

# Applying the Bioaccumulation Assessment Tool for Medium-Chain Chlorinated Paraffins (MCCPs)

Prepared for:  
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## Executive Summary

This document provides a summary overview of a bioaccumulation (B) assessment of Medium-Chain Chlorinate Paraffins (MCCPs) using the Bioaccumulation Assessment Tool (BAT) Ver.2.0. There are various B-metrics in various species and different criteria for B hazard classification. Some B-metrics are from laboratory models such as bioconcentration factors (BCFs) and biomagnification factors (BMFs). Some B-metrics are calculated from measurements in the environment including field BMFs, bioaccumulation factors (BAFs), and trophic magnification factors (TMFs). A weight of evidence (WOE) approach is recommended in regulatory programs (e.g., REACH Annex XIII) to consider various B-metrics and their reliability for B assessment.

The BAT provides a quantitative WOE approach for B assessment using multiple B-metrics, or Line(s) of Evidence (LOE), following OECD guidance for conducting a WOE approach. A total of 113 measured LOE for MCCPs are included in the BAT. Each of these LOE were subject to reliability scores using the BAT Data Evaluation Templates (DETs). The data reliability assessment methods and criteria are derived from OECD testing guidelines and published guidance for evaluating measured lab and field bioaccumulation data. Seventy-seven of the 113 measured LOE were deemed reliable for B assessment. In addition to the measured LOE, the bioaccumulation models in BAT provide an additional seven LOE (e.g., model calculated lab BCF, field BAF, field BMF) to compare against measured data. Eighty-two percent of the measured reliable quality LOE classify MCCPs as “nB” compared to 18% of reliable quality measured LOE that classify MCCPs as “vB”. While there is uncertainty in the strength of evidence, the majority of currently available, reliable quality measured LOE indicate that MCCPs are not bioaccumulative in aquatic food webs.

An additional WOE using fugacity ratios is included in this report. The fugacity ratio approach seeks to address whether a chemical biomagnifies in the environment or not. Seventy-seven reliable quality LOEs for MCCPs were converted to fugacity ratios and 92% of these data were below the biomagnification threshold of 1 indicating it is unlikely that MCCPs biomagnify in fish and the aquatic environment.

The appendices to this report include (i) a BAT Summary Output Report and (ii) a Microsoft Excel™ file entitled “BATv2\_MCCP\_disabled\_07122020.xlsx”. This Excel file is a disabled version of the BAT that documents the details of the various LOE, associated data reliability assessments, and the BAT analysis for MCCPs.

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## Background

Chemicals are undergoing bioaccumulation (“B”) hazard assessment as part of national and international regulatory programs including the REACH legislation in Europe [1-4]. Bioaccumulation is broadly defined as a process by which the concentration of a chemical in an organism exceeds that in the respiratory medium (e.g., water for fish, air for mammals), or in the diet, or both [5]. Bioaccumulation is the net result of competing rates of chemical uptake and elimination in an organism under a defined set of exposure conditions [5-7]. Fish are commonly used as a model organism for B assessment. Bioaccumulation assessment can be a scientific and regulatory challenge in some cases because there are various metrics for assessing bioaccumulation in aquatic and terrestrial organisms and food webs (e.g., BCF, BMF, BAF, TMF [5, 8]), various “B” criteria (threshold values for “B” classification), variability and uncertainty in bioaccumulation data, and sometimes conflicting “B” classification results.

All B data are uncertain whether they are derived from measurement or models. A weight of evidence (WOE) approach is commonly recommended in most regulatory programs (e.g., REACH Annex XIII [9]). However, there is often no clear implementation guidance and/or WOE strategy [10], making it difficult for stakeholders to collect, generate, integrate, evaluate, and compare various Line(s) of Evidence (LOE) for ‘B’ assessment decision-making. Weight of Evidence is a process of assembling, evaluating, weighing, and integrating evidence to come to a scientifically defensible conclusion and the WOE approach is used when scientific questions can only be answered by using multiple LOE [11]. The WOE approach provides a consistent framework for decision-making and needs to be transparent. Recently the Organization for Economic Cooperation and Development (OECD) developed “Guiding Principles and Key Elements for Establishing a Weight of Evidence for Chemical Assessment” [12].

The Bioaccumulation Assessment Tool (BAT) is a formal means for applying a WOE approach [13]. The BAT is a user-friendly spreadsheet-based tool to guide the collection, generation, evaluation, and integration of various LOE to aid bioaccumulation assessment decision-making for aquatic and terrestrial organisms. The BAT provides a consistent WOE approach that includes critical evaluations of data confidence. The WOE approach in BAT follows the WOE guidance developed by the OECD [12]. LOE that can be included in the BAT are bioaccumulation metrics currently used in most B assessment programs (i.e., BCF, BAF, BMF, TMF [5, 8]). LOE can be obtained from field data (e.g., BAF, BMF, or TMF) or laboratory data (e.g., BCF or BMF) or in silico (model) calculations (e.g., quantitative structure-activity relationships, QSARs) or from a combination of in vitro measurements and in silico (TK model) calculations (e.g., in vitro biotransformation rates used to calculate BCFs). Each LOE is assigned a relevance weight (from 0 to 5). The LOE are subject to data quality evaluations using Data Evaluation Templates (DETs) to determine reliability scores (from 0 to 5). The DETs in BAT are developed based on OECD testing guidance, e.g., OECD 305 [14] and critical reviews, e.g., for field endpoints [15]. The Strength of Evidence in BAT is determined by the frequency of “B” classifications based on all LOE. For example, if all LOE result in a “nB” classification the Strength of Evidence for the chemical being “nB” is 100% and the Strength of Evidence for the chemical being classified as “B” or “vB” is 0%.

More details of the BAT are available here: <https://arnotresearch.com/models/> and in the User Manual embedded in the BAT, e.g., [13].

Medium-Chain Chlorinate Paraffins (MCCPs) are a mixture of chemicals, considered an unknown or variable composition, complex reaction products or biological materials (UVCB substance), registered for evaluation under a single CAS No (85535-85-9) [16]. The range of chemical properties for the MCCP constituents is large [17-19]. For example, measurements and predictions for the octanol-water partition coefficient ( $K_{ow}$ ) for MCCP constituents span a few orders of magnitude ( $\log K_{ows}$  from  $\sim 7$  to  $>9.0$  [20] or  $\sim 5.5$  to  $8.2$  [16]). The very high  $K_{ows}$  reflect the fact that these chemicals are very hydrophobic (“water-hating”) and hence partition from water to organic and biological phases. MCCPs are undergoing B assessment as a part of REACH legislation as summarized in the United Kingdom Competent Authority (UK CA) submission evaluation conclusion and report [21]. The UK CA finding was that the “substance meets the Annex XIII criteria for bioaccumulation (B), with some constituents meeting the very bioaccumulative criteria (vB)” [21].

Previous reports prepared by ARC relating to the B assessment of MCCP provide some background to this current report [22, 23]. The previous reports present background technical knowledge regarding bioaccumulation in fish, critical summary reviews of laboratory experimental data and field data commonly considered in the B assessment of MCCPs [22, 23]. This document provides an overview regarding the bioaccumulation (B) hazard assessment of MCCPs using the Bioaccumulation Assessment Tool (BAT) WOE approach [13] and the fugacity ratio WOE approach.

The BAT Ver.2.0 was applied using available measured and modelled data for MCCPs. The data used include data in the REACH substance evaluation document [21] and associated studies including recent peer-reviewed literature, e.g., [24] related to the B assessment of MCCP constituents. Details of the information included in the BAT WOE results are provided in a series of spreadsheets included as an appendix to this report (i.e., a non-operational version of the BAT). These spreadsheets document the details of 113 currently available LOE and the data quality scores calculated by the DETs as well as 7 new LOE generated by the BAT. A summary report generated by the BAT is included in the [Appendix](#). A Microsoft Excel™ file entitled “BATv2\_MCCP\_disabled\_07122020.xlsx” accompanies this report. This Excel file is a disabled version of the BAT that documents the details of the various LOE, associated data reliability assessments, and the BAT analysis for MCCPs.

## Applying the BAT to MCCPs

Because the BAT is only applicable to discrete organic chemicals and MCCP is a mixture some simplifying assumptions were necessary. Two representative structures were selected to represent the mixtures ([Table 1](#)). These representative structures reflect the recent experimental work that was conducted as part of the on-going evaluations of MCCP under REACH (i.e., C14 50% Cl by wt), i.e., [25]. The two representative structures seek to approximate the chlorine

weight in the recently tested MCCP mixture (i.e., C14Cl5.5). It is recognized that field data and historic B testing for MCCPs reflect a much broader range of chemical structures and associated properties. Fortunately, recent testing shows that the range of  $K_{ow}$  values for the C14 50% Cl mixtures is relatively small ( $\log K_{ows} \sim 5.98 - 6.96$  [26]) compared to earlier estimates by QSARs and other methods [16, 20]. For example, the range in  $\log K_{ow}$  is 5.98-6.96 and a median value of 6.58 is derived from the estimates of the two representative structures. *The only structural information used in the BAT bioaccumulation models are the physical-chemical properties, i.e.,  $K_{ow}$ , for aquatic B assessment and biotransformation half-life predictions in fish that are based on QSARs.*

**Table 1.** Representative structures selected to derive a  $\log K_{ow}$  for BAT input.

Representative structures	Formula	MW	$\log K_{ow}$ [26]
<chem>CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CC</chem>	C14 H25 Cl5	370.62	6.32
<chem>CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC</chem>	C14 H24 Cl6	405.07	6.66

### Sample “screenshots” of the BAT application for MCCPs.

Below are some examples of the data summaries and evaluations that can be accessed in the BAT Ver.2.0 Excel file entitled “BATv2\_MCCP\_disabled\_07122020.xlsx” that accompanies this report.

LABORATORY DIETARY EXPOSURE TEST (OECD 305)									
DET 1							Author(s):		EAG 305
Name	MCCP C14, 5Cl and 6Cl						Year:	2019	
CAS	85535-85-9						Title:		
SMILES	CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CC CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C						Source:		
Key Test Details and Quantitative Information							Species	Oncorhynchus mykiss	
	Value						Value		
Uptake Period	14		d		Concentration in diet	15		mg/kg	
Depuration Period	56		d		Concentration in fish at end of uptake	0.184		mg/kg	
Mass (start)	5.85		g		LD50			mg/kg	
Mass (end)	17.88		g		Feeding rate (l)	0.015		g food/g fish/d	
Fish lipid content	6.5		%		Composition of Diet				
Temperature	15		°C		Lipid	18		%	
pH	7				Protein	66.3		%	
TOC			mg/L		Water	15.7		%	
Dissolved O <sub>2</sub>	9.03		mg O <sub>2</sub> /L		Assumed Food Absorption Efficiencies				
BMF <sub>SS</sub>	+				Lipid	92		%	
BMF <sub>K</sub>	0.0388				Protein	75		%	
BMF <sub>KG</sub>	0.169	Growth-corrected			Water	70		%	
BMF <sub>KL</sub>	0.107	Lipid-normalized			Body-gut partitioning (K <sub>BG</sub> )	1			
BMF <sub>XLG</sub>	0.468	Growth-corrected			Diet-gut partitioning (K <sub>DG</sub> )	2.29			
E <sub>D</sub> (α)	6.77	%			BMF <sub>MAX</sub>	0.113			
k <sub>T</sub>	0.0262	1/d			time to 95% steady state	115		d	
k <sub>G</sub>	0.0202	1/d							

**Figure 1.** The EAG 305 fish lab BMF study input sheet.

Quality Criteria for Data Reliability of a fish BMF Study

1. Were the BMF units clearly reported (e.g., kg/kg wet weight)?	<input checked="" type="radio"/> Yes <input type="radio"/> No
2. BMF for parent chemical reported	<input checked="" type="radio"/> Yes <input type="radio"/> No
3. If BMF was calculated as $C_{fish}/C_{diet}$ , was the steady state assumption ( $\pm 20\%$ ) confirmed?	<input type="radio"/> Yes <input type="radio"/> No <input checked="" type="radio"/> N/A
4. If BMF was calculated as $(I-ED)/KT$ , were the rate constants with units clearly reported?	<input checked="" type="radio"/> Yes <input type="radio"/> No <input type="radio"/> N/A
5. Organism concentration measured directly for chemical of interest	<input checked="" type="radio"/> Yes <input type="radio"/> No
6. Dietary uptake efficiency (ED or alpha) $\leq 100\%$	<input checked="" type="radio"/> Yes <input type="radio"/> No
7. For ionising chemicals: was pH reported and within 0.5 log units of average?	pH 6 - 8.5 <input checked="" type="checkbox"/> $< > 0.5$ log mean <input type="checkbox"/>
8. Diet concentration measured directly for chemical of interest?	<input checked="" type="checkbox"/>
9. Diet lipid content reported?	<input checked="" type="checkbox"/>
10. Was growth rate reported?	<input checked="" type="checkbox"/>
11. Mortality/adverse effects in test/control group $< 5\%$	<input type="radio"/> Yes, both <input type="radio"/> No, ctrl <input checked="" type="radio"/> No, test
12. Whole body fish lipid content reported	<input checked="" type="radio"/> Yes <input type="radio"/> Partial <input type="radio"/> No
13. Test species reported?	Check OECD species <input checked="" type="radio"/> Yes, OECD <input type="radio"/> Yes, not OECD <input type="radio"/> No
14. Fish mass reported? Yes, Partial (start or end) or No	<input checked="" type="radio"/> Yes <input type="radio"/> Partial <input type="radio"/> No
15. Whole body of fish analyzed? Tissue: Whole Body Lipid %: 6.5	<input checked="" type="radio"/> Yes <input type="radio"/> Partial <input type="radio"/> No
16. Feeding rate reported in the range of 1-3% body weight per day?	<input checked="" type="checkbox"/>
17. Was there a control group?	<input checked="" type="checkbox"/>
18. What was the chemical purity?	<input type="radio"/> $\geq 98\%$ <input checked="" type="radio"/> $\geq 95\%$ <input type="radio"/> $< 95\%$ <input type="radio"/> NR
19. LOQ reported?	<input checked="" type="checkbox"/>
20. Conducted according to recognized international standard, e.g. OECD?	<input checked="" type="radio"/> Yes <input type="radio"/> with some mods. <input type="radio"/> No
21. Study consistent with GLP or guiding principles?	<input checked="" type="radio"/> Yes <input type="radio"/> with some mods. <input type="radio"/> No
22. Test design	flow through <input checked="" type="radio"/> semi-static <input type="radio"/> static <input type="radio"/> NR
23. Water temperature reported AND appropriate for species AND constant ( $\pm 2^\circ\text{C}$ )	<input checked="" type="checkbox"/>
24. Diet concentration $< 1\%$ reported acute toxicity?	<input checked="" type="checkbox"/>
25. For neutrals: was pH reported and within 0.5 log units of average?	pH 6 - 8.5 <input type="checkbox"/> $< > 0.5$ log mean <input type="checkbox"/>
26. Was dissolved oxygen reported and $> 60\%$ ?	<input checked="" type="checkbox"/>
27. All organisms in study of similar size ( $\pm 30\%$ wt. or vol.)?	<input type="checkbox"/>
28. Acclimatization for at least 14 days under test conditions?	<input type="checkbox"/>
29. Minimum of 4 fish per sampling event?	<input checked="" type="checkbox"/>
30. Water hardness is reported AND 10-250 mg/L?	<input checked="" type="checkbox"/>
31. Light-dark cycle reported AND 12-16 h illumination (or otherwise appropriate?)	<input checked="" type="checkbox"/>
CRITICAL FAIL (Overall Reliability Score = 0), brief justification required:	
<div></div>	
Assess Study Reliability	

Figure 2. The BAT fish lab BMF DET corresponding to the EAG BMF study.



**FIELD BIOACCUMULATION AND BIOMAGNIFICATION FACTORS (BAFs, BMFs)**

**DET 1**  
Name: MCCP C14, 5CI and 6CI  
CAS: 85535-85-9  
SMILES: CC(C)CC(C)CC(C)CC(C)CCCC(C)CC CC(C)CC(C)CC(C)CC(C)C

Author(s): Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S.  
Year: 2008  
Title: Bioaccumulation and trophic magnification of short- and medium-chain chlorinated paraffins in food webs from Lake Ontario and  
Source: Environ. Sci. Technol. 42: 3893-3899

**Environmental input parameters required for BAT-calculated BAF entries only:**  

POC

mg/L

DOC

mg/L

100

% freely dissolved

or TOC

mg/L

Water Conc total

µg/L

3.1

freely dissolved (µg/L)

pH

7

Temp

15

Method Detection Limit (MDL) or equivalent

DO

9.93

Water (µg/L)

Biota (µg/kg)

Lipid Content (%)

C<sub>BIOTA</sub> (µg/kg)

Org. Type

BAF (L/kg)

BAF<sub>5%</sub> (L/kg)

BAF<sub>105%</sub> (L/kg)

# Species: 8	Mass (kg)					
plankton						
Alewife						
Smelt						
Diporeia						
Sculpin-Diporeia LO C14Cl6						
Lake Trout-Alewife LO C14Cl6						
Lake Trout-Smelt LO C14Cl6						
Lake Trout-Sculpin LO C14Cl6						

Lake Ontario

C14Cl6 only

Reliability Score:

73.44%

Once Test Details and Quality Criteria are entered:

1. Assess Input and Reliability

2. Add Data to BAT

Input Cell Color Coding BAF entries:

Minimal user input for BAF and/or BAF<sub>L</sub> entry

Input Cell Color Coding BMF entries:

Minimal user input for BMF and/or BMF<sub>L</sub> entry

User input for BAT to calculate BAF/BMF

Input for BAT to calculate BAF, BAF<sub>5%</sub>, BAF<sub>105%</sub>

Input for BAT to calculate BMF, BMF<sub>L</sub>

BAT calculated or user input values

Enter BMFs and/or BMF<sub>L</sub> ↓ or %lipid in diet and diet conc ↓, or calculate using → and organism lipid content and C<sub>BIOTA</sub> ↑

Species:

%lipid in diet

diet conc µg/kg

Org. Type

BMF

BMF<sub>L</sub>

plankton			Invertebrate		
Alewife			Fish		
Smelt			Fish		
Diporeia			Invertebrate		
Sculpin-Diporeia LO C14Cl6			Fish		
Lake Trout-Alewife			Fish		0.64
Lake Trout-Smelt			Fish		0.29
Lake Trout-Sculpin			Fish		0.24

Feeding Preferences (Fraction of Diet) for BMF calculations

Consumer ↓

Diet Choices

	plankton	Alewife	Smelt	Diporeia	Sculpin-Diporeia	Lake Trout	Lake Trout	Lake Trout
plankton								
Alewife								
Smelt								
Diporeia								
Sculpin-Diporeia								
Lake Trout								
Lake Trout								
Lake Trout								

**Figure 3.** The BAT field BMF input sheet.



Quality Criteria for Data Reliability of a BMF/BAF Field Study

**For each criterion below, either check box if statement is true or select best option as stated. All unanswered criteria are scored "0".**

1. Were field blanks used in the sampling?	<input checked="" type="checkbox"/>
2. Was a randomized sampling design employed?	<input type="checkbox"/>
3. Enter a score (0-30) representing confidence that water (for BAF) and dietary (for BMF) samples used in B-metric are co-located and considered representative of the exposures?	28
4. Enter a score (0-30) representing confidence that biological and environmental (e.g. water) samples used in B-metric obtained in the same year and season?	28
5. Enter a score (0-30) representing confidence that steady-state is approximated (e.g. +/-~20%) with 30 being analytical confirmation of this assumption).	28
6. For neutral chemical BMFs: lipid contents in predator and prey are reported?	<input checked="" type="checkbox"/>
7. Were analytical standards used in the analysis?	<input checked="" type="checkbox"/>
8. For the numerator (organism) concentrations: What was the frequency of detects? --> Sample size (=>20 or <20 or <=5)?	<input type="radio"/> 80-100% <input checked="" type="radio"/> 50-<80% <input type="radio"/> <50% or unknown <input type="radio"/> =>20 <input checked="" type="radio"/> <20->5 <input type="radio"/> <=5
9. For the denominator (water or diet) concentrations: What was the frequency of detects? --> Sample size (=>20 or <20 or <=5)?	<input type="radio"/> 80-100% <input checked="" type="radio"/> 50-<80% <input type="radio"/> <50% or unknown <input type="radio"/> =>20 <input checked="" type="radio"/> <20->5 <input type="radio"/> <=5
10. How are measurements below the MDL addressed? Using statistical or replacement methods, or unknown?	<input type="radio"/> Statistical <input checked="" type="radio"/> Replacement <input type="radio"/> Unknown
11. Are sampled species names reported?	<input checked="" type="checkbox"/>
12. For each sampled species (i.e. fish or within a taxa/TL for lower TLs) is organism mass (or length or age) reported and similar (i.e. minimal differences)?	<input type="checkbox"/>
13. Is environmental temperature reported?	<input type="checkbox"/>
14. For ionisables: is pH reported?	<input type="checkbox"/>
15. CRITICAL FAIL (Overall Reliability Score = 0), brief justification required:	<input type="checkbox"/>
<div style="border: 1px solid black; height: 40px; width: 100%;"></div>	
Assess Study Reliability	

**Figure 4.** The BAT DET for a BAF/BMF study.

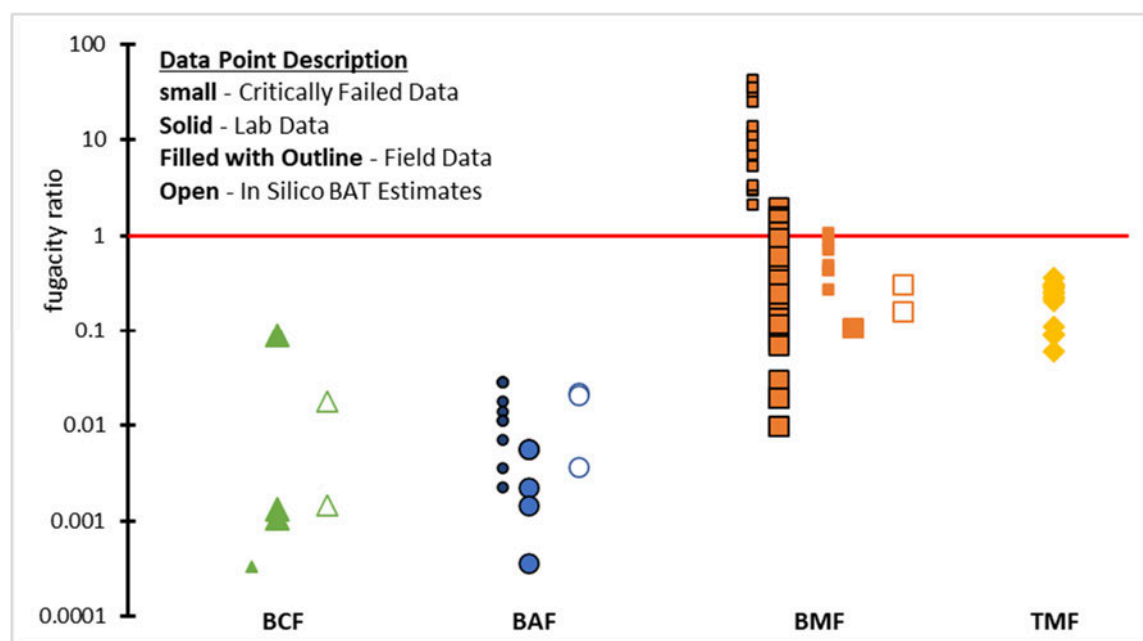
## Fugacity Ratios

Following a bioaccumulation expert workshop co-sponsored by the US EPA, SETAC and ILSI-HESI, Burkhard and colleagues [8] a framework to assess bioaccumulation and biomagnification in food webs using a weight of evidence approach that maximizes the application of various available B assessment metrics (i.e., BCFs, BAFs, BMFs, TMFs) was developed. Briefly, the approach converts measurements of laboratory and field B assessment metrics (i.e., BCFs, BAFs, BMFs, TMFs) into a “common currency” in terms of fugacity ratios enabling direct comparisons of different B-metrics for B assessment [8]. In this manner the data can be compared against a single B-hazard criterion of 1. ***Fugacity ratio data points > 1 indicate biomagnification, data points ≤ 1 indicate no biomagnification.*** The additional benefit of the fugacity ratio approach is that it can be conveniently summarized in a figure [8]. The fugacity ratio WOE approach seeks to address the question “Does the chemical biomagnify in the environment?” This is a different problem formulation than the more general question “Does the chemical bioaccumulate in the environment?”; however, it has been argued that biomagnification is the fundamental hazard that regulatory programs should be seeking to address [5, 27]. In addition to the data reliability analyses that we have conducted for all LOE in this report, a WOE approach can provide some indication of potential error in certain data points, e.g., outliers. Previous analyses we have conducted [22] include a WOE approach for the B assessment of MCCPs using the fugacity ratio approach as detailed by Burkard et al. [8].

The BAT requires chemical information for a discrete organic chemical and MCCPs are a mixture. For BCFs and BAFs used in the fugacity ratio approach, chemical specific  $K_{ow}$  values are required for a fugacity ratio calculation [8].  $K_{ow}$  is not a parameter required for calculating fugacity ratios using BMF and TMF data [8]. The fugacity ratio summary presented in this section of the report is slightly different than the fugacity ratio summary conducted in the BAT Ver.2.0 (see Appendix). The limitation in the BAT fugacity ratio analysis is because some of the reported B data for MCCPs are for different homologues (and hence different  $K_{ow}$ ) than the representative value used in the BAT. In this section we used  $K_{ow}$  values for different MCCP congeners (homologues) when calculating fugacity ratios for the BCFs and BAFs. The BAT utilizes the user-entered  $K_{ow}$  to automatically make predictions of the fugacity ratios of the entered B-metric data, however, because there are many different homologues and mixtures of these homologues considered in this study, it is prudent to manually recalculate the fugacity ratios for the entered BCF and BAF studies using specific literature or reported  $K_{ows}$ .

**Figure 5** shows the fugacity ratios for each LOE included in the BAT calculated manually including some instances in which different  $K_{ow}$  values were used for BCFs and BAFs to better reflect the properties relating to B-metrics reported in the literature. Small symbols are LOE that were deemed to have a significant data reliability issue and were deemed not reliable for the WOE approach. The “critically failed” (not reliable) LOE are included in the figure for completeness and transparency. Reasons for critical fails are included in the BAT and a few additional points for clarification for some LOE are provided below, as detailed earlier [22, 23].

The larger filled symbols reflect LOE that are reliable for the B assessment. There is general agreement from the multiple LOE in terms of fugacity ratios: 92% of the measured, reliable quality fugacity ratios are < 1 providing a strong WOE that MCCPs are not likely to biomagnify in the aquatic environment. The invertebrate fugacity ratios for BCFs for daphnia magna (0.001-0.091) [24] are higher than fish fugacity ratios for BCFs (0.003) [28]. This is also captured in the BAT bioaccumulation model calculated fugacity ratios (open triangles) for BCFs for generic lab organisms as well (i.e., 0.018 for invertebrates and 0.001 for fish). The higher fugacity ratios in invertebrates may reflect the limited capacity for biotransformation that aquatic invertebrates have as compared to fish. Figure 5 shows that the fugacity ratios calculated with the bioaccumulation models in the BAT (open symbols) are in general agreement with the empirical fugacity ratio estimates model estimates for these metrics are representative of the observed data (within an order of magnitude and showing similar trends).



**Figure 5.** Fugacity ratios for all LOE used in the BAT for MCCPs.

The BCFs determined by Hurd and Vaughn (2010) [28] used a mixture that was qualified as C<sub>14</sub>Cl<sub>4.5</sub>. Here the geometric mean of recent K<sub>OW</sub> measurements for C<sub>14</sub>Cl<sub>4</sub> and C<sub>14</sub>Cl<sub>5</sub> [26] was used to estimate a log K<sub>OW</sub> = 6.43. The BCFs (LOE) from this study was deemed not reliable for B assessment (“critical fail”) because it used radiolabeled chemical and did not explicitly quantify parent chemical in the B experiment [22, 23]. LOE that were deemed not reliable for B assessments by our data reliability analyses in the BAT appear in Figure 5 as the smaller symbols (e.g., green triangles for this BCF). The BCF study by Thompson et al. (2000) [29] did not report fish lipid contents so fugacity ratios could not be calculated and do not appear in the above plot. Invertebrate BCFs recently reported for CP mixtures (Cerechlor50LV, CP-52 and CerechlorS45) by Castro et al. [24] calculated representative K<sub>OW</sub>s for each mixture (log K<sub>OW</sub> = 6.24, 8.07, 7.88, respectively). The K<sub>OW</sub>s were calculated by the authors using KOWWIN [20] for 224 congeners and the relative composition of each mixture to determine their selected values. For

transparency we calculated the fugacity ratios here using the  $K_{OW}$  values the selected. (three larger solid triangles). The log  $K_{OW}$  values for the fugacity ratio calculations for the BAFs for MCCPs reported by Houde et al. (2008) [19] were selected as:

- $C_{14}Cl_6$ : log  $K_{OW}$  = 6.66 based on recent measurements [26].
- $C_{15}Cl_5$  and  $C_{15}Cl_6$ : assumed a log  $K_{OW}$  of 6.75 for  $C_{15}$  congeners

**This additional, more explicit method of calculating fugacity ratios “manually” using congener- and homologue-specific  $K_{OW}$  estimates rather than the approach in the BAT using a single  $K_{OW}$ , does not change the outcome of the B assessment using fugacity ratios. It is included here only for sake of completeness. Both the BAT and manual WOE approaches using fugacity ratios show that 92% of the measured LOE are below a threshold of 1. This indicates that MCCPs are not likely to biomagnify in aquatic food webs.**

## Summary

This B assessment for MCCP constituents uses B data included in the REACH substance evaluation (SEV) document [21] and the peer-reviewed literature. The current assessment only considers LOE for fish and aquatic invertebrates. The LOE include: 4 fish BCFs, 4 invertebrate BCFs, 8 lab BMFs, 13 field fish BAFs, 5 field invertebrate BAFs, 70 field fish BMFs and 14 field TMFs. The food web bioaccumulation models included in BAT were used to calculate an additional 7 LOE. The bioaccumulation models in BAT were parameterized using a combination of in vivo (n=1) and in silico (n=6) fish biotransformation half-life estimates and 3 in vivo measurements of the chemical uptake efficiency from the diet for fish.

The data reliability evaluations raise a few points worth mentioning in this summary report. Details of the data quality issues are in the “BATv2\_MCCP\_disabled\_07122020.xlsx” file and many of these issues have been mentioned in previous reports [22, 23]. Some of the laboratory data BCF and BMF data were deemed unreliable (“critically failed”) because only total radioactivity was used, rather than direct and explicit chemical analysis. In one of the two BCF experiments by Thompson et al. [29], the water concentration exceeded the water solubility of the chemical and the study length was shown to be insufficient to reach steady state. These data reliability issues are recognized as key sources of uncertainty in B data [7, 30]. For field studies, including Houde et al. (2008) [19], several BAF and BMF calculations relied on a single observation above the method detection limit (MDL). For example, Sculpin-Diporeia BMFs in Lake Ontario had only one quantifiable sample for the denominator (Diporeia). MCCP homologues  $C_{15}Cl_5$  and  $C_{15}Cl_6$  were quantifiable in only one of 7 water samples from Lake Ontario. This value (29 pg/L) was averaged with 6 replacement values of one half the detection limit (0.5 pg/L). The BAFs for these homologues are therefore unreasonably uncertain and deemed unreliable for B assessment.

**Table 2** summarizes the strength of evidence results for B-hazard classifications considering different permutations of the LOE included in this study. In total 120 LOE were considered in the current BAT WOE approach. 61% of the LOE indicate MCCPs are “not bioaccumulative” (nB) while 38% of the LOE indicate MCCPs are “very bioaccumulative” (vB) with the remaining 1% classified

as “bioaccumulative” (B). The BAT DETs document the study details and reliability scores (see accompanying file “BATv2\_MCCP\_disabled\_07122020.xlsx”). As a result of the data reliability evaluations 32% (or 36 of 113) measured LOE were determined to have at least one key source of uncertainty (“critical fails”) that renders these LOE unreliable for B assessment. The 77 reliable quality measured LOE had reliability scores ranging from 52-88%. **Eighty-two percent of the measured reliable quality LOE classify MCCPs as “nB” compared to 18% of reliable quality LOE that classify MCCPs as “vB” (Table 2).** While there is uncertainty in the strength of evidence, the majority of currently available, reliable measured LOE indicate that MCCPs are not bioaccumulative in aquatic food webs.

**Table 2.** A summary of the Strength of Evidence for the B hazard classification of MCCP using currently available lines of evidence (LOE).

	<b>nB</b>	<b>B</b>	<b>vB</b>	<b><i>n</i></b>
<b>All data (incl. BAT B model calculations)</b>	61%	1%	38%	120
<b>All measured LOE</b>	63%	1%	36%	113
<b>Measured LOE with reliability &gt;50%</b>	82%	0%	18%	77
<b>Unreliable LOE</b>	22%	3%	75%	36

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## Appendix – BAT Summary Output Report for MCCPs

**The Bioaccumulation Assessment Tool (BAT) ver2.0-BETA**

developed by ARC Inc. with support from CEFIC-LRI

Prepared by:

Organization:

ARC Inc.

Report created on:

2020-12-08 15:24

**Bioaccumulation Assessment Report****Project Summary****MCCP C14, 5CI and 6CI****CAS #: 85535-85-9****Neutral****SMILES: CC(CI)CC(CI)CC(CI)CC(CI)CCCC(CI)CC CC(CI)CC(CI)CC(CI)CC(CI)CC(CI)CC(CI)CC****Summary REACH Scenario****B****vB****Relevance****Line of Evidence****Threshold****Threshold****Weight**

Laboratory Fish BCF

2000

5000

3

Laboratory Invertebrate BCF

2000

5000

3

Field BAF

2000

5000

3

In Silico BCF

2000

5000

3

In Silico BAF

2000

5000

3

Laboratory BMF

1

1

3

Laboratory Mammal TK-BMF

1

1

3

Field BMF

1

1

3

In Silico Aq BMF

1

1

3

In Silico Terr BMF

1

1

3

Field TMF

1

1

3

**Status:****Chemical Summary****MCCP C14, 5CI and 6CI****85535-85-9****Neutral****User  
Entered****spLFER/  
ppLFER****Used in  
BAT**

Molecular Weight (g/mol)

387.90

387.90

Water Solubility (mg/L)

6.10E-03

6.10E-03

Vapor Pressure (Pa)

1.95E-05

1.95E-05

Henry's Law Constant (Pa/m<sup>3</sup>·mol)

1.24E+00

1.24E+00

logK<sub>AW</sub>

-3.30

-3.30

logK<sub>OW</sub>

6.58

6.58

logK<sub>OA</sub>

9.88

9.88

logK<sub>POC</sub>

6.12

6.12

logK<sub>DOC</sub>

5.48

5.48

logK<sub>StorageLipidW</sub>

6.77

logK<sub>MembraneLipidW</sub>

7.10

7.10

log<sub>ProteinW</sub>

5.31

logK<sub>CarbohydrateW</sub>

5.31

logK<sub>SerumAlbuminW</sub>

5.32

5.32

Solubility in Octanol (mol/m<sup>3</sup>)

59.80

59.80

MCCP C14, 5CI and 6CI, CAS #: 85535-85-9

Reliability

### Biotransformation Estimate Summary

	hours	days	CF	n
Standardized Half-life in Fish (10g, 15°C)	1.27E+03	5.28E+01	7.3	7
Standardized Half-life in Mammals (70kg)	-	-	-	-

Biotransformation summary	0.01 kg FISH $k_B$	70 kg MAMMAL $k_B$	Reliability Score
$k_B$			
Amot (2013) Comments on Preliminary B Assessment of	6.80E-04		80.00%
USEPA-EPISuite BCFBAF v3.0	2.62E-03		100.00%
QSARINS-Fish HLb M1	3.01E-04		100.00%
QSARINS-Fish HLb M2	4.60E-04		66.67%
QSARINS-Fish HLb M3	3.28E-04		100.00%
OPERA-Fish HL	1.42E-03		100.00%
IFS-fhlb.qsarpred	1.21E-04		100.00%

	Fish	Herbivore	Carnivore
Dietary absorption efficiency (%)	9.06	79.06	100
Confidence Factor	2.7	1	1











































Dietary absorption efficiency summary	0.01 kg FISH $E_D$ %	HERBIVORE $E_D$ %	CARNIVORE $E_D$ %	Reliability Score
EAG 305 report-rainbow trout	6.77			80.00%
Fisk 2000-rainbow trout	10			80.00%
Fisk 2000-rainbow trout	11			80.00%











































3  
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MCCP C14, 5CI and 6CI, CAS #:  
85535-85-9











































					Strength of Evidence:			Outcome nB, B, vB	Reliability 1,2,3,4,5	Relevance 1,2,3,4,5	
					ALL:	nB:	B:				vB:
					No BAT-calc:	62.80%	0.90%				36.30%
					All Aquatic:	60.80%	0.80%				38.30%
Bioaccumulation Estimate Summary											
B-metric	LOE Source	Sheet Ref.	Value	Category							
BAF: Aquatic-Fish-BAT Generic Field Low TL Fish	BAT Estimate	N/A	6.98E+04	vB>5000	● 4	●	●	●	3		
BAF: Aquat. Invert.-BAT Generic Field Aquat. Invert.	BAT Estimate	N/A	2.52E+05	vB>5000	● 4	●	●	●	3		
BAF: Aquat. Invert.-BAT Generic Field Benthic Invert.	BAT Estimate	N/A	1.61E+05	vB>5000	● 4	●	●	●	3		
BMF: Aquatic-Fish-BAT Generic Field Upper TL Fish	BAT Estimate	N/A	0.302	nB≤1	● 2	●	●	●	3		
BMF: Aquatic-Fish-BAT Generic Lab Fish	BAT Estimate	N/A	0.158	nB≤1	● 2	●	●	●	3		
BCF: Aquatic-Fish-BAT Generic Lab Fish	BAT Estimate	N/A	2.81E+04	vB>5000	● 4	●	●	●	3		
BCF: Aquat. Invert.-BAT Generic Lab Invert	BAT Estimate	N/A	1.35E+05	vB>5000	● 4	●	●	●	3		
BCF: Aquatic-Fish-Oncorhynchus mykiss	Hurd, KS and Vaughan, M (2010)	BCF Fish Lab 1	4.44E+03	B>2000	● 3	○	○	●	3		
BCF: Aquatic-Fish-Oncorhynchus mykiss	Thompson RS, Caunter JE, Gillings E. (2000)	BCF Fish Lab 2	1.09E+03	nB≤2000	● 2	○	○	●	3		
BCF: Aquatic-Fish-Oncorhynchus mykiss	Thompson RS, Caunter JE, Gillings E. (2000)	BCF Fish Lab 3	349	nB≤2000	● 2	○	○	●	3		
BMF: Aquatic-Fish-Oncorhynchus mykiss	EAG 305 (2019)	BMF Lab 1	0.107	nB≤1	● 2	●	●	●	3		
BCF: Aquat. Invert.-daphnia magna	Castro, M, Sobek, A, Yuan, B, Breitholtz, M (2019)	BCF Invert Lab 1	7.94E+04	vB>5000	● 4	●	●	●	3		
BCF: Aquat. Invert.-daphnia magna	Castro, M, Sobek, A, Yuan, B, Breitholtz, M (2019)	BCF Invert Lab 2	7.94E+04	vB>5000	● 4	●	●	●	3		
BCF: Aquat. Invert.-daphnia magna	Castro, M, Sobek, A, Yuan, B, Breitholtz, M (2019)	BCF Invert Lab 3	5.01E+04	vB>5000	● 4	●	●	●	3		
BMF: Aquatic-Fish-LakeTrout-Alewife LO C14CI6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 1	0.64	nB≤1	● 2	●	●	●	3		











































BMF: Aquatic-Fish-LakeTrout-Smelt LO C14Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 1	0.29	nB≤1		2		4		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C14Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 1	0.24	nB≤1		2		4		3
BMF: Aquatic-Fish-LakeTrout-Alewife LO C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 2	0.64	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 2	0.48	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 2	0.35	nB≤1		2		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 3	2	vB>1		4		3		3
BMF: Aquatic-Fish-LakeTrout-Alewife LM C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 3	0.16	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 3	0.84	nB≤1		2		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C14Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 4	1.6	vB>1		4		3		3
BMF: Aquatic-Fish-LakeTrout-Alewife LM C14Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 4	0.22	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C14Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 4	0.95	nB≤1		2		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C14Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	2.1	vB>1		4		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C14Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	3	vB>1		4		3		3
BAF: Aquat. Invert.-plankton	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	7.92E+04	vB>5000		4		3		3











































BAF: Aquatic-Fish-Alewife	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	5.00E+05	vB>5000		4		3		3
BAF: Aquatic-Fish-Smelt	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	1.26E+06	vB>5000		4		3		3
BAF: Aquatic-Fish-Sculpin-Diporeia	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	1.26E+06	vB>5000		4		3		3
BAF: Aquatic-Fish-Lake Trout	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 5	3.15E+05	vB>5000		4		3		3
BAF: Aquat. Invert.-plankton LO C15C15	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	3.15E+05	vB>5000		4		0		3
BAF: Aquatic-Fish-alewife LO C15C15	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	3.97E+05	vB>5000		4		0		3
BAF: Aquatic-Fish-sculpin LO C15C15	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	7.92E+05	vB>5000		4		0		3
BAF: Aquatic-Fish-rainbow smelt LO C15C15	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	5.00E+05	vB>5000		4		0		3
BAF: Aquatic-Fish-lake trout LO C15C15	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	1.99E+05	vB>5000		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C15C15	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	3.1	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C15C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	7	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C15C17	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 6	12	vB>1		4		0		3
BAF: Aquat. Invert.-plankton LO C15C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	6.29E+04	vB>5000		4		0		3
BAF: Aquatic-Fish-alewife LO C15C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	3.15E+05	vB>5000		4		0		3











































BAF: Aquatic-Fish-sculpin LO C15C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	7.92E+05	vB>5000		4		0		3
BAF: Aquatic-Fish-rainbow smelt LO C15C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	7.92E+05	vB>5000		4		0		3
BAF: Aquatic-Fish-lake trout LO C15C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	9.98E+04	vB>5000		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C15C19	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	43	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C15C110	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	25	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C17C117	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 7	11	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C14C17	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	5.3	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C14C18	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	8.9	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C14C19	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	14	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C14C110	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	11	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C16C16	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	3.4	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C16C17	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	32	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C16C19	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	35	vB>1		4		0		3
BMF: Aquatic-Fish-Sculpin-Diporeia LO C16C110	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 8	8.8	vB>1		4		0		3
























BMF: Aquatic-Fish-LakeTrout-Alewif LO C14CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 9	0.86	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C14CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 9	0.27	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C14CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 9	0.28	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LM C14CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 9	0.16	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C14CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 9	1.2	vB>1		4		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C14CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 9	0.52	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LO C14CI8	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 10	0.43	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C14CI8	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 10	0.23	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C14CI8	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 10	0.18	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LM C14CI8	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 10	0.14	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C14CI8	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 10	0.61	nB≤1		2		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C14CI8	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 10	1.5	vB>1		4		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LO C14CI9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 11	0.31	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C14CI9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 11	0.28	nB≤1		2		3		3

BMF: Aquatic-Fish-LakeTrout-Sculpin LO C14CI9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 11	0.11	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LM C14CI9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 11	0.18	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C14CI9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 11	1.1	vB>1		4		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C14CI9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 11	0.23	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LO C14CI10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 12	0.23	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C14CI10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 12	0.31	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C14CI10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 12	0.08	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LM C14CI10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 12	0.17	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C14CI10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 12	0.92	nB≤1		2		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C14CI10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 12	0.1	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LO C16CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 13	0.22	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C16CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 13	0.01	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C16CI7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 13	0.01	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewif LM C15CI5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 13	0.4	nB≤1		2		3		3

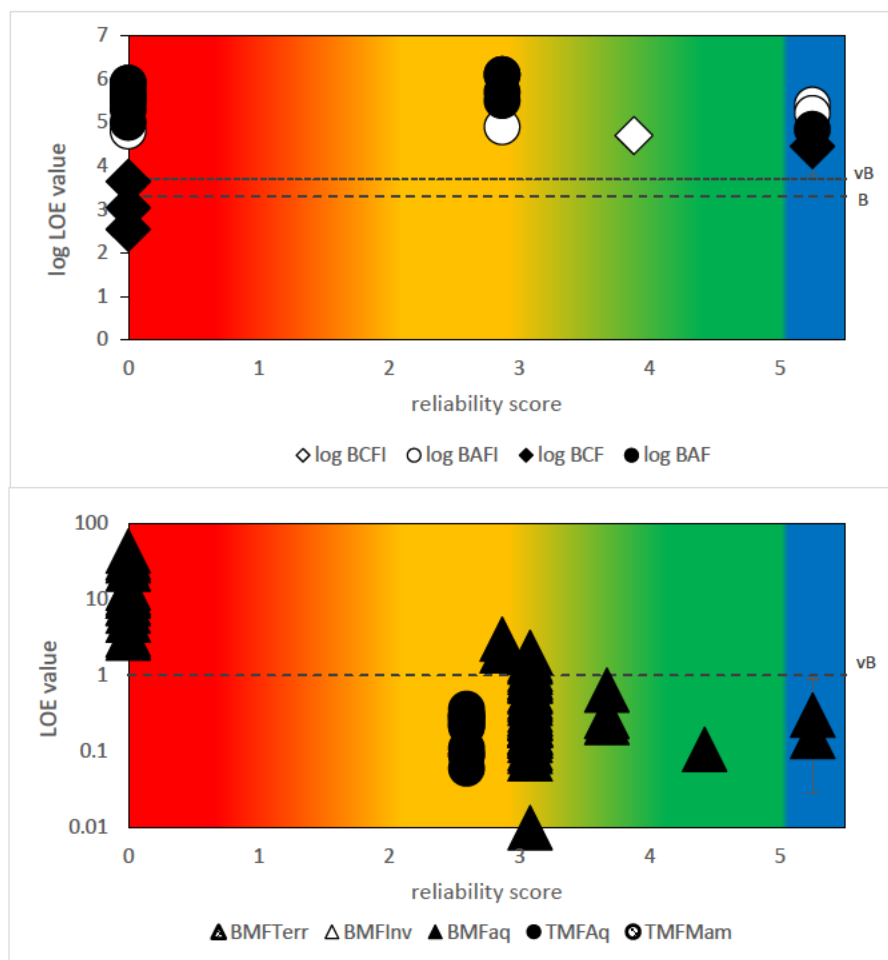
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BMF: Aquatic-Fish-Sculpin-Diporeia LM C15Cl5	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 13	0.5	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewife LO C15Cl7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 14	0.25	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C15Cl7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 14	0.07	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C15Cl7	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 14	0.12	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewife LM C15Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 14	0.35	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LM C15Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 14	0.93	nB≤1		2		3		3
BMF: Aquatic-Fish-Sculpin-Diporeia LM C15Cl6	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 14	0.62	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewife LO C15Cl	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 15	0.03	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C15Cl9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 15	0.02	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C15Cl9	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 15	0.02	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Alewife LO C15Cl10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 15	0.02	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Smelt LO C15Cl10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 15	0.02	nB≤1		2		3		3
BMF: Aquatic-Fish-LakeTrout-Sculpin LO C15Cl10	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	BAF BMF Field 15	0.02	nB≤1		2		3		3

TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 1	0.31	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 2	0.28	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 3	0.36	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 4	0.29	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 5	0.26	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 6	0.21	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 7	0.3	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 8	0.25	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 9	0.23	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 10	0.11	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 11	0.09	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 12	0.09	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 13	0.22	nB≤1		2		3		3
TMF: Aquatic-Fish	Houde, M, Muir, DCG, Tomy, GT, Whittle, DM, Teixeira, C, Moore, S. (2008)	TMF Field 14	0.06	nB≤1		2		3		3

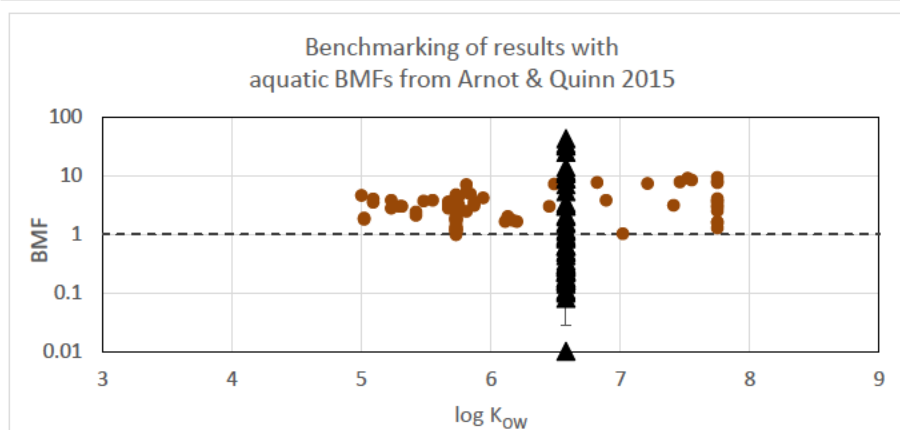
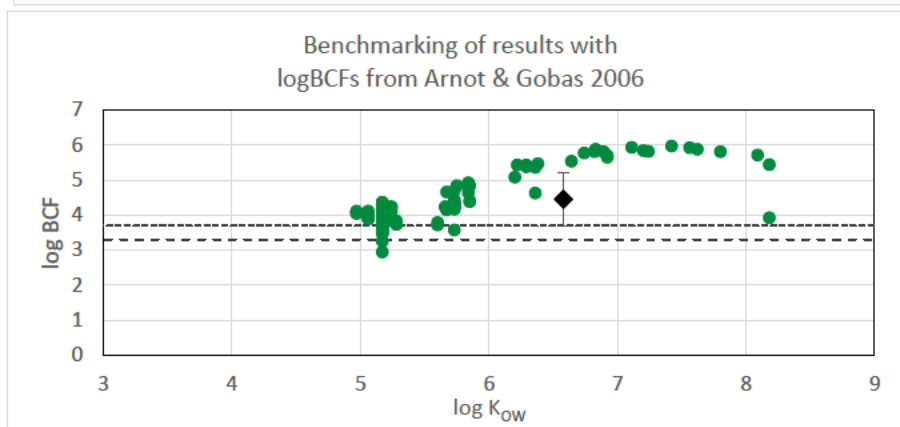
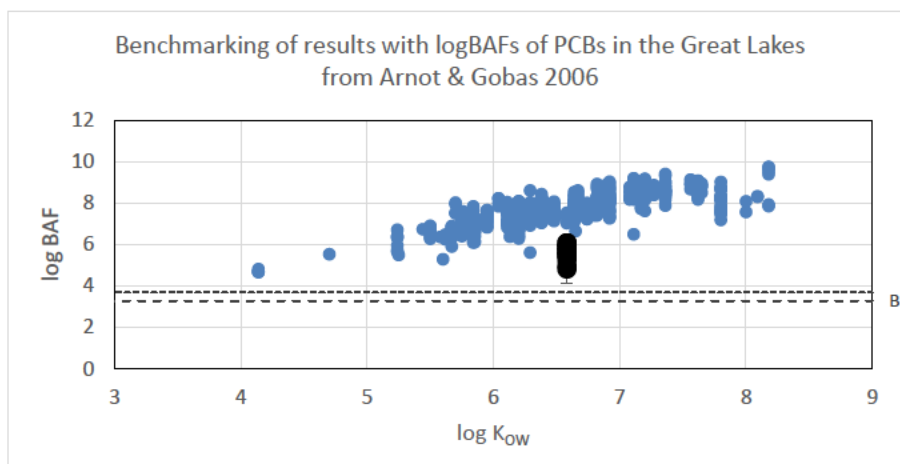
BMF: Aquatic-Fish-onocorhynchus mykiss	Fisk, A, Cymbalisty, CD, Bergman, A., Muir, DCG (1996)	BMF Lab 2	1.07	$vB>1$		4		0		3
BMF: Aquatic-Fish-onocorhynchus mykiss	Fisk, A, Cymbalisty, CD, Bergman, A., Muir, DCG (1996)	BMF Lab 3	0.9	$nB\leq 1$		2		0		3
BMF: Aquatic-Fish-onocorhynchus mykiss	Fisk, A, Cymbalisty, CD, Bergman, A., Muir, DCG (1996)	BMF Lab 4	0.72	$nB\leq 1$		2		0		3
BMF: Aquatic-Fish-onocorhynchus mykiss	Fisk, A, Cymbalisty, CD, Bergman, A., Muir, DCG (1996)	BMF Lab 5	0.44	$nB\leq 1$		2		0		3
BMF: Aquatic-Fish-onocorhynchus mykiss	Fisk, A, Cymbalisty, CD, Bergman, A., Muir, DCG (1996)	BMF Lab 6	0.5	$nB\leq 1$		2		0		3
BMF: Aquatic-Fish-oncorhynchus mykiss	Fisk, AT, Tomy, GT, Cymbalisty, CD, Muir, DCG (2000)	BMF Lab 7	0.43	$nB\leq 1$		2		0		3
BMF: Aquatic-Fish-oncorhynchus mykiss	Fisk, AT, Tomy, GT, Cymbalisty, CD, Muir, DCG (2000)	BMF Lab 8	0.27	$nB\leq 1$		2		0		3

MCCP C14, 5CI and 6CI, CAS #: 85535-85-9

### Benchmarking Figures



Benchmarking Figures





## MCCP C14, 5Cl and 6Cl, CAS #: 85535-85-9

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