Controls on the Trophic Magnification Factor of Organic Chemicals in Aquatic Foodwebs

Matthew MacLeod, Jon Arnot, Katrine Borgå & Michael McLachlan

Department of Applied Environmental Science, Stockholm University, Sweden
Arnot Research and Consulting, Toronto, Ontario, Canada
Norwegian Institute for Water Research (NIVA), Oslo, Norway

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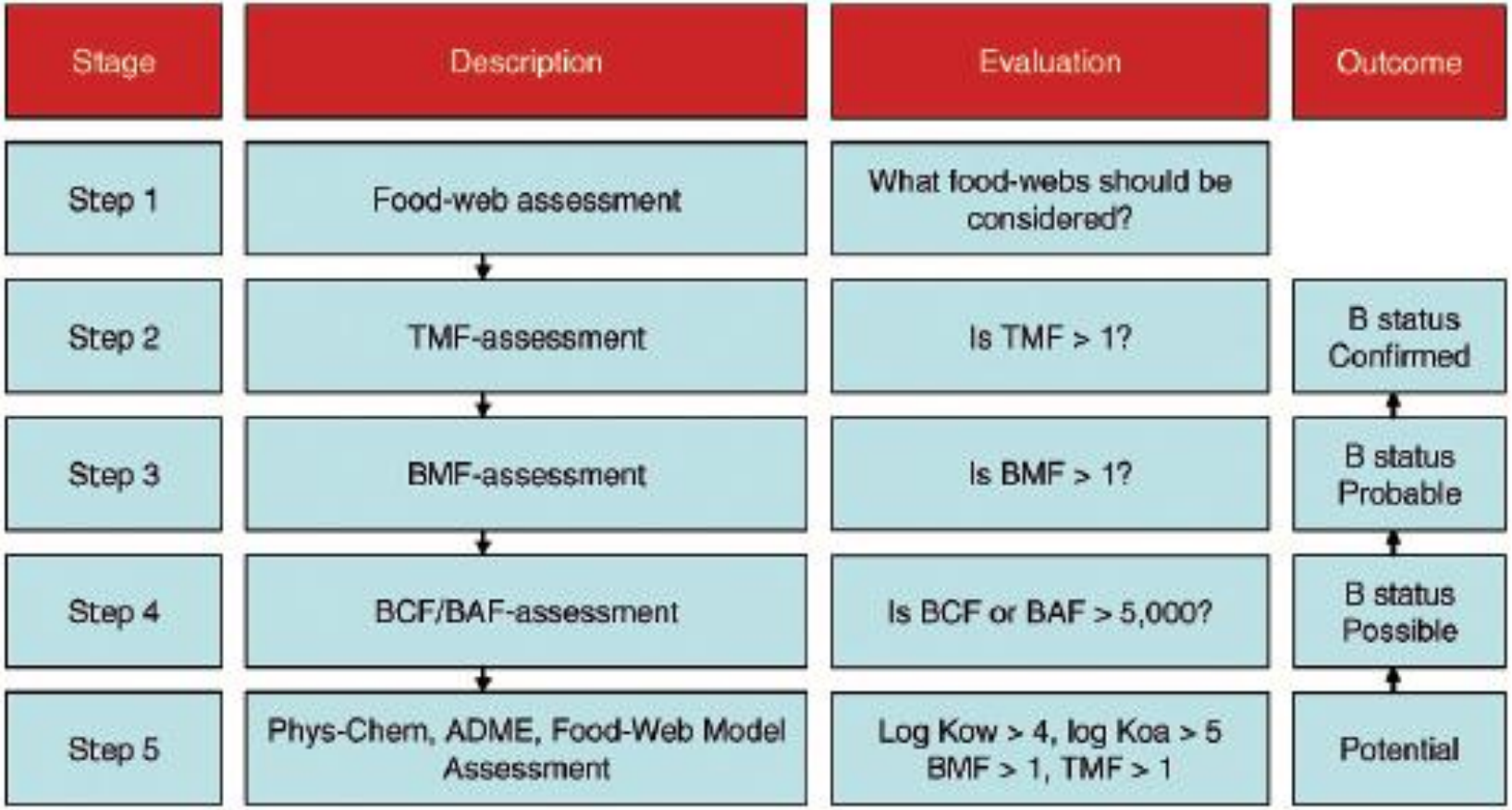
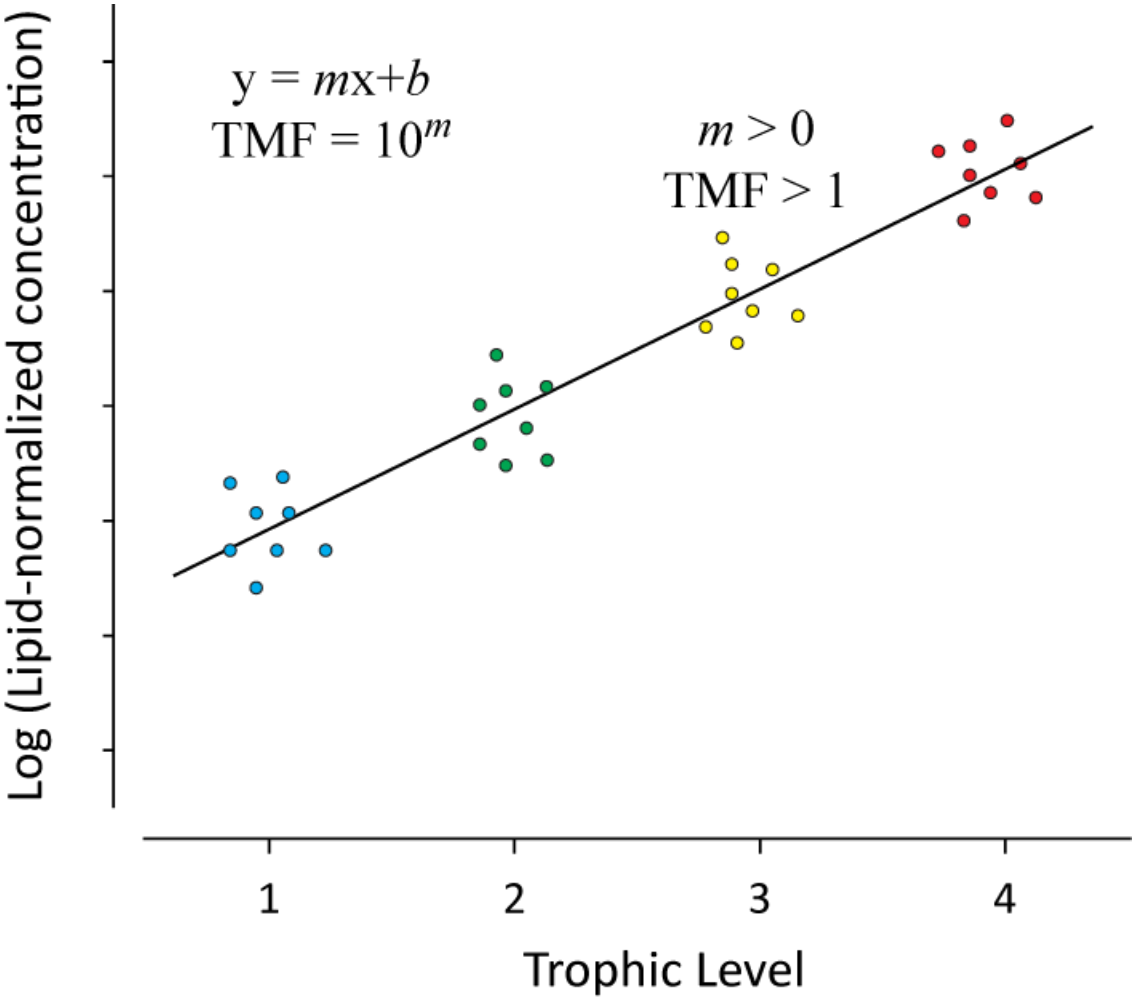
“The TMF is the most conclusive evidence of the bioaccumulative nature of the compound”

- Gobas, de Wolf, Burkhard, Verbruggen & Plotzke. IEAM, 5(4), 2009.



What is the Trophic Magnification Factor?



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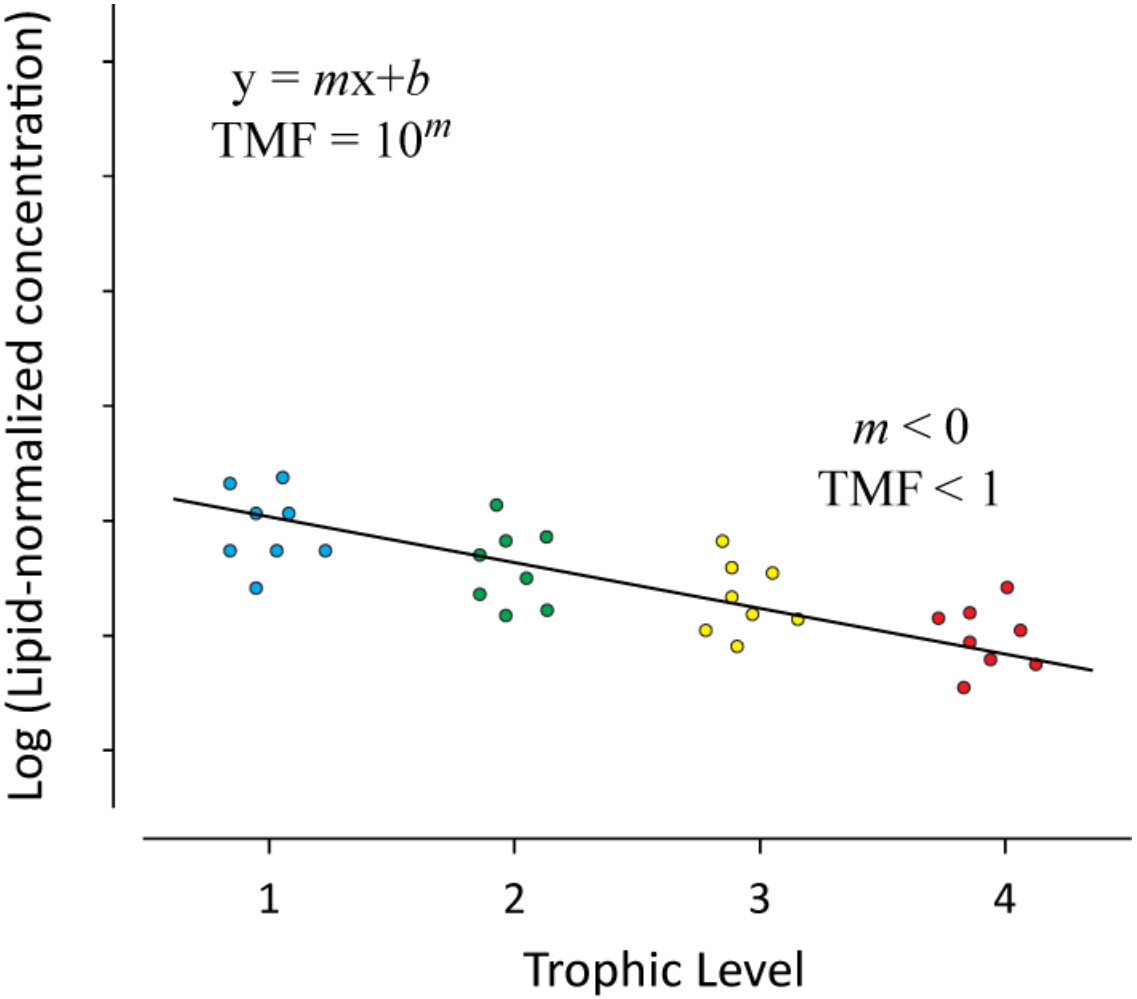

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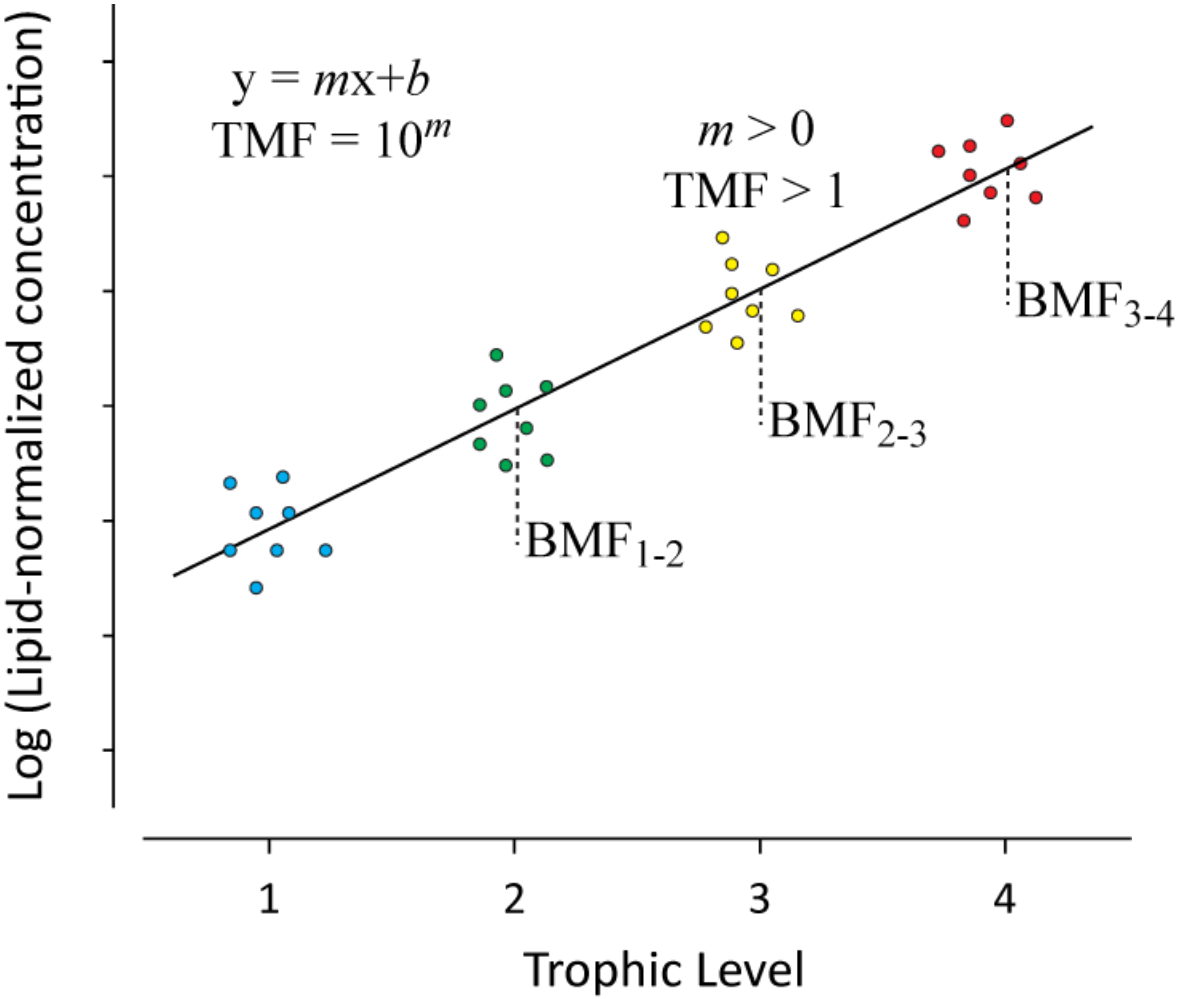

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Special Issue Honoring Don Mackay

A FOOD WEB BIOACCUMULATION MODEL FOR ORGANIC CHEMICALS IN AQUATIC ECOSYSTEMS

JON A. ARNOT and FRANK A.P.C. GOBAS*
School of Resource and Environmental Management, Simon Fraser University, 8888 University Drive, Burnaby, BC V5A 1S6, Canada

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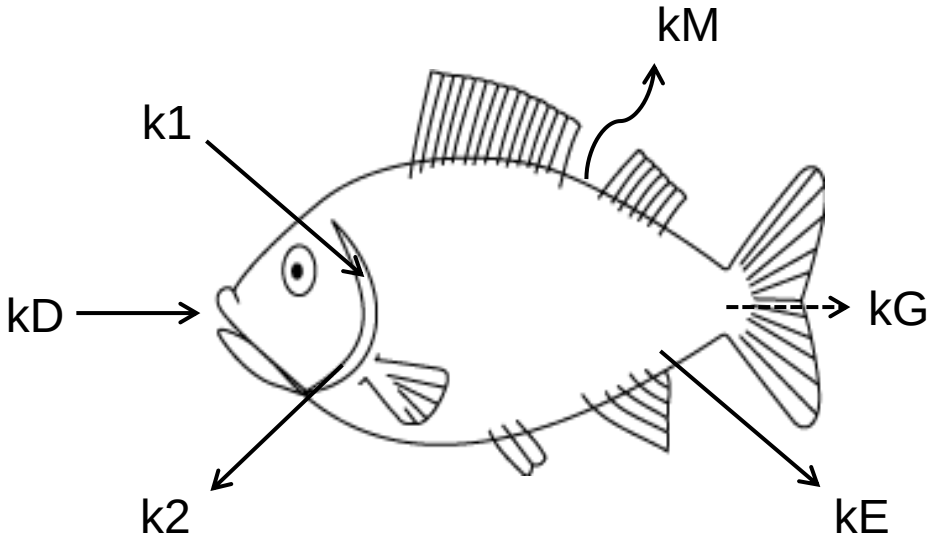
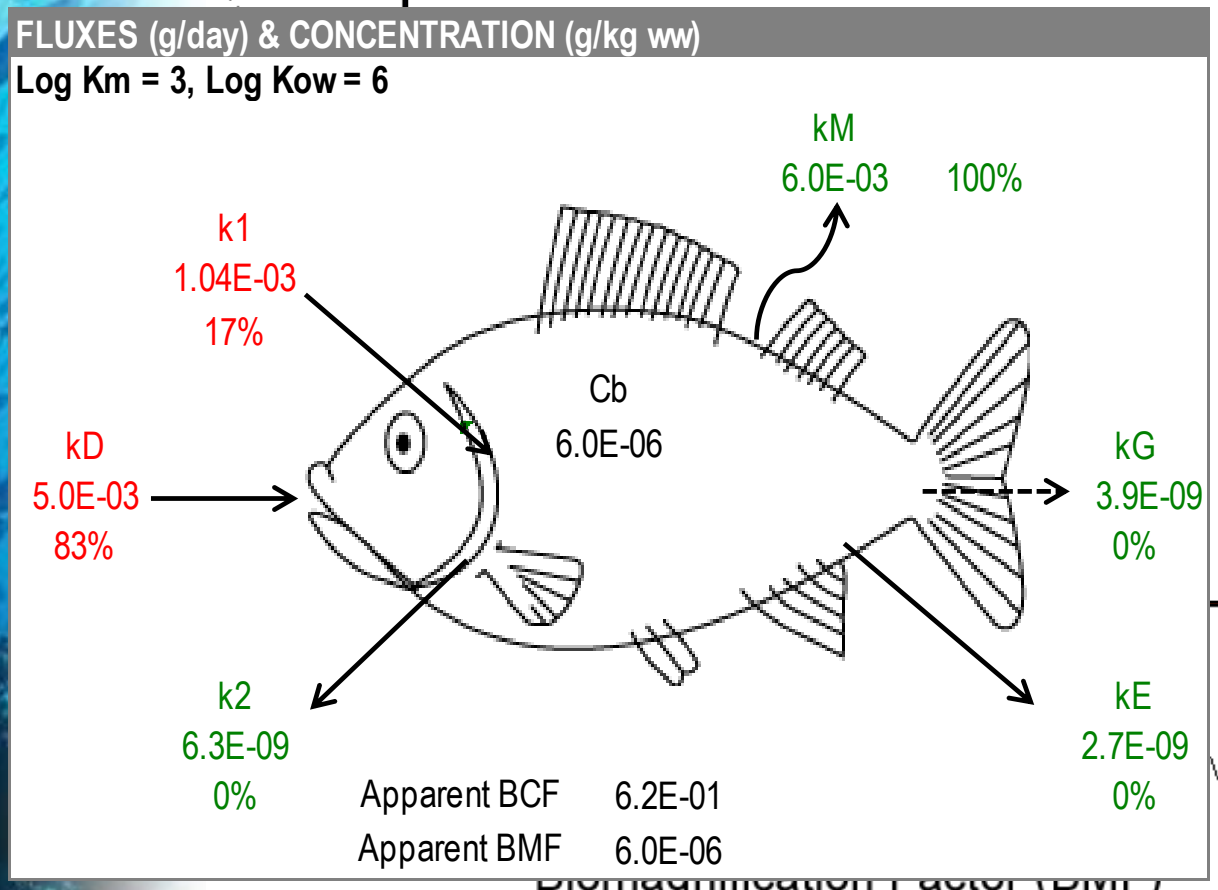


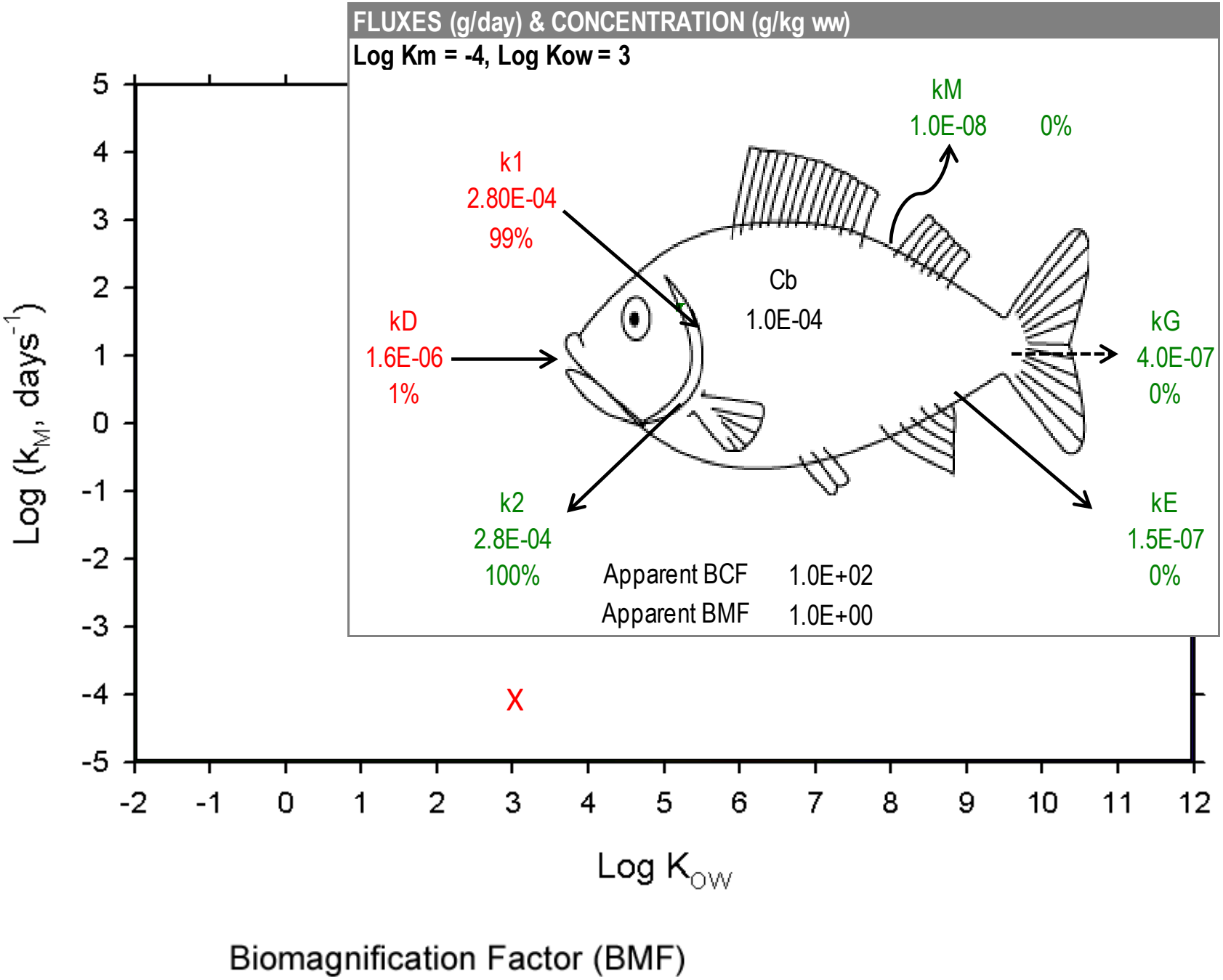
Methods and Goals

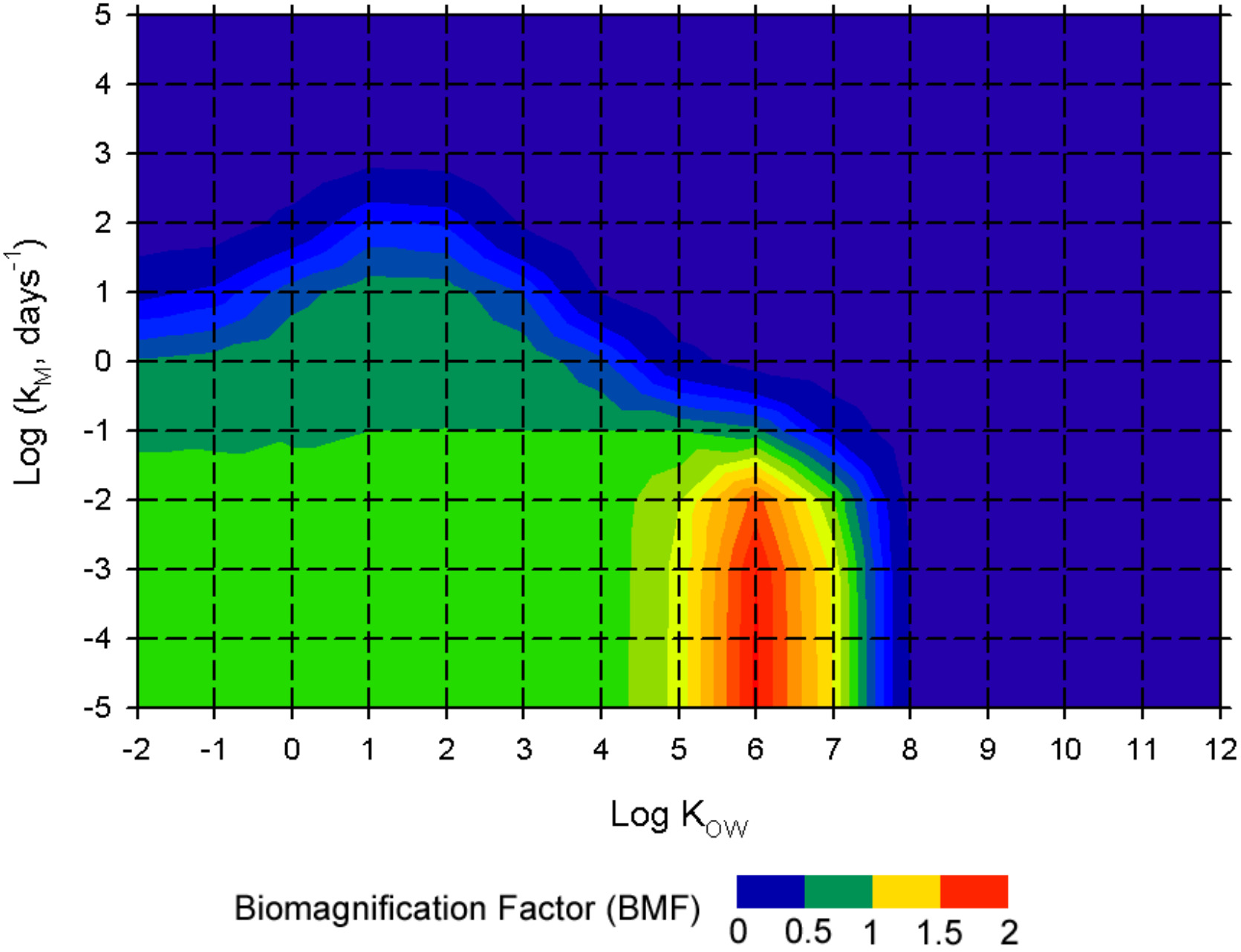
- Apply the A&G fish bioaccumulation model to explore the controls on BMF (and thus TMF) of chemicals
- Identify tools and future research that could enable laboratory → field extrapolation of TMFs for “new” chemicals
- Key model input parameters:

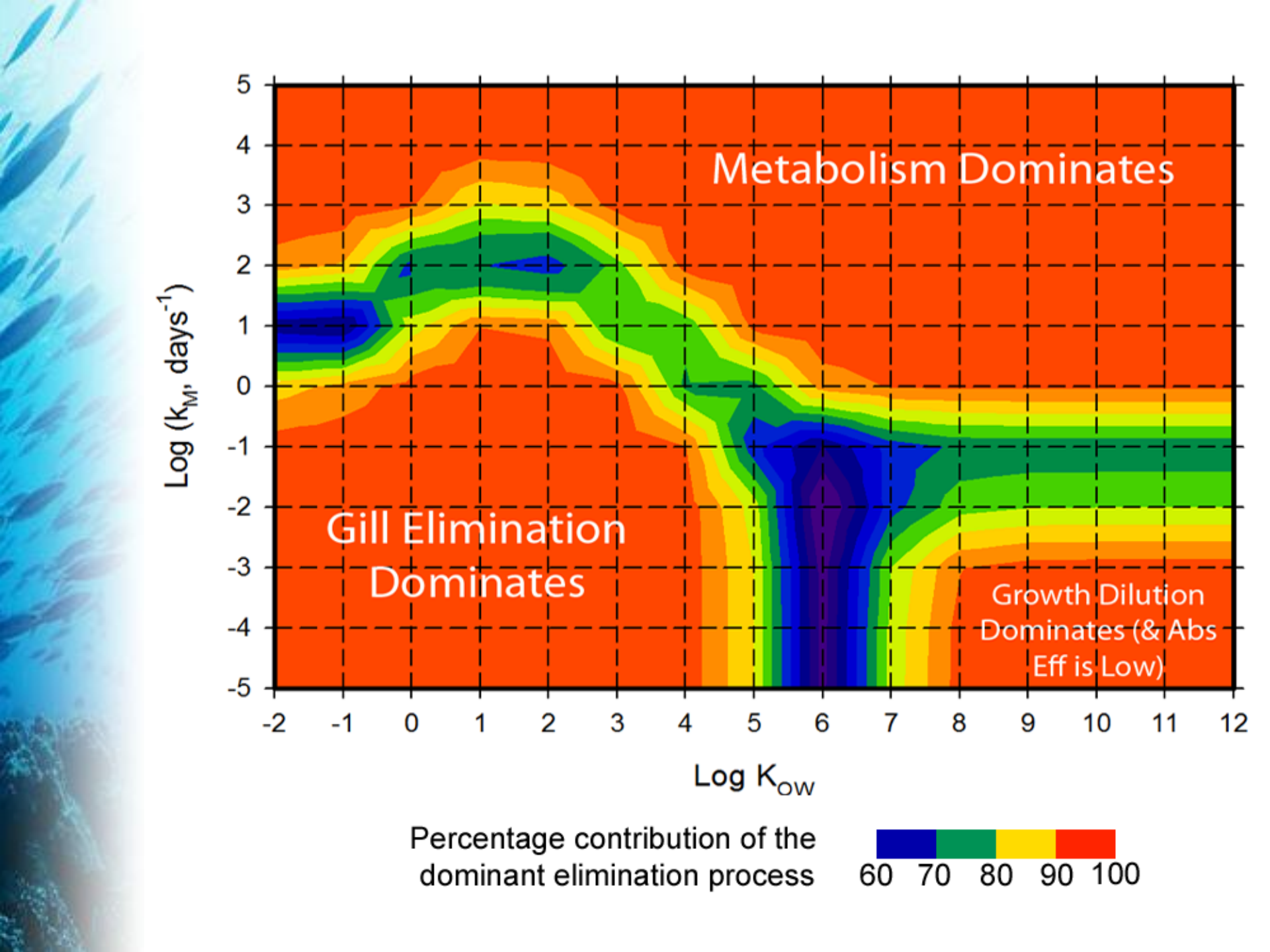
  Log Kow and kM


FLUXES (g/day) & CONCENTRATION (g/kg ww)
Log Km = 3, Log Kow = 6
kM
6.0E-03
100%
k1
1.04E-03
17%
Cb
6.0E-06
kD
5.0E-03
83%
kG
3.9E-09
0%
k2
6.3E-09
0%
kE
2.7E-09
0%
Apparent BCF
6.2E-01
Apparent BMF
6.0E-06

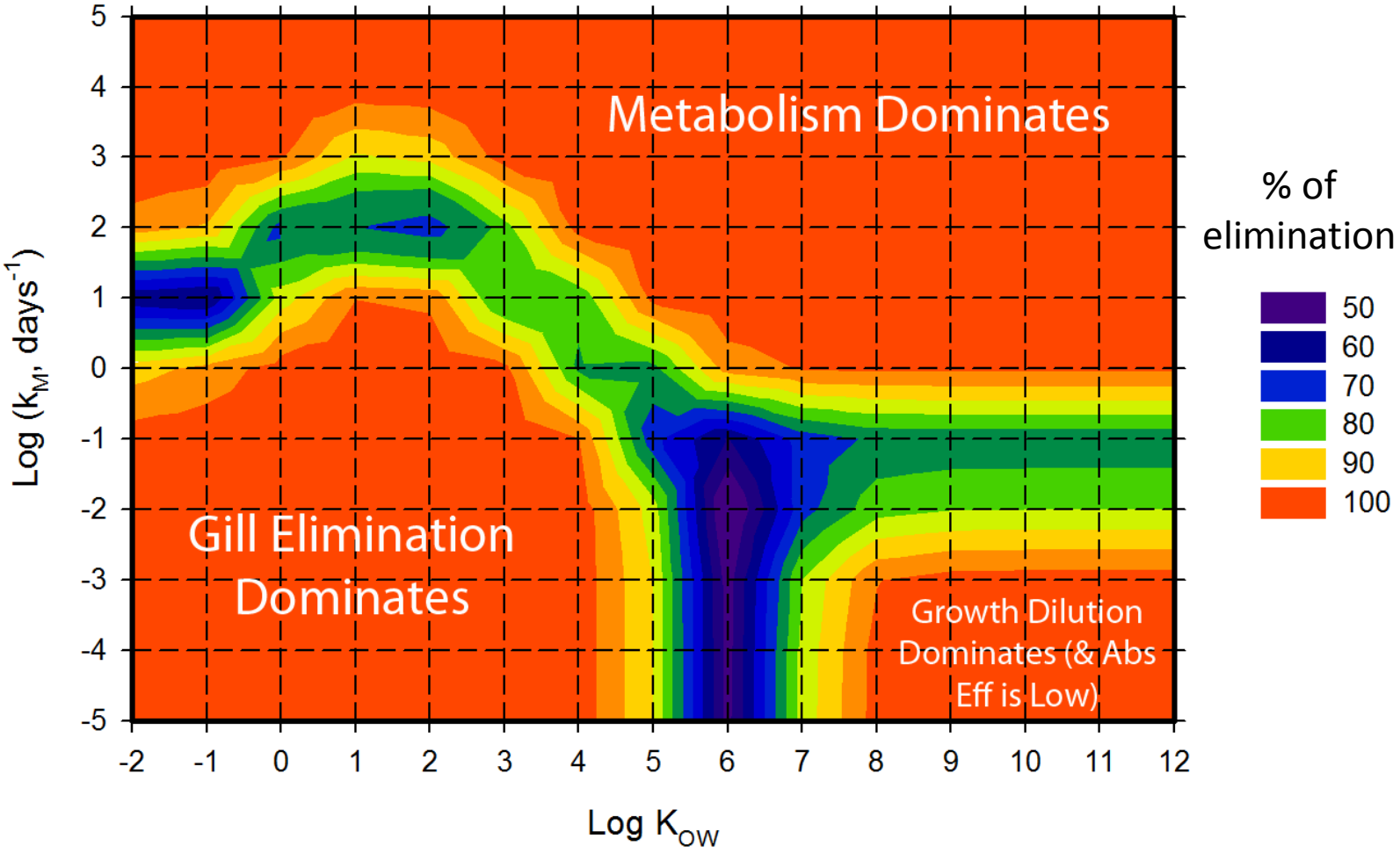
5
4
3
2
X
6
7
8
9
10
11
12


FLUXES (g/day) & CONCENTRATION (g/kg ww)
Log Km = -4, Log Kow = 3
kM
1.0E-08
0%
k1
2.80E-04
99%
Cb
1.0E-04
kD
1.6E-06
1%
kG
4.0E-07
0%
k2
2.8E-04
100%
kE
1.5E-07
0%
Apparent BCF 1.0E+02
Apparent BMF 1.0E+00
X
Log (k_M, days^-1)
Log K_OW
Biomagnification Factor (BMF)


Log (k_M, days^{-1})
5
4
3
2
1
0
-1
-2
-3
-4
-5
-2
-1
0
1
2
3
4
5
6
7
8
9
10
11
12
Log K_{OW}
Biomagnification Factor (BMF)
0
0.5
1
1.5
2


Metabolism Dominates
Gill Elimination Dominates
Growth Dilution Dominates (& Abs Eff is Low)
Log (k_M, days^{-1})
Log K_{OW}
5
4
3
2
1
0
-1
-2
-3
-4
-5
-2
-1
0
1
2
3
4
5
6
7
8
9
10
11
12
Percentage contribution of the dominant elimination process
60
70
80
90
100

What tools could screen chemicals for potential TMF > 1?



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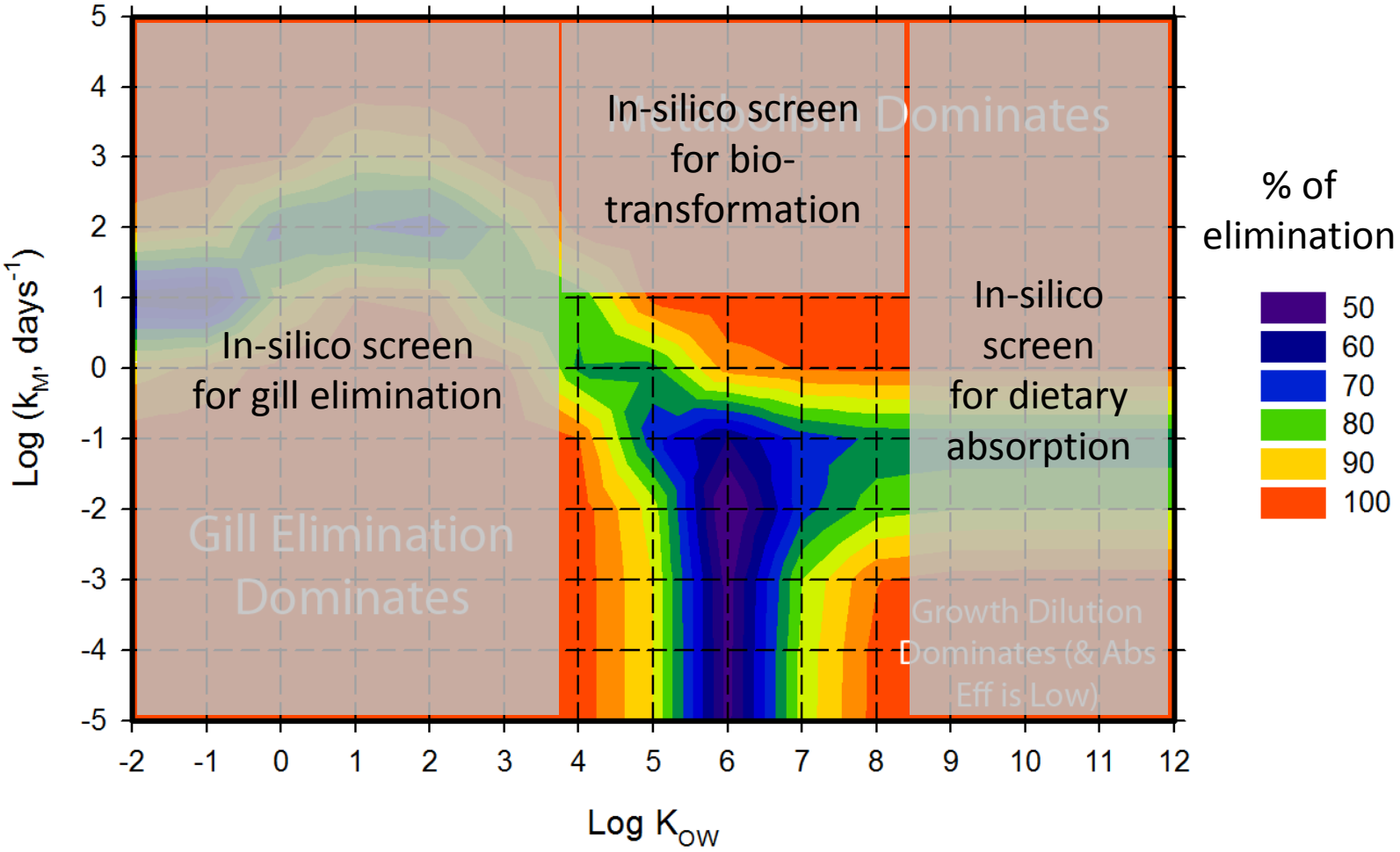
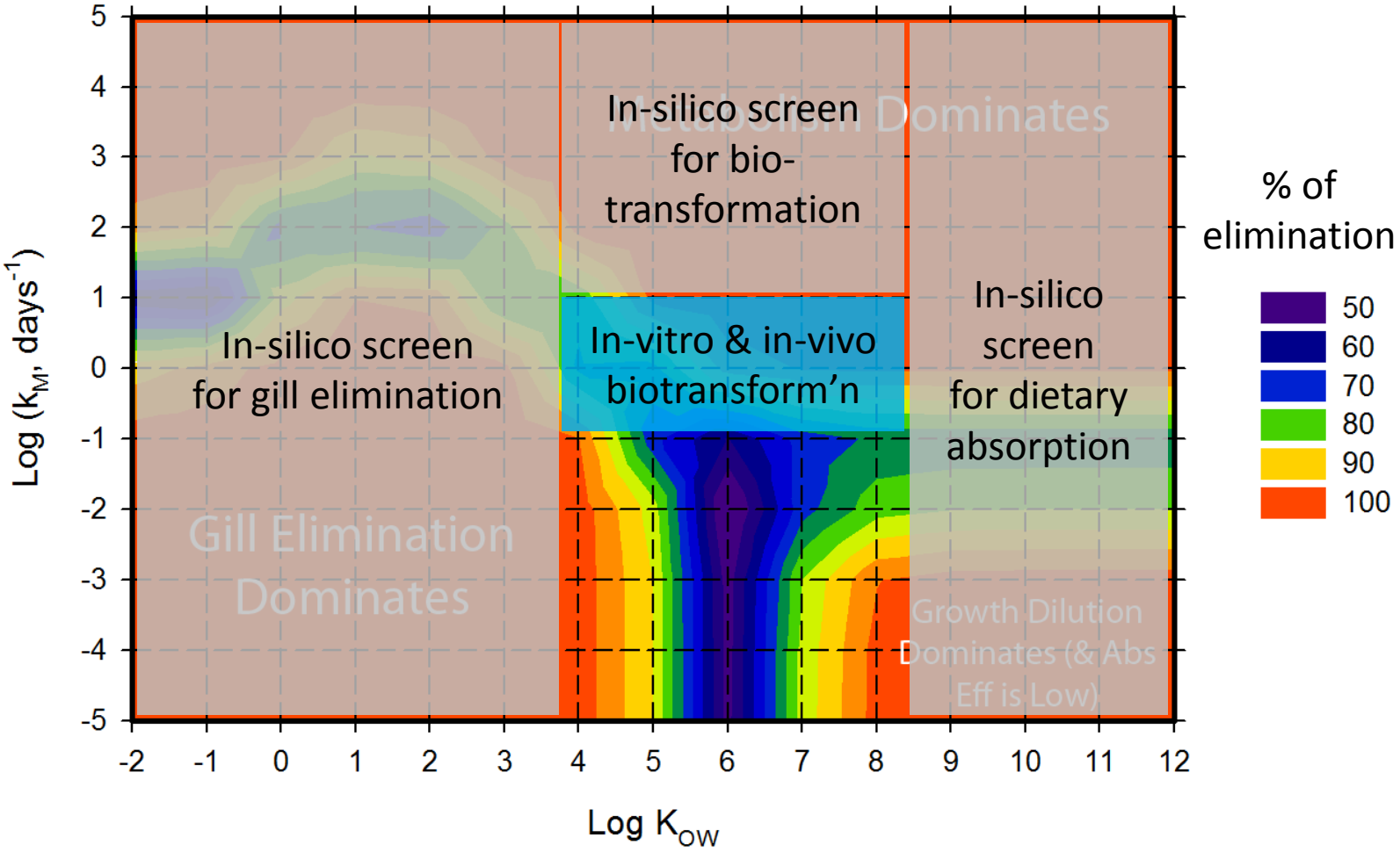
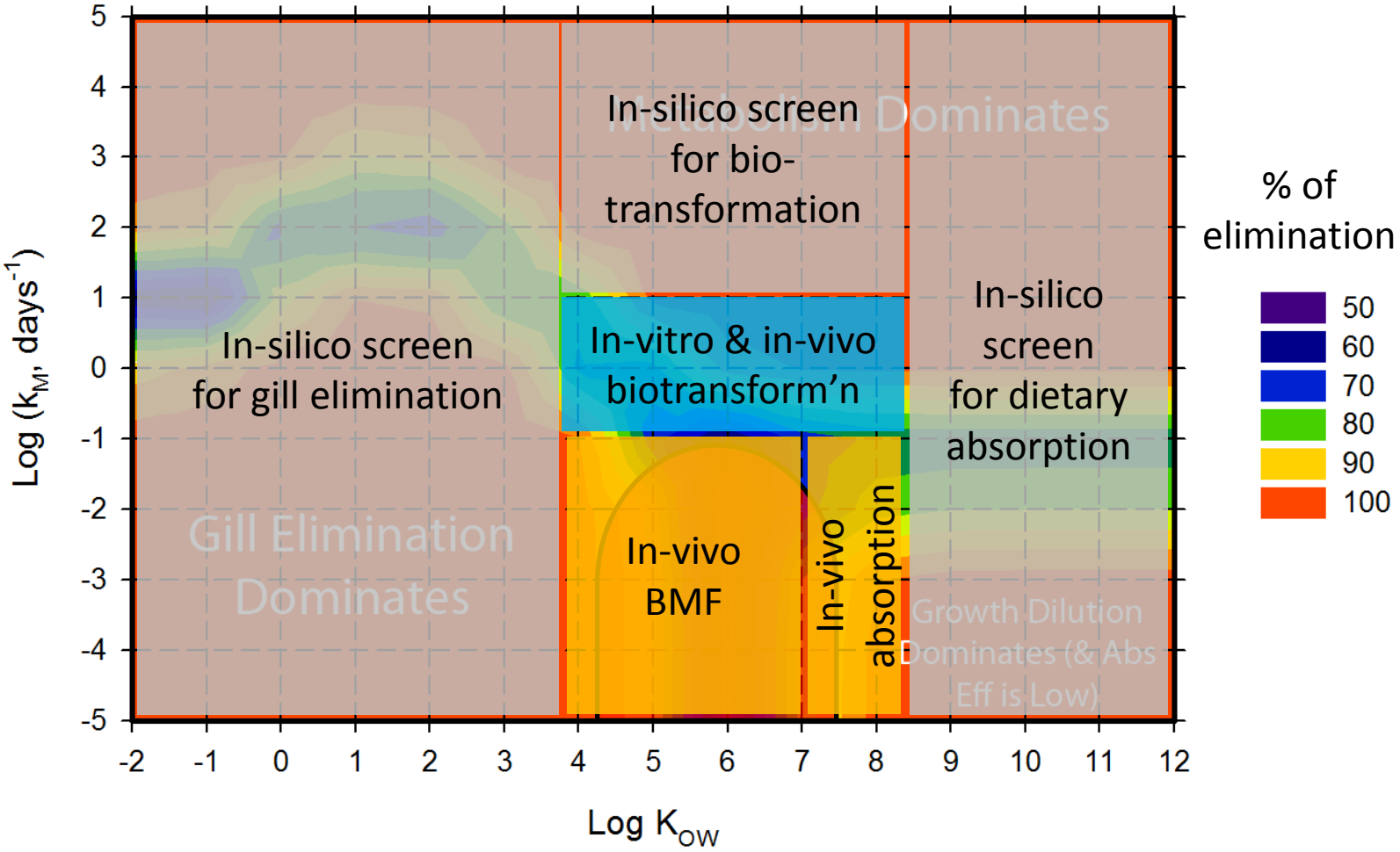


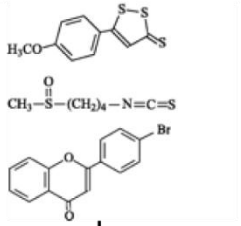
What tools could screen chemicals for potential TMF > 1?



What tools could screen chemicals for potential TMF > 1?



A Tiered Strategy for Screening for TMF



in-silico gill elimination

in-silico absorption

in-silico biotransformation

in-vitro biotransformation

in-vivo absorption

biomagnification test

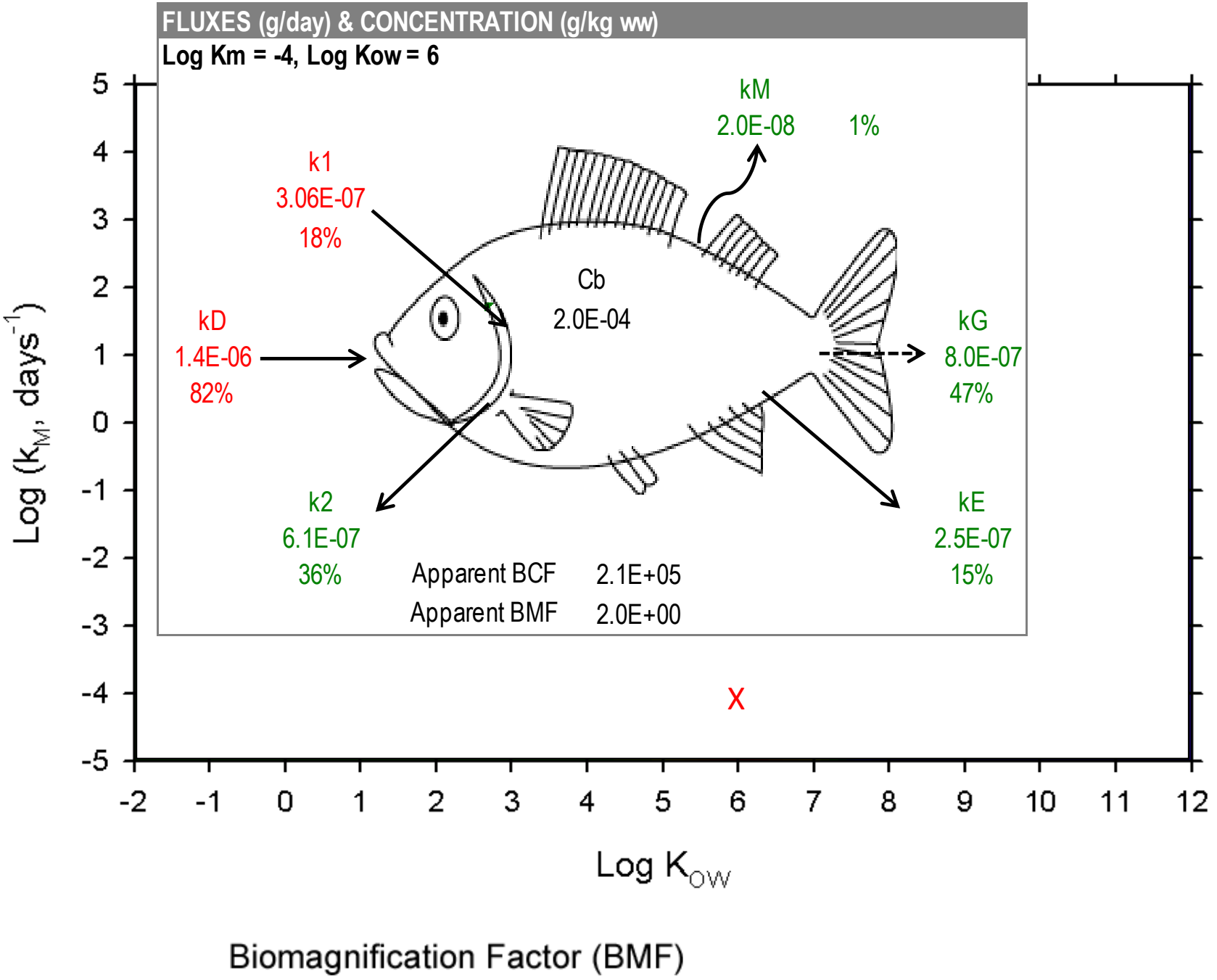
extrapolated TMF > 1

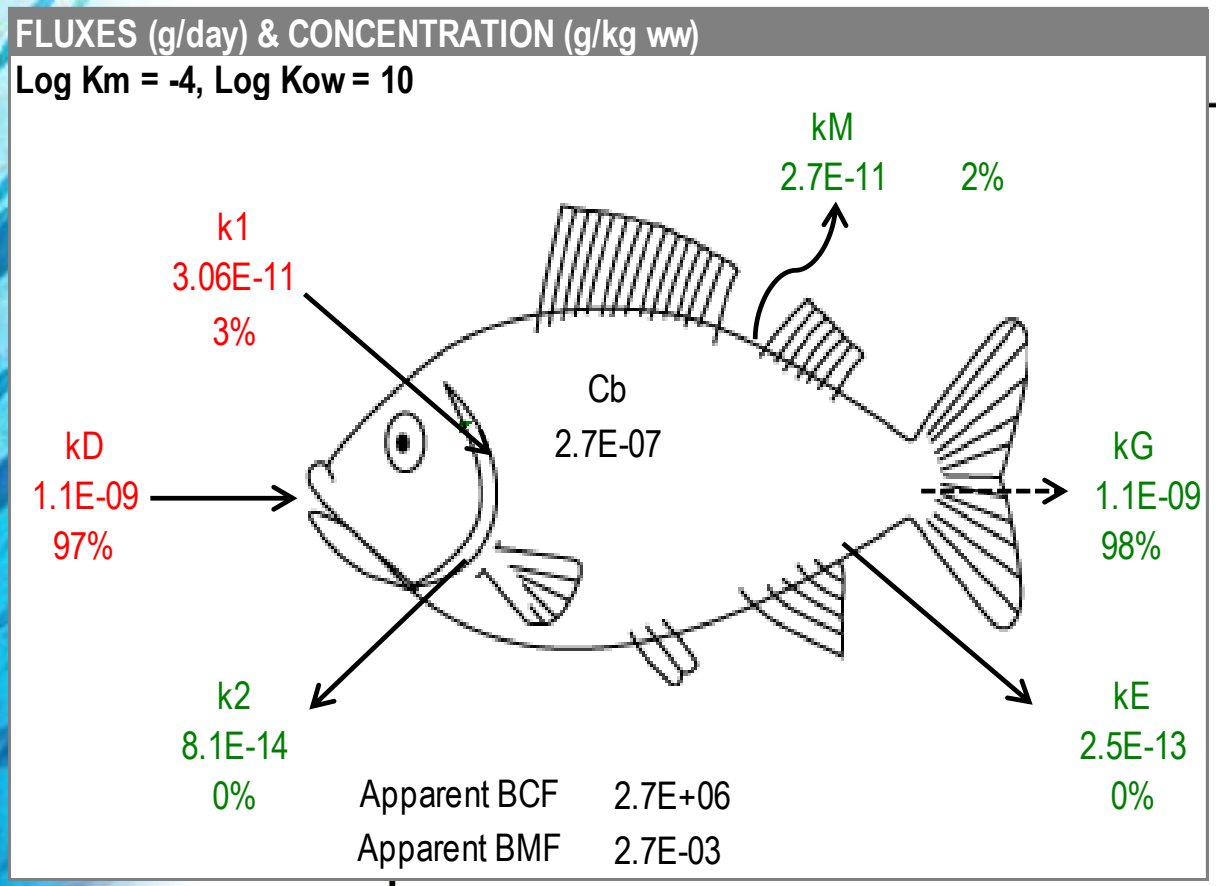
TMF < 1

Acknowledgments

- Philipp Mayer & John Nichols

- CEFIC Long Range Initiative ECO 15 (TMF^2)


FLUXES (g/day) & CONCENTRATION (g/kg ww)
Log Km = -4, Log Kow = 6
kM
2.0E-08
1%
k1
3.06E-07
18%
Cb
2.0E-04
kD
1.4E-06
82%
kG
8.0E-07
47%
k2
6.1E-07
36%
kE
2.5E-07
15%
Apparent BCF 2.1E+05
Apparent BMF 2.0E+00
X
Log (kM, days-1)
Log KOW
Biomagnification Factor (BMF)



Biomagnification Factor (BMF)