LTLS
FRESHWATER
ECOLOGY

Prediction of the impacts of chemical mixtures and how we will use this within LTLS-FE

SL, 20.07.23

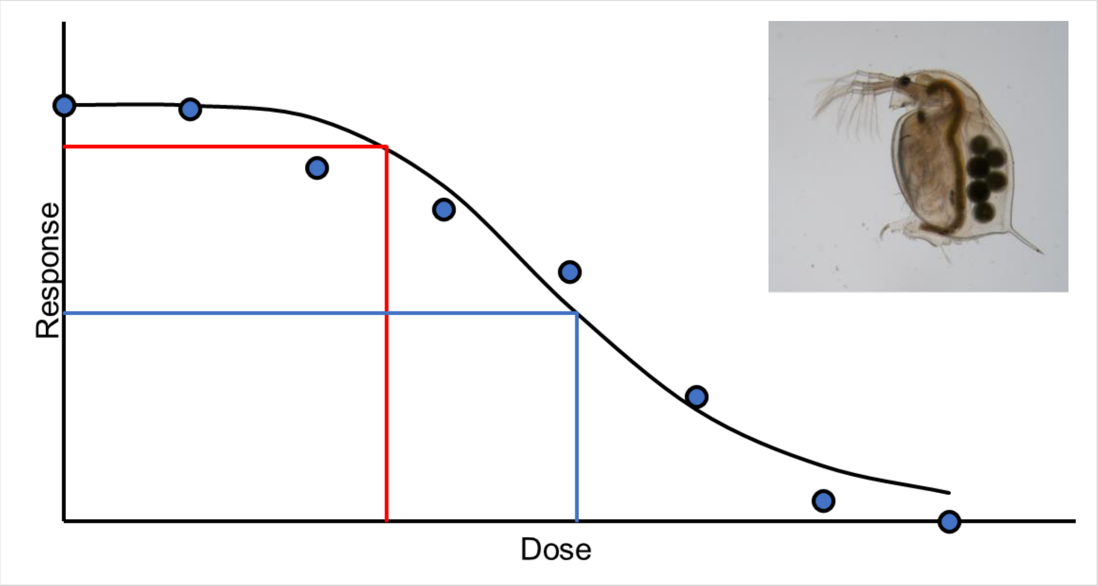
The problem

- Completed LTLS-FE IM will predict concentrations of many chemical variables, each potentially exerting a stress on the ecosystem
- For ecological prediction,
- useful to reduce the number of explanatory variables
  - Reduce the cocktail of chemical concentrations to the smallest possible number of variables
- Can this be done???
  - **YES**
  - There are established methods/models for doing this

- IMPORTANT!
  - This only applies to the toxic chemicals – not the nutrients

Background: chemical risk assessment

- A key goal of chemical RA is to generate 'safe concentrations' of chemicals
  - ➢ Below the 'safe concentration', risk is considered negligible
  - ➢ 'Safe concentrations' are the basis for Environmental Quality Standards
- The risk assessment is based around data on the toxicity of the chemical to single species in controlled laboratory tests



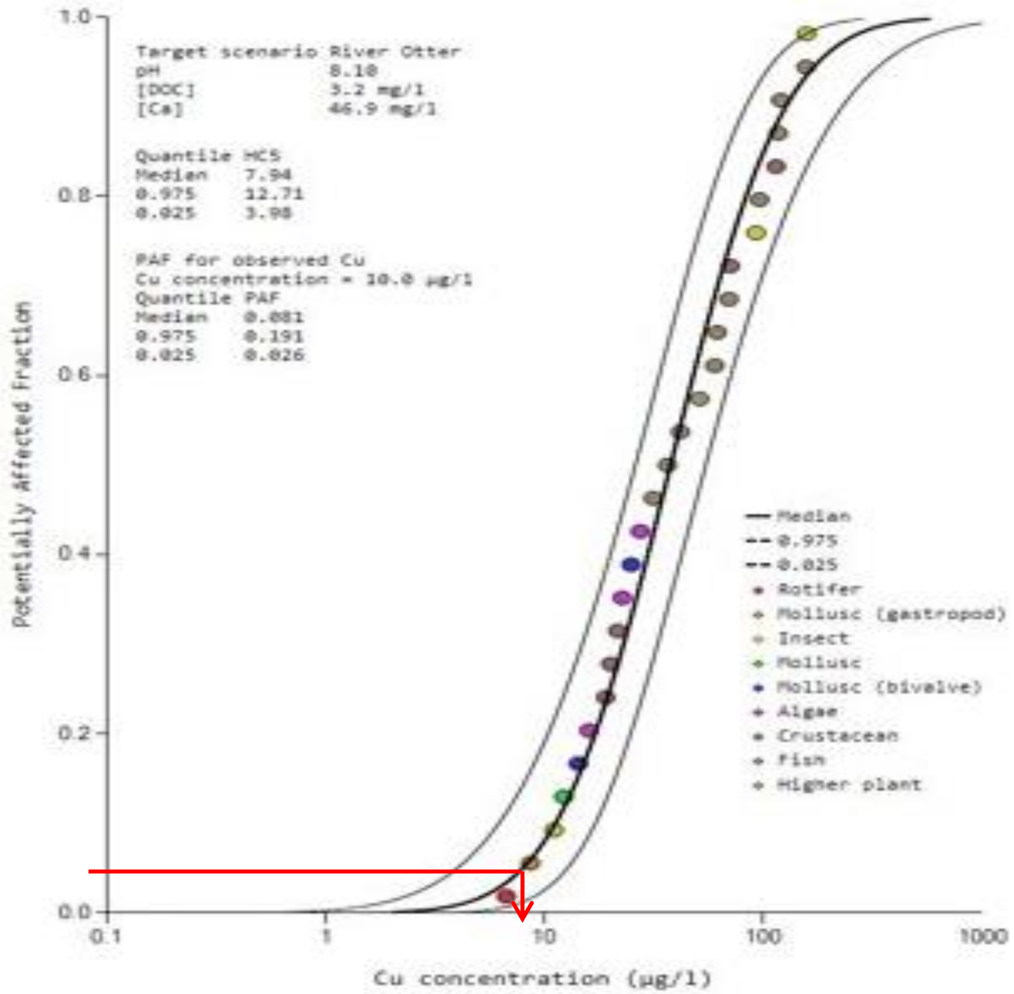
Toxic endpoint concentration

e.g.

10% effect (L(E)C10)
50% effect (L(E)C50)

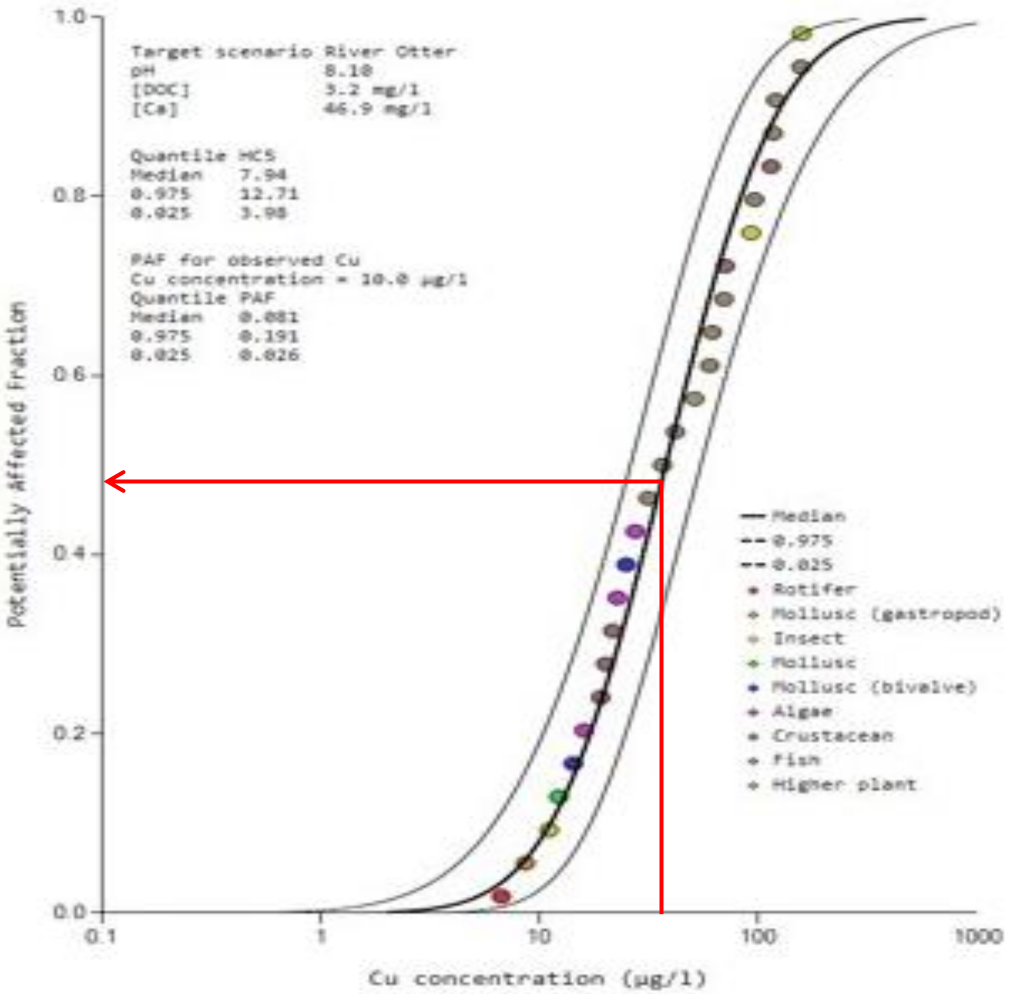
Background: chemical risk assessment (2)

- How to bring the data for single chemical effects on multiple species together?
  - ➢ Species sensitivity distribution (SSD)
  - ➢ Fit statistical distribution (typically lognormal) to the toxic endpoints
- ‘Safe concentration’ typically taken as the concentration impacting 5% of the species (HC5 – hazardous concentration impacting 5% of species)
- So what…?

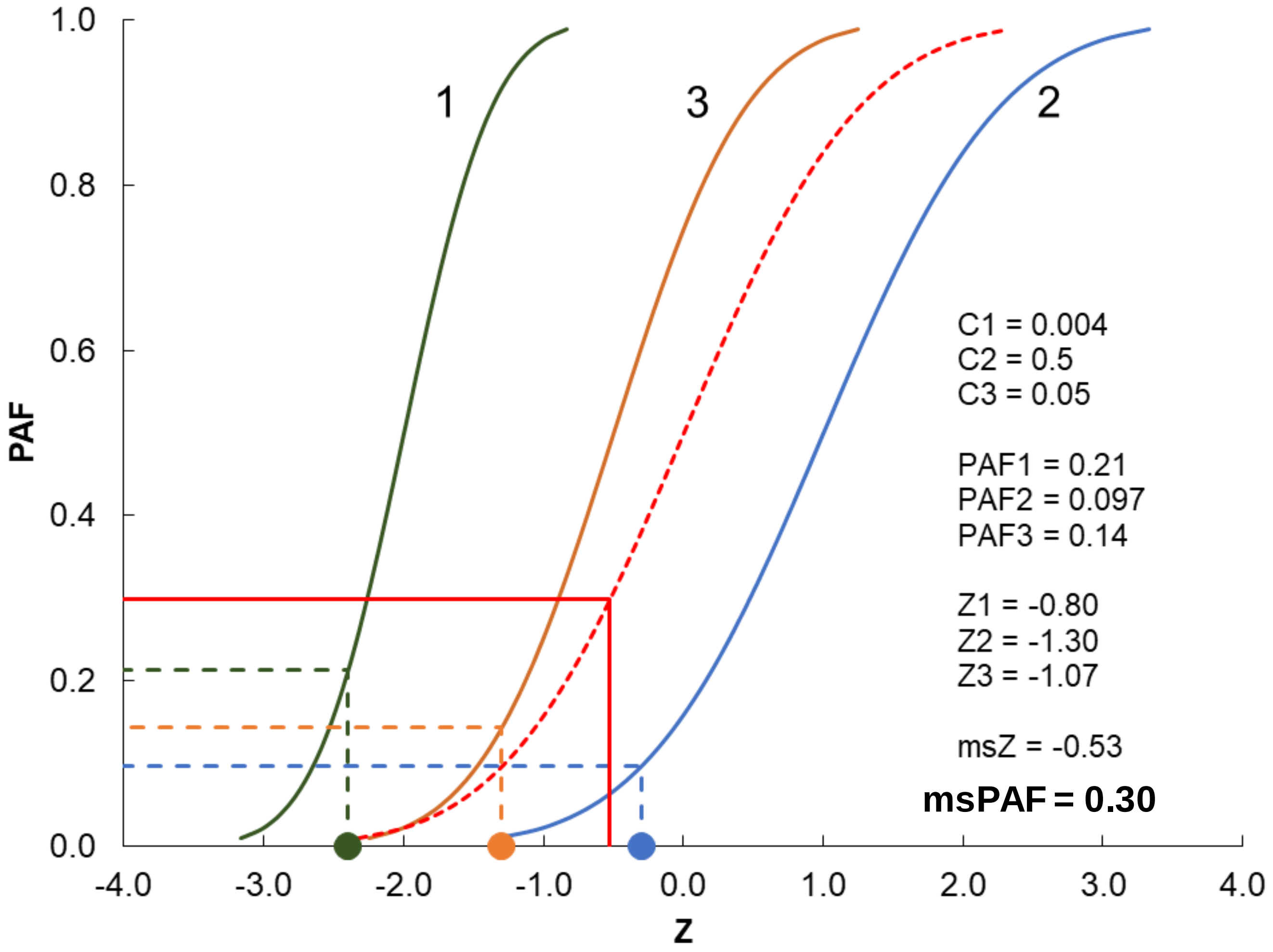


Mixtures

- We want to predict the *combined* impact of multiple chemicals
- There is an approach that allows us to do this, using lognormal SSDs
- Based on the *concentration addition* concept
- “Adds” chemical concentrations, correcting for the differences in their *potency*



Example



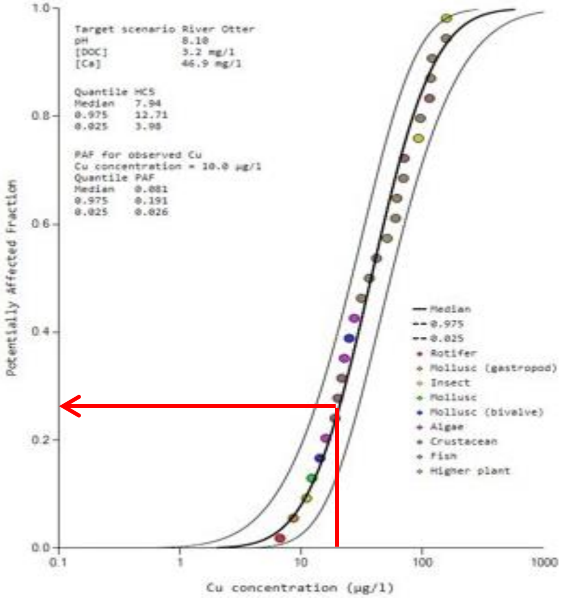
<u>Other information:</u>

- PAFs for the individual chemicals…
    - Hotspots of individual chemical risk
    - Ranking of chemicals by impact

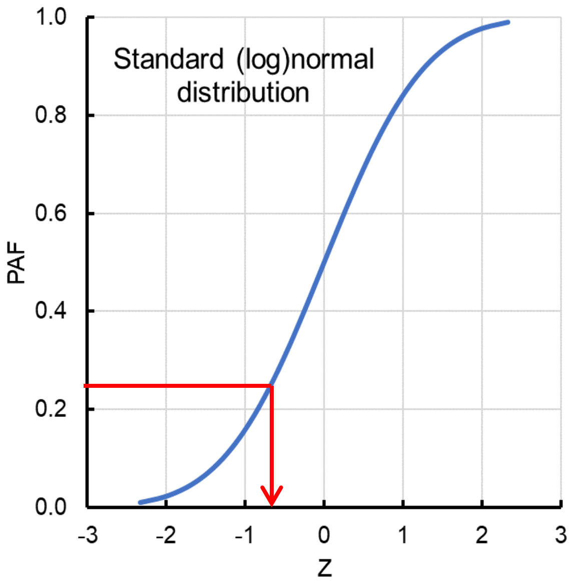
<u>Data source:</u>

- 'Posthuma database'
    - SSD parameters (mean, SD of lognormal distribution)
    - > 10,000 chemicals(!)

Background: chemical risk assessment (2)



Calculate PAFs for all chemicals in the mixture

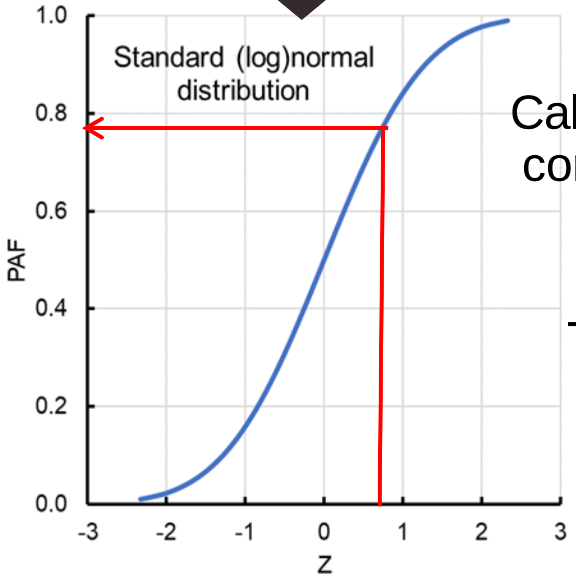


Calculate **Z values** for all chemicals in the mixture

Z is the logged chemical concentration, normalised against hazard

$$\text{msZ} = \log_{10} \sum 10^{Z_i}$$

Sum the Z values



Calculate the PAF corresponding to the msZ

- the **msPAF**

LTLS FRESHWATER ECOLOGY · UK Centre for Ecology & Hydrology · ROTHAMSTED RESEARCH · BGS British Geological Survey · CARDIFF UNIVERSITY PRIFYSGOL CAERDYDD · Bowburn Consultancy

Bioavailability modelling and WHAM-F_{TOX}

Organism effect (single metal) ∝ occupancy of binding sites on organism by metal

Occupancy can be modelled using chemical equilibrium principles

Geochemical speciation model e.g. WHAM7

Binding model for organism

BLM
Binding at a specific 'receptor'

WHAM-F_{TOX}
'Metabolically active' bound metal

Uses **humic acid** as surrogate for organism binding

Fractional occupancy (θ)

Binding of multiple metals

Proton (H^+) included as toxicant

WHAM-F_{TOX}: predicting impacts

For *i* 'taxa':

Toxicity function - single species concentration addition model

θ_H, θ_M →

$$F_{tox,i} = \theta_H + \Sigma\, \alpha_{M,max,mean} \times \beta_i \times \theta_M$$

Laboratory ecotoxicity test data → intrinsic metal potency average across species, infinite time $\alpha_{M,max,mean}$

Fitting to field data → Species-specific sensitivity term lognormally distributed β_i

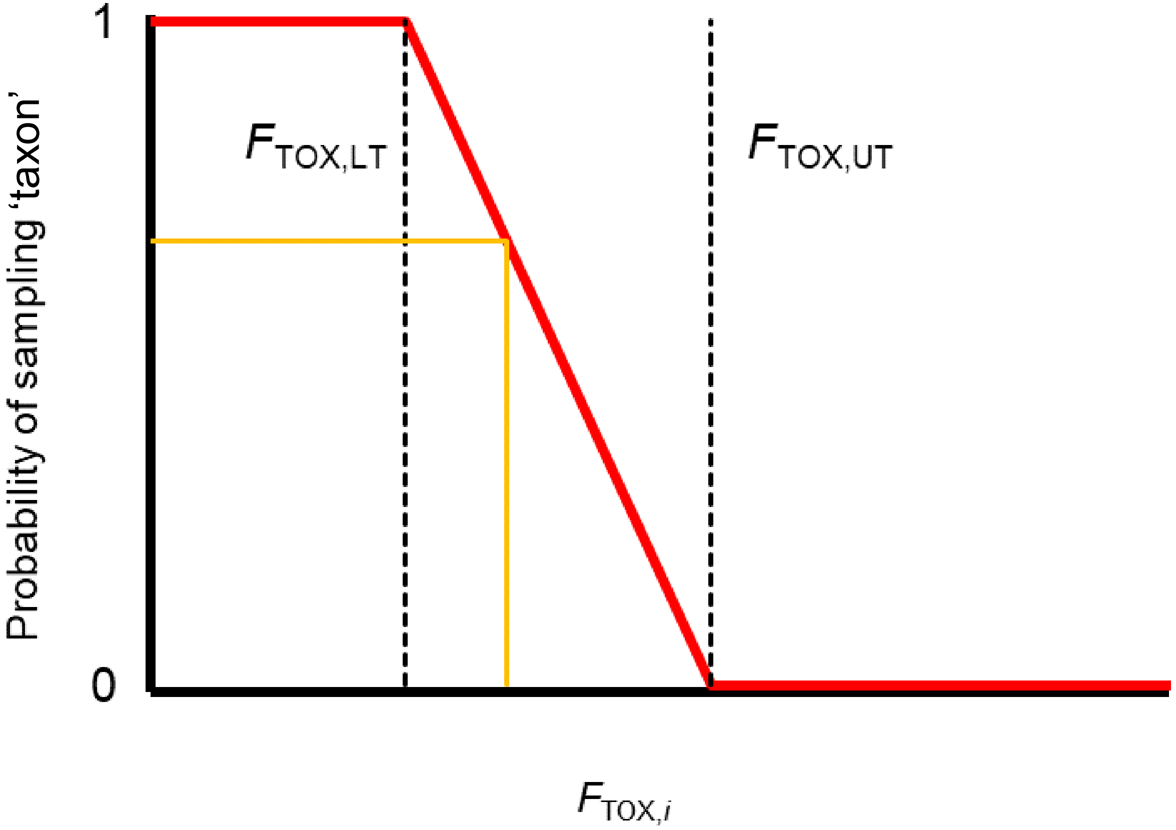
Cation	*n*	$\alpha_{M,max,mean}$	SE
H		(1.0)	
Al	7	2.6	0.0
Ni	79	31.1	3.4
Cu	1543	34.6	0.7
Zn	118	17.0	1.3
Cd	152	673	35
Hg	5	621	347
Pb	33	126	24

The value for H is set to 1.0;
n = number of data;
SE = standard error.

Tipping et al., Aquat. Toxicol 231, 105708 (2021). https://doi.org/10.1016/j.aquatox.2020.105708

Tipping et al., Aquat. Toxicol 212, 128-137 (2019). https://doi.org/10.1016/j.aquatox.2019.04.022

Relating toxicity to 'taxon' response



Fixed relationship between $F_{TOX,i}$ and effect (the probability of finding the 'taxon', Pr_i)

if $F_{TOX,i} < F_{TOX,LT}$ → $Pr_i = 1$ ('taxon' present)

if $F_{TOX,i} > F_{TOX,UT}$ → $Pr_i = 0$ ('taxon' absent)

if $F_{TOX,LT} < F_{TOX,i} < F_{TOX,UT}$ → $Pr_i = 0 - 1$

Predicted number of 'taxon', $n_{sp} = \Sigma Pr_i$

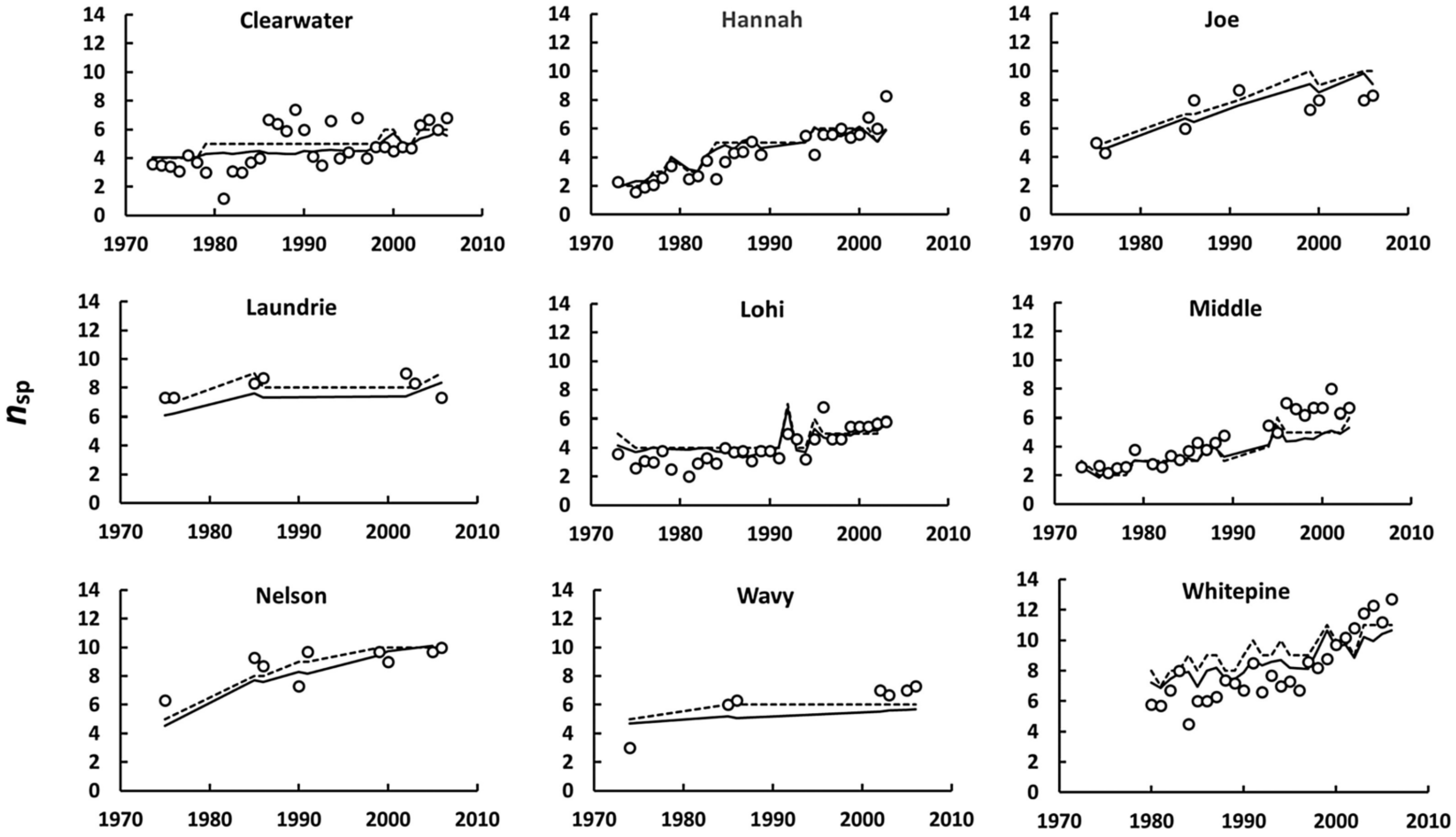
$F_{TOX,LT}$, $F_{TOX,UT}$ fixed, independent of 'taxon', obtained from laboratory data

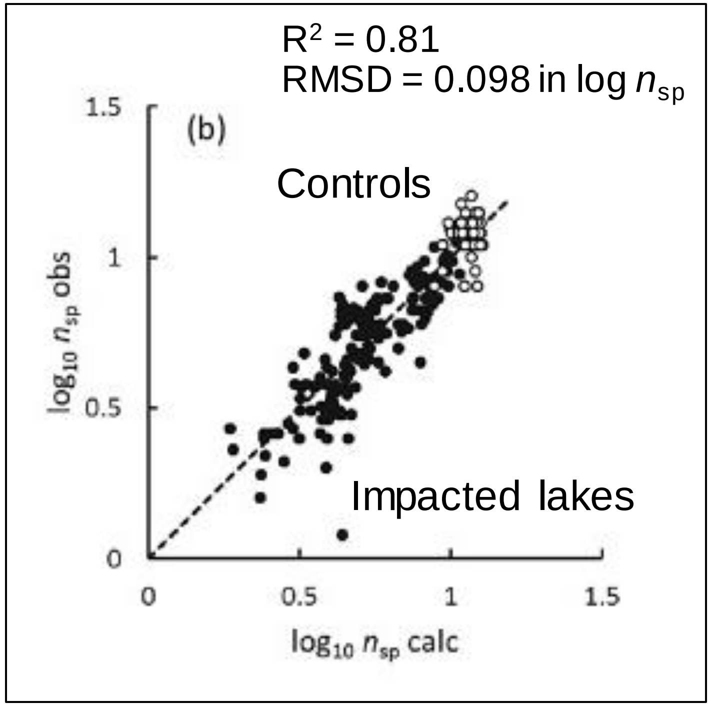
The ‘taxon’

- Theoretical rather than real
  - ➢ More like a ‘niche’ in which a taxon may be present
- If the number of ‘taxa’ used is large then the proportional response (number of taxa present is independent of the number of ‘taxa’
  - ➢ Use a large number of taxa to obtain a proportional response (0-1) – corresponds to msPAF

Results

Tipping et al., Aquat. Toxicol 231, 105708 (2021).
https://doi.org/10.1016/j.aquatox.2020.105708





n_{sp} = 13

from observations on 'control' lakes

LTLS FRESHWATER ECOLOGY

UK Centre for Ecology & Hydrology

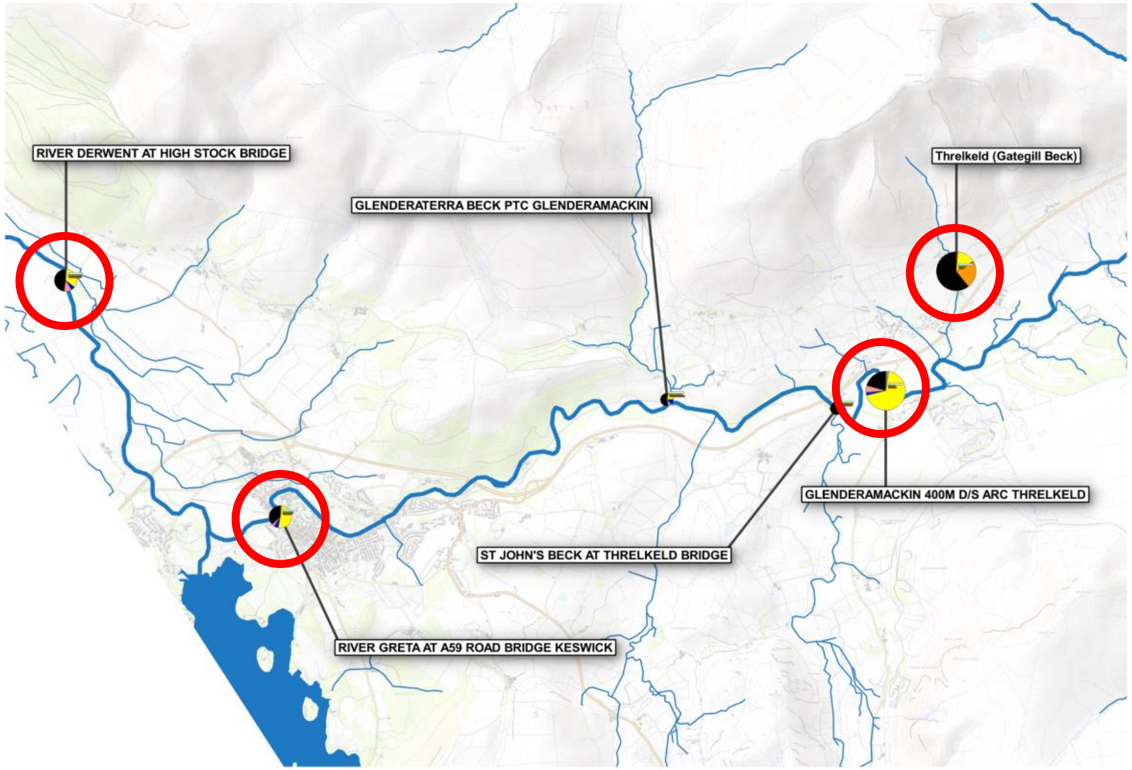
ROTHAMSTED RESEARCH

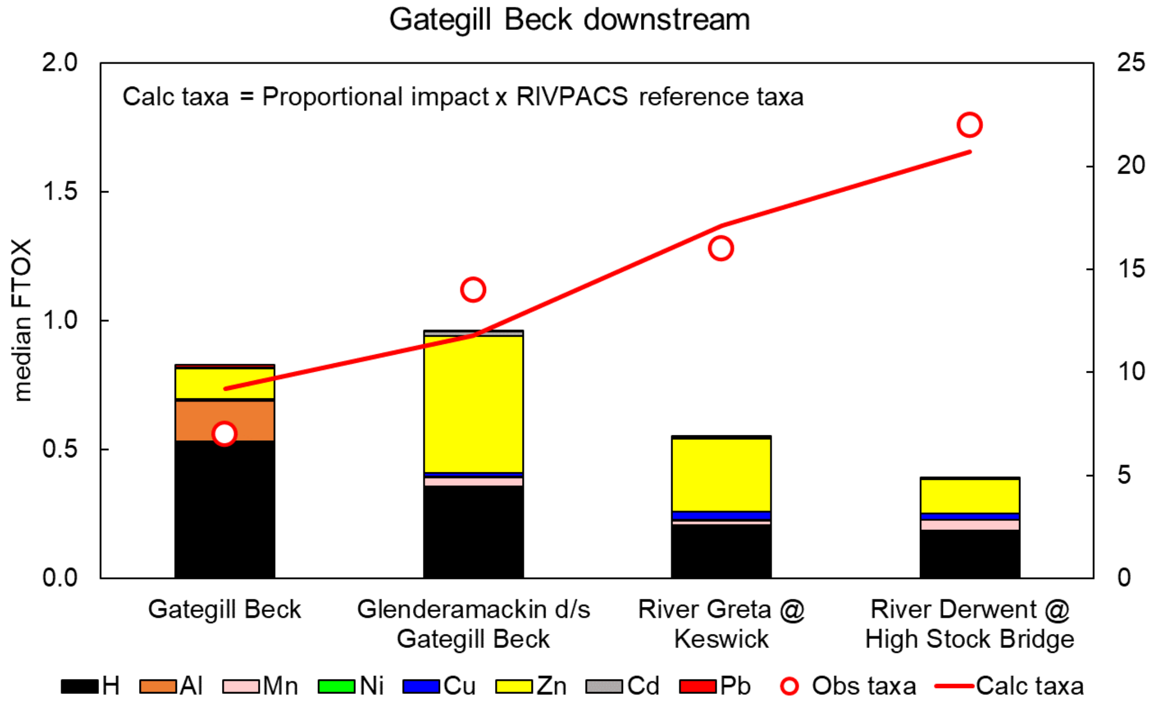
BGS British Geological Survey

CARDIFF UNIVERSITY PRIFYSGOL CAERDYDD

Bowburn Consultancy

Results


RIVER DERWENT AT HIGH STOCK BRIDGE
GLENDERATERRA BECK PTC GLENDERAMACKIN
Threlkeld (Gategill Beck)
GLENDERAMACKIN 400M D/S ARC THRELKELD
ST JOHN'S BECK AT THRELKELD BRIDGE
RIVER GRETA AT A59 ROAD BRIDGE KESWICK


Gategill Beck downstream
Calc taxa = Proportional impact x RIVPACS reference taxa
median FTOX
2.0
1.5
1.0
0.5
0.0
25
20
15
10
5
0
Gategill Beck
Glenderamackin d/s Gategill Beck
River Greta @ Keswick
River Derwent @ High Stock Bridge
H
Al
Mn
Ni
Cu
Zn
Cd
Pb
Obs taxa
Calc taxa

Summary

- We can derive separate ‘stress metrics’
  - ➢ Organic micropollutants
  - ➢ Metals & acidity
- Internally consistent measures of combined stress
- At the moment I am *not* considering combining these further…
  - ➢ Different derivation methods