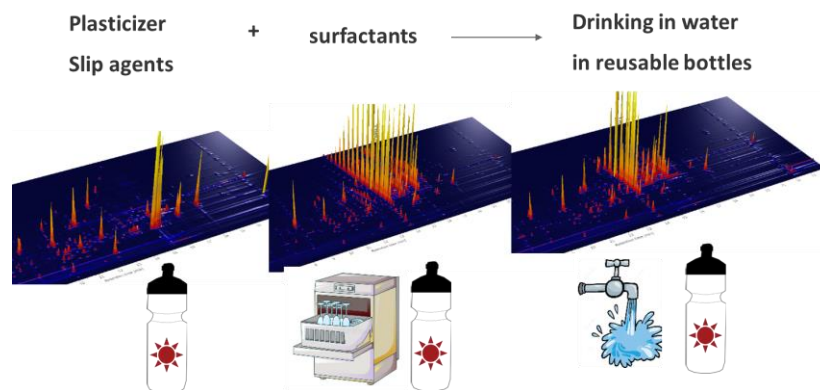


Migration of Compounds from Reusable Plastic Bottles into Drinking Water



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KØBENHAVNS UNIVERSITET



Background

Reusable plastic sports bottles

- widespread use in different sports
- So far, plastic bottles are only analyzed for well-known contaminants (e.g. bisphenol A)
- complains about the smell



Biodegradable polyethylene

The bottle made of biodegradable polyethylene decomposes in the landfill. The flexibility of this material means it is much more recyclable. On one hand because it is simply made of polyethylene, you can dispose of this bottle in the plastics bin to be 100% recycled. On the other hand, the bottle is biodegradable.

This is achieved by adding a bio-batch to the material that changes the molecular structure of the bottle. This had no effect on the use of the bottle until it is in the landfill or is accidentally left behind during a ride through the forest. In the middle of the landfill or under a layer of leaves and soil in the forest, there is heat and humidity. At the correct temperature, the bio-batch additive activates and the bottle decomposes into water, humus and gas. It does not degrade into small pieces of plastic as in oxo-biodegradable materials. The whole composting process in a landfill takes about one to five years. In nature this takes longer. Furthermore, in the landfill the gas can be recaptured for use as an energy source.



Shiva Bio 500ml & 750ml

100% biodegradable

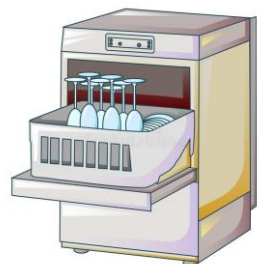
6 bottle colours, 6 cap colours

<https://bottlepromotions.com/biobased-bottles/>

Experimental setup



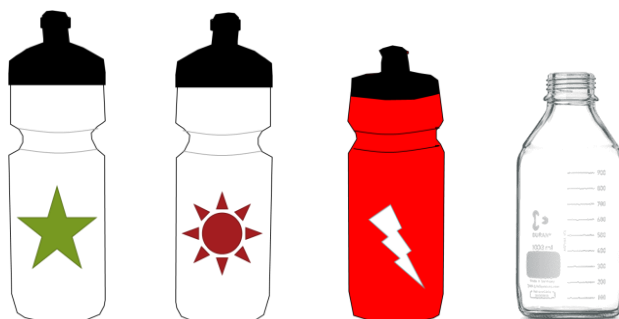
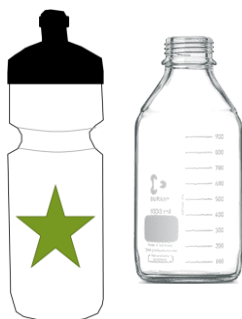
New



After the dishwasher



Bottles were flushed thoroughly after the dishwasher



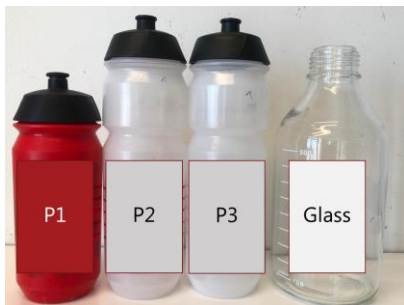
Previously used bottles



Previously used bottles

drinking water stored for 24 hours in the bottles

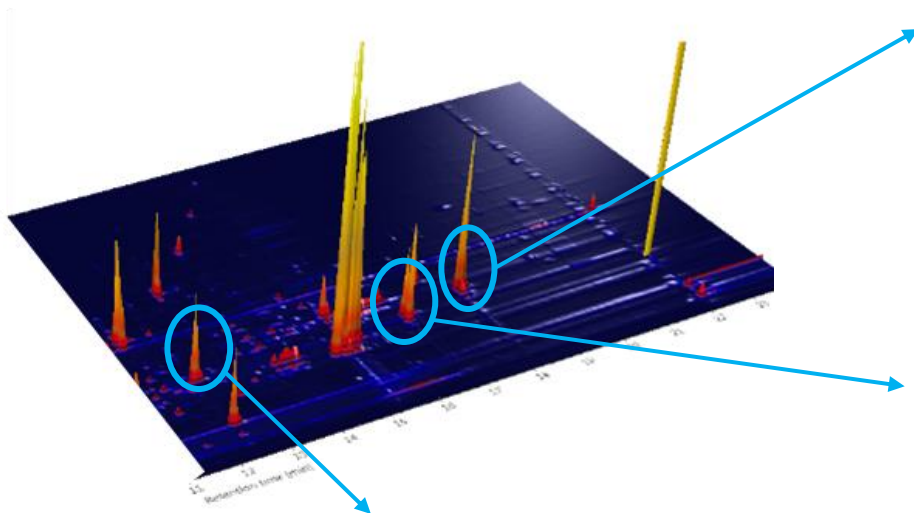
Liquid chromatography coupled to high resolution mass spectrometry



analysis of water sample

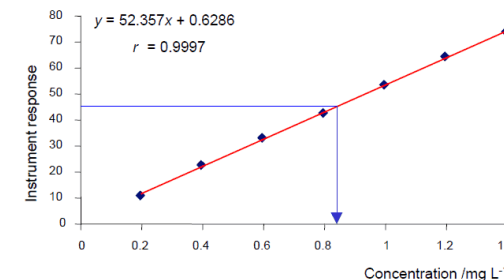
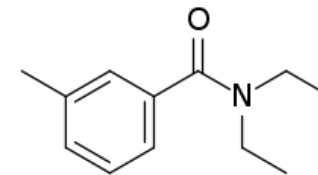


Method: Chemical fingerprinting



Target screening :

quantification of known chemicals

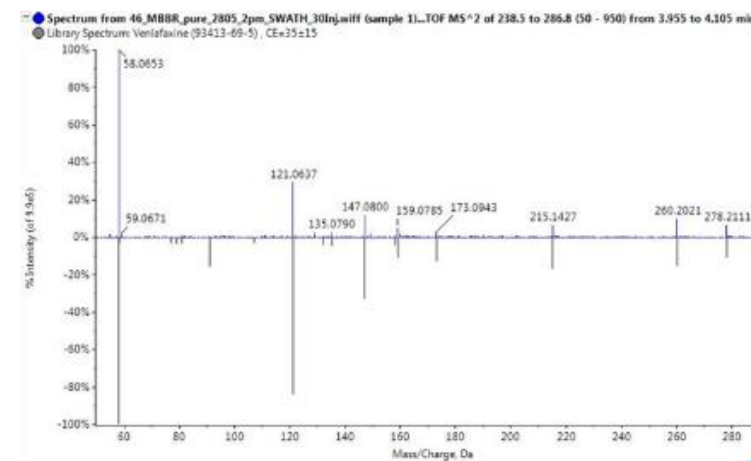
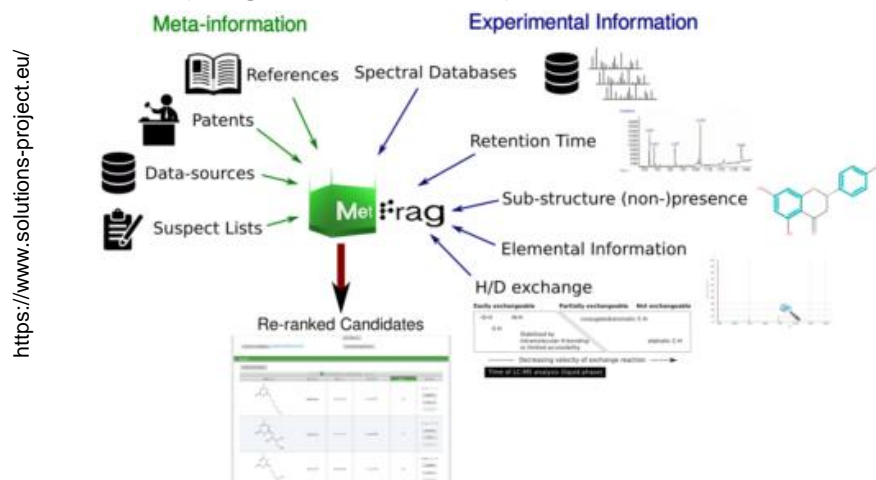


Suspect screening:

Identify compounds by comparison with databases

Non-target screening:

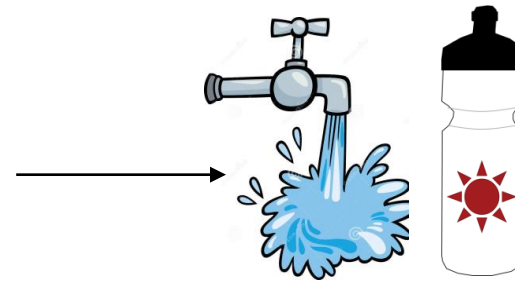
Identifying unknowns by prioritization



Non-target screening



+

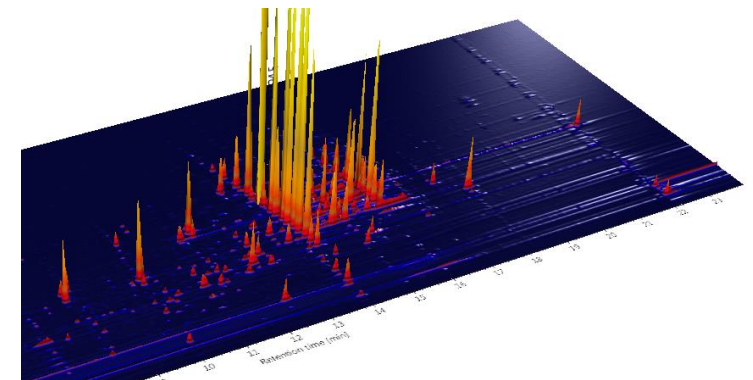
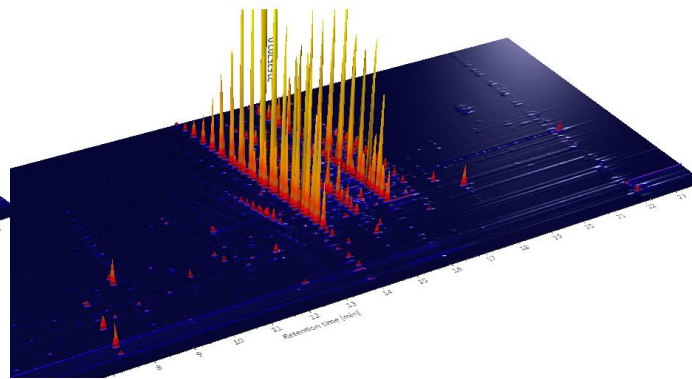
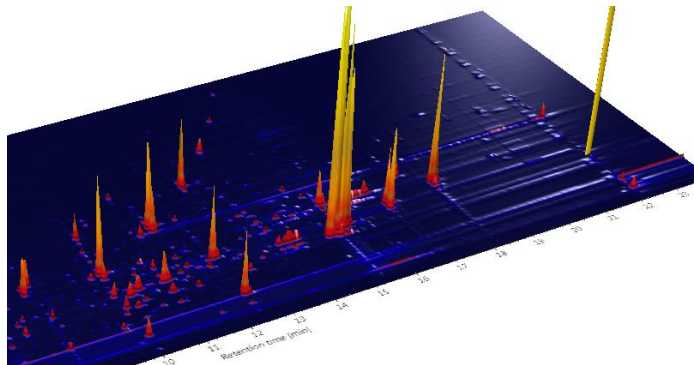


from reusable plastic bottles itself

from dishwasher (soap)

Remaining compounds after thoroughly flushing

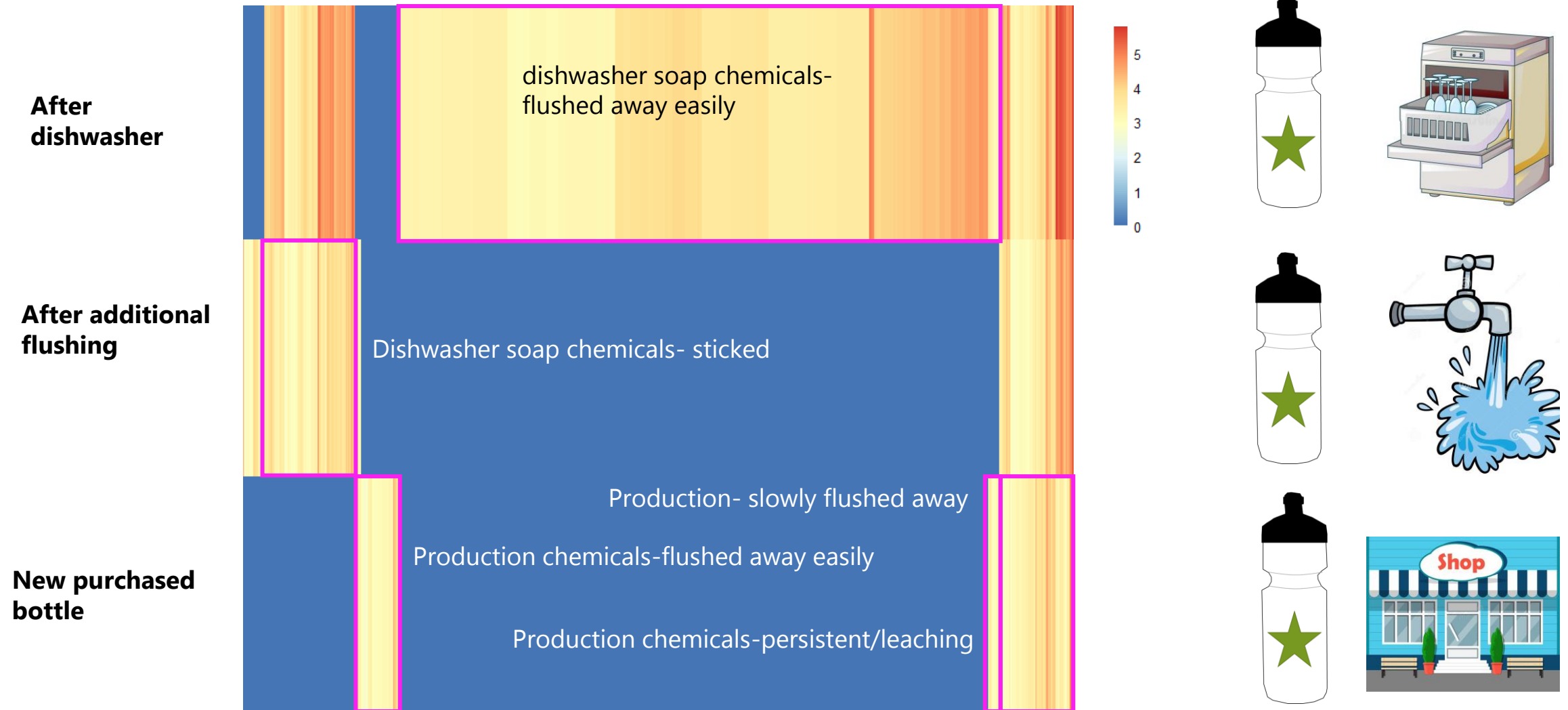
Compounds migrating into drinking water



→ Several thousand peaks detected – originating from plastic or dishwasher process

Non-target screening results: New reusable plastic bottle

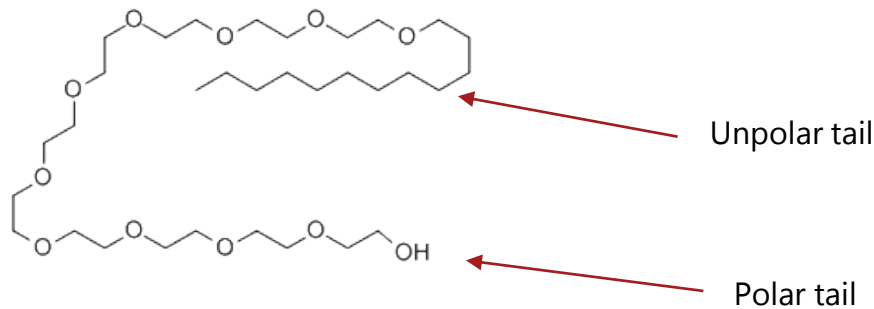
Each line represents one chemical (2000 chemicals presented here)



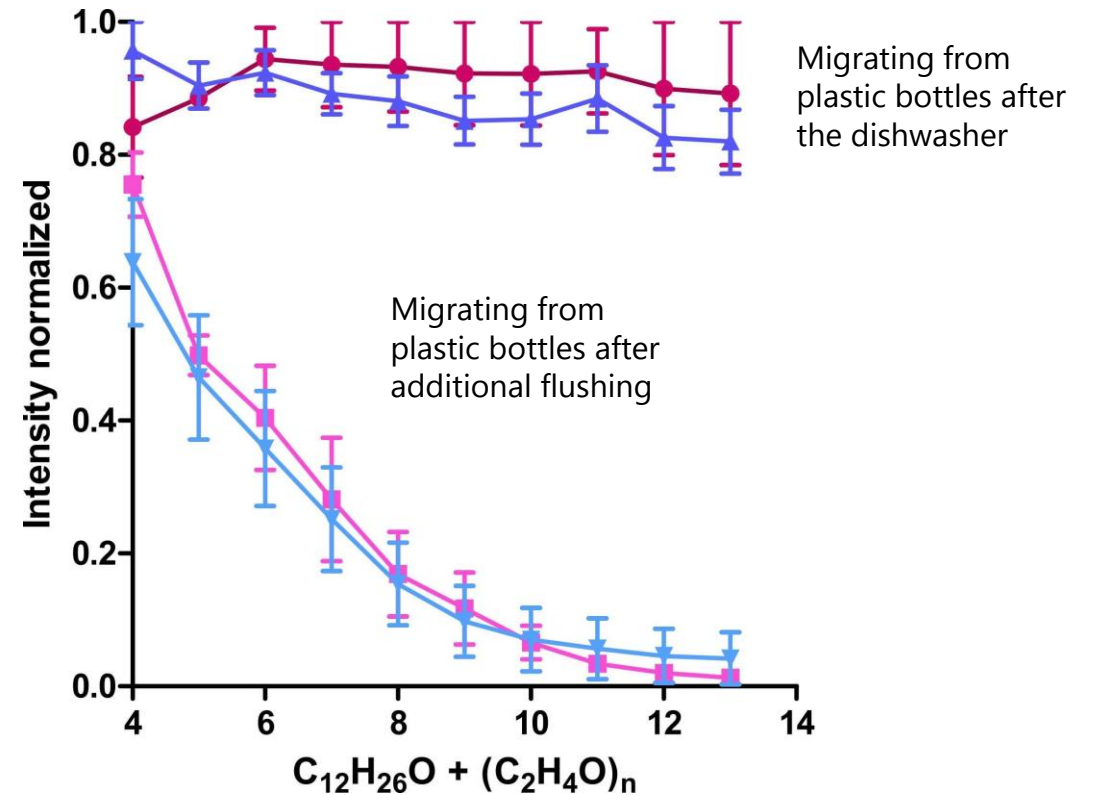
Compounds migrating from the dishwasher

Most of the identified compounds are detergents

Example: Polyoxyethylene lauryl ether
non-ionic surfactant



Homologous series, different lengths of ethylene oxide (EO) (C₂H₄O) groups
→ The more EO groups, the more polar is the compounds



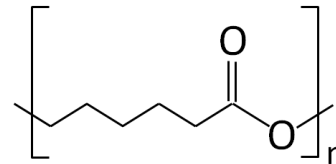
→ Unpolar compounds are sticking more to the plastic and migrate into the drinking water even after additional flushing

Compounds migrating from plastic itself

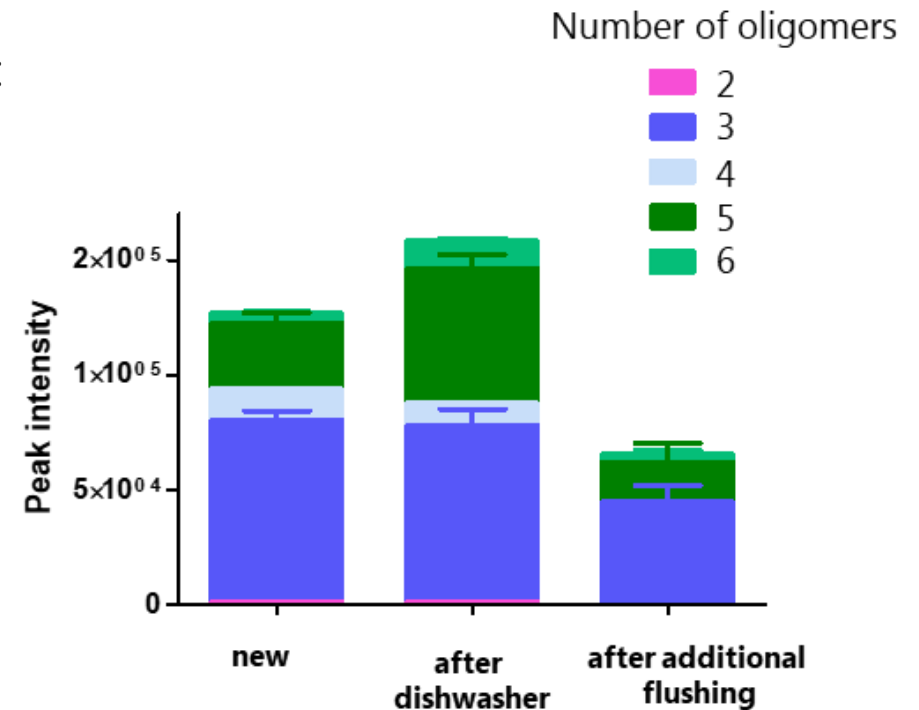
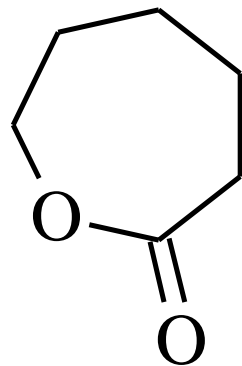
Plasticizer

e.g. Polycaprolactone

Biodegradable polyester for elastic properties

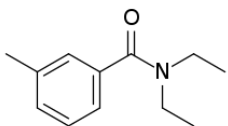


It degrades into smaller molecules during the use of the bottle:

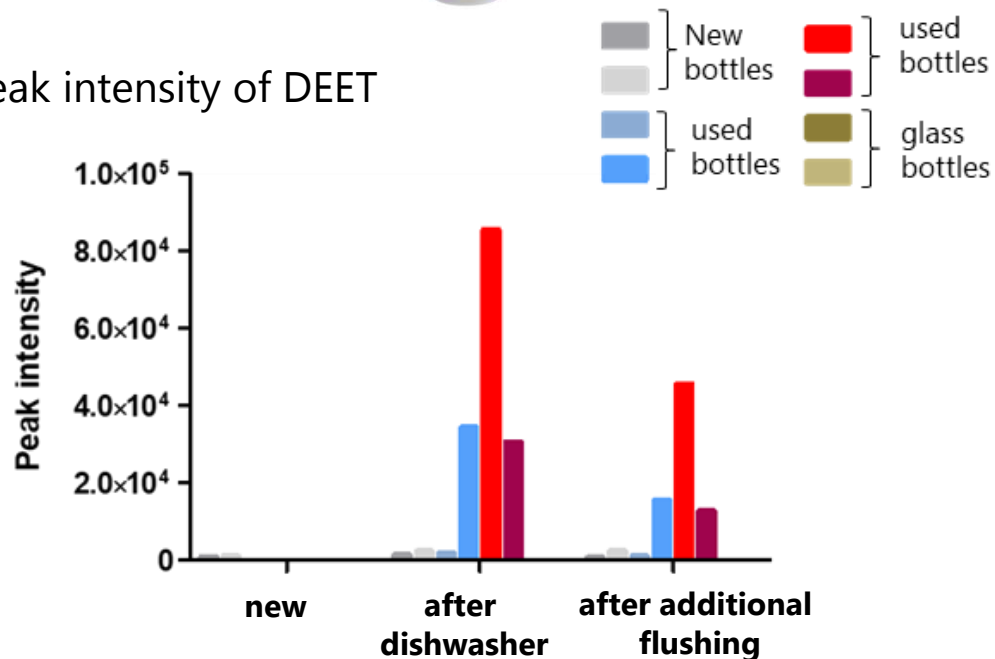


Compounds migrating from plastic itself

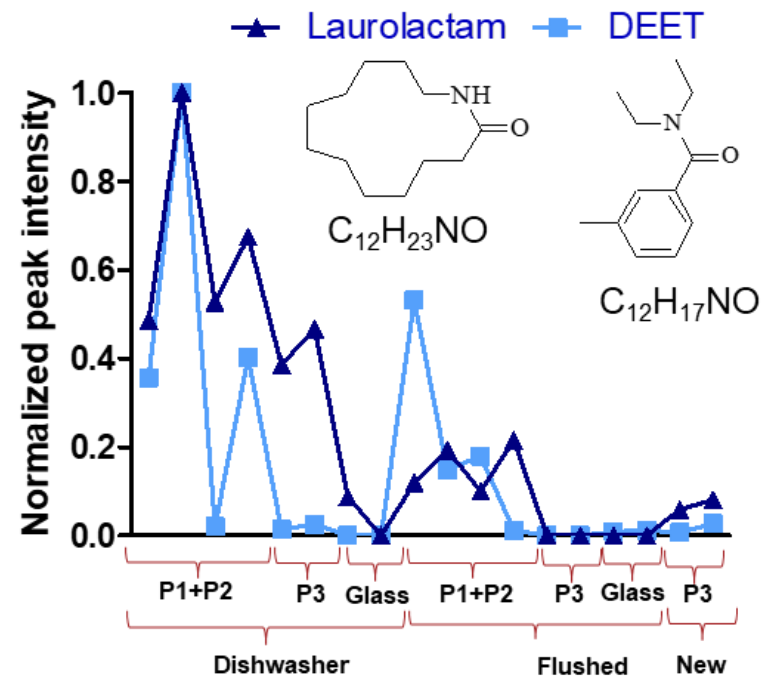
DEET



Peak intensity of DEET



- DEET was not detected in glass bottles
- small concentrations in new bottles, high concentrations in used bottles

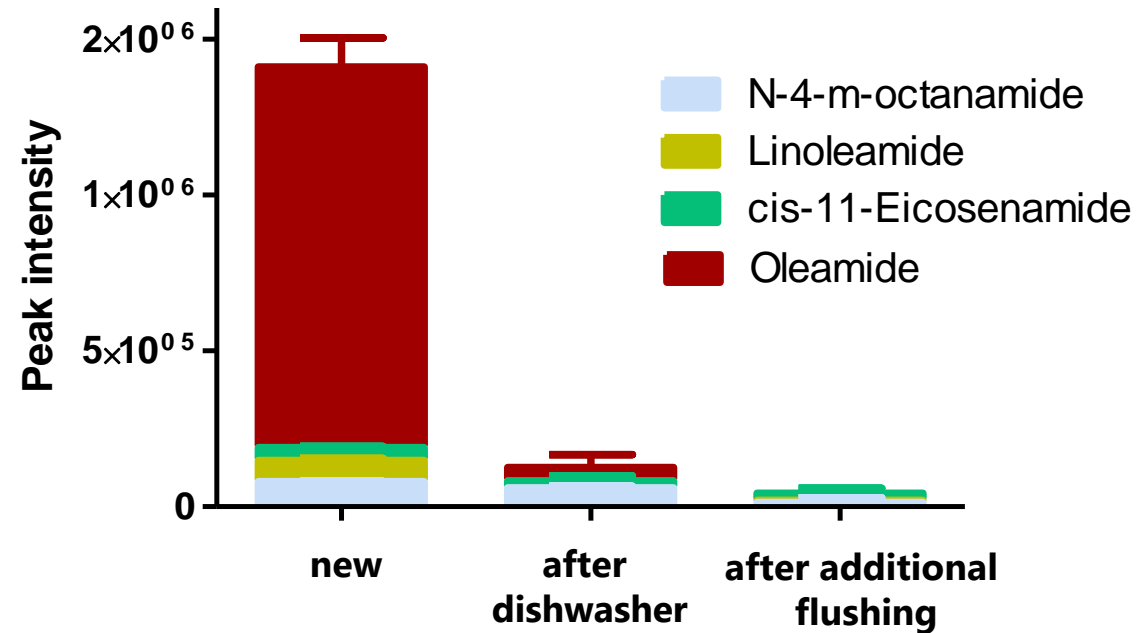
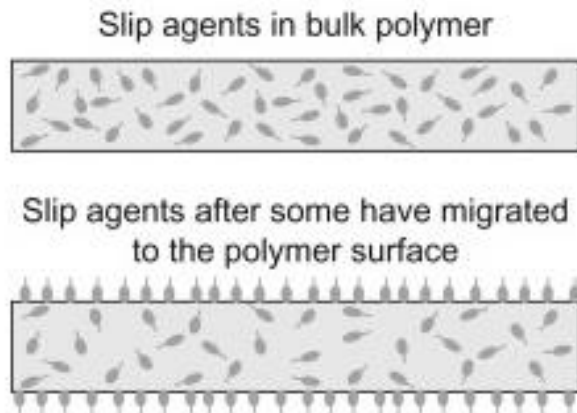


DEET- probably a plasticizer or a transformation product of a plasticizer

Compounds migrating from plastic itself

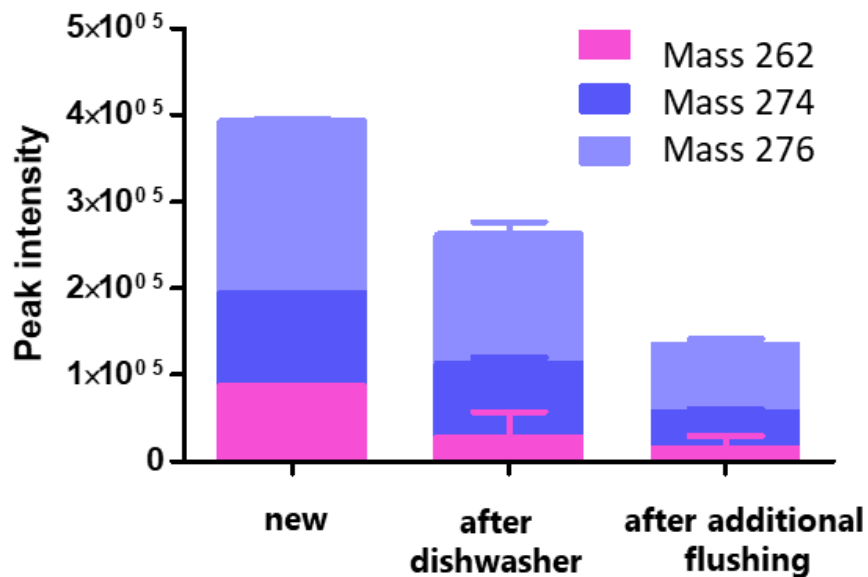
Slip agents

Fatty amides, they migrate or bloom to the surface where they form a microcrystalline structure that decreases friction

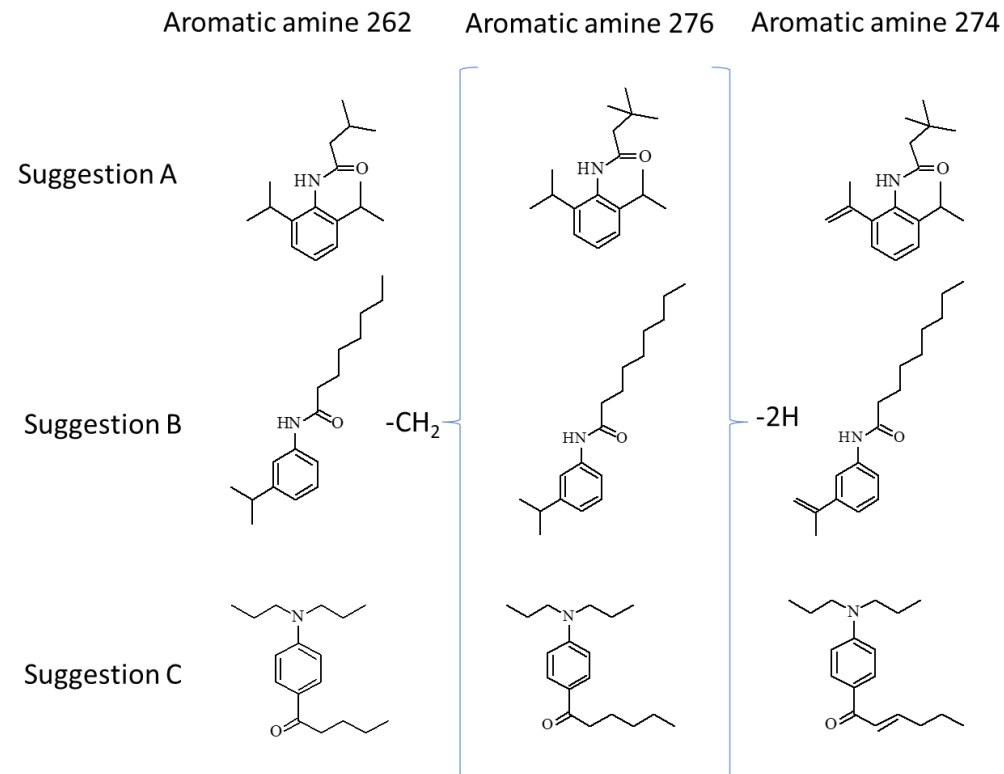


→ Important to wash new bottles before use!

Aromatic amines of unknown origin



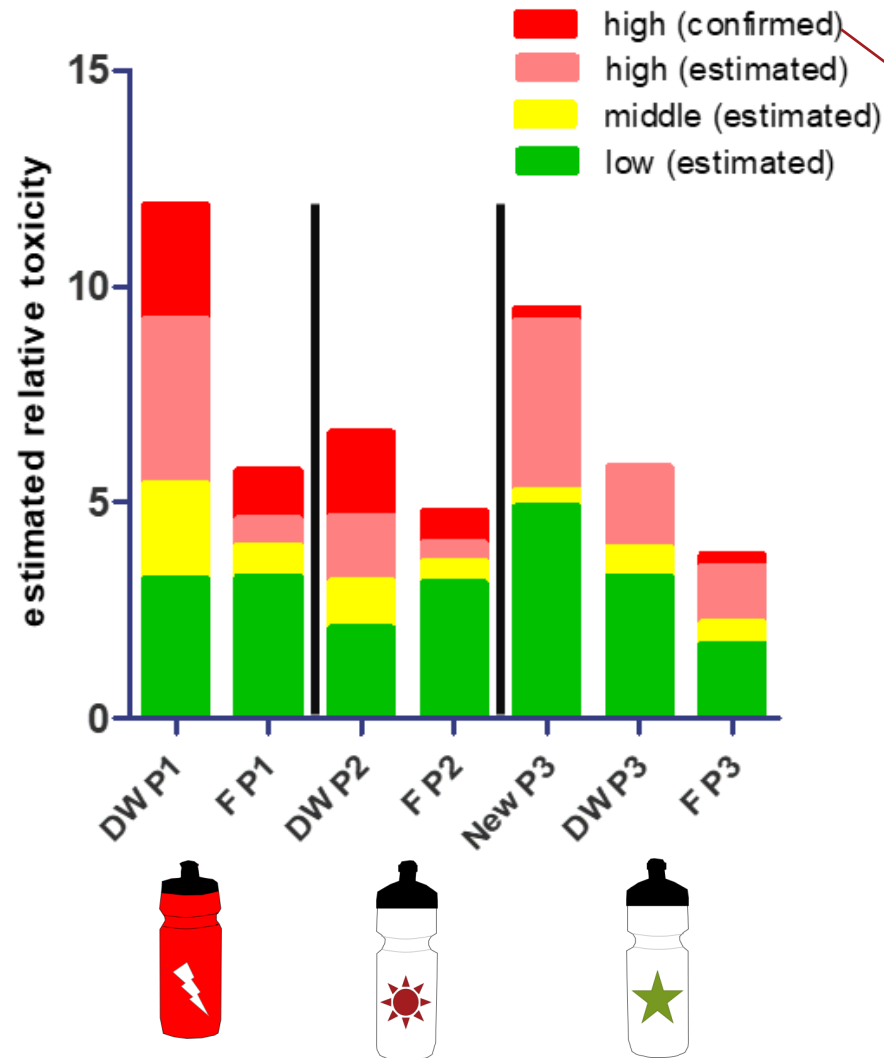
Proposed structures



→ No literature about these compounds available

→ Could be formed as transformation products from antioxidants or slip agents or introduced in the production process

Estimated toxicity for the sum of the 42 identified compounds



Toxicity estimated by Cramer rules (predicted toxicity based on structure) and literature review

Photoinitiators were the dominant group for high confirmed toxicity:

- ☐ Irgacure 369 well-known for endocrine disrupting effects
- ☐ 4-methylbenzophenone carcinogenicity, reproductive toxicity

→ no concentrations were determined so far-risk of the compounds unknown!

Summary of identified compounds

Plasticizer
Slip agents
Photo initiators

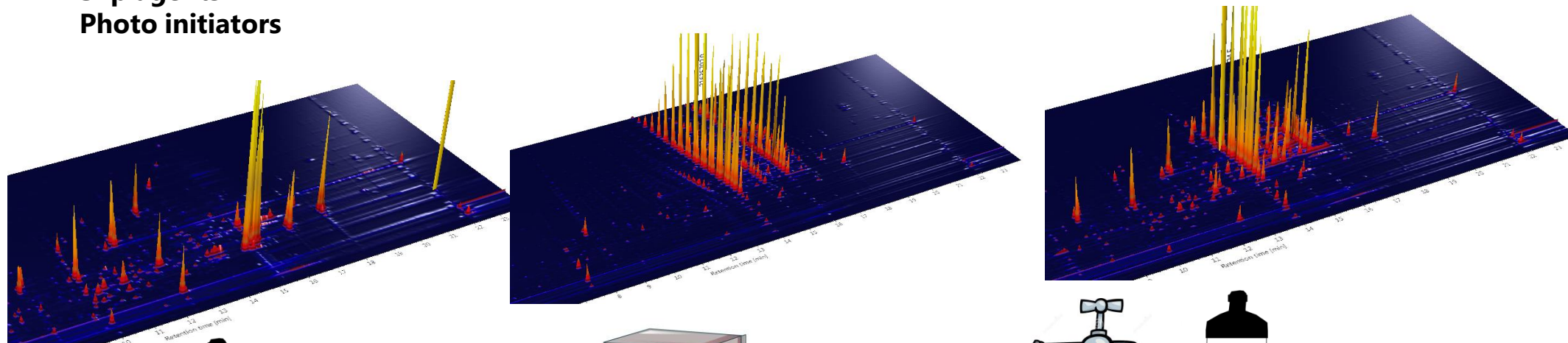
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Surfactants



Drinking water
in reusable bottles

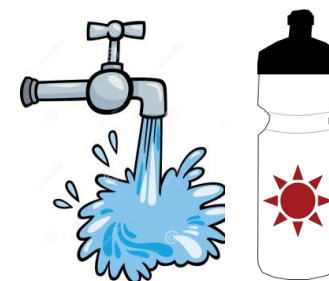
Compounds
migrating into
drinking water



from reusable plastic bottles itself



from dishwasher soap



Remaining compounds after
thoroughly flushing

Conclusion

- Study under real consumer use revealed **thousands of compounds** migrating from the **plastic bottles**- 42 contaminants could be identified
- **Risk** of using these bottles **is unknown** at the current stage- research for quantifying non-target compounds is ongoing in our group
- Are plastic bottles suitable for re-use, especially when they are labelled as biodegradable plastic?

Acknowledgment

ACN Group from the University of Copenhagen



Research Paper

Non-target screening for the identification of migrating compounds from reusable plastic bottles into drinking water

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HIGHLIGHTS

- Migration of > 400 plastic related and > 3500 dishwasher related compounds.
- The dishwashing process increased the migration of plastic related compounds.
- Oligomers suspected from polycaprolactone (PCL) were migrating.
- Three of the identified photoinitiators have possible endocrine disrupting effects.
- Diethyltoluamide (DEET) may have been formed from the plasticizer lauro lactam.

GRAPHICAL ABSTRACT

