

# Non-target screening analyses of organic contaminants in river systems as a base for monitoring measures

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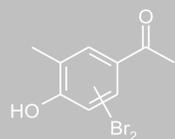
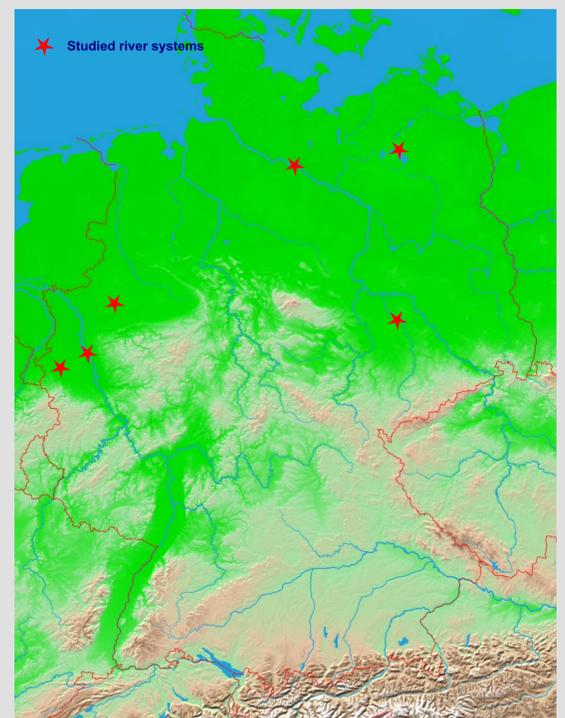
## Aims and Scope

Organic contaminants discharged to the aquatic environment exhibit a high diversity with respect to their molecular structures and the resulting physico-chemical properties. The chemical analysis of anthropogenic contamination in river systems is still an important feature, especially with respect to (i) the identification and structure elucidation of novel contaminants, (ii) to the characterisation of their environmental behaviour and (iii) to their risk for natural systems.

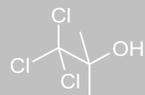
A huge proportion of riverine contamination is caused by low-molecular weight organic compounds, like pesticides, plasticizers, pharmaceuticals, personal care products, technical additives etc. Some of them, like PCB or PAH have already been investigated thoroughly and, consequently, their behaviour in aqueous systems is very well described. Although analyses on organic substances in river water traditionally focused on selected pollutants, in particular on common priority pollutants which are monitored routinely, the occurrence of further contaminants, e.g. pharmaceuticals, personal care products or chelating agents has received increasing attention within the last decade. Accompanied, screening analyses revealing an enormous diversity of low-molecular weight organic contaminants in waste water effluents and river water become more and more noticed. Since many of these substances have been rarely noticed so far, it will be an important task for the future to study their occurrence and fate in natural environments. Further on, it should be a main issue of environmental studies to provide a comprehensive view on the state of pollution of river water, in particular with respect to lipophilic low molecular weight organic contaminants. However, such non-target-screening analyses has been performed only rarely in the past.

## German river systems

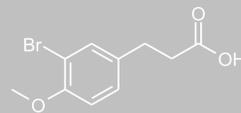
Investigated river systems comprised: Rur, Rhine, Havel/Spree and Mulde rivers. Numerous organic substances have been identified, which can be characterised to be rarely reported, unnoticed or still unknown contaminants. Some of them can act as river specific compounds due to their unique structure and the singular appearance.



Brominated methylhydroxyacetophenones  
(unknown emission source)

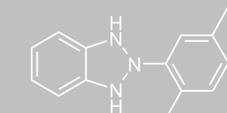
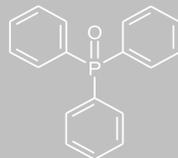


Chlorobutanol (antiseptic)

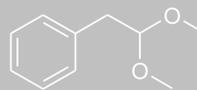


Brominated (methoxyphenyl)propionic acids  
(unknown emission source)

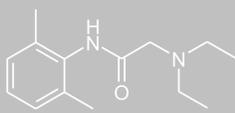
Triphenylphosphine oxide  
(unknown emission source)



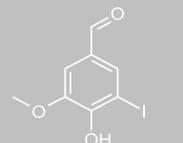
Drometrizol (UV-absorber)



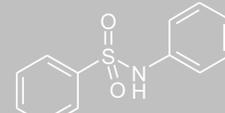
Viridine (fragrance)



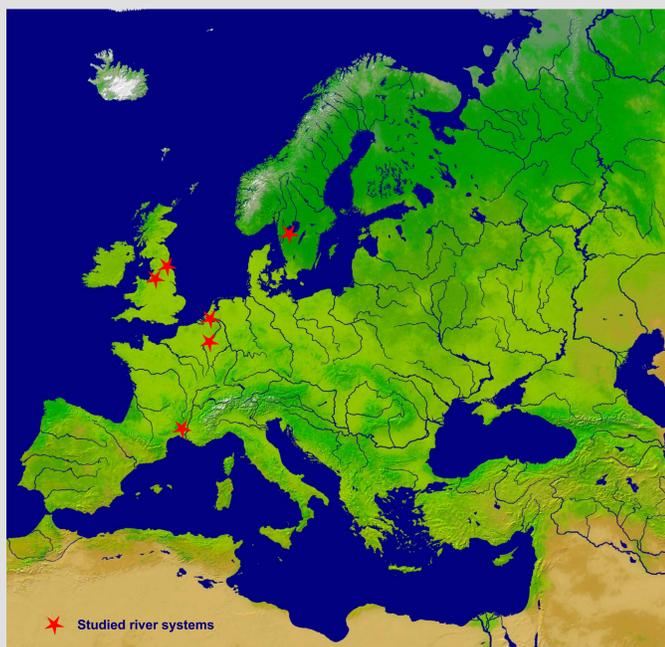
Lidocain (pharmaceutical)



Hydroxyiodomethoxybenzaldehyde  
(unknown emission source)

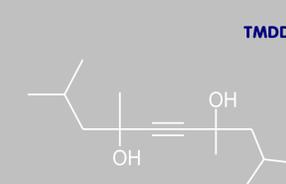


Benzenesulfonic acid N-phenylamide  
(unknown application)

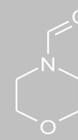


## European river systems

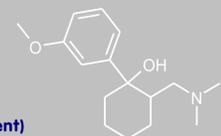
Investigated river systems comprised: Maas, Ems, Göta Älf, Scheldt, Tess, Mersey and Rhône rivers. Also in these river systems numerous organic compounds were identified for the first time as environmental contaminants. Some of these pollutants (e.g. TMDD) appeared concurrently in different European rivers indicating a general and widespread contamination.



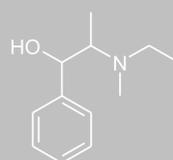
TMDD (surfactant)



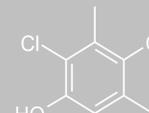
N-Formylmorpholine (solvent)



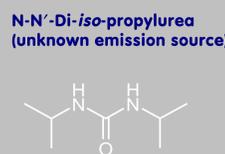
Tramadol (pharmaceutical)



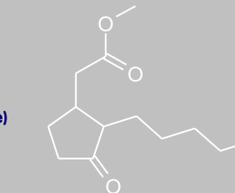
Etafedrine  
(pharmaceutical)



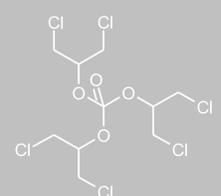
Dichlorodimethylphenol  
(unknown emission source)



N-N'-Di-iso-propylurea  
(unknown emission source)



Dihydrojasmonate (fragrance)



Tris(dichloropropyl)phosphate  
(flame retardant ?)

## Conclusions

The application of extended non-target screening analyses on German and European rivers on the base of GC/MS analyses revealed complex pattern of anthropogenic contaminants comprising a lot of still unnoticed pollutants (e.g. specific sulfones, phosphorous containing substances, nitrogen heterocycles etc.) or still unidentified compounds (such as selected brominated aromatics) of obviously high environmental relevance.

Generally, this investigation demonstrated the need to expand our analytical focus on a broader spectrum of organic contaminants, in particular to build up an adapted base for advanced monitoring studies. Base for such appropriate monitoring measures should be comprehensive and detailed screening analyses to depict the real state of pollution in river systems.