE (“Input” to the BAT) are evaluated using Data Evaluation Templates (DETs) – **Figure 4**
- LOE are subject to data quality evaluations using DETs – **Figure 5**
- Primary “Output” includes a suite of “B” assessment endpoints presented against user-defined criteria and thresholds (e.g., $BCF > 5,000 \text{ L/kg} = \text{“vB”}$) – **Figure 6**
- Information is compared for “B” assessment, e.g., half-lives in terrestrial organisms vs. fish BCFs, and summarized using a Quantitative Weight of Evidence (QWOE) Approach – **Figure 7**
- The chemical undergoing assessment can also be compared against measurements for benchmark chemicals for the various metrics

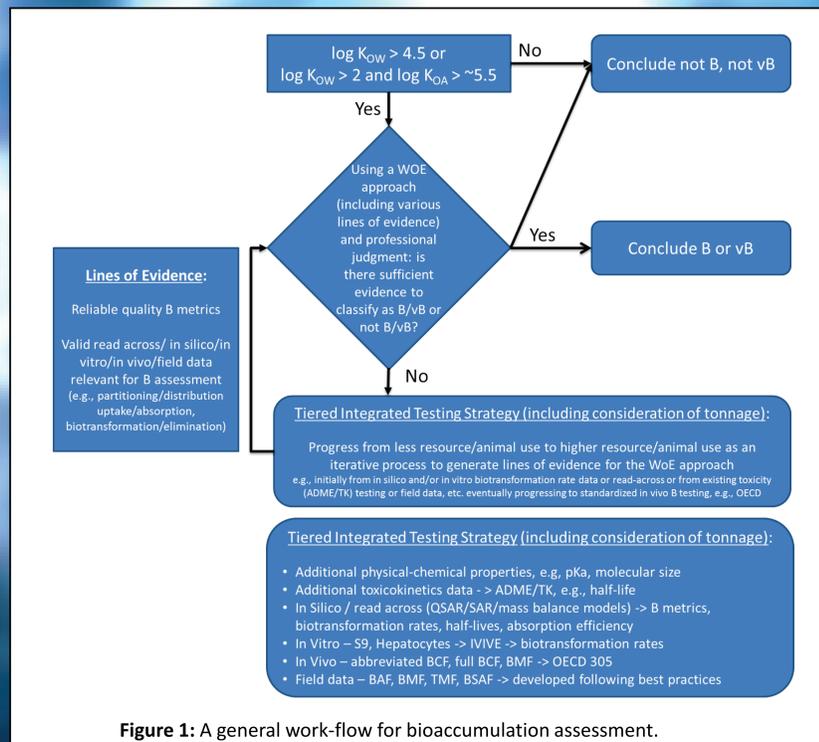


Figure 1: A general work-flow for bioaccumulation assessment.

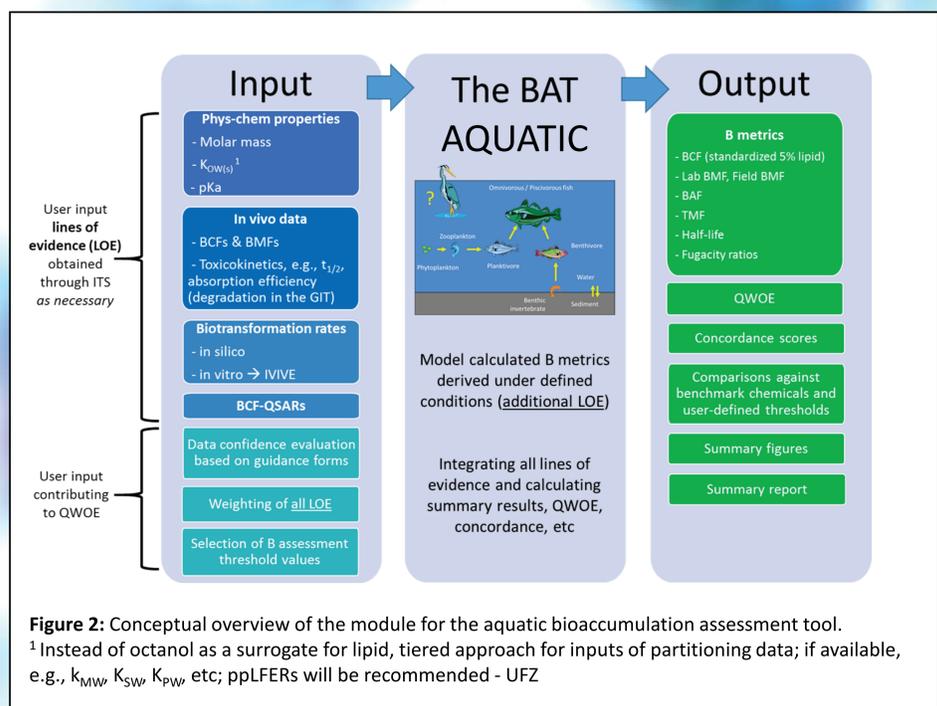


Figure 2: Conceptual overview of the module for the aquatic bioaccumulation assessment tool.
¹ Instead of octanol as a surrogate for lipid, tiered approach for inputs of partitioning data; if available, e.g., K_{MW} , K_{SW} , K_{PW} ; etc; pPLFRs will be recommended - UFZ

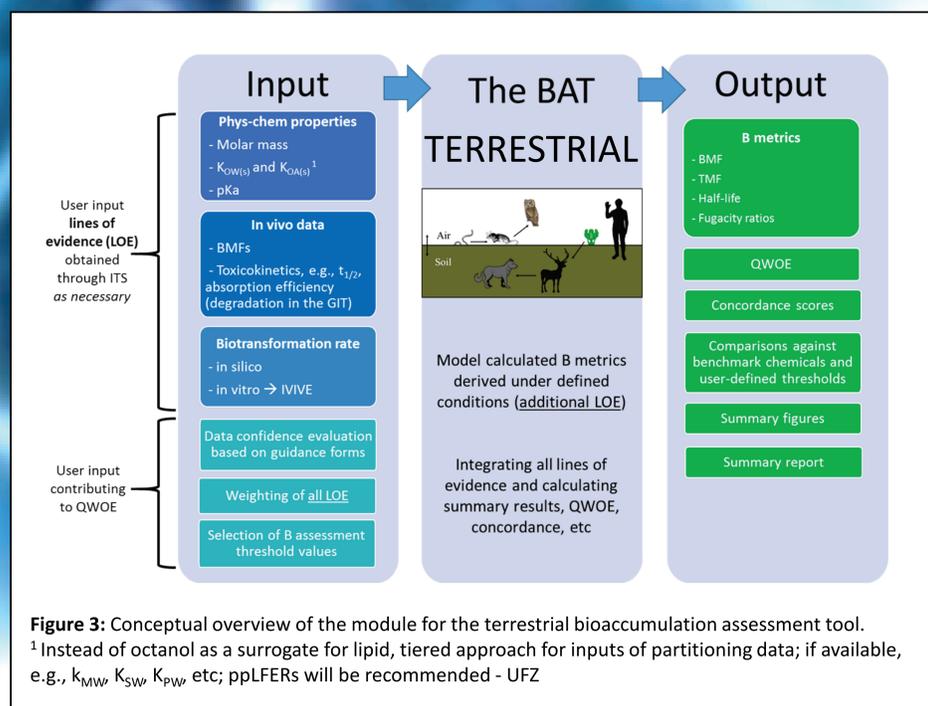


Figure 3: Conceptual overview of the module for the terrestrial bioaccumulation assessment tool.
¹ Instead of octanol as a surrogate for lipid, tiered approach for inputs of partitioning data; if available, e.g., K_{MW} , K_{SW} , K_{PW} ; etc; pPLFRs will be recommended - UFZ

Figure 4: Lab BMF Data Entry Template (DET)

Quality Criteria for data reliability of a (flow-through) fish bioaccumulation study		
Relevant Criteria		
1	Flow through test	
2	Mass reported	
3	Lipid content reported	
4	Temperature reported	
5	Gut uptake efficiency	
6	Total depuration	
7	Growth rate	
8	GLP Certificate	
9	OECD 305	
10	Substance purity	Greater than 95%
11	Test species	One of recommended species? <input type="checkbox"/> Check OECD species
12	Similar age?	
13	Similar length?	
14	Acclimatization period	Minimum of 14 d under test conditions
15	Water Hardness	Total hardness 10-250 mg/L CaCO ₃
16	pH	Reported and between pH 6 and 8.5
17	TOC	Reported and less than 2 mg/L
18	Co-solvent present	The use of solvents/dispersants not recommended
19	Length of uptake phase	28 d or until steady-state achieved
20	% of steady-state reported?	
21	% of steady-state	
22	Length of depuration phase	Less than twice the length of uptake phase
23	Number of animals	Minimum = 4 fish/sampling event
24	Weight of smallest > 2/3 of the largest Control group?	
25	Loading of tanks	In range of 0.1 - 1 g fish/L water?
27	Dissolved oxygen	Greater than 60%? <input type="checkbox"/> Check link
28	Feeding rate	In range of 1 - 2% of body weight/d
29	Light-dark cycle	12 to 16 h illumination/d
30	Test temperature	Appropriate for test species
31	pH deviation	Within +/- 2 °C
32	pH deviation	Within 0.5 log units of average
33	Analytical	Fish concentration measured directly
34	Analysis interval	Fish at least 5 times during uptake & 4 times during depuration
35	Mortality	Mortality/adverse effects in control group < 10%
36	Mortality	Mortality/adverse effects in test group < 10%
37		

Figure 5: Lab BMF data quality evaluation criteria in Lab BMF DET

Metric	Metric Weight	Threshold value	(Units)
BCF - Lab			L/kg
BMF - Lab			kg/kg
BAF - Field			L/kg
BMF - Field			kg/kg
TMF - Field			-

Figure 6: User-defined criteria and thresholds for B assessment metrics

Data (LOE)	LOE Weight	Data confidence score (from DET)	Classification	Metric Weight
Measured BCF	2	75%	nB < 2,000	4
QSAR BCF	1	60%	B > 2,000	4
BAT BCF - Lab	1	75%	B > 2,000	4
BAT BMF - Field	1	70%	nB < 1	2
BAT TMF - Field	1	70%	nB < 1	2

Figure 7: Example of summary QWOE information

Discussion

- Stakeholder involvement (e.g., industry, academia, regulatory scientists) included during development - **BAT Advisory Team**
- Biotransformation rate constants obtained from in vivo, in silico and in vitro methods are included for aquatic and terrestrial
- The BAT (Ver.1.0) will be freely available and accompanied by supporting documentation (e.g., tool description and user's guide)
- The BAT can continue to evolve with the emerging science and from practical experience in its application and evaluation

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