



Miljøministeriet
Miljøstyrelsen

Miljøstyrelsens holdning til ”Non target” og suspect screening

ATV møde
10. maj 2022
Helle Rüzsz Hansen

Miljøstyrelsens syn på sagen i dag

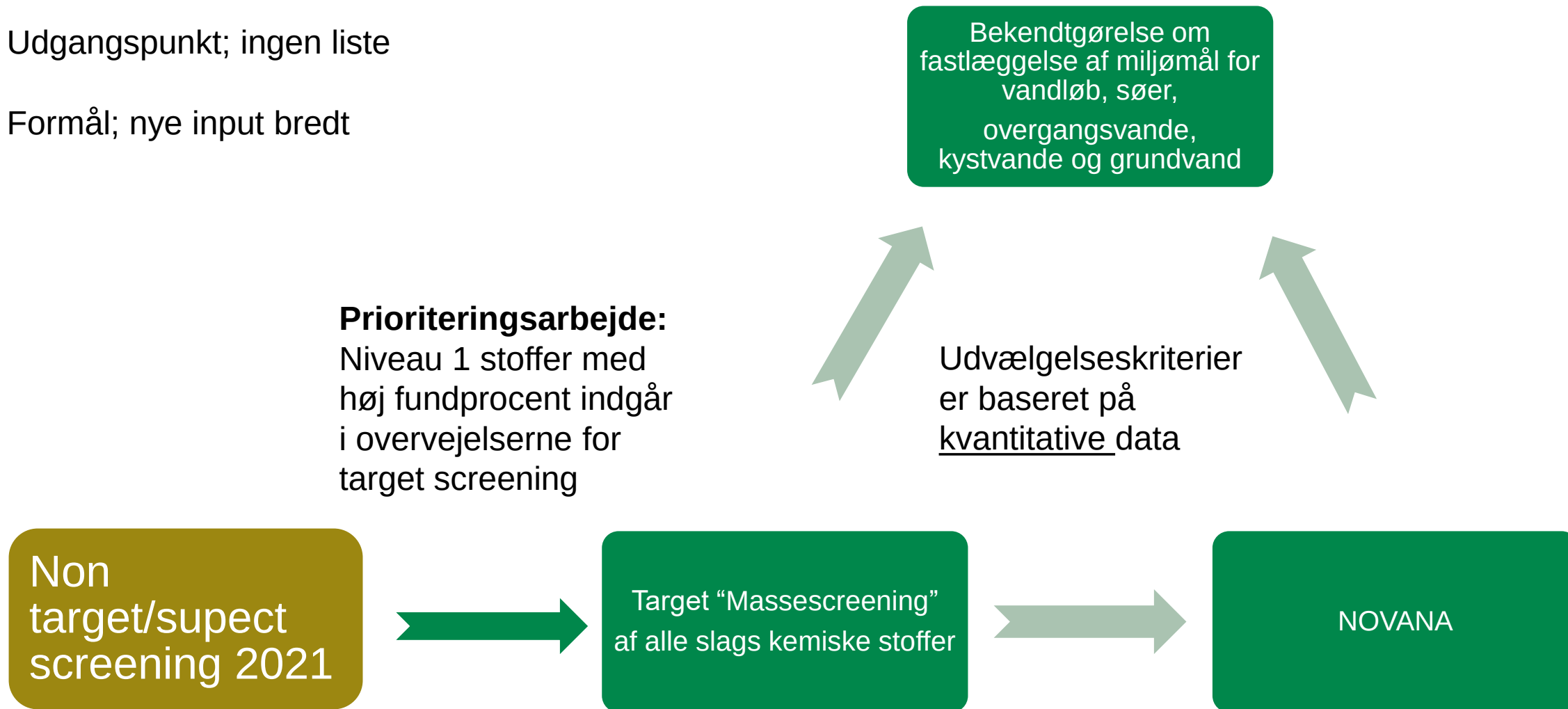
Non target og suspect screening ses som et kvalitativt værktøj, der.....

- **KAN BIDRAGE MED NY VIDEN – MÅLER VI FOR DET RIGTIGE?**
- **Kan bidrage til at afdække hvilke kemiske parametre, der potentielt bør medtages i overvågningsprogrammer, bekendtgørelser og udledningstilladelser.....**
- **Altid bør bekræftes med en opfølgende kvantitativ target analyse**

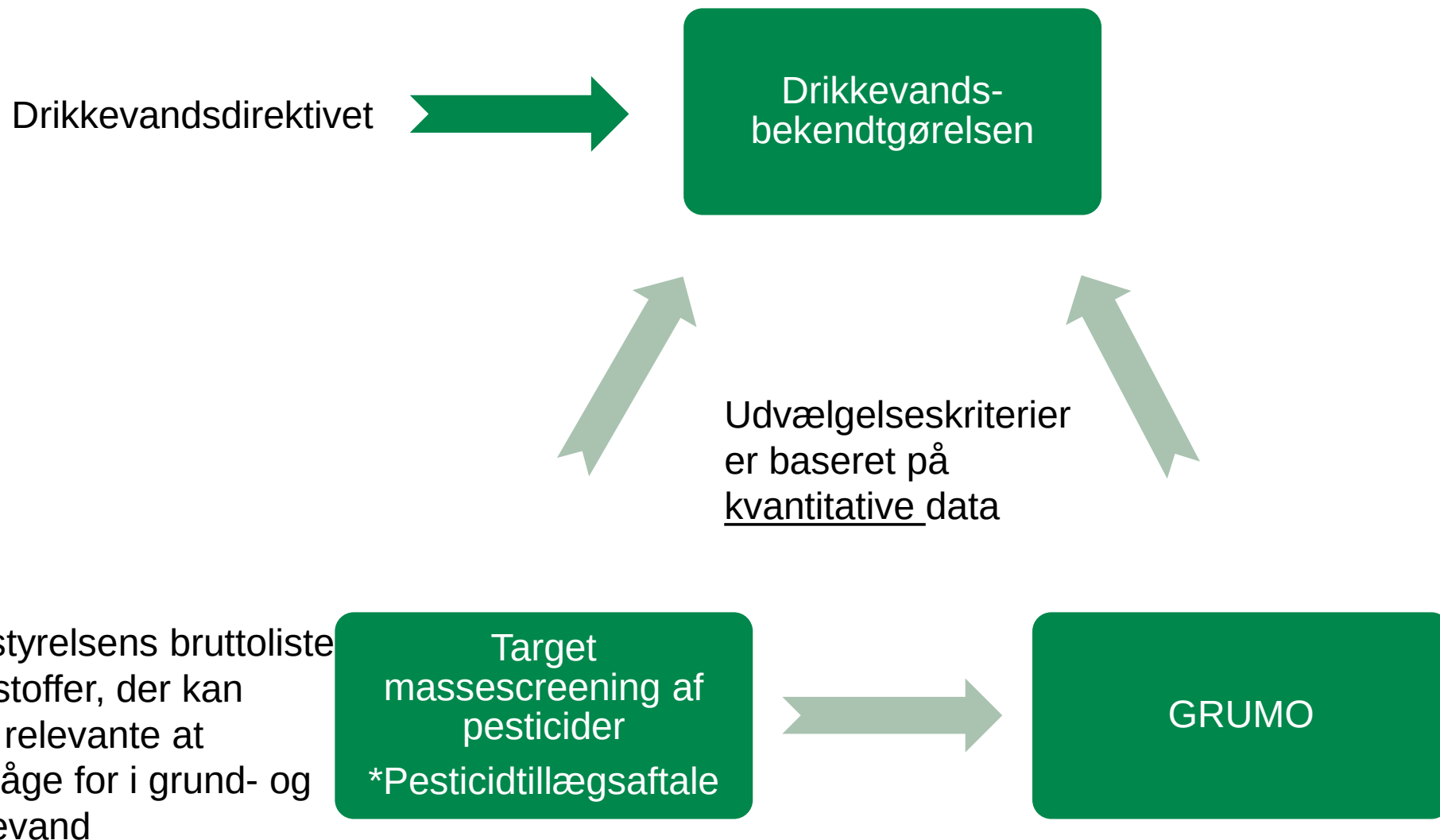
Pilot projekt – strategi på overfladevand

Udgangspunkt; ingen liste

Formål; nye input bredt



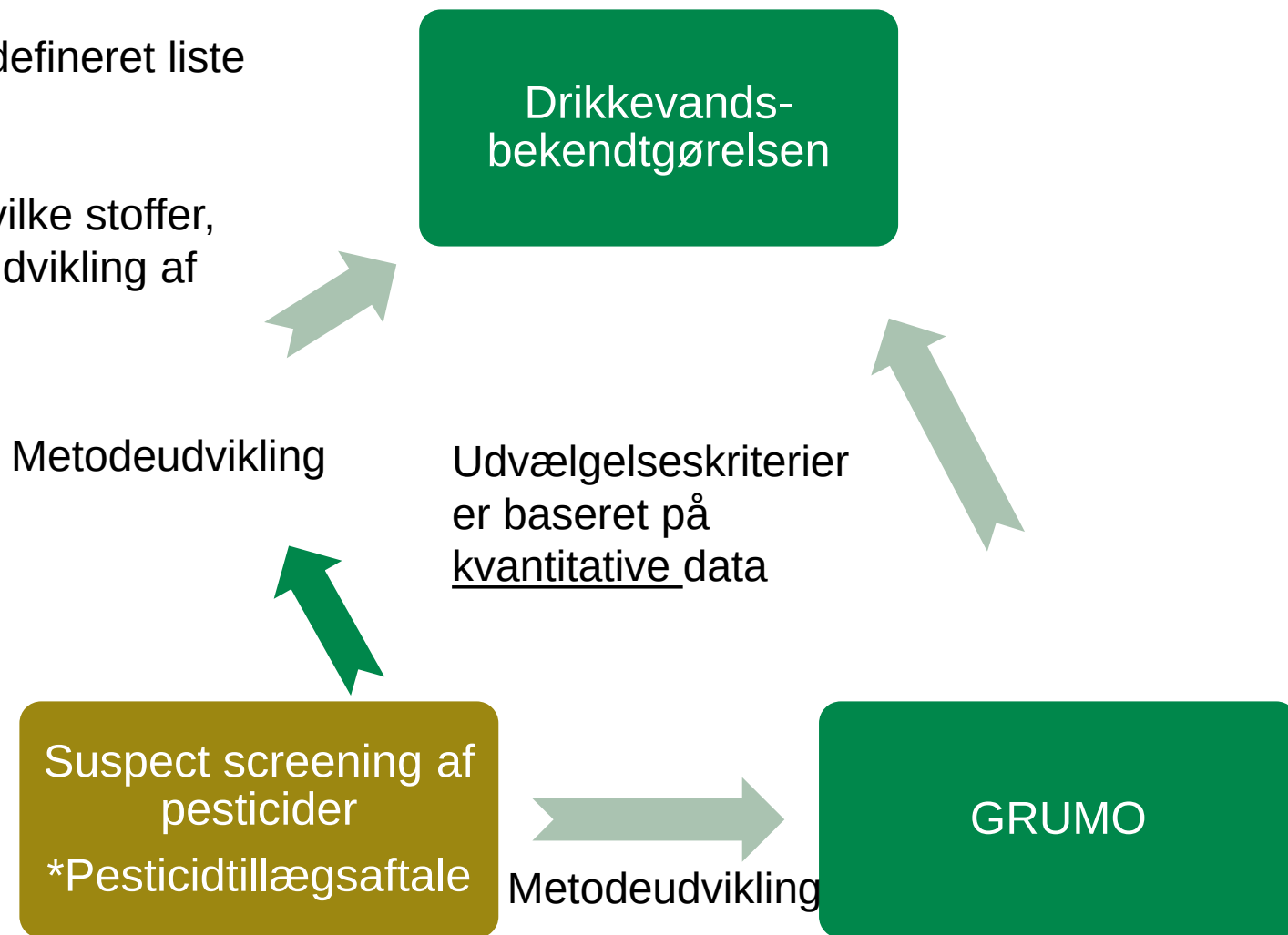
Hvordan kommer kemiske stoffer på Drikkevandsbekendtgørelsens bilag



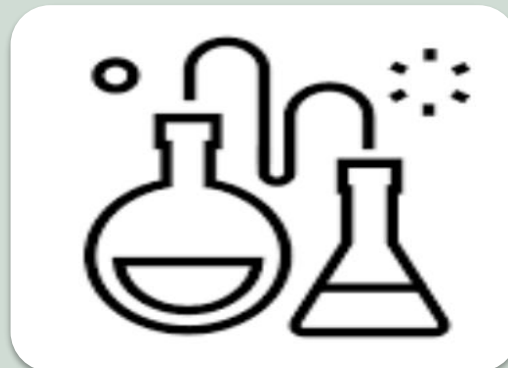
Strategi på grund- og drikkevandsområdet

Udgangspunkt: en defineret liste af relevante stoffer

Formål: Afdække hvilke stoffer, der bør prioriteres udvikling af target-metoder for



Udfordringer set fra Miljøstyrelsen



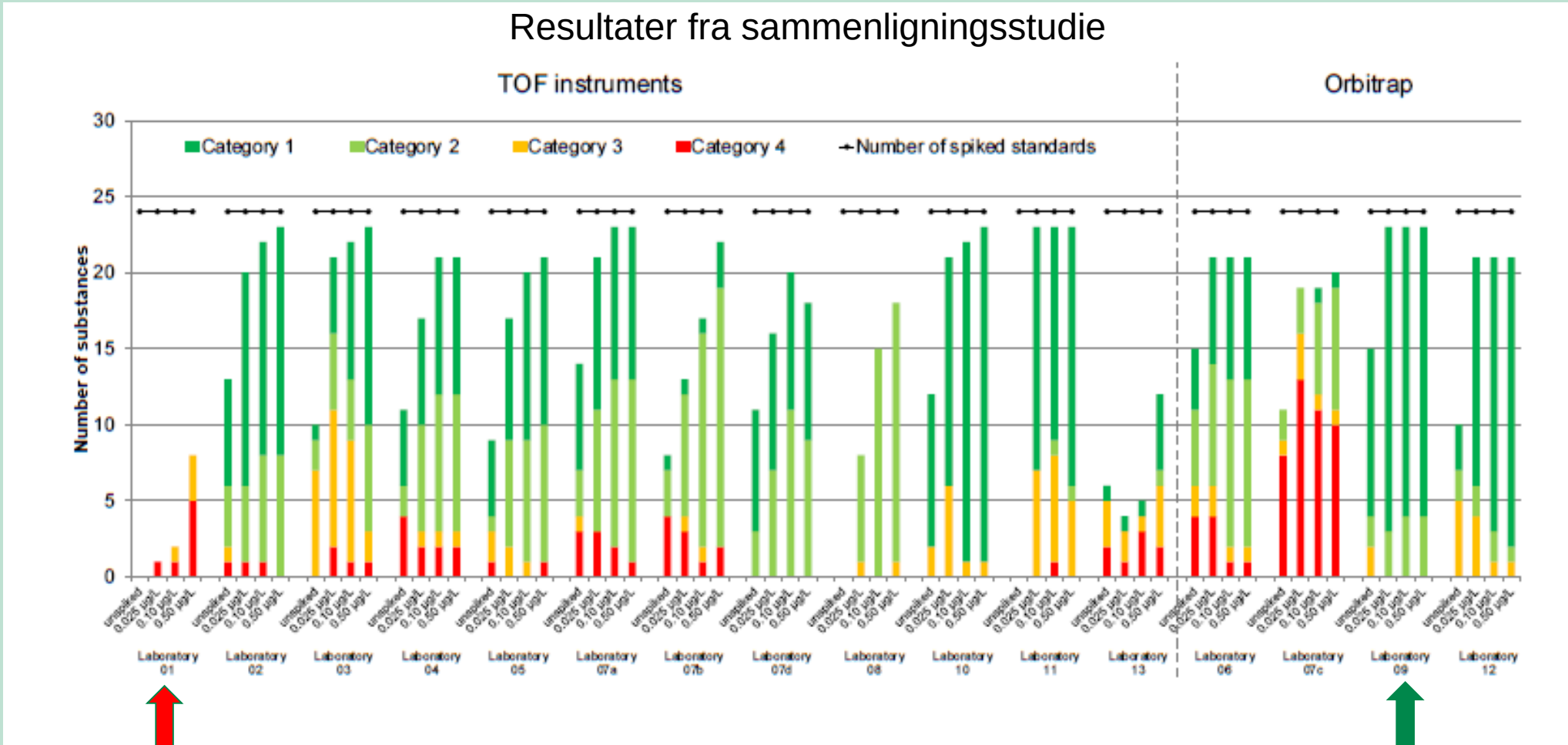
Udbud

Analyse og
data
process-
sing

Report:
Data og
resultater

Handle-
muligheder

Hvordan sikrer vi os, at vi ikke hyrer laboratorie 1?



Kilde: Use of non-target screening by means of LC-ESI-HRMS in water, Water Chemistry Society 2019



Kravspecifikationerne:

Er en udfordring fordi, der er ingen.....

- "plejer"

- ISO/CEN standarder for analyse og afrapportering

- opskrift at hente fra udlandet (forskningssamarbejder uden udbud)

Inspiration er hentet fra metabolomics-området

Bedste udgangspunkt er et rapporteringsværktøjet udviklet til videnskabelige undersøgelser af US-EPA-forskere og andre (<https://nontargetedanalysis.org/srt/>)



BP4NTA
BENCHMARKING AND PUBLICATIONS
FOR NON-TARGETED ANALYSIS

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NTA Study Reporting Tool (SRT)

Want to use the Study Reporting Tool to guide your study design, evaluate your own manuscript, or conduct a peer-review?

You're in the right place! You can download Excel or PDF versions of the SRT on this page. The image below shows a preview of the SRT. In the downloadable versions (available via links above the image), you can use the Scoring dropdown menus to assign color/numeric scores and use the Rationale column to explain your selection. The Excel file also has a tab in which you can easily plot scores from multiple reviewers.

Download the SRT as an Excel file

Note: The Excel file includes the SRT, a plotting functionality to easily view scores from multiple reviewers, and a table that explains the scoring levels.

Download the SRT as a PDF file

Note: The scoring drop-down colors will not work when viewing the PDF in an Internet browser or in Mac Preview – please use a PDF application such as Adobe.

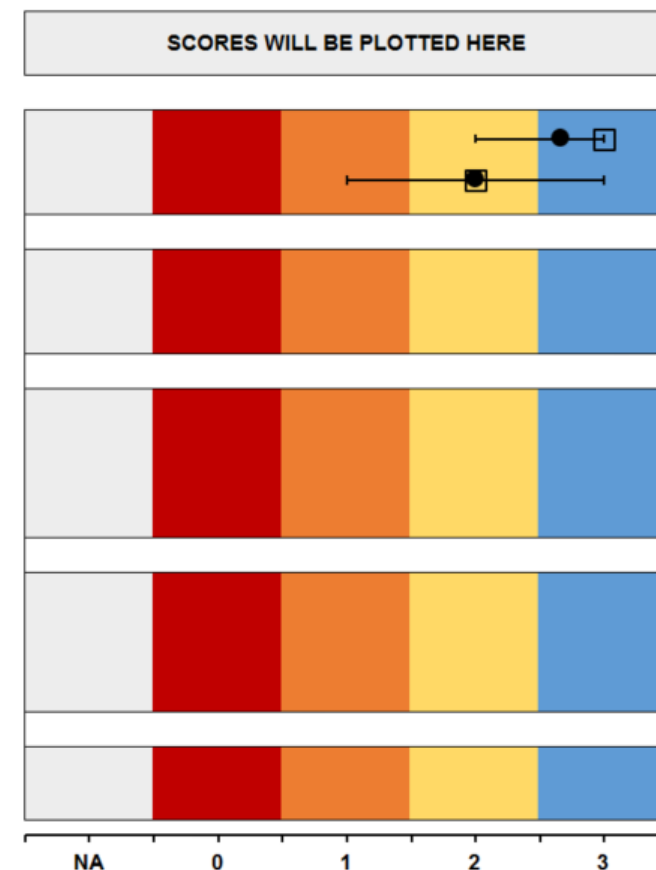
How (and why) to use the
The Non-Targeted Analysis Study Reporting Tool (SRT):
A framework to improve research transparency and reproducibility

Video produced by:
Benchmarking & Publications for Non-Targeted Analysis (BP4NTA) working group
2021

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SRT giver input til at stille krav til analyse og afrapportering.

Section	Category	Sub-Category
Methods	Study Design	1. Objectives & Scope
		2. Sample Information & Preparation
		3. QC Spikes & Samples
	Data Acquisition	4. Analytical Sequence
		5. Chromatography
		6. Mass Spectrometry
	Data Processing & Analysis	7. Data Processing
		8. Statistical & Chemometric Analysis
		9. Annotation & Identification
		10. Quantification
Results	Data Outputs	11. Statistical & Chemometric Outputs
		12. Identification & Confidence Levels
		13. Quantification
		14. Processed data
	QA/QC Metrics	15. Data Acquisition QA/QC
		16. Data Processing & Analysis QA/QC

[illegible]

Katherine T. Peter, Allison L. Phillips, Ann M. Knolhoff, Piero R. Gardinali, Carlos A. Manzano, Kelsey E. Miller, Manuel Pristner, Lyne Sabourin, Mark W. Sumarah, Benedikt Warth, Jon R. Sobus. The Non-Targeted Analysis Study Reporting Tool (SRT): A Framework to Improve Research Transparency and Reproducibility. *Analytical Chemistry*, **2021**. DOI: [10.1021/acs.analchem.1c02621](https://doi.org/10.1021/acs.analchem.1c02621)

Behandlet rådata har fået værdi - retrospektivanalyse

Lai et al. *Environ Sci Eur* (2021) 33:43
<https://doi.org/10.1186/s12302-021-00475-1>

 Environmental Sciences Europe

RESEARCH

Open Access



Retrospective non-target analysis to support regulatory water monitoring: from masses of interest to recommendations via in silico workflows

Adelene Lai^{1,2*} , Randolph R. Singh^{1,3} , Lubomira Kovalova⁴, Oliver Jaeggi⁴, Todor Kondić¹  and Emma L. Schymanski^{1*} 

- Hvem ejer rådata?
- Hvordan sikrer vi os adgang?
- Hvem skal have adgang?
- Hvor skal rådata gemmes?
- Hvilke metadata skal sikres?

Miljøstyrelsen er i dialog med Danmarks Miljøportal om videreudvikling af en løsning startet i et samarbejde med Københavns Universitet

De fortolkede data - resultaterne

Niveau 1

Name	CAS	Concentration (ng/L)		Detection frequency
		Min	Max	
2-Hydroxyatrazine	2163-68-0	0.67	2.50	13%
4-Methylbenzotriazole	29878-31-7	2.32	2.98 · 10 ³	53%
5-Methyl-1H-benzotriazole	136-85-6	138	794	29%
Atenolol	29122-68-7	1.17	66.6	45%
Atrazine	1912-24-9	0.26	0.77	24%
Atrazine-Desethyl	6190-65-4	0.56	4.89	16%
Azoxystrobin	131860-33-8	0.29	0.72	11%
Bentazone	25057-89-0	3.49	61.4	11%
Bicalutamide	90357-06-5	1.87	33.0	26%
Boscalid	188425-85-6	0.17	0.92	50%
Butyl Benzyl Phthalate	85-68-7	4.92	44.6	16%
Caffeine	58-08-2	22.3	2.49 · 10 ⁴	61%
Candesartan	139481-59-7	0.73	3.39	24%
Carbamazepine	298-46-4	0.12	3.69	47%
Cetirizine	83881-51-0	0.11	0.74	39%
Citalopram	59729-33-8	0.12	0.94	26%
Citroflex 2	77-93-0	152	1.69 · 10 ³	32%
Clopidogrel	113665-84-2	0.46	46.2	34%
Cotinine	486-56-6	4.53	16.2	5%
Coumarin	91-64-5	4.89 · 10 ⁵	4.89 · 10 ⁵	3%
Diethyltoluamide (DEET)	134-62-3	0.67	52.8	79%
Dibutyl phosphate	107-66-4	3.38	11.4	21%
Diclofenac	15307-86-5	1.41	75.8	58%
Diffufenican	83164-33-4	0.25	8.2	10%
Dinoseb	88-85-7	1.69	1.7	1%
Dinoterb	1420-07-1	17.9	1	1%
Fexofenadine	83799-24-0	0.12	0.1	0%
Fluconazole	86386-73-4	19.5	1	1%
Fluopyram	658066-35-4	0.53	1	1%
Furosemide	54-31-9	11.3	8	0%
Hydrochlorothiazide	58-93-5	18.6	1	1%
Lamotrigine	84057-84-1	4.89	7.2	1%
Losartan	114798-26-4	0.12	2	2%
MCPA	94-74-6	6.37	2	2%
Mecoprop	93-65-2	6.17	2	2%
Metazachlor	67129-08-2	6.49	6	6%
Metazachlor-ESA	172960-62-2	2.82	4	4%
Metoprolol	51384-51-1	4.98	3	3%
Oxcarbazepine	28721-07-5	1.39	2.4	2%
Propiconazole	60207-90-1	0.11	0	0%
Propranolol	525-66-6	0.19	0	0%
Propyphenazone	479-92-5	0.26	4.22	45%
Prosulfocarb	52888-80-9	0.12	1.56	100%

Niveau 2

Substance	C _{max} (ng/L)	Substance	C _{max} (ng/L)
(-)-Caryophyllene oxide	2.20E+01	Dimethachlor ESA	5.57E+00
(2E)-3-(Dodecylsulfonyl)acrylic acid	1.55E+04	Diphenamid	2.33E-01
(2R)-2,3-Dihydroxypropanoic acid	2.51E+01	DL-Malic acid	4.12E+01
(3β,5α,9α)-3,6,19-Trihydroxyurs-12-en-28-oic acid	4.66E+03	DL-Stachydrine	6.01E+01
(R)-3-Hydroxy myristic acid	4.30E+00	Docosahexaenoic acid	2.21E+04
1-Adamantanamine	4.07E+01	Eicosapentaenoic acid	1.59E+06
1-Phenyl-1H-pyrazole	1.20E+01	Enzacamene	1.78E+04
1,2,3,4-Tetramethyl-1,3-cyclopentadiene	4.03E+02	Ethyl myristate	3.56E+01
10-Hydroxycarbazepine/Licarbazine	8.66E+01	Ethyltriglycol	1.94E+06
10,11-Dihydro-10,11-dihydroxycarbamazepine	8.81E+02	Farnesene	3.04E+00
12-Hydroxydodecanoic acid	9.53E+01	Flecainide	4.02E+01
14(S)-HDHA	4.13E+01	Galaxolidone	6.43E+04
15-deoxy-Δ12,14-Prostaglandin A2	1.39E+01	Gluconic acid	7.78E+01
15(S)-HpEPE	3.68E+02	Glycerol 3-phosphate	3.25E+01
19-Nortestosterone	8.74E+03	Guanosine	2.90E+02
2-[(1S)-1-Hydroxyethyl]-4(1H)-quinazolinone	7.27E+02	Hexadecanedioic acid	5.69E+03
2-Amino-6-methylmercaptapurine	1.85E+03	Hexamethoxymethyl melamine	1.30E-01
2-Azaspiro[4.5]decan-3-one	1.10E+03	Hydrocodone	1.03E+00
2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine (EDDP)	2.95E-03	Hydromorphenol	1.06E+01
	7.97E+00	Hydromorphone	7.19E+00
	2.32E+00	Hydroxyterbutylazine	1.84E+00
	2.56E+02	Ibuprofen	4.47E+06
	8.76E+02	Iminostilbene	2.89E-01
	2.05E+06	Isotretinoin	1.11E+06
	7.49E+01	Ketamine	5.73E+01
	1.14E+02	L-Norleucine	1.29E+04
	5.59E+00	L-Threonine	1.13E+02
	1.22E+03	Limonene-1-OH	1.91E+05
	7.44E+01	Malonic acid	7.09E+00
	3.70E+01	Memantine	7.66E+00
	2.60E+01	Methabenzthiazuron	1.42E+00
	2.39E+01	Methyl cinnamate	1.54E+06
	2.76E+01	Methylphenidate	7.15E-01
	1.36E+01	Myristic acid	2.96E+01
	8.65E+01	N-[(S)-(+)-1-Ethoxycarbonyl-3-phenylpropyl]-L-alanine	1.90E+01
	1.79E+01	N-Acetyl-DL-serine	8.86E+00
	1.91E+05	N-Desmethyltramadol	1.52E+00
	8.92E+00	N-Desmethylvenlafaxine	5.41E-01
3-tert-Butyladipic acid			

Citat af Juliane Hollender:
In our studies for the Swiss federal offices for the environment at the moment only compounds identified with level 1 (reference compounds) trigger further action such inclusion in future monitoring programs.



Handlemuligheder som regulerende myndighed fremadrettet

Der er ikke noget "plejer" ift. regulering pba. "Non target" og suspect screening

- Handlemulighederne ligger derfor ikke fast
- Handlemulighederne afhænger af niveauet for identifikation (identifikationssikkerhed)

Data på niveau 1

- Semikvantitative data
- kan måske understøtte regulering direkte uden yderligere data – fx inkludering af stoffet på drikkevandsbekendtgørelsen eller i GRUMO
- der formodes ikke at være langt til måling ved target metoder

Data på niveau 2

- Kvalitative data
- kan ikke understøtte regulering direkte uden yderligere data
- Anvendes til fx prioritering af, hvilke stoffer, der bør udvikles target analyser for

Spørgsmål?

