Integrated Approaches to Improve Water Quality in Surface and Drinking Water

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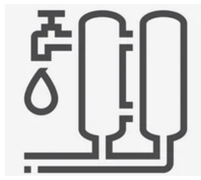
Problem, Aim & Approach

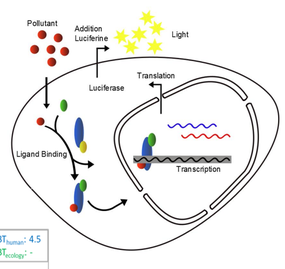
- **Problem**: Single-compound chemical monitoring misses emerging/unknown contaminants and mixture effects in drinking water sources. This limits water authorities in assessing risks and designing effective measures.
- **Aim:** Integrate analytical approaches to support actionable and inclusive water quality management.
- **Approach:** Integrated use of **in vitro bioassays**, **high-resolution MS (HRMS) targeted screening**, **multivariate statistics** and **effect-directed analysis (EDA).**
- **Samples:** wastewater treatment plant (WWTP) effluent, surface water (SW), process water (PW) and drinking water (DW) of 4 DW companies in the Rhine and Meuse catchments in the Netherlands[a].

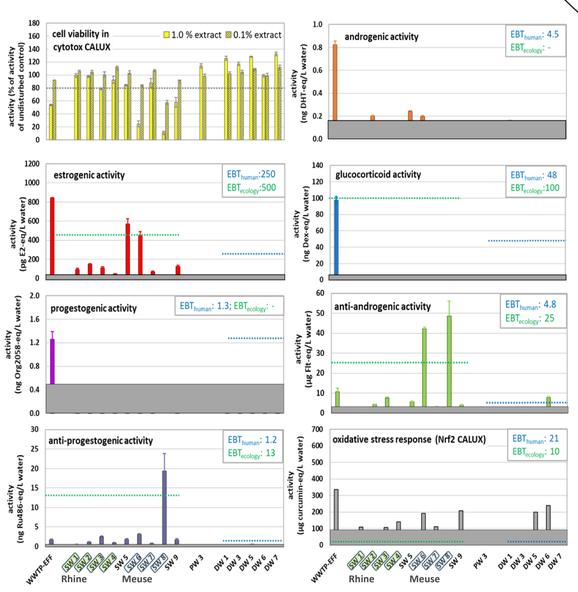
Workflow & Key Findings

Samples: 1x  9x  1x  5x 

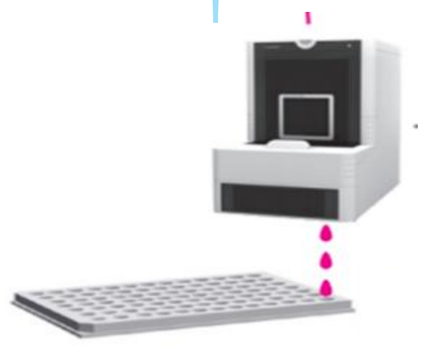
Analyses:

CALUX® bioassays
10 endpoints



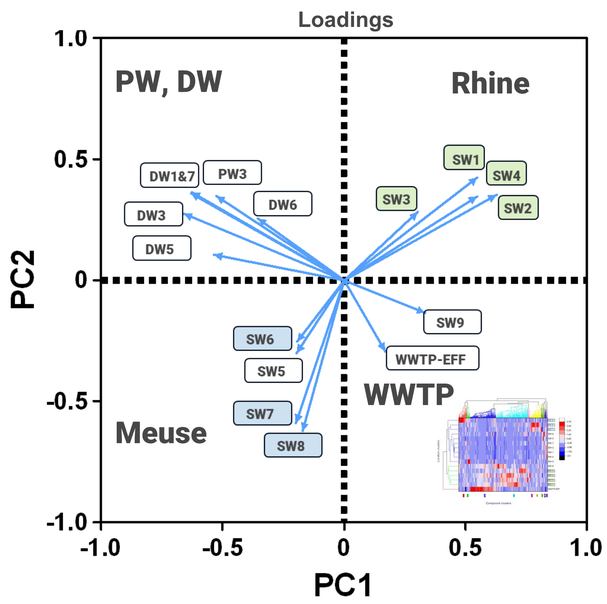


- Eight bioactivity types detected in SWs[b]
- Most bioactivities removed during DW treatment
- EDA if:
  - EBT exceeded
  - limited removal
  - unknown drivers



HRMS-targeted screening
>2000 compounds

Multivariate statistics
PCA & HCA



EDA: fractionation & activity confirmation

AR: Dihydrotestosterone, 17α-methyl-testosterone, Androstenedione

ER: Estriol, 17α-estradiol, 17β-estradiol, Estrone, 17α-ethynylestradiol

Anti-AR: Diuron, Cyproconazole*, Dimethenamid *, Fenoxycarb, Fluopicolide, Myclobutanil *, Boscalid, Fipronil *, Metolachlor*, Omeprazole

Anti-PR: Diuron, Cyproconazole*, Dimethenamid*, Fenoxycarb*, Fluopicolide, Myclobutanil*, Boscalid, Fipronil*, Metolachlor*

GR: Dexamethasone, Budesonide, Rimexolone, Prednicarbate, Amcinonide

PR: 19-norethindrone, Cyproterone-acetate, Medroxy-progesterone, Progesterone

Oxidative stess response: Omeprazole, Glipizide

Cytotoxicity: All anti-AR & anti-PR-compounds with *

➢ causative compounds feed risk assessment[c]

Data integration for decision support: e.g.:
- emission reduction
- upgrade of water treatments

➢ Catchment specific pollution profiles[b]:
- Rhine: pharmaceuticals dominant
- Meuse: pesticides, steroids
- WWTP: pharmaceuticals, stimulants

From Complex Chemical Pollution to Management-Relevant Insights:

Method	Component	Key insight for management
• Bioassay panel	• Biological effects	• Identifies mixture toxicity & health relevant activity
• HRMS-screening	• Chemical presence	• Reveals thousands of contaminants and catchment-specific profiles
• Multivariate statistics	• Pattern identification	• Clusters locations & prioritizes compound groups
• EDA	• Causality	• Pinpoints compounds driving observed bioassay effects
• Data integration	• Decision support	• Enables actionable risk-based water quality management

a: This study was performed within the framework of the Joint Research Program of four Dutch dune water companies: Dunea, PWN, Waternet, and Evides (DPWE)
b: Houtman et al., Env. Int. (2025): https://doi.org/10.1016/j.envint.2025.109740
c: Houtman et al., Env. Int. (2025): https://doi.org/10.1016/j.envint.2025.109782

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