Application of target, suspect and non-target screening approach for a comprehensive characterisation of micropollutants in environmental samples from the Nordic countries

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Norwegian Studies 2013-2014

Target, suspect and non-target screening approach is a good tool for prioritisation of environmental contaminants

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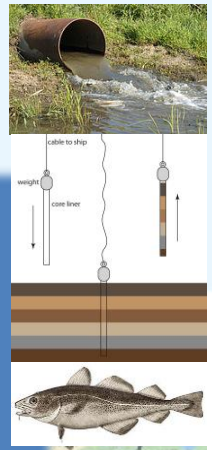
Joint Nordic NTScreening



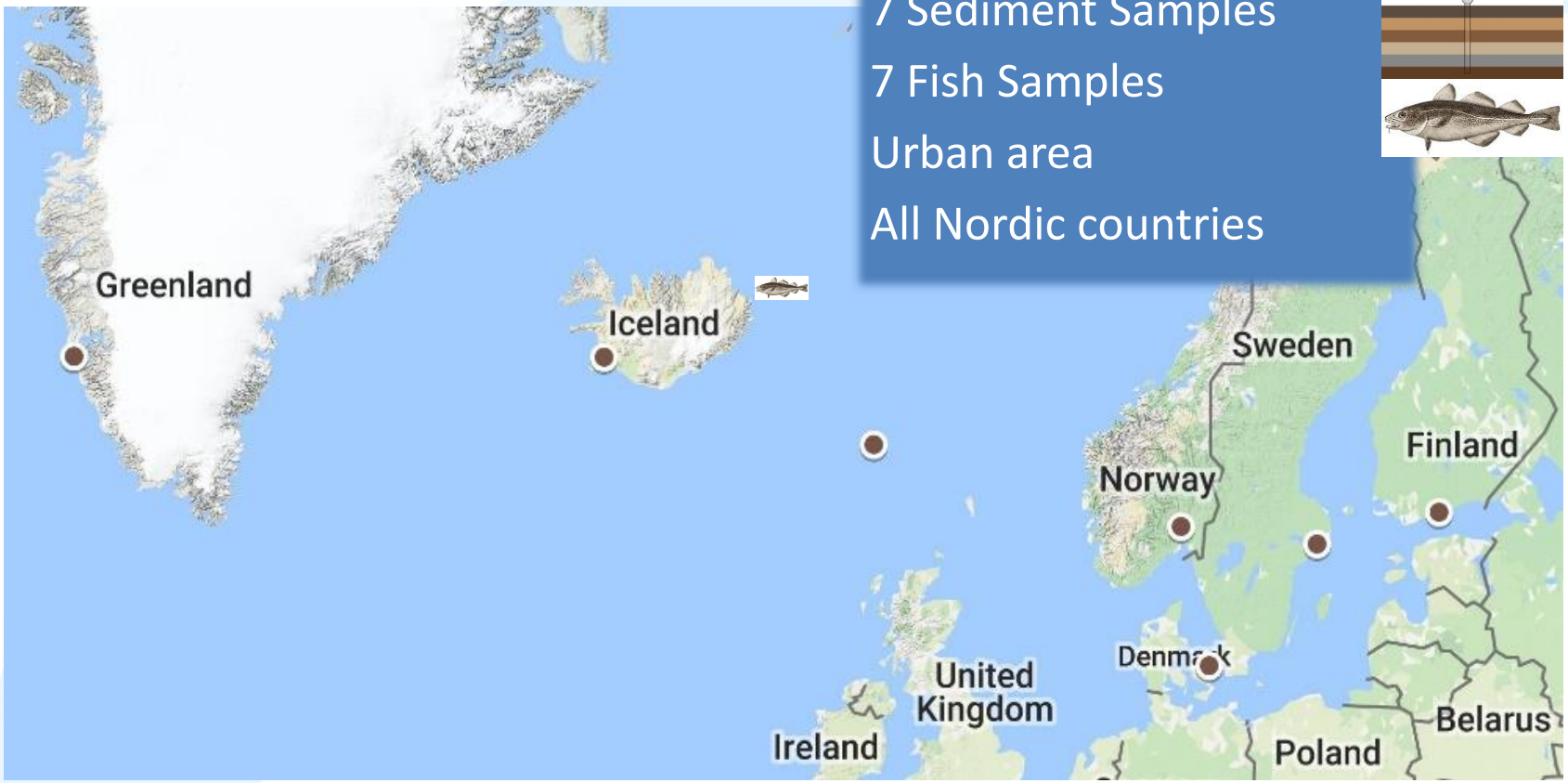
7 Effluent Samples

7 Sediment Samples

7 Fish Samples

Urban area

All Nordic countries



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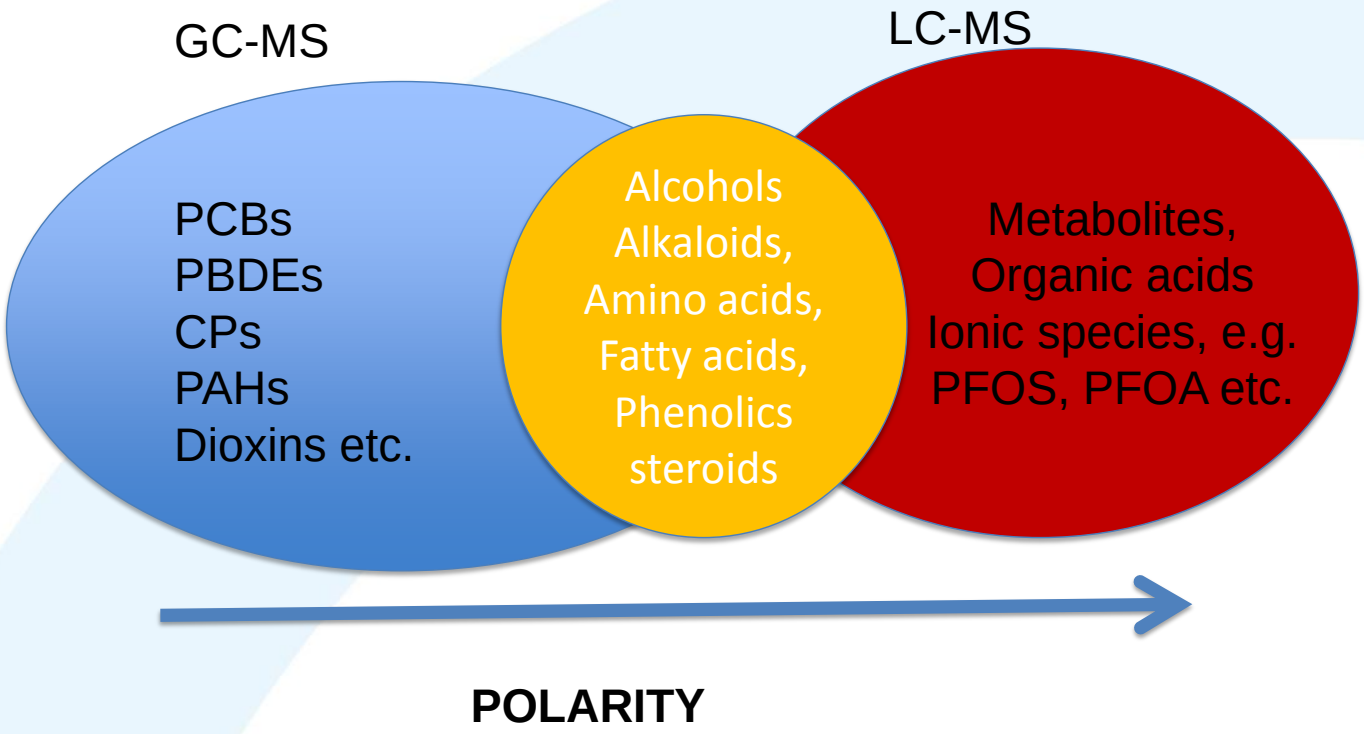
Properties of chemicals and the analytical techniques with which they are the most compatible



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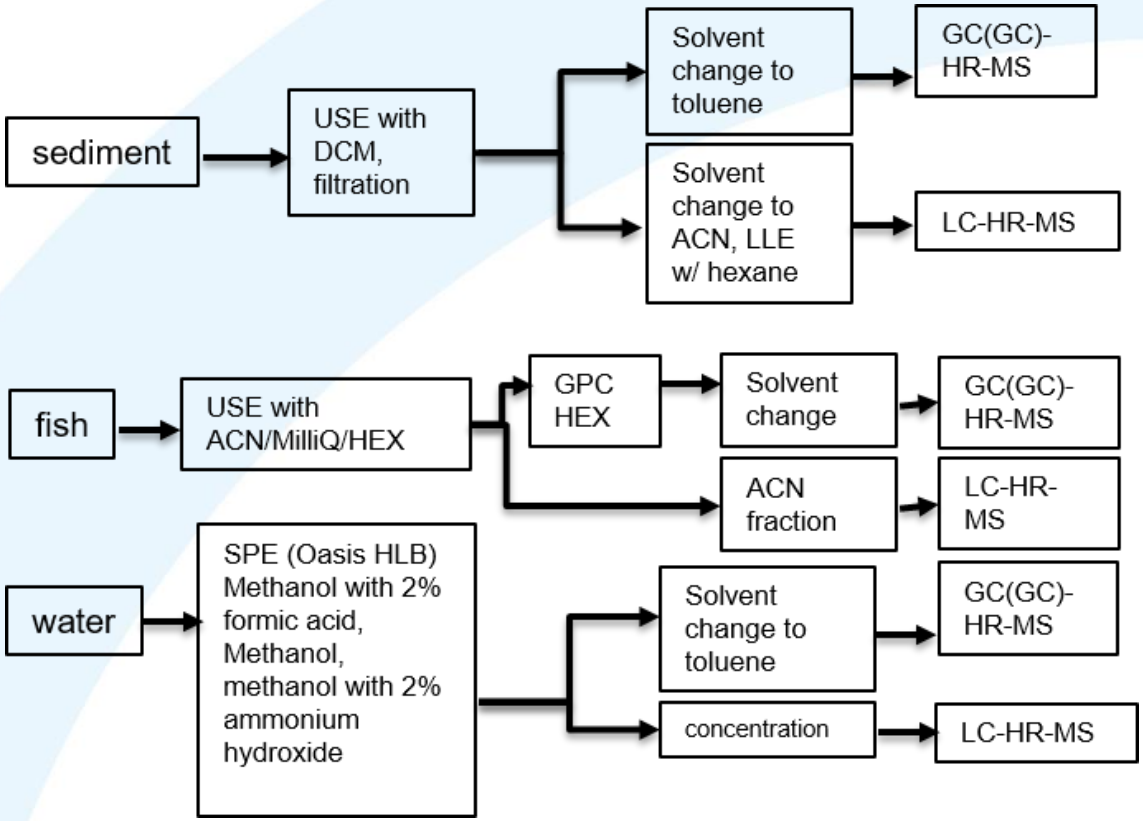
Sample preparation methods



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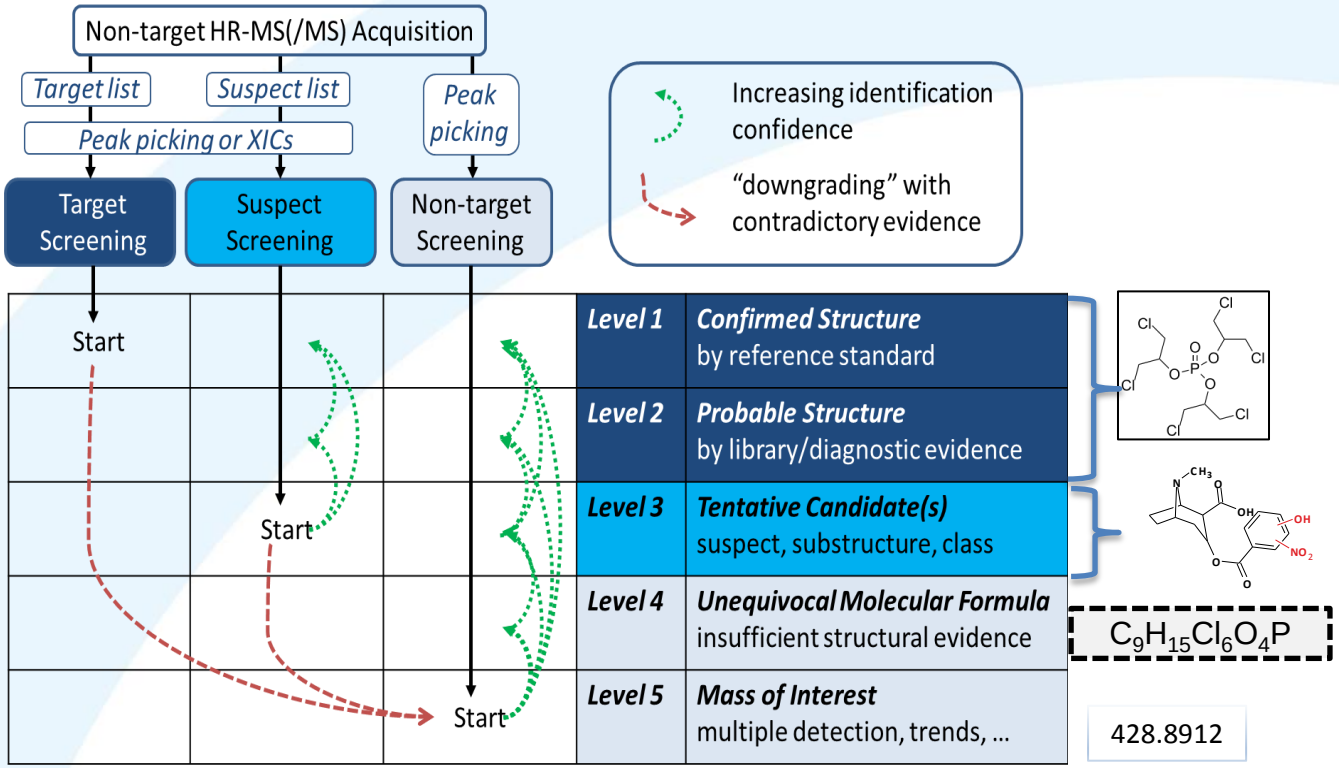
Workflow Norman approach



Adapted from Schymanski et al., 2015

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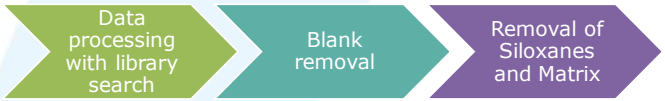
GC-MS

GCxGC-HR-TOF
Ionisation: EI

GC-HR-TOF
Ionisation: NCI

Workflow 1



S/N >10 Tolerance: 200% Classifications

Workflow 2

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LC-MS

LC-HR-QTOF-MS(MS)

ESI+ and ESI-

Pick picking → Suspect screening: vendor databases and Norman suspect lists → Verification with MSMS data → in silico (MetFrag), querying ChemSpider → Confirmation with standards for most interesting compounds

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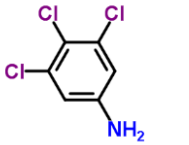
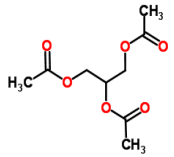
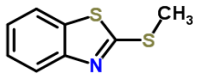
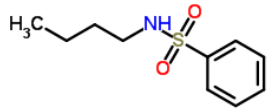
Interesting compounds – Joint Nordic NTS

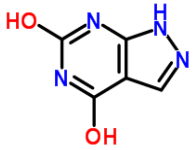
Compound/Compound group	CAS	Matrix	Frequency
PFAS:			
PFHxPA	40143-76-8	Effluent	2
C6/C6-PFPIA	40143-77-9	Sediment	2
Perfluoroctylsulfonamide	754-91-6	Sediment	1
4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,13-henicosafluoro-2-hydroxytridecyl dihydrogen phosphate	94158-70-0	Sediment	1
Halogenated:			
2,3-dichloro aniline	608-27-5	Sediment	1
3,4,5-dichloro aniline	634-91-3	Sediment	1
Natural Cl3Br3-monoterpene		Fish	2
Biocides:			
1-[(1-Butoxy-2-propanyl)oxy]-2-propanol	29911-28-2	Effluent	5
1-[(1-Butoxy-2-propanyl)oxy]-2-propanol	29911-28-2	Fish	1
Triacetin	102-76-1	Effluent	4
Triacetin		Sediment	3
Different bisphenols		All	1-7
Industrial additives:			
2-(Methylthio)benzothiazole	615-22-5	Water, sediment, biota	2-5
N-Butylbenzenesulfonamide	3622-84-2	Effluent	3
PPCPs:			
Oxypurinol	2465-59-0	Fish	5
Lamotrigine	84057-84-1	Effluent	7
Cetirizine	83881-51-0	Effluent	7
Paroxypropione	70-70-2	Fish	5
Carvone	99-49-0	Effluent	5

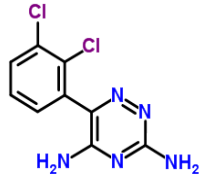












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Summary

- Wide range of compounds detected
- Occurrence in different matrices and in all Nordic countries can be used as a prioritisation factor in planning traditional monitoring campaigns
- Raw data is being stored and is subjected to further analyses

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Thank you for your attention!

Questions?

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