THE BIOACCUMULATION ASSESSMENT TOOL

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Outline

Rationale & Objectives

Bioaccumulation Assessment Tool (BAT) Overview

Examples of Input and Output

Summary
Rationale

Why develop a tool?

Various regulatory programs for B assessment, e.g.:
- REACH, TSCA, CEPA, CSCL
- Various **metrics** for B assessment
  - Kow, lab BCF, lab BMF, field BMF, field BAF, field TMF, etc
- Various **criteria (thresholds)**, e.g., REACH Annex XIII

Fig from Gobas

| 5,000 | 2,000 |
| 1,000 |
| 500  |
| 1    |
General Project Objectives

To develop a spreadsheet tool which can be used to:

- **collect**, **evaluate** and **integrate** various lines of evidence (LOE) relevant to B-assessment (i.e., TK, ADME data streams)

- provide **consistent** and **transparent** results by means of a quantitative weight of evidence (QWOE) approach.

- **guide** and **inform** B-assessment decision-making
Quantitative Weight of Evidence (QWOE)

B-metric

Threshold

Relevance

Outcome

Reliability

Weighted Outcome

nB / B / vB

* Data Evaluation Template
Conceptual overview (aquatic)

1. Initialization
   - Define B and vB thresholds

2. Chemical data input
   - Molar mass
   - $K_{\text{ow}}$
   - pKa (ionogenic)

3. Biotransformation rates LOE, DETs
   - in vitro → IVIVE
   - in silico

4. Bioaccumulation LOE input and generated, DETS

5. Output
   - B metrics summary (Study & BAT-generated LOEs -standardized)
   - Compare LOE value against defined thresholds
   - Compare LOE value against benchmark chemicals (figures)
   - Reliability Scores (DETs)
   - WOE scores
   - Overall QW/OE
   - Concordance scores
   - Summary figures
   - Summary report

The BAT
- Model calculated B metrics derived under defined conditions (additional LOE)
  - BCF/BMF Lab conditions
  - Generic Lab conditions
  - Generic Field conditions
    - Aquatic/terrestrial

Integrating all lines of evidence and calculating summary results, QW/OE, concordance, etc.
1. Initialization
2. Chemical Data Input

Minimum input:
1. MW
2. $K_{OW}$
3. $K_{OA}$ (or $K_{AW}$)

Tiered approach for inputs of partitioning data; if available or calculated if not e.g., $k_{MW}$, $K_{SW}$, $K_{PW}$, etc. ppLFERs
3. Biotransformation Rates

Default → “no biotransformation”

**Collect** biotransformation information such as:

- In Vitro S9, hepatocyte or microsome studies
  - Fish and Rodent
  - *In vitro-in vivo* extrapolation → $k_M$
- Biotransformation rate QSARs
  - Link to EPISuite (others)

Study conditions
Key values
DETs assess study methods → reliability
3. Biotransformation rates

Data collection and evaluation
4. Bioaccumulation Studies

**Collect** information, enter (if available):

- Laboratory BCF
- Laboratory BMF
- Field TMF
- In silico BCF, BMF, BAF

Study conditions
Key Values
DETs → reliability

- BAT generated results
- Simulated Lab and Field, aquatic and terrestrial
  - BCF, BAF, BMF, TMF
4. Bioaccumulation Studies

sample: Lab BCF

BAT simulates
- Experiment
- Generic lab
5. Output

**Evaluate and Integrate**

Each B assessment metric outcome → assigned value reliability → assigned value sorted by relevance

QWOE to determine B-classification outcome
5. Output

Summary plots

Benchmarking

Formatted PDF

Summary

Bioaccumulation Assessment Tool
developed by ARC Inc.
with funding from CEFIC
Prepared by: Ulisa Toose
Organization: ARC Inc

Bioaccumulation Assessment Report

Project Summary
11/13/2017  Hypothetical Neutral  123-45-6

Results Summary
Summary

BAT:

- User-defined relevance for each B metric and threshold value
- Collect and generate Lines of Evidence for a single chemical
- Evaluate data reliability using LOE-specific criteria (based on TGD)
- Compare B metrics against user-defined thresholds
  - “B classification outcome, nB, B, vB”
- Integrates Relevance, Reliability and Outcome of the assessments
- Generate summary output, figures, benchmarking, report
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