Application of retrospective analyses in identification and monitoring of contaminants of emerging concern

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Analytical approaches

- Traditional targeted screening approach
- Targeted screening with full scan HR-MS

 Non-targeted (nonspecific) screening approach









Targeted screening with full scan HR-MS

Samples extracted and pre-cleaned to cover specific group(s) of compounds

- Good sensivity and reliable identification and quantification of the target compounds
- Suspect screening/retrospective analyses possible (LCMS only with analytical standard available)
- The scope of retrospective analyses limited by sample preparation method



Increasing interest in non-target analyses

Search Web of Science for: Non target* AND mass spectrometry OR non-target* AND mass spectrometry (29 February 2016)



Approx. 5200 publications



Target/Suspect/Non-target screening

Samples extracted to cover widest possible range of compounds. Minimum cleanup to avoid losses

- Allows to detect wide range of compounds in a single analysis,
- but is often less sensitive for some compounds than targeted screening and often not quantitative
- Effective tool in identification of emerging compounds
- Retrospective analyses possible



Storing and processing HR-MS data







Retrospective analysis - The sucralose case

- 2007 NILU was asked about sucralose in environment?
- 2006 NILU analysed PPCPs in environmental samples with LC-HRToF-MS
- New treatment of old raw data revealed sucralose as an environmental







Ruus et al., 2015





Ruus et al., 2015



Conclusions

- Tool for identification and prioritisation of environmental contaminants for routine monitoring
- Supplement to ESBs
- International collaboration:
- NORMAN network:
 - MassBank
 - NormaNEWS
 - Common approach & protocols



Thank you for your attention!

Questions?

