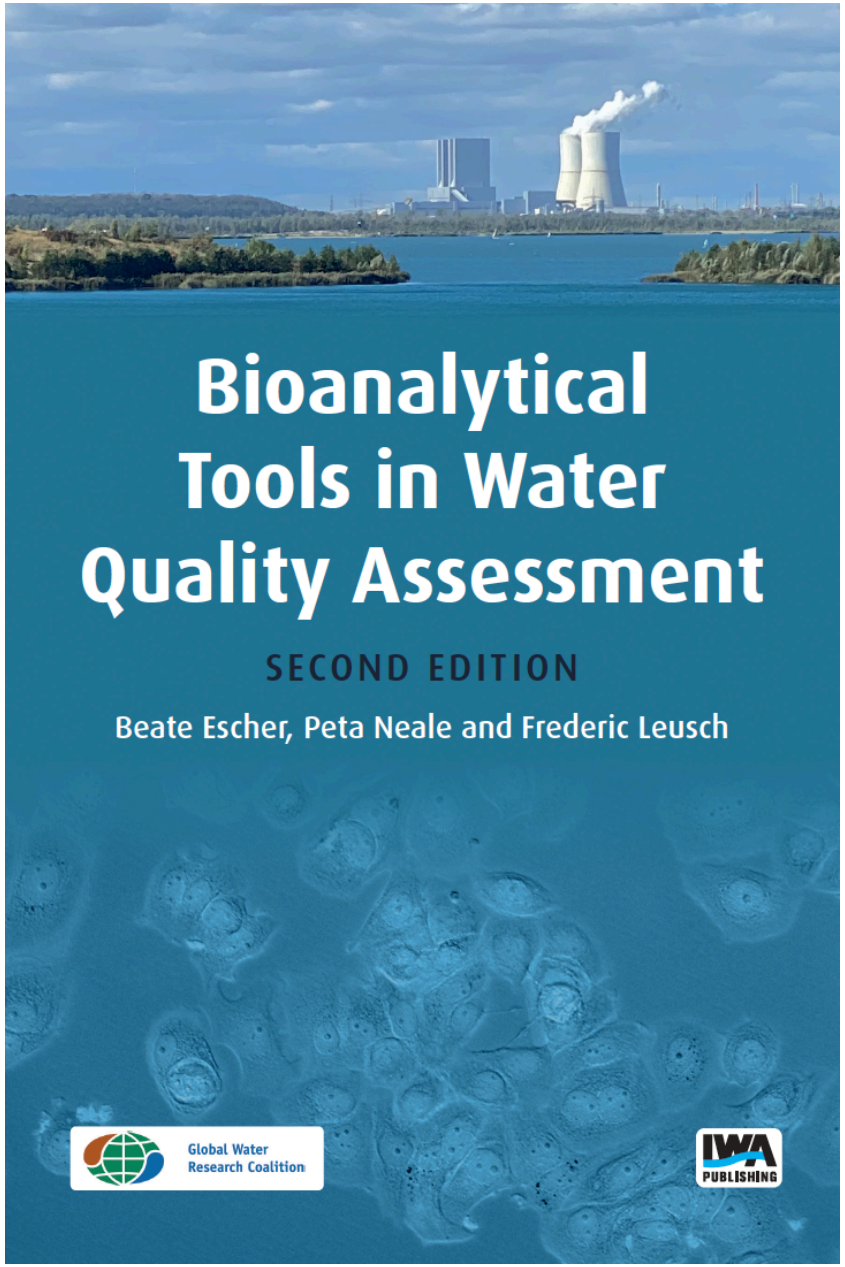
Chapter 1
Introduction to bioanalytical tools in water quality assessment

This presentation accompanies Chapter 1 of
“Bioanalytical Tools in Water Quality Assessment”
This unit gives an introduction to the topic and an overview about all book chapters

Exercises and more material can be found at
www.ufz.de/bioanalytical-tools

Questions? please send an e-mail to bioanalytical-tools@ufz.de



Learning goals

- You are familiar with the essentials of bioassays as they are applied for water quality assessment
- You can appreciate how chemical analysis and bioassays complement each other to characterise mixtures of chemicals in the environment

The chemicals' challenge

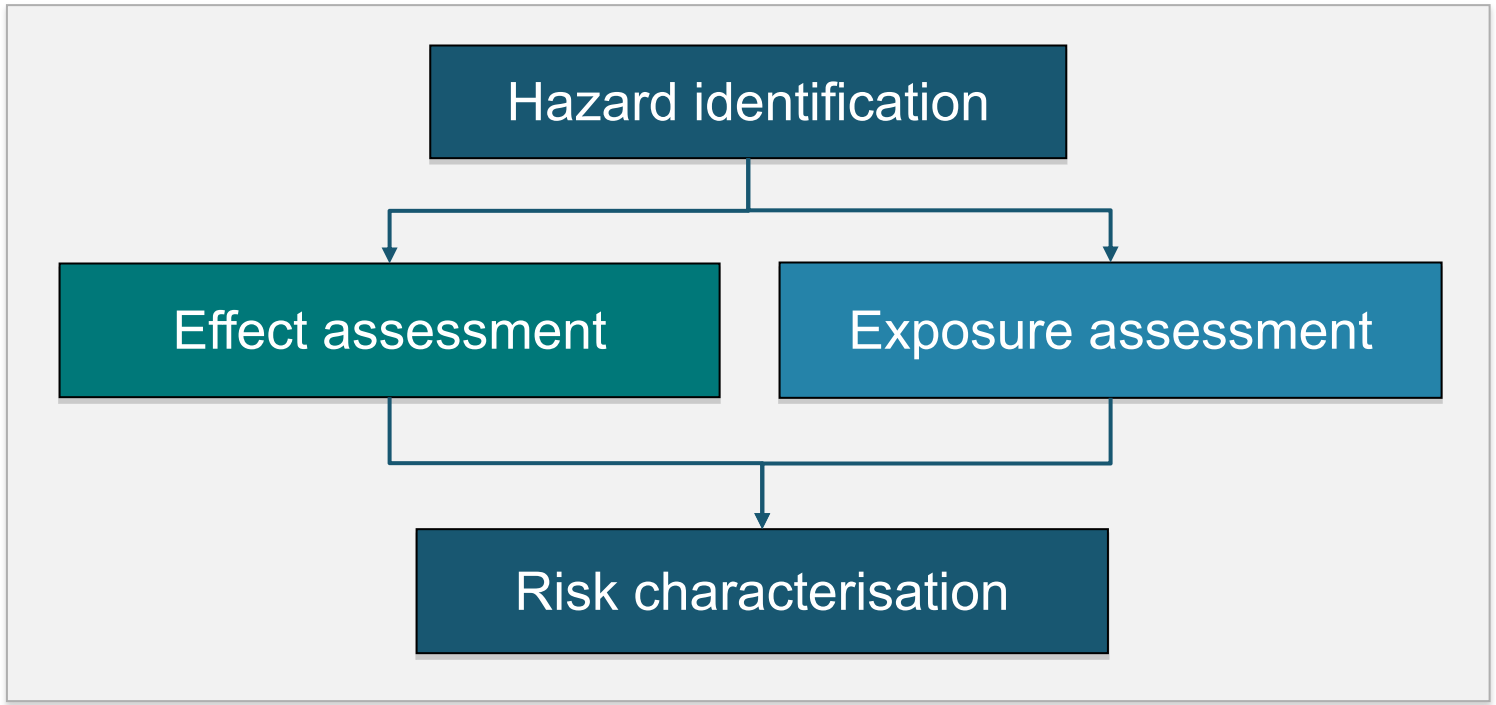
- Many chemicals! >180 Mio CAS #
  - >340,000 in commercial use (Wang 2020)
  - > 100,000 registered under REACH –191 SVHC (substances of very high concern)
  - 25000 to 84000 in commerce in the US

- Low concentrations
- Transformation products
- Mixtures

Chapter 2

Chapter 3

Challenge for risk assessment and monitoring



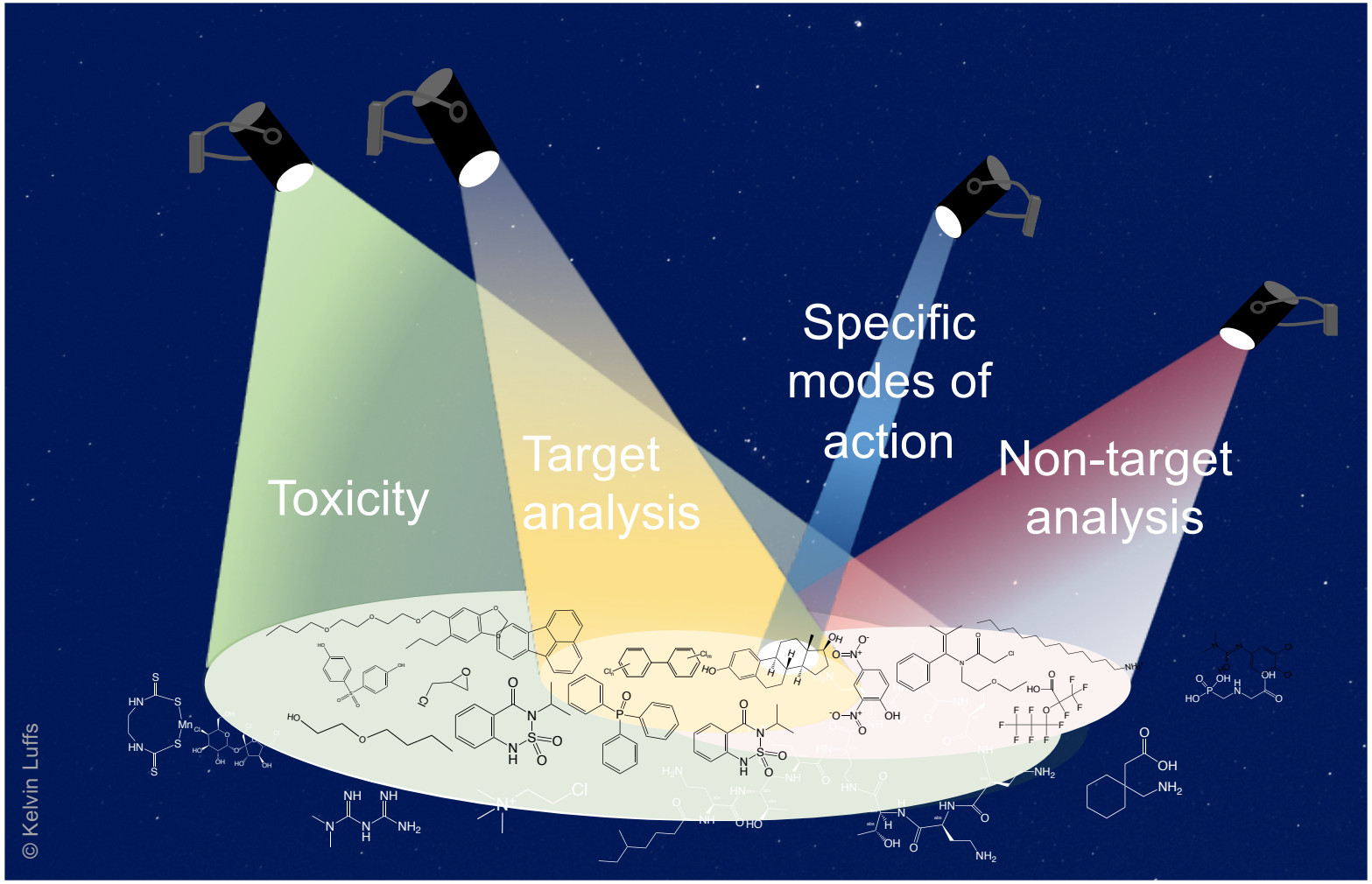
The chemicals' challenge

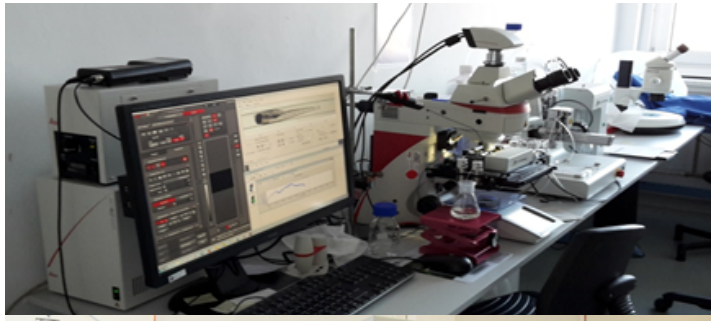
- Chemicals detected in the environment, biota and humans
- Chemicals with known effects
- Mixture effects

- Chemicals below detection limits
- Unknown chemicals
- Chemicals without analytical methods
- Transformation products
- Mixture effects

Bioanalytical tools can capture
and characterise the entire iceberg

Combining chemical analysis and bioassays

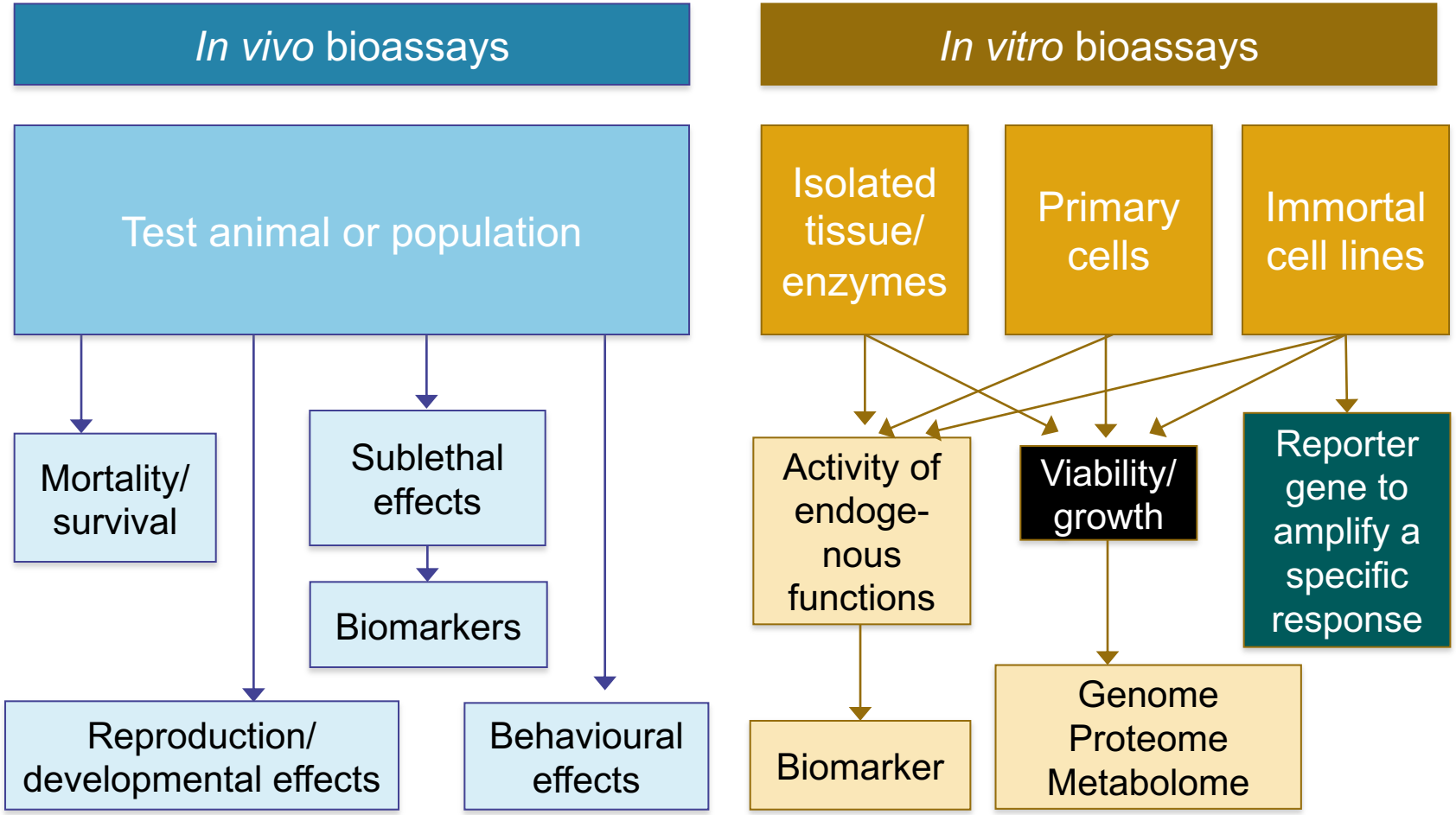




Bioassays

In vivo: Chapter 3

In vitro: Chapter 9

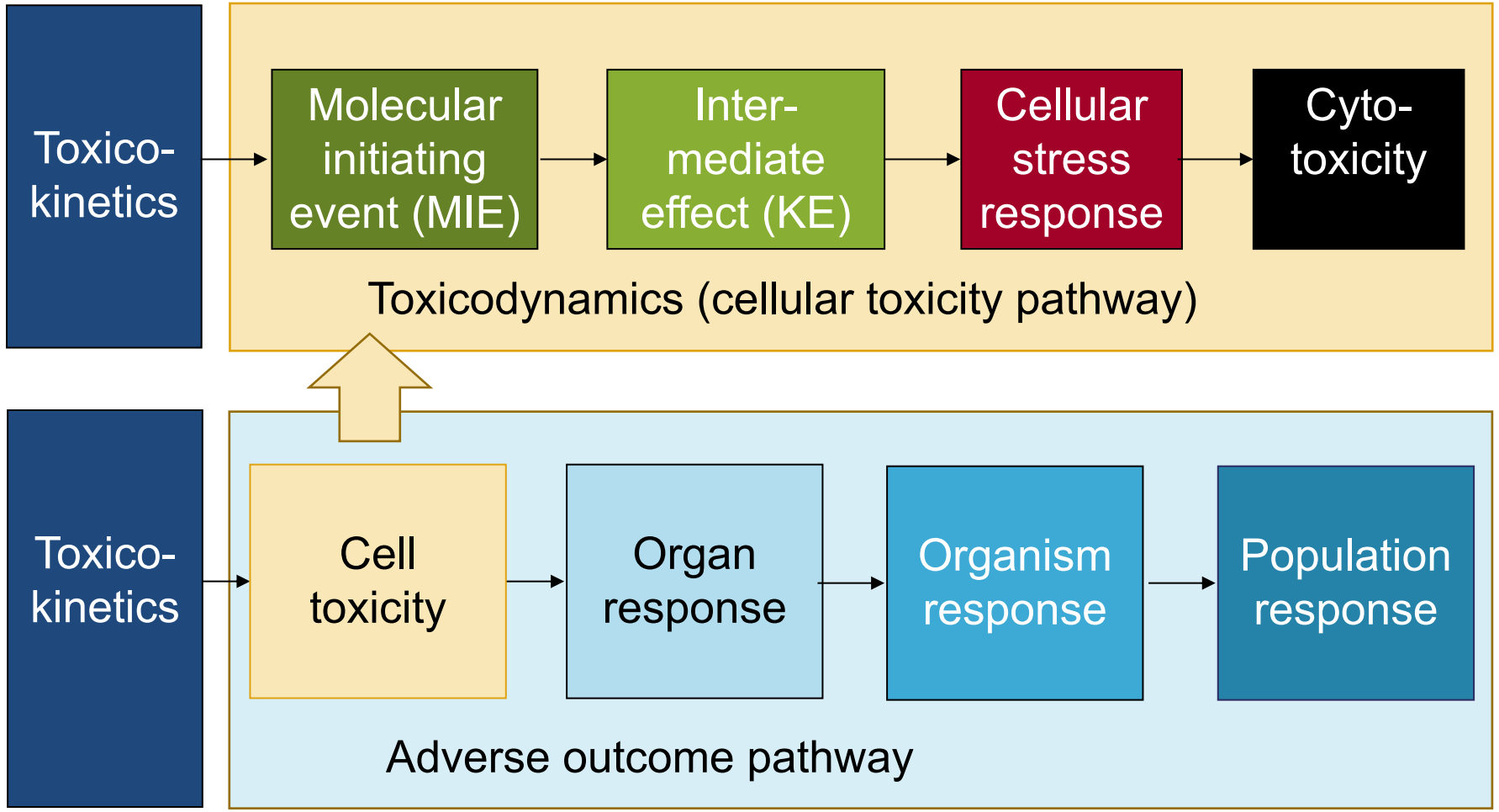


AOPs
Chapter 4

Human Health
Chapter 5

Environmental
Chapter 6

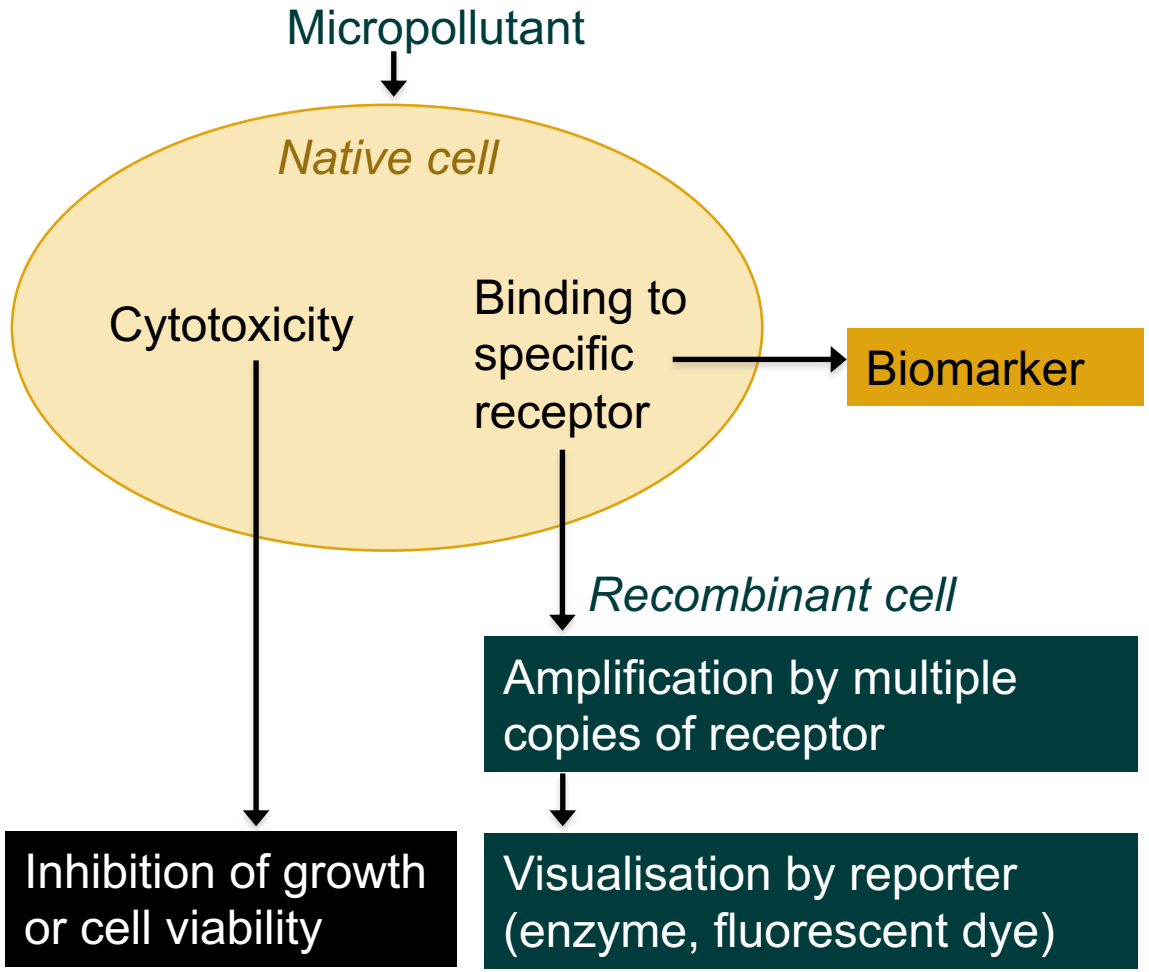
Mechanistic basis for choosing bioassays



Cellular assays

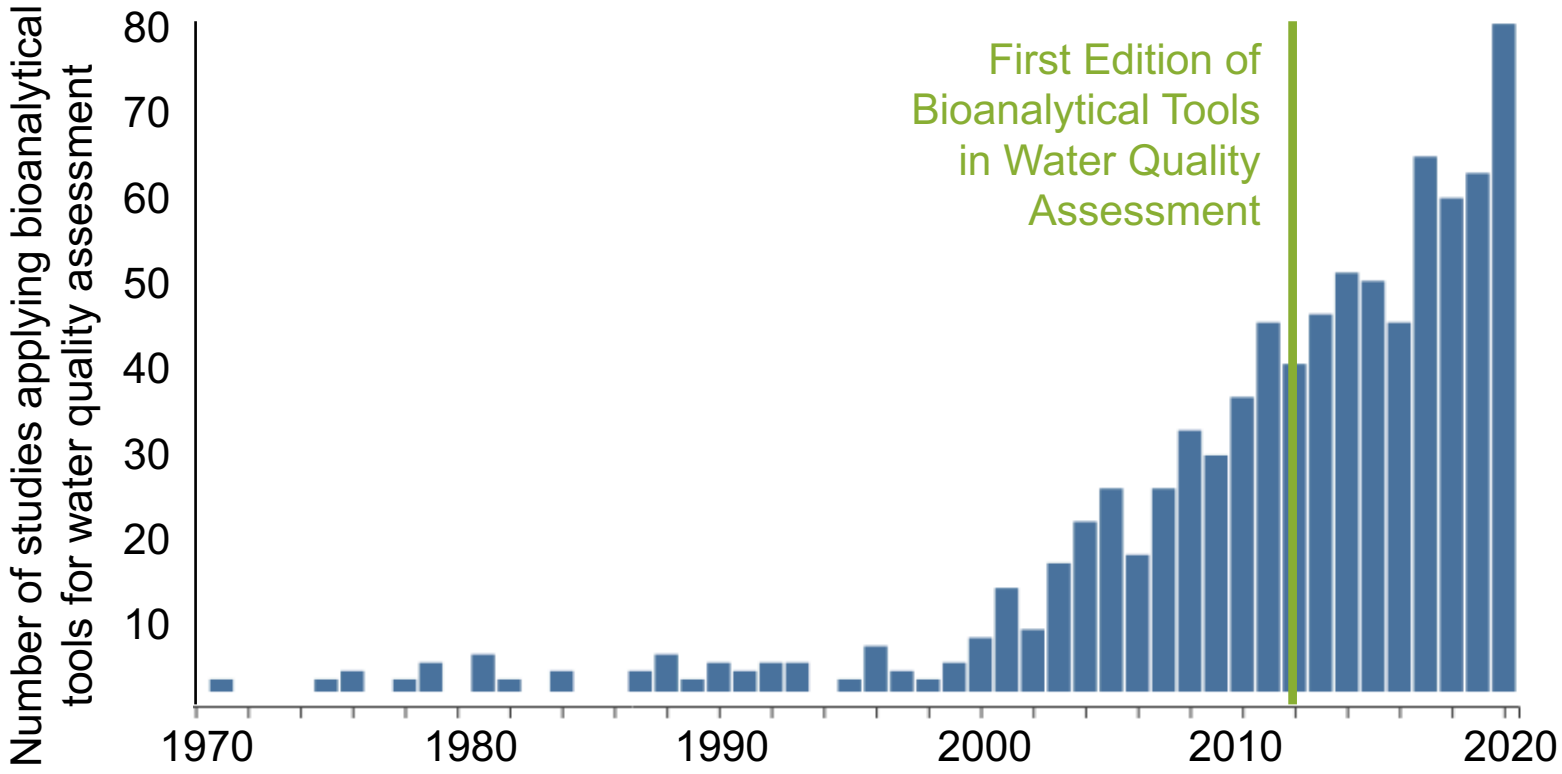
Cell-based bioassays target particular endpoints or mechanisms of toxicity and can be divided into two groups:

- Bioassays with native cells (primary cells and immortal cell lines)
- Bioassays with recombinant cell lines (reporter gene cell lines)



The use of bioanalytical tools for water quality monitoring is growing

Search in Web of Science with the keywords “(*in-vitro* or *vitro* or bioanalytical) and battery and bioassay* and water and quality” on 18 November 2020



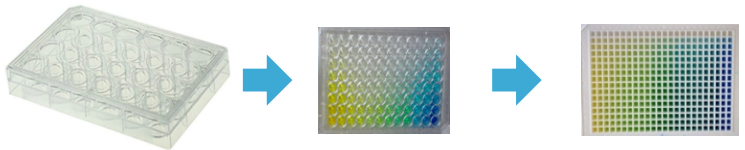
Selection of test batteries of bioassays

Test batteries can be purpose-built for specific applications (modular set up)

- Profiling of single chemicals for chemical risk assessment (ToxCast, Tox21)
- Assessment of treatment efficacy of natural and engineered treatment systems
- Surveillance and compliance monitoring of water quality (effect-based trigger values (EBT))
- Benchmarking chemicals in diverse environmental samples (sediment, biota)

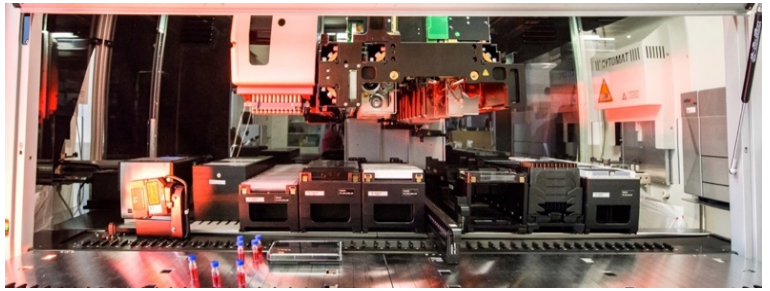
High throughput screening (HTS)

- Pipetting robots: large numbers of bioassays
- Well-plates: low volume requirement
  - Bacteria (30 min, 40-200 µL, 96/384)
  - Cell-based bioassays (24h, 40-100 µL, 96/384)
  - Algae (24-74h, 300 µL, 24/96)
  - Daphnia (48h, 1 mL, 12/24)
  - Fish Embryo Toxicity (FET) (24-120h, 2 mL, 12/24/96)

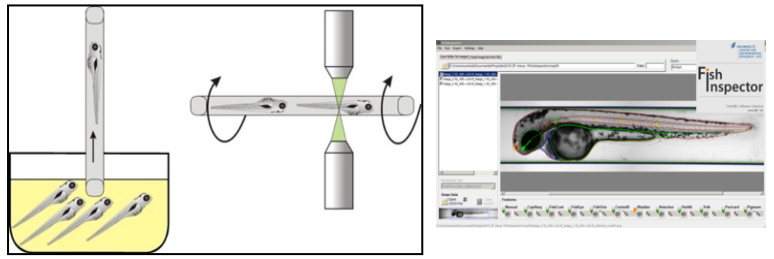


12/24 well plates 96 well plates 384 well-plates

HTS robotic system for cellular assays



HTS system for fish embryo toxicity test (VAST imager)



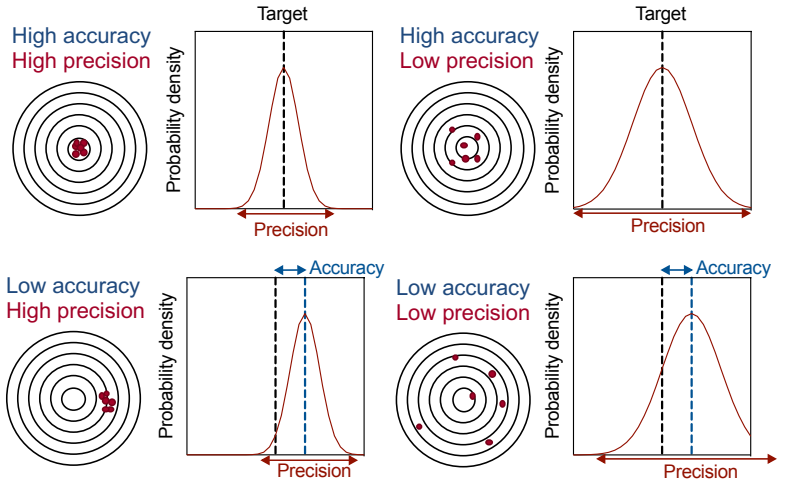
Making sense out of the experiments ……and good housekeeping

Dose-response
Chapter 7

Exposure
Chapter 9

QC/QA
Chapter 11

- Concentration-response modelling
- Derivation of benchmark concentrations
- Toxic units and bioanalytical equivalent concentrations
- Exposure in cellular assays
- Quality assurance and quality control (QA/QC)
  - Accuracy, precision, robustness, sensitivity
  - Bioassay quality, matrix interferences
  - Practicalities in the laboratory

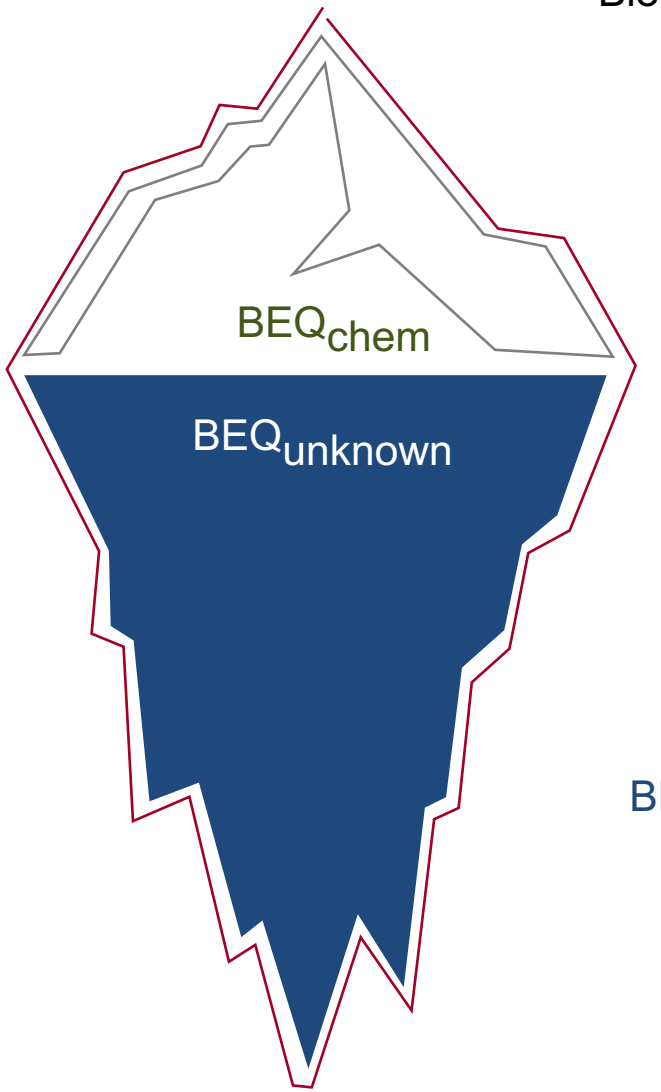


Linking chemical analysis and bioassays through “iceberg modelling”

Mixtures: Chapter 8

Iceberg modelling: Chapter 13

Biological Equivalent Concentrations (BEQ)



$$BEQ_{chem} = \sum_{i=1}^{n} REP_i \cdot C_i$$

Chemical analysis

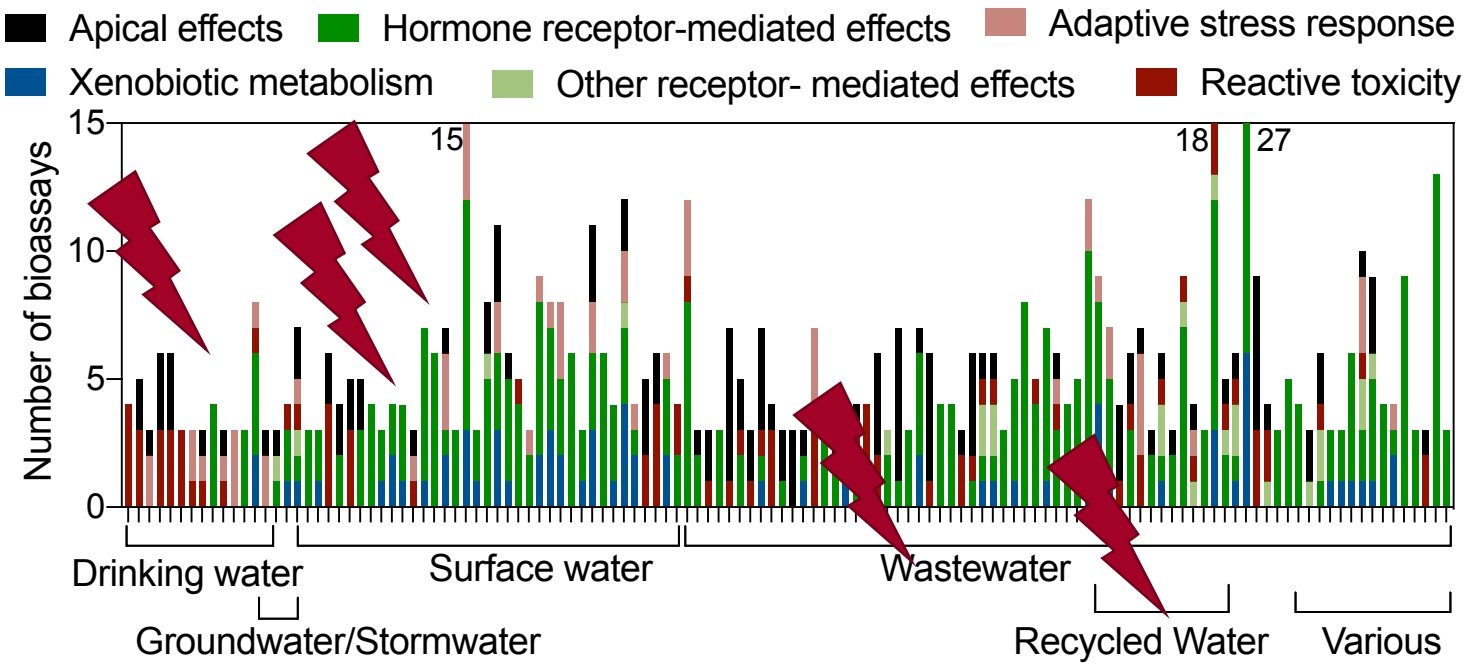
$$BEQ_{bio} = \frac{EC_y\ (ref)}{EC_y\ (sample)}$$

Bioassay data

$$BEQ_{unknown} = BEQ_{bio} - BEQ_{chem}$$

Practical applications

- Overview of studies published that have applied test batteries of *in vitro* and *in vivo* assays



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You can work through the chapters individually – they are self-contained

Some useful combinations

- For the novice: 1-3-10-13-14
- For the regulator: 1-2-3-9-10-13-16
- For the practitioner: 1-10-11-7
- If you plan a field study: 12-10-13-14
- For the mixture modeller: 1-7-8-13
- If you know it all and want to know what's on the horizon: 15-16

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