

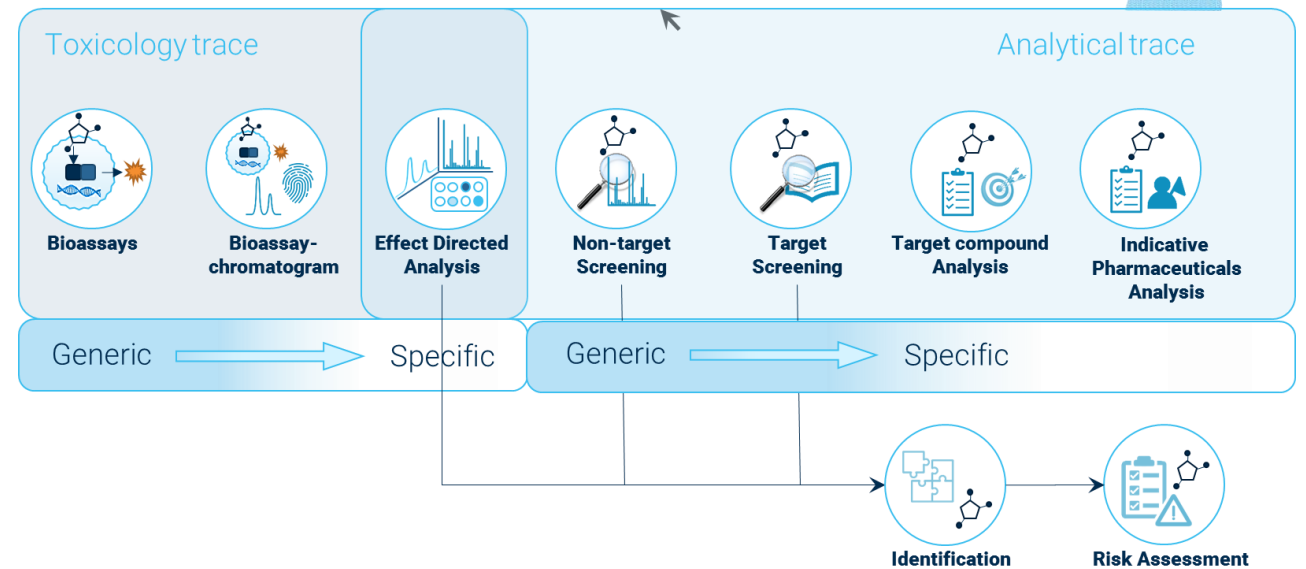
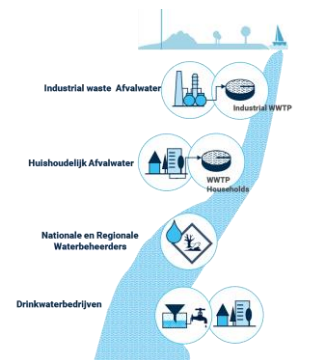
# Bioactive compounds in water



Corine Houtman  
Bio Detectors 2022, September 13 Prague

# The Water Laboratory:

- Central laboratory for 3 Dutch Drinking Water companies
  - Use surface water from rivers Rhine, Meuse and Lake Yssel to prepare drinking water
- Monitoring and Research on presence and toxicology of chemical contaminants in the water cycle
- Using:
  - Bioassays
  - Chemical target analysis
  - Screening
  - Combination: Effect Directed Analysis



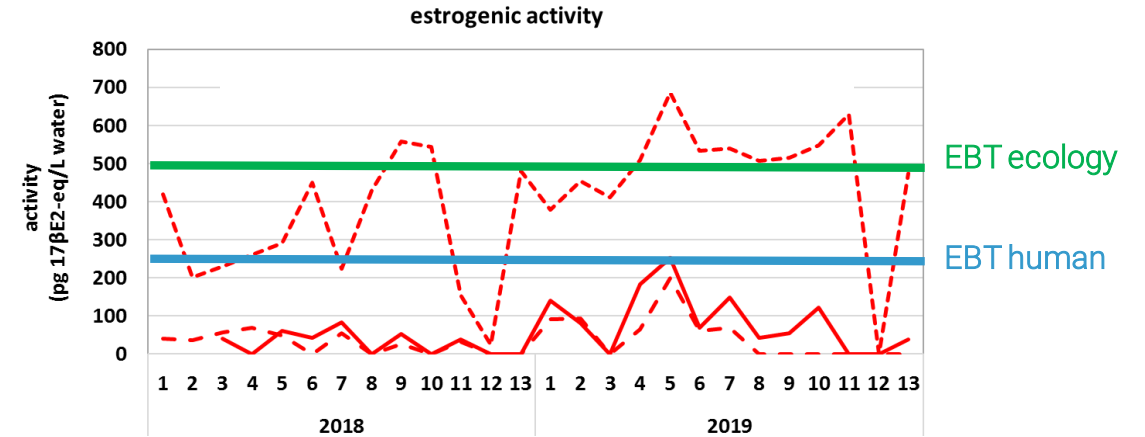
# The Water Laboratory:

## Bioassay Policy:

- EU DW Legislation: Risk Based Monitoring
- => prioritization of compounds using bioassays & screening

## Bioassays in routine monitoring:

- Surface waters (13x/y)
- Drinking water (4x/y)
  - compare concentrations with Effect based Trigger Values
  - 2 consecutive exceedances & unknown cause? => start [Effect Directed Analysis](#) => characterize / identify active compounds



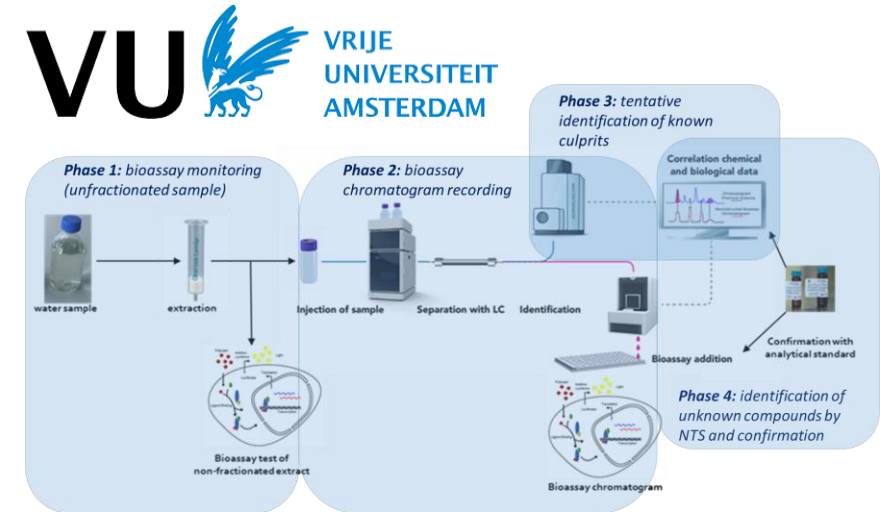
# Effect Directed Analysis

## EDA Platform Developed in cooperation with VU

- Jonker et al., 2015 & Zwart et al., 2020

## Implemented at the Water Laboratory:

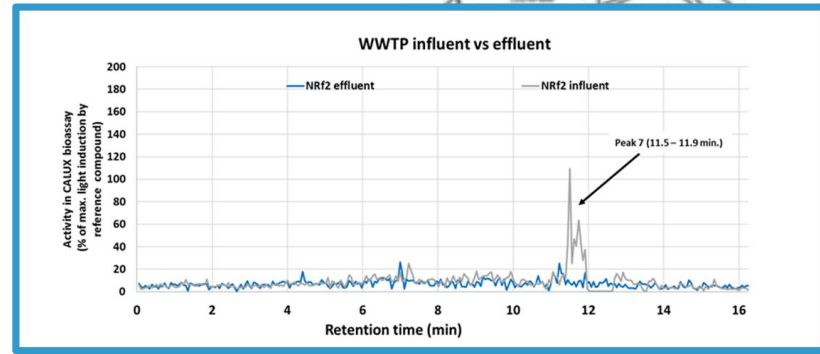
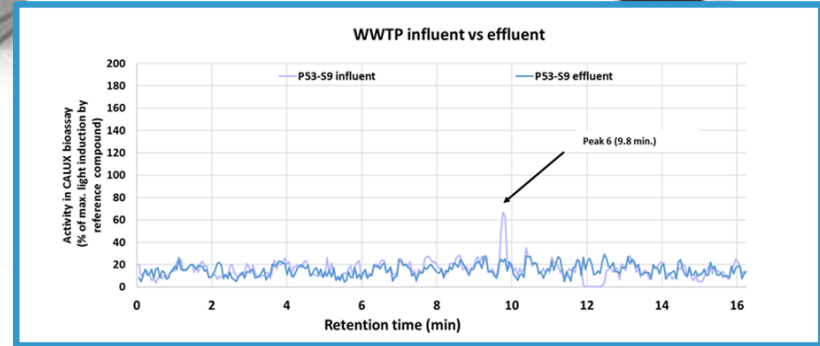
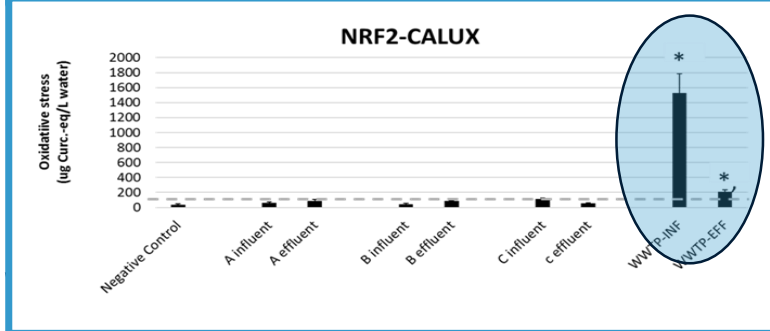
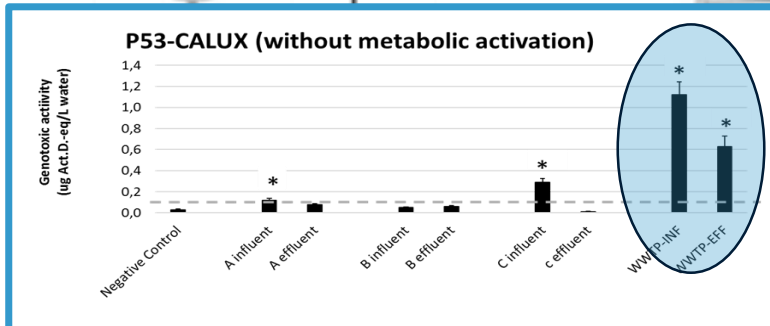
- Application to sources DW and WWTP effluent:
  - AR, ER, GR (Houtman et al., ETAP 2020)
  - PR, AR, anti-AR, anti-PR, cytotox-CALUX (Houtman et al., Env. Int. 2021)
- Coupling new bioassays to Effect-directed Analysis platform:
  - P53-CALUX
  - NRF2-CALUX



# Effect Directed Analysis with P53- and NRF2-CALUX



water sample



Identification responsible compounds:

Genotoxicity (P53-CALUX):

- One peak
- 10 candidates

Oxidative stress:

- One peak
- 5 candidates

=>activity to be confirmed with pure standards

# EDA in sources and DW of 4 DW companies

- Companies:

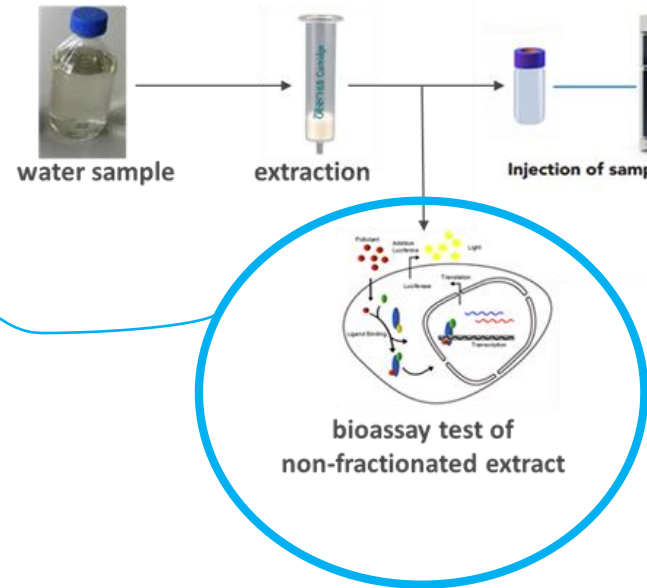


- common research program



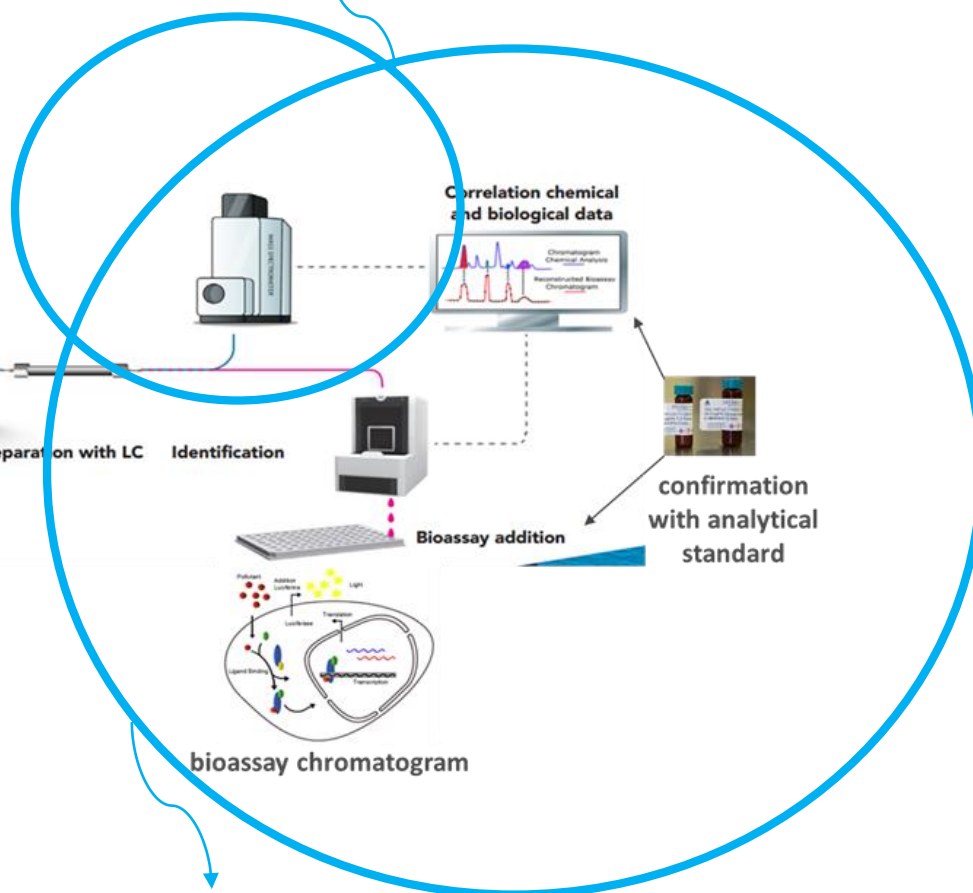
### 1. CALUX 10 endpoints

- |                              |                                 |                                  |
|------------------------------|---------------------------------|----------------------------------|
| Hormone like effects:        | Hormone antagonism:             | Reactive MoAs:                   |
| 1. Androgenic (AR)           | 5. Anti-androgenic (anti-AR)    | 8. Cytotoxicity (cell viability) |
| 2. Estrogenic (ER $\alpha$ ) | 6. Anti-estrogenic (anti-ER)    | 9. Oxidative stress (NRF2)       |
| 3. Glucocorticoid (GR)       | 7. Anti-progestogenic (anti-PR) | 10. Genotoxicity (P53 $\pm$ S9)  |
| 4. Progestogenic (PR)        |                                 |                                  |



### 3. Targeted hr-QToF screening

>2000 compounds



### 2. EDA: for a selection of locations / endpoints

# Conclusions

- Bioactive compounds are the ones that matter for WQ, especially for DW
- Bioassays are very valuable instruments for Risk Based Monitoring
- Combination with high resolution chemical screening enables:
  - identification of bioactive compounds
  - pattern analysis to understand spatial differences



# Thanks!



BioDetection  
Systems



# You !





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