

# Non-target analysis of PMT compounds and transformation products in drinking water in and around Luxembourg

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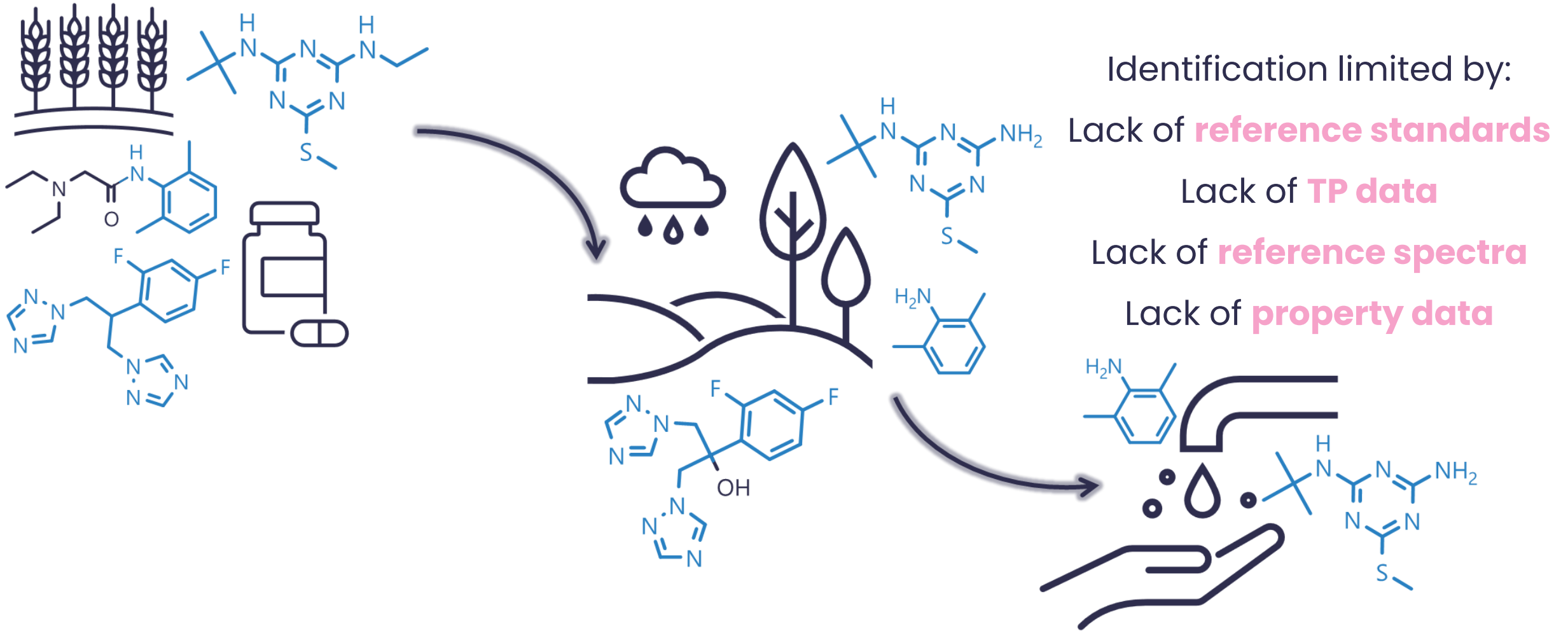
Luxembourg Centre for Systems Biomedicine (LCSB) University of Luxembourg

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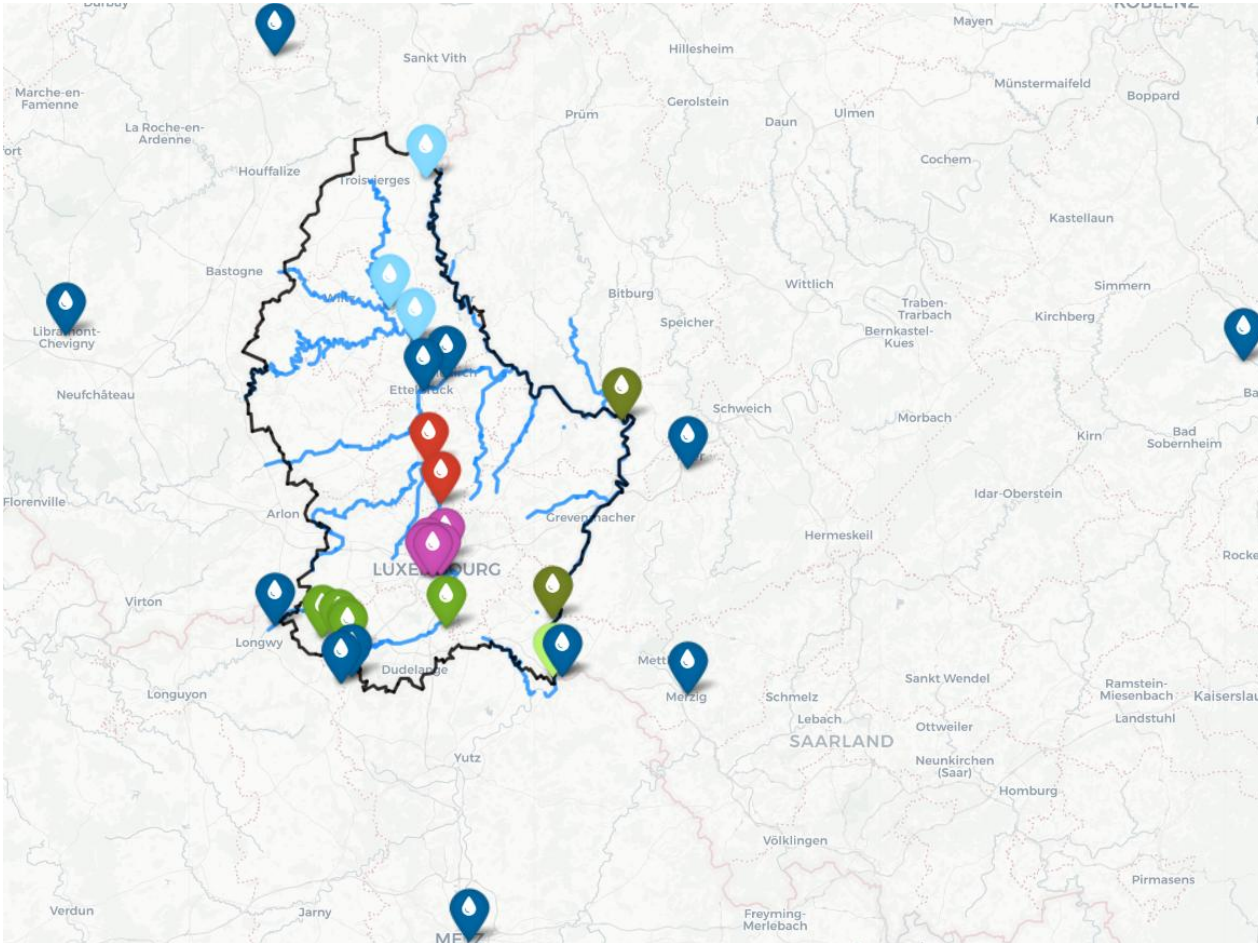
2026-05-21

# Introduction



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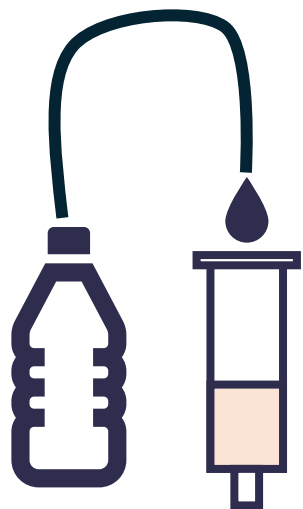
Tap water samples from 31 locations in  
Luxembourg, France, Belgium and Germany  
Samples once per month for 3 months



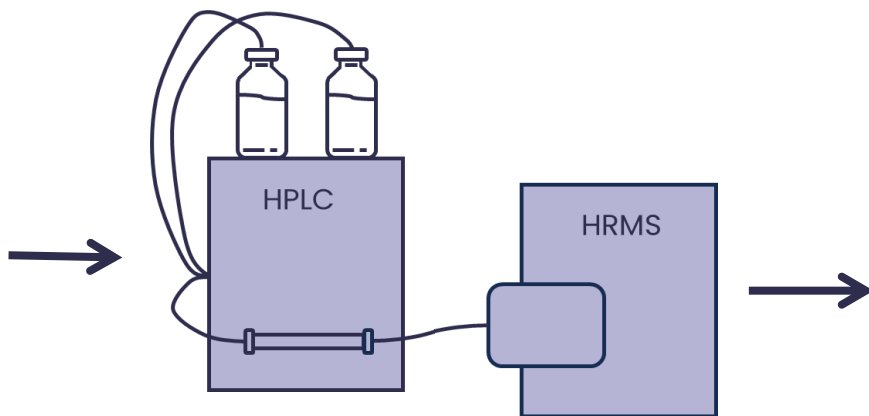
Still bottled water from local  
supermarket  
6 brands



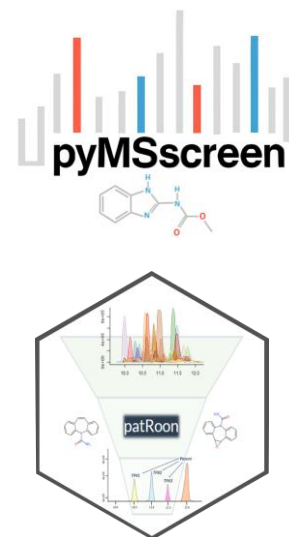
# Workflow



Preconcentration with  
SPE



HPLC-HRMS analysis



Data processing

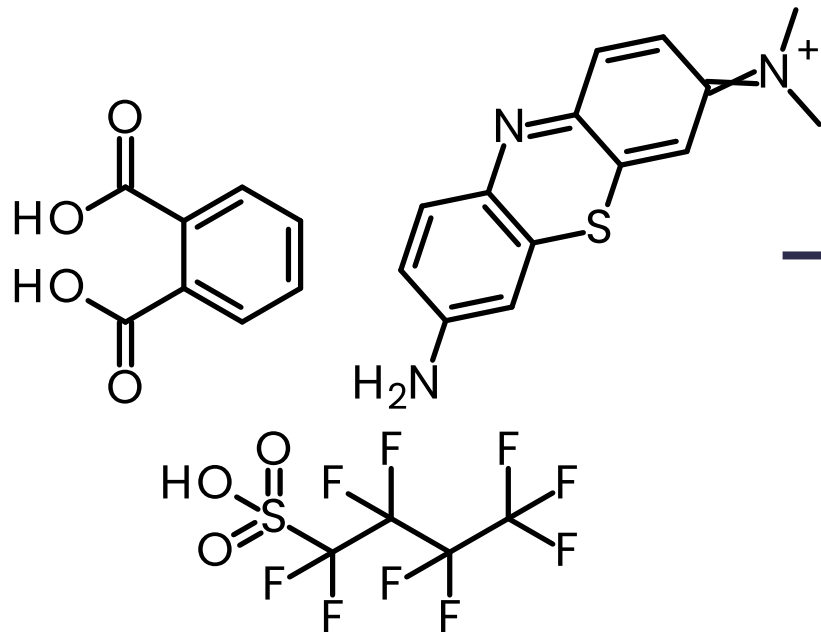


TP identification and  
PMT property  
predictions

# Transformation products filtering

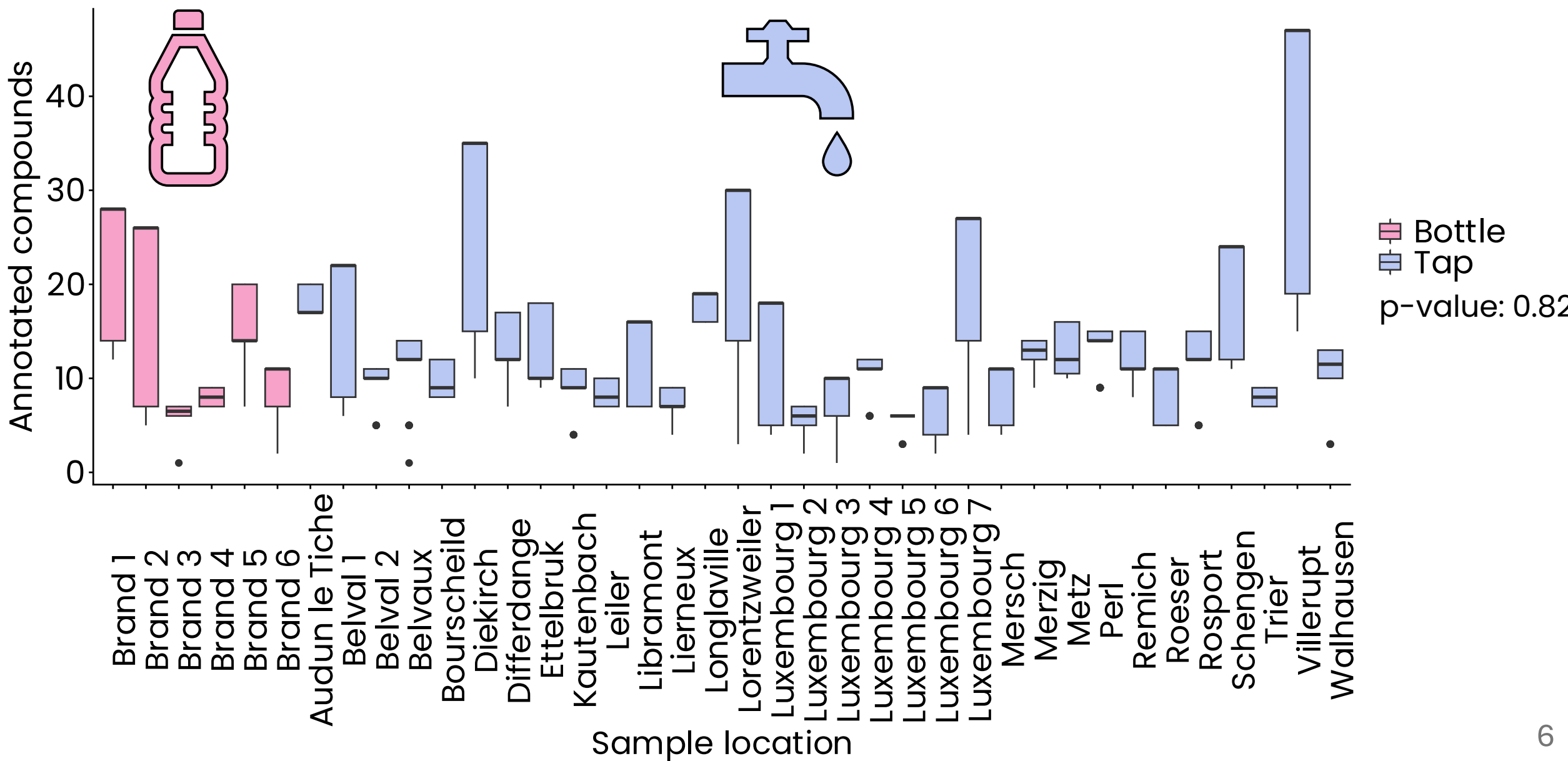
**Annotated TPs**

**Compare against  
NORMAN-SLE REACH list**

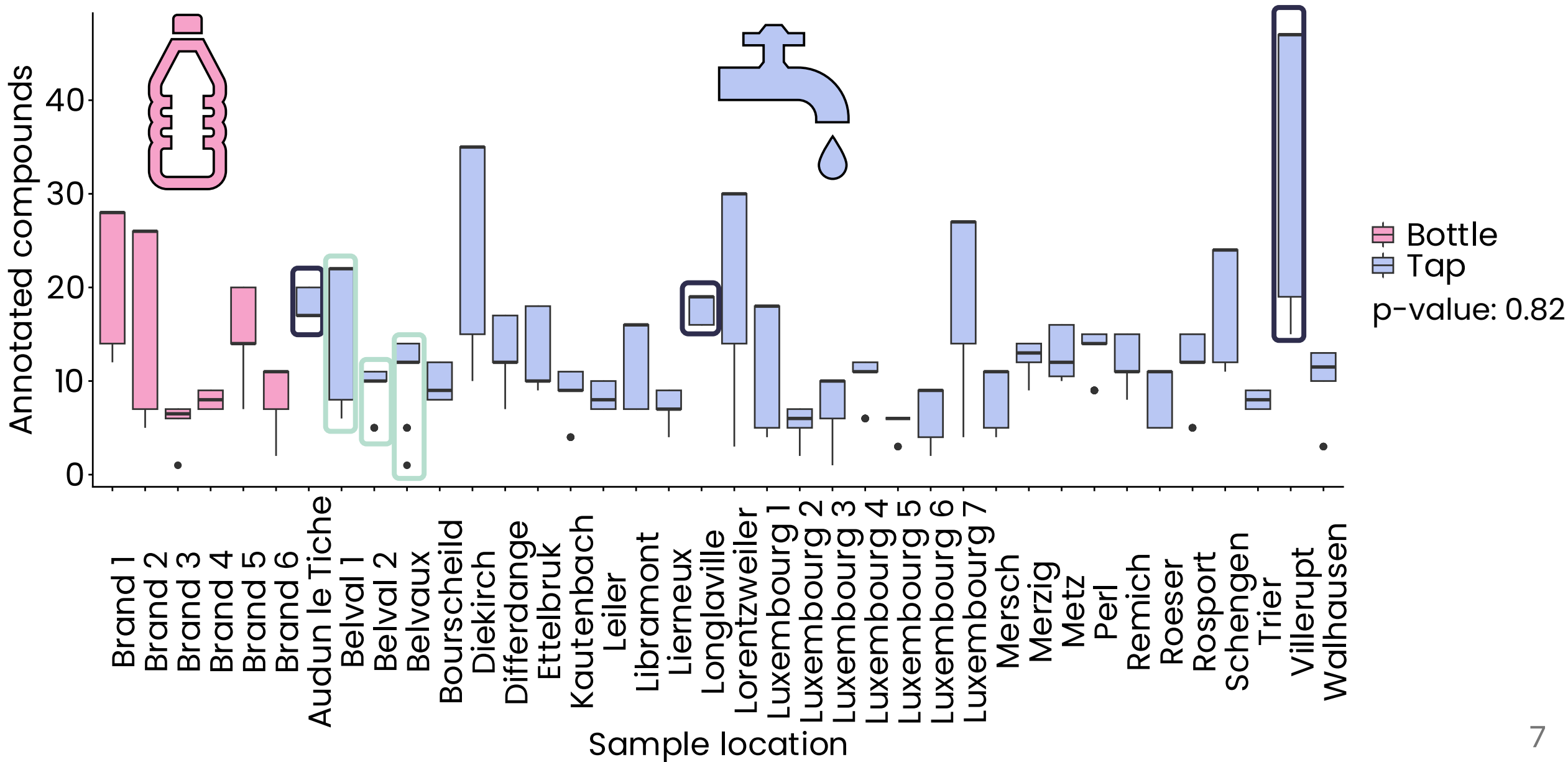


**TPs with no  
other use**

# Number of annotated compounds

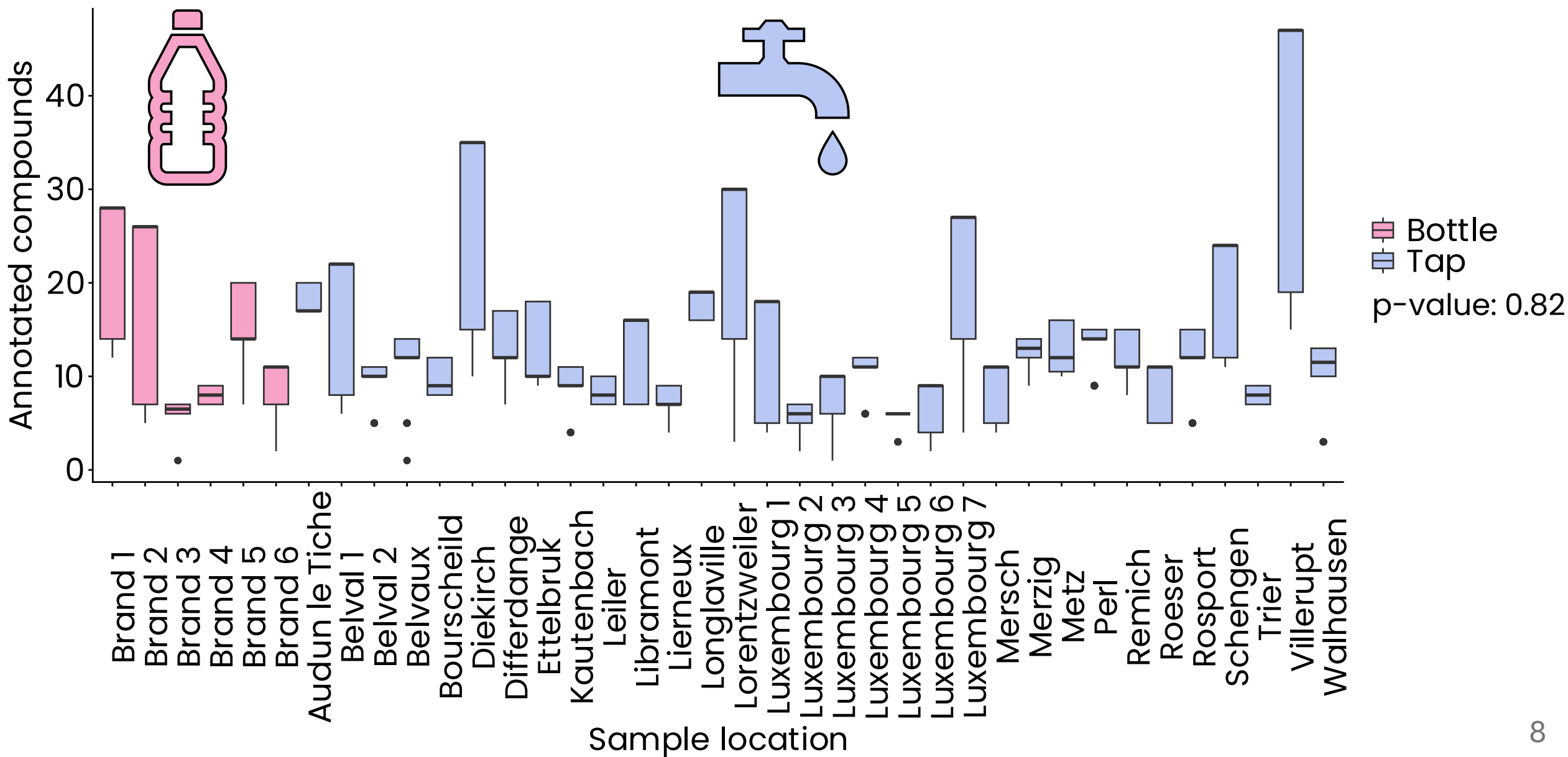


# Number of annotated compounds



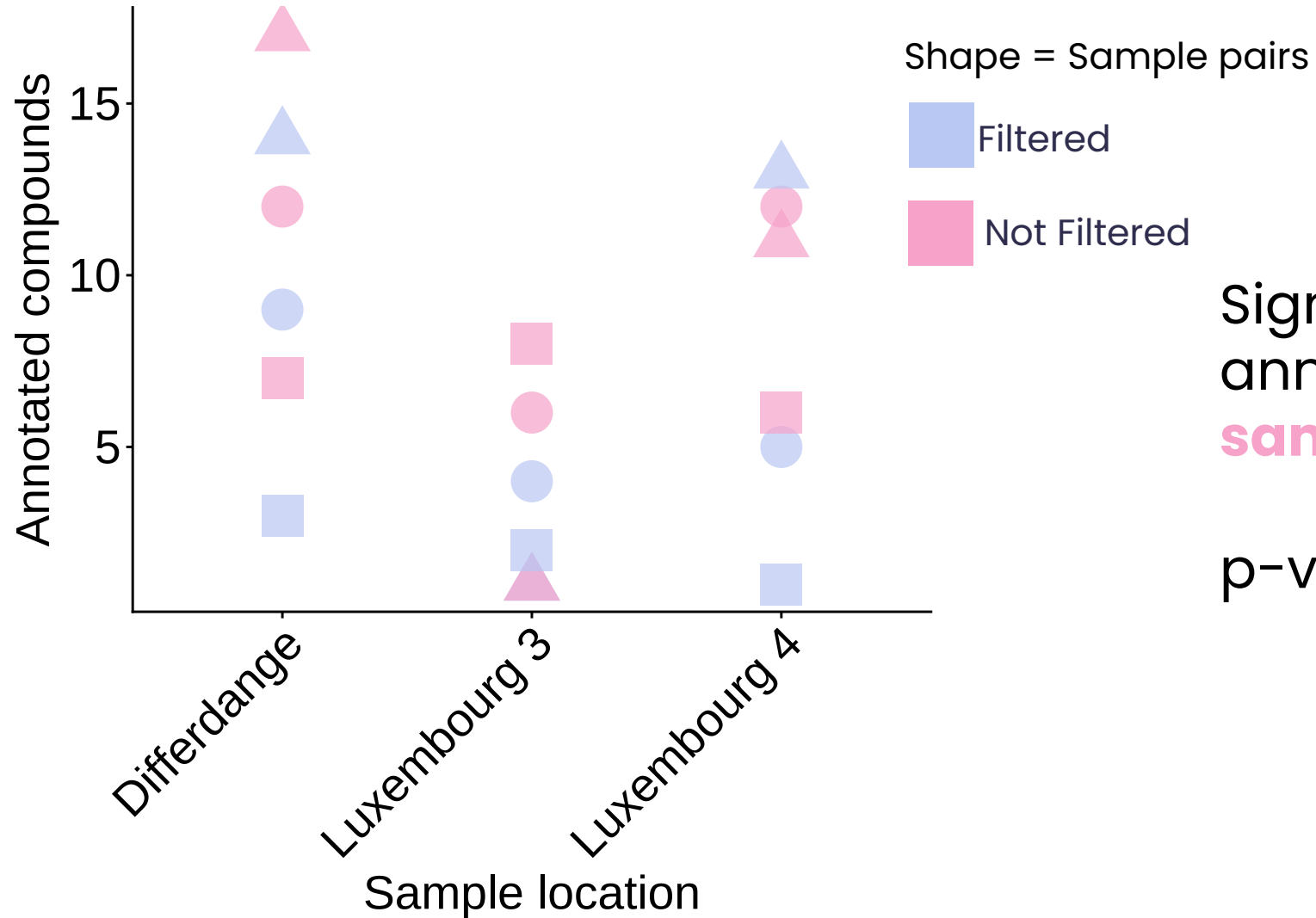


# Number of annotated compounds





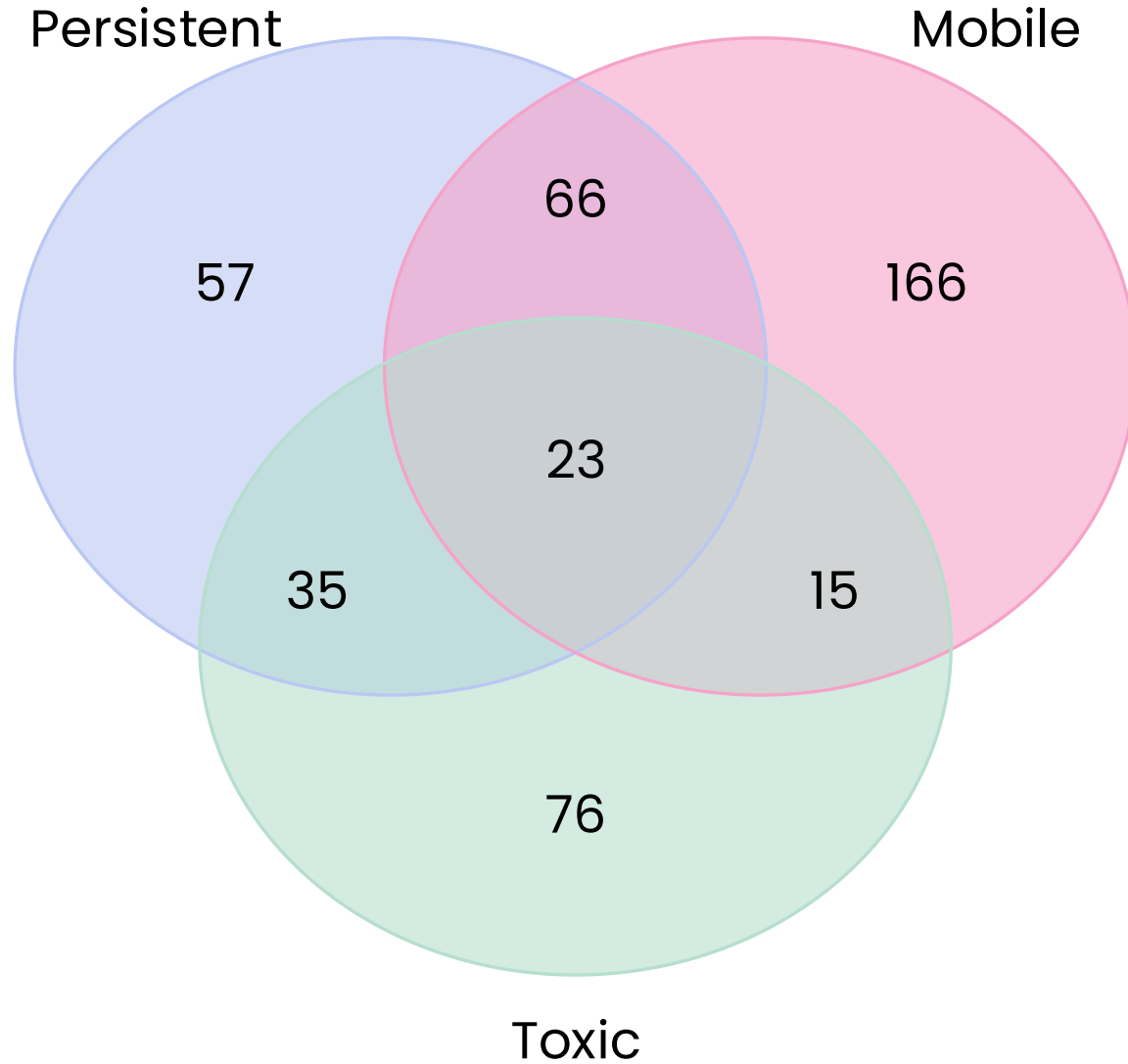
# Filtered vs unfiltered water



Significantly **fewer compounds** annotated in the **filtered water samples**

p-value: 0.03

# Predicted PMT properties



**Inside model applicability domains:**

**58% persistent**

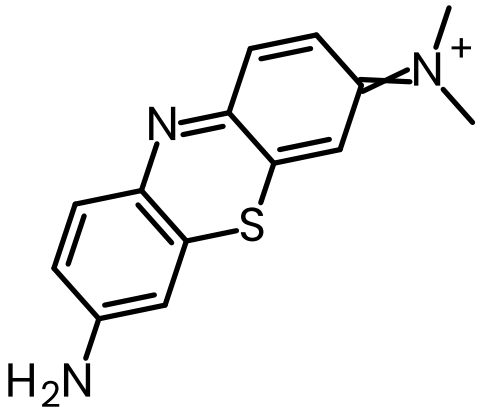
**83% mobile or very mobile**

**35% endocrine disrupting**

# Transformation products

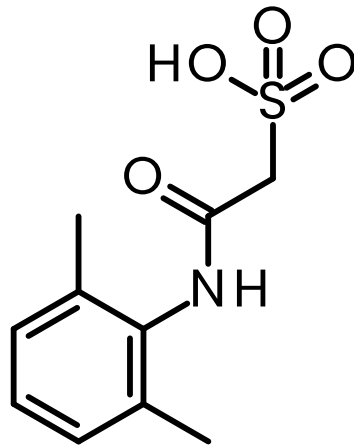
**148 (38%)** compounds annotated as TPs

**36** have no other known uses in REACH



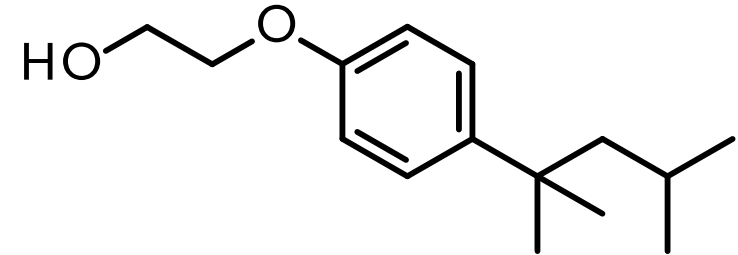
**Azure A cation**  
**9 Samples**  
**Conf. 3b**

PMT



**Dimethachlor CGA369873**  
**14 Samples**  
**Conf. 2a**

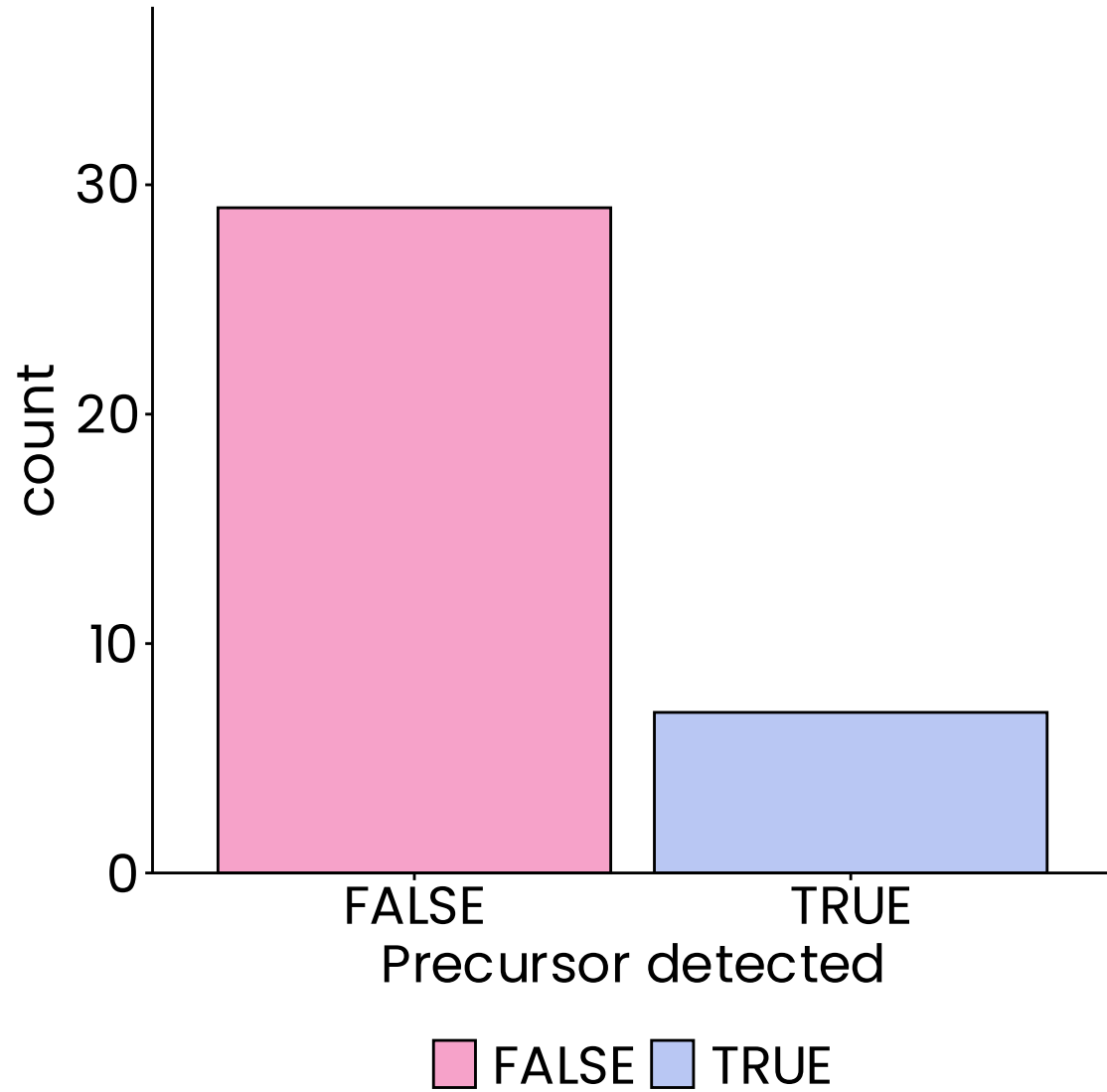
PM



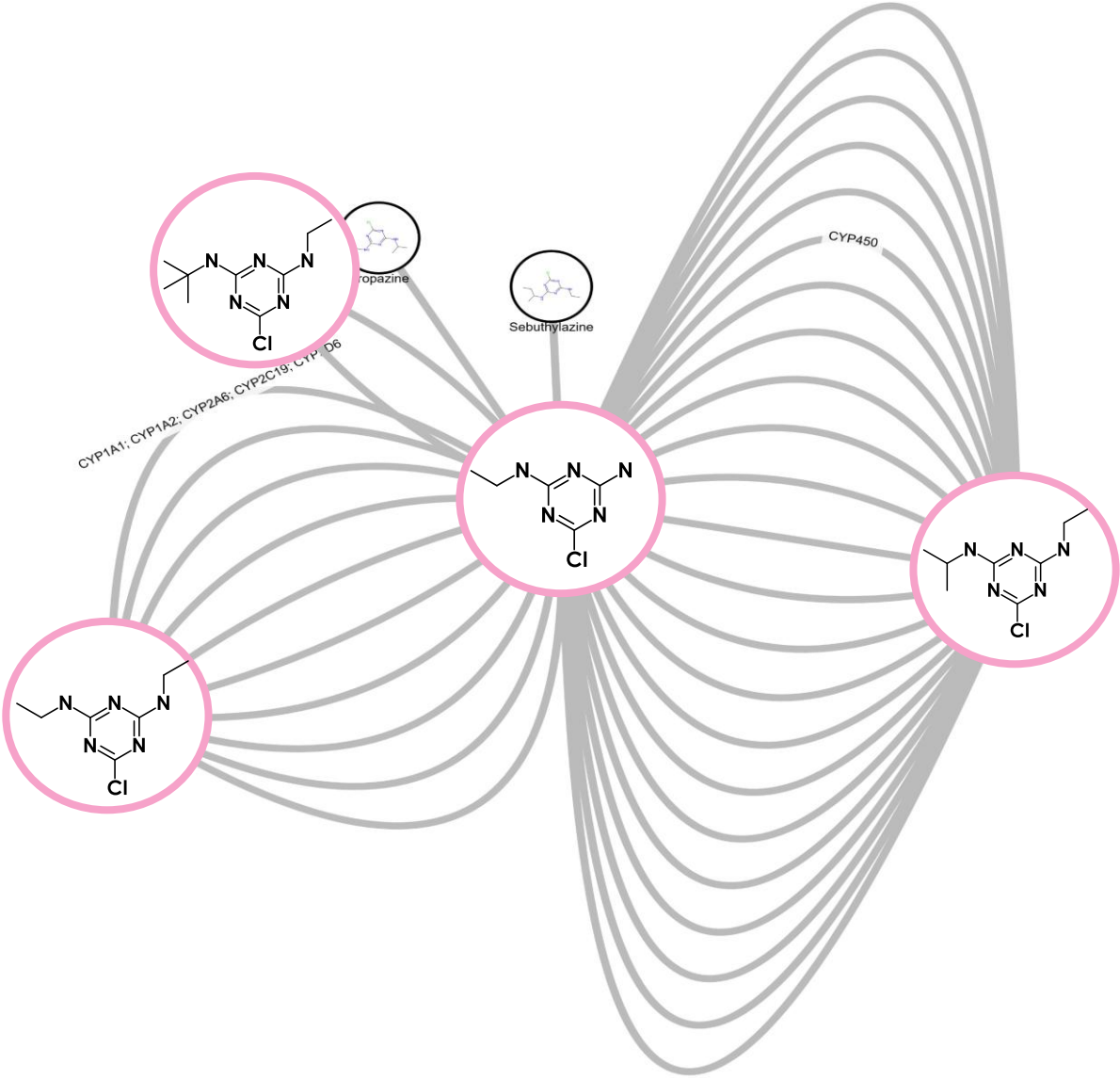
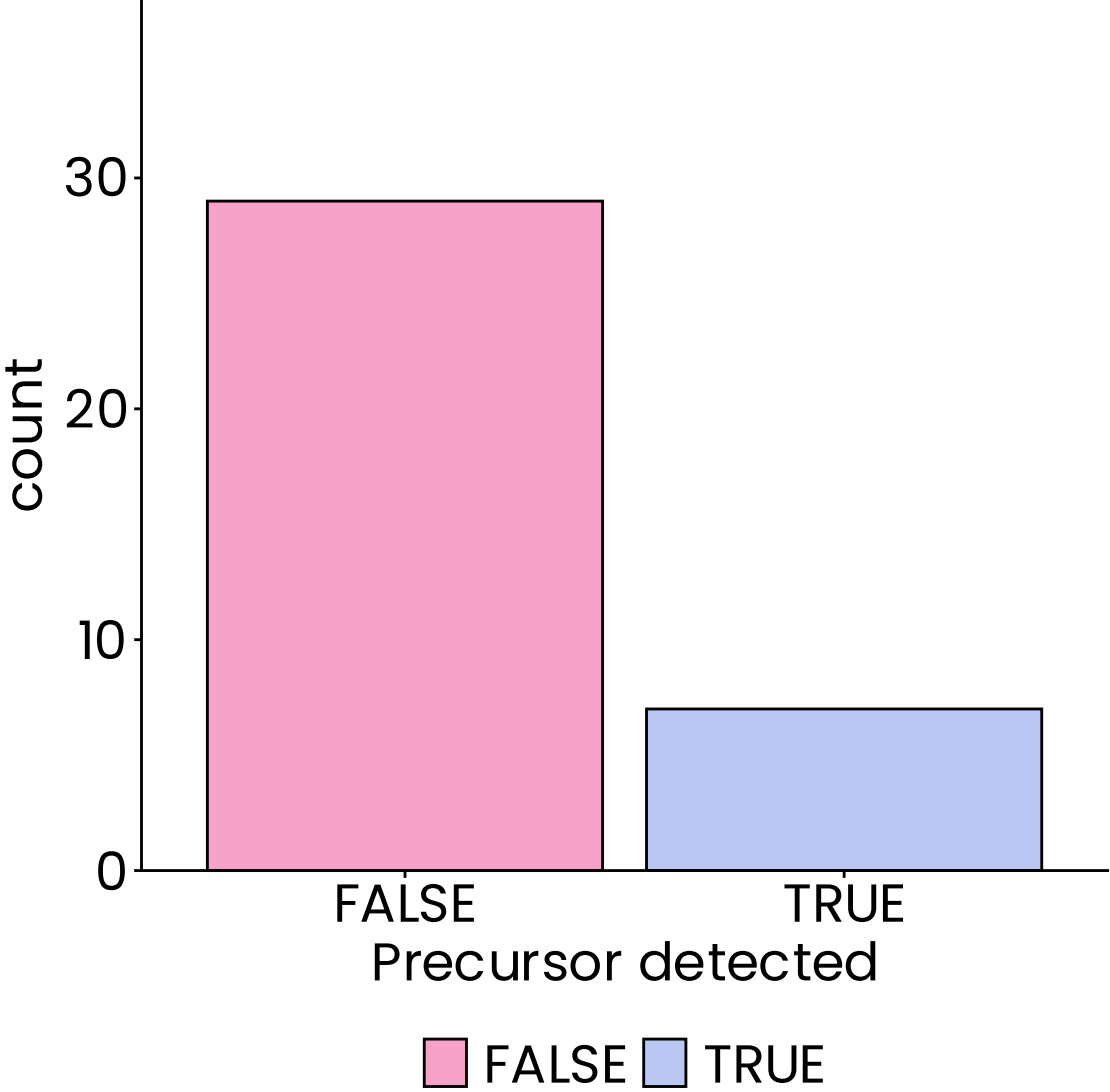
**Triton X 100**  
**7 Samples**  
**Conf. 3b**

PT

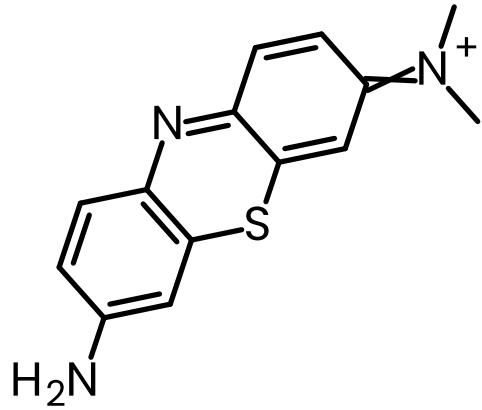
# Precursor annotation



# Precursor annotation



# Precursor identification without annotation?



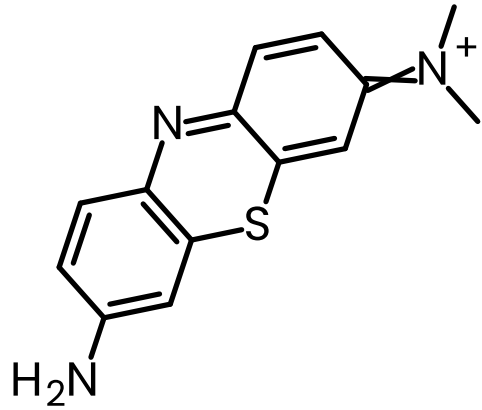
**Azure A cation**

**9 Samples**

**Conf. 3b**

PMT

# Precursor identification without annotation?

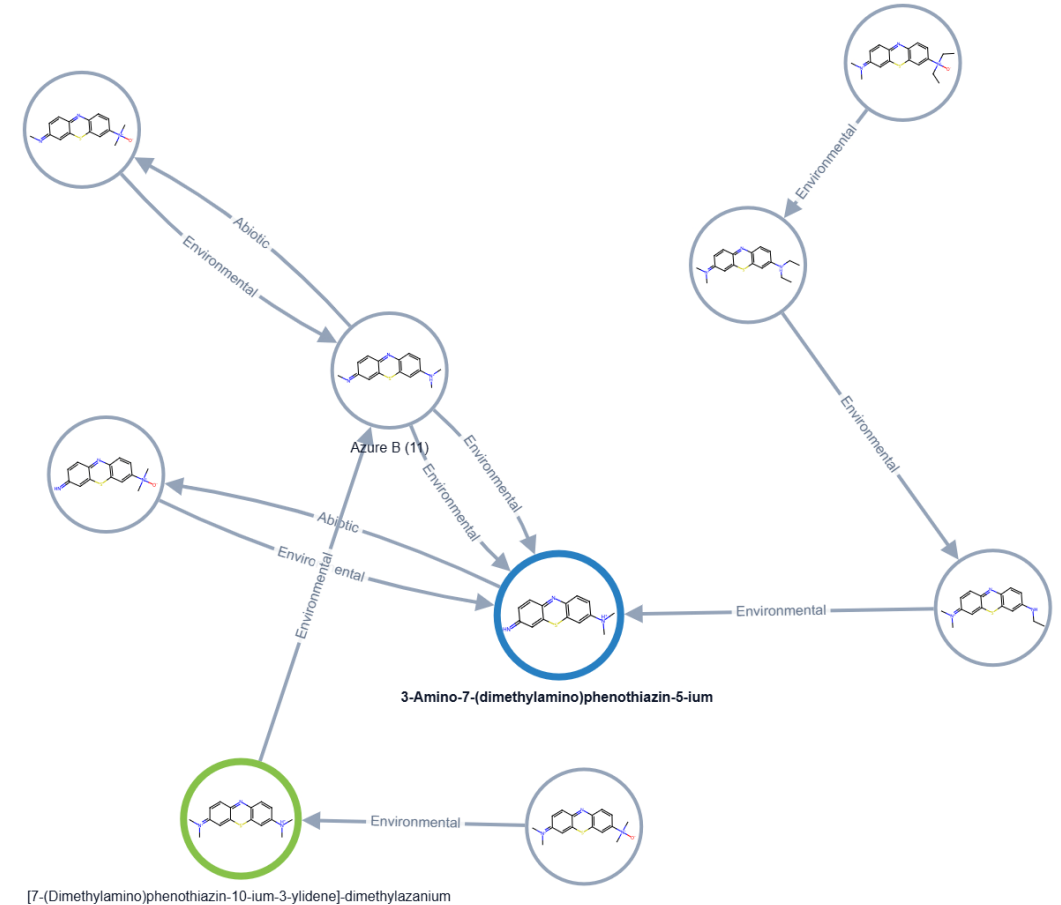


# Azure A cation

## 9 Samples

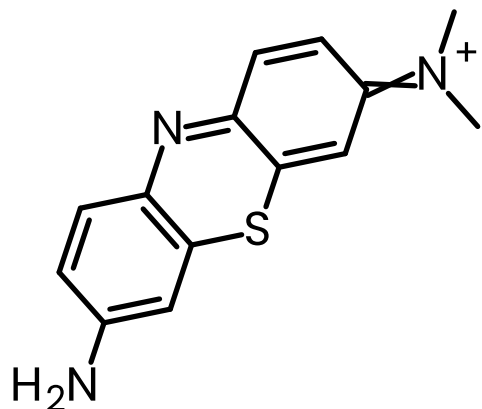
### Conf. 3b

PMT



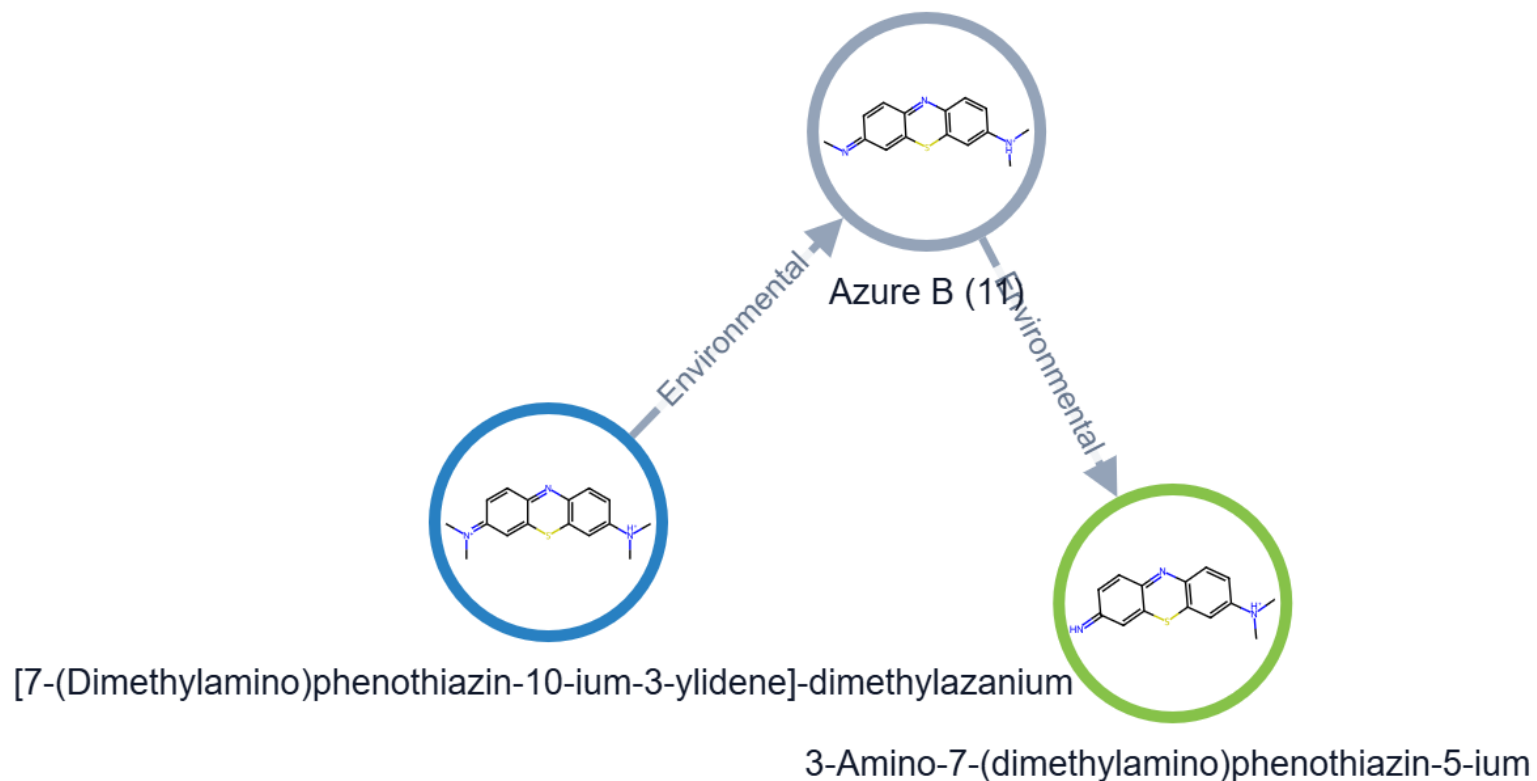


# Precursor annotation

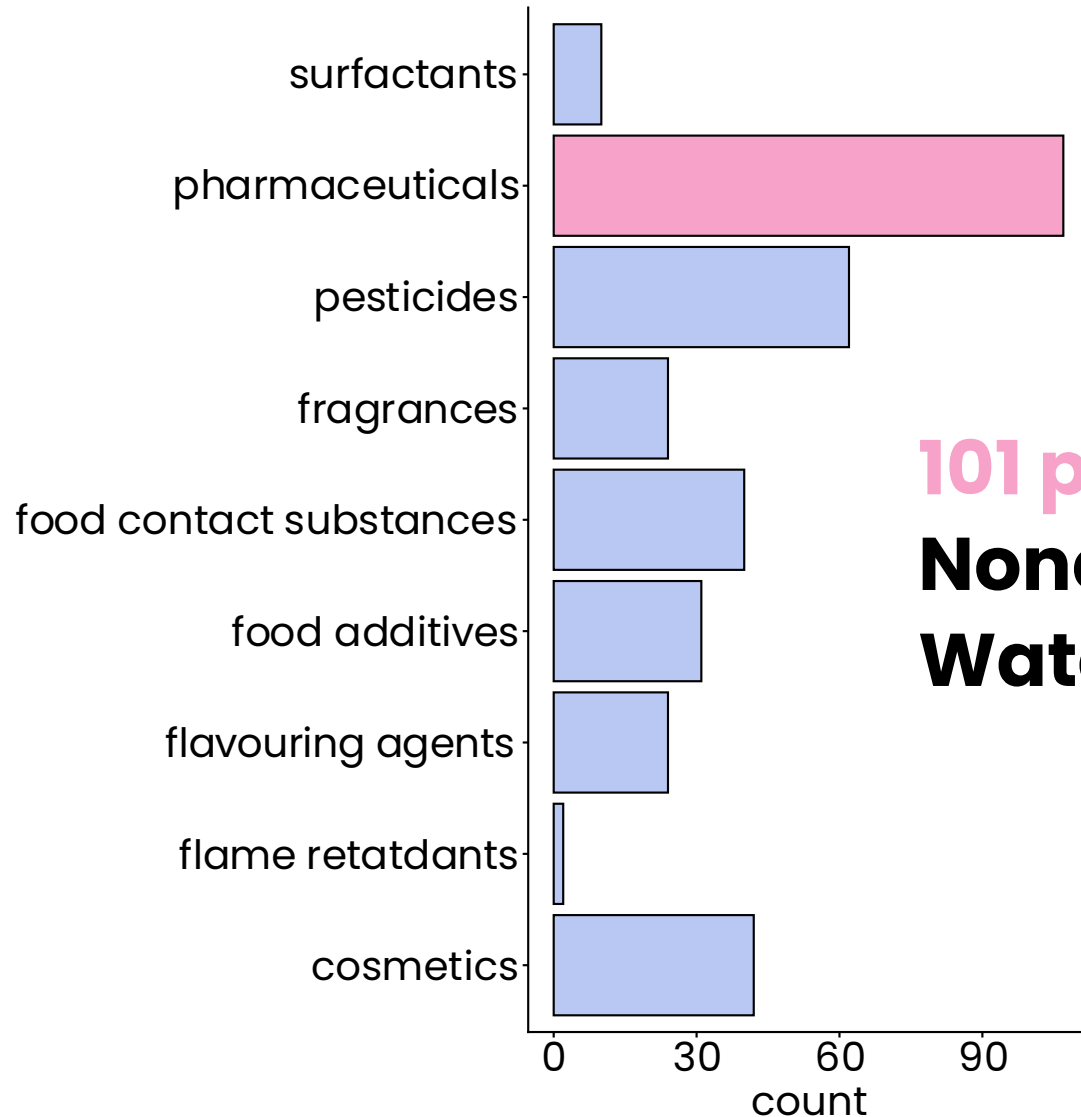


**Azure A cation**  
**9 Samples**  
**Conf. 3b**

PMT



# Compound classes



**101 pharmaceuticals** annotated.  
**None** are included in the **EU Drinking Water Directive**

# Acknowledgements



Many thanks to my sampling volunteers

## Thank you for listening!



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