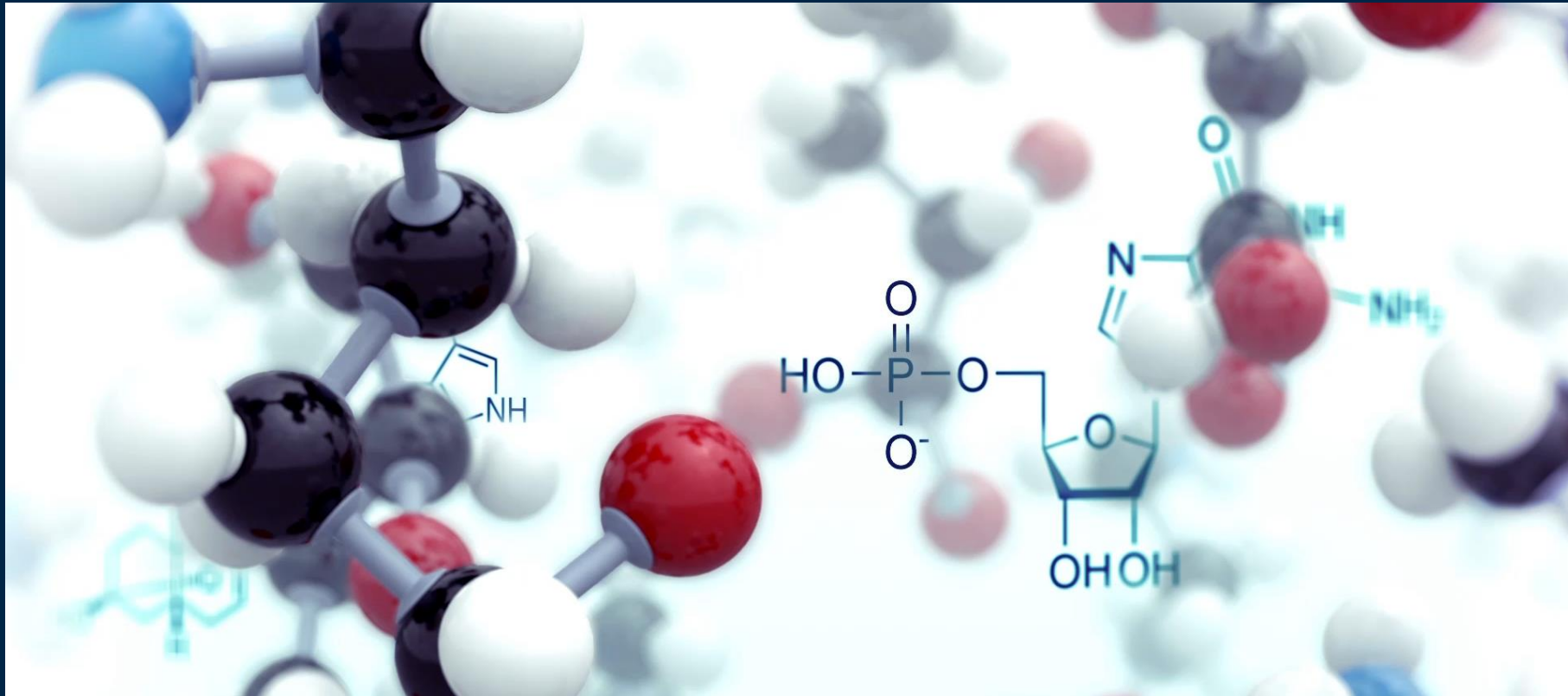


PRIORITIZATION OF CHEMICALS OF CONCERN

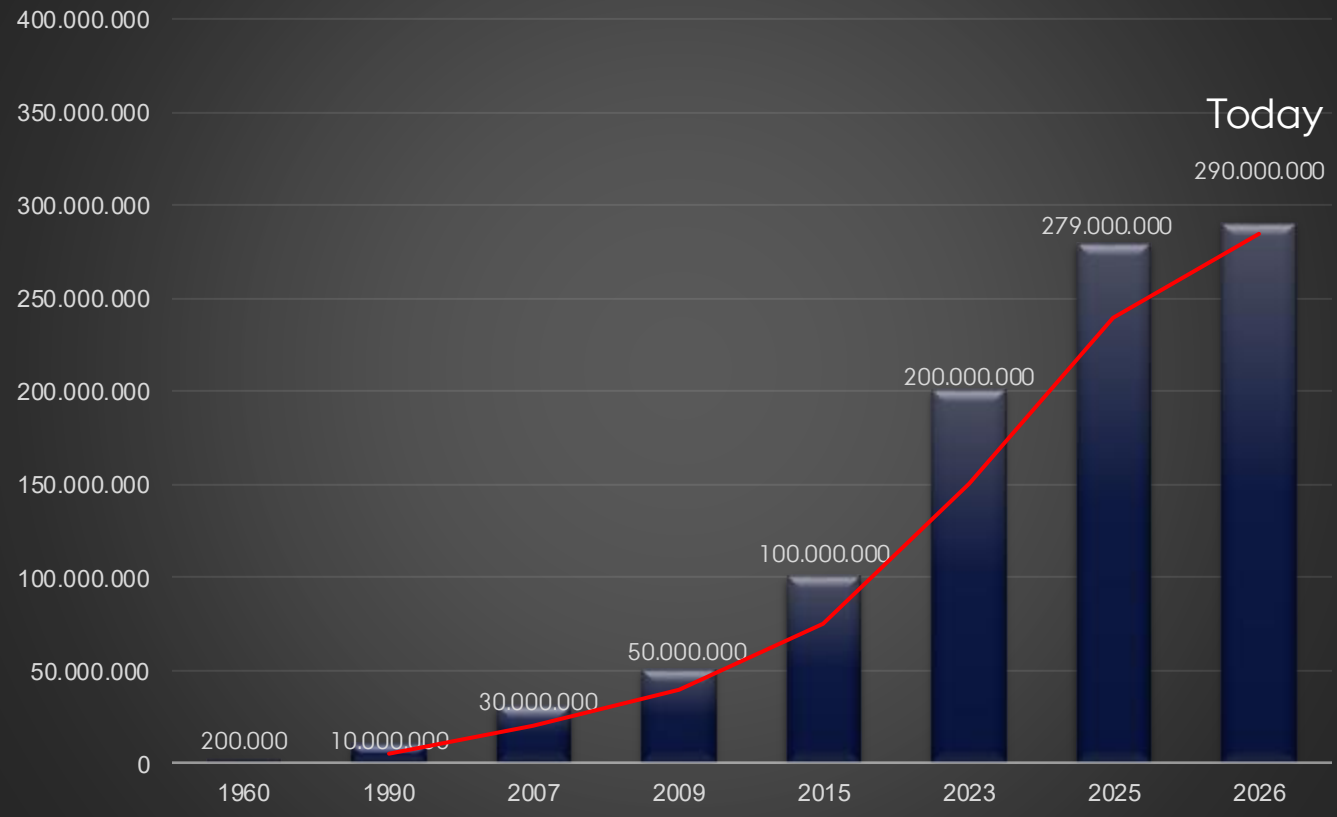


Hans Sanderson



CHEMICAL CONTEXT

Number of substances in CAS Registry

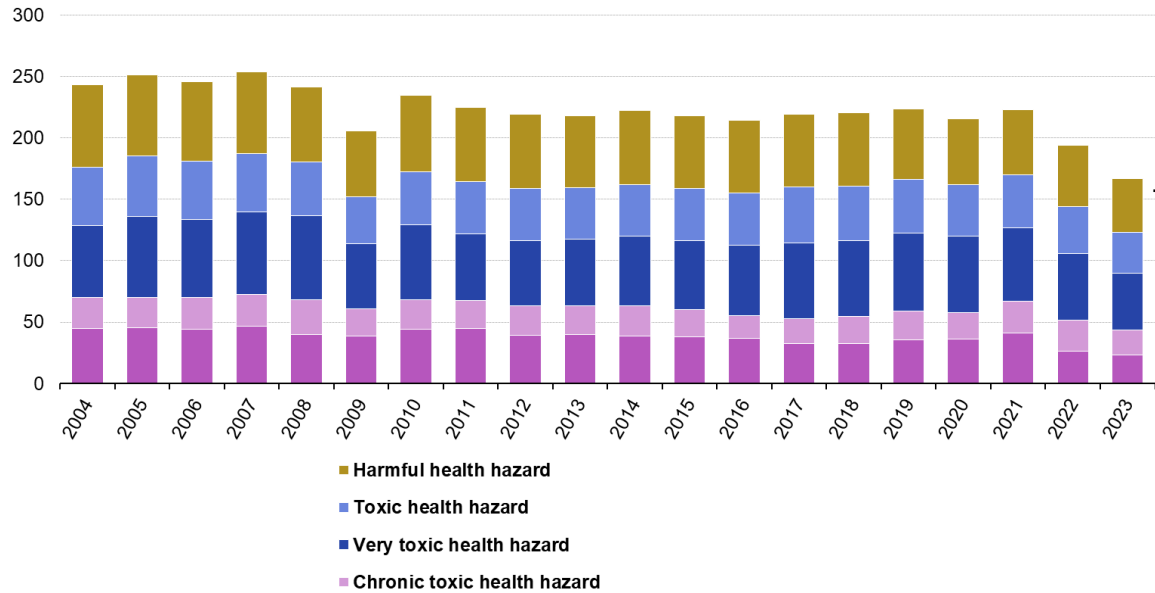


- The global chemical industry was valued at approximately **\$5.5 trillion** in 2022.
- The total volume of chemicals produced globally in 2022 was about **4.1 billion metric tons**.
- The chemical industry accounts for roughly **7%** of the **world's** gross domestic product (**GDP**) and approx. **10%** of **GHG emissions**.
- In 2019, in the WHO European Region, **269 500 deaths** were attributable to exposure to several selected **chemicals**.
- A 2020 Eurobarometer survey showed that **84 %** of Europeans are **worried** about the impact on their **health** of chemicals present in everyday products.

CHEMICAL PROFILE

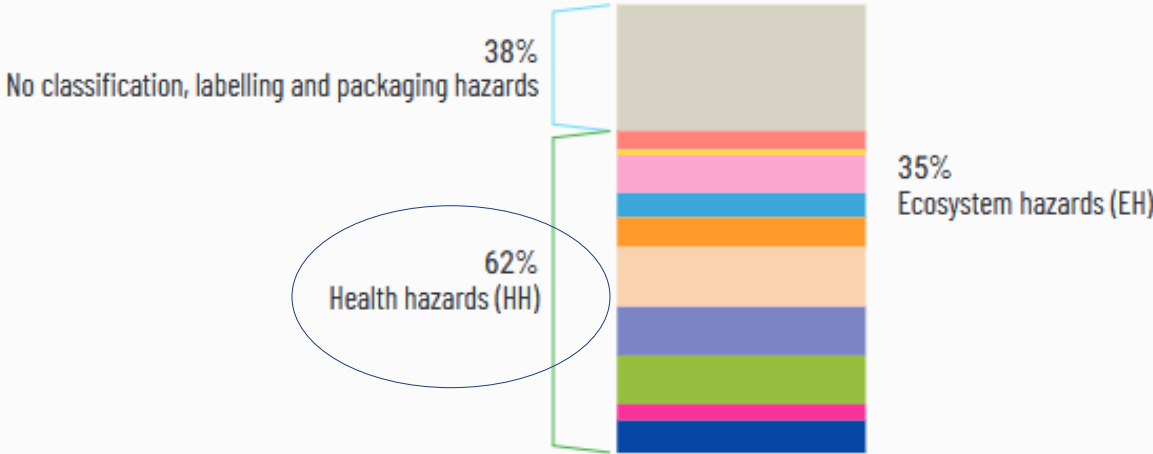


Consumption of chemicals hazardous to health, EU, 2004-23
(million tonnes)

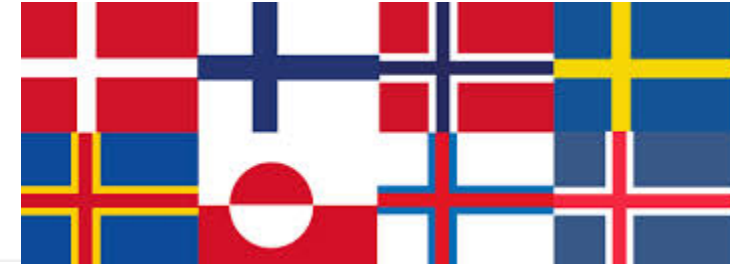


167 million tonnes

Note: The different classes of chemicals are ranked according to their toxicity from the most dangerous (bottom class) up to the least dangerous (top class).
Source: Eurostat (online data code: env_chmhaz)



STUDY OUTLINE



- Funded by the Nordic Council of Ministers (2020-2021) and the DK-EPA (2024-2025):

Study 1) The Nordic countries (SWE; FIN; NOR; DEN) have registered, assessed and monitored chemicals in decades – but what about **new compounds (CECs)**?

Study 2) DK-EPA are we looking for the right active pharmaceutical ingredients (**APIs**)? (Short summary)

Aims:

- Identify knowledge gaps and **monitoring needs** for **new** contaminants of emerging concern (**CECs**) in the **environment** and potentially reaching **people**
- Rank** and **prioritize** the CECs based on an objective **quantitative risk** screening
- Propose monitoring updates across the Nordic countries



PROBLEMATIC COMPOUNDS



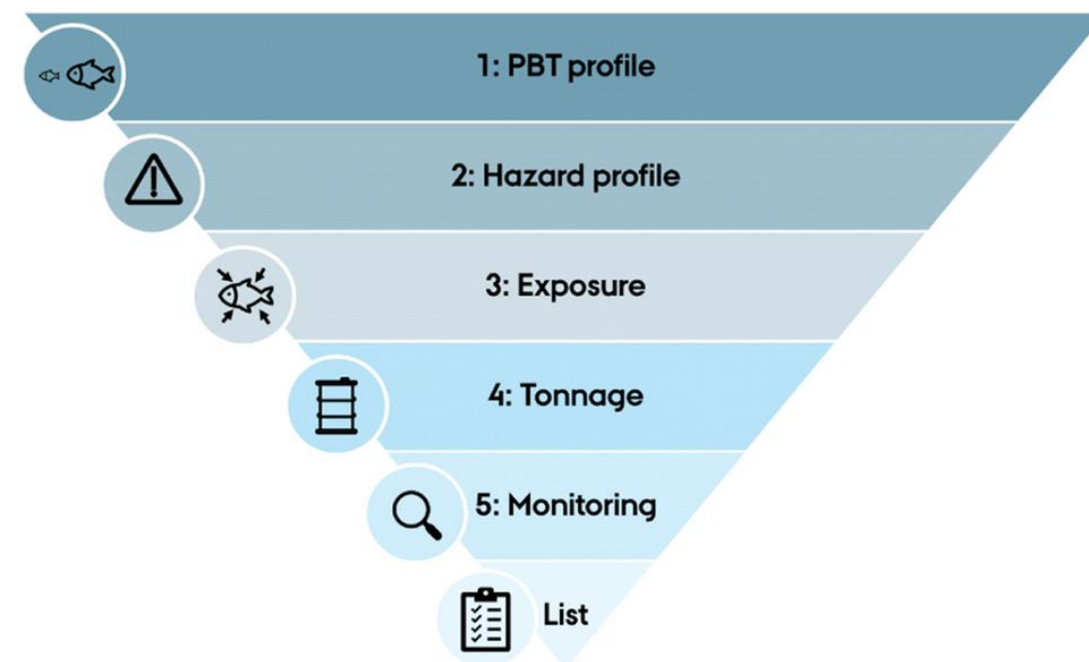
Cite this: RSC Sustainability, 2024, 2, 558

Semi-quantitative risk-based prioritisation scheme for chemicals of concern in the Nordic countries†

Hans Sanderson, * Patrik Fauser, Linda Bengtström and Katrin Vorkamp

Table 1 Lists of chemicals used to generate the initial list of chemicals for the prioritisation scheme as well as weighting factors applied to the scoring in Filter 2

List	Number of entries	Source
REACH article 59 candidate list	194	(https://echa.europa.eu/en/cand
REACH annex XIV authorisation list	55	(https://echa.europa.eu/da/auth
REACH annex XVII restriction list	125	(https://echa.europa.eu/da/subs
Community rolling action plan (CoRAP) list of the european chemical agency (ECHA)	307	(https://echa.europa.eu/da/infor-action-plan/corap-table)
Substitute it now! (SIN) list	761	(https://chemsec.org/buisness-t
List of possible endocrine disrupting compounds (EDC)	430	(https://edlists.org)
Total	1871	
Subtraction of metals and intermediate chemicals	343	
Initial list for prioritisation	1528	



Scoring and weighting of the endpoints

Cut-off values for further consideration/concern

Ranking the most problematic CECs

FILTER 1: PBT PROFILE

- PBT; vPvB;
- Screen compounds on lists - aggregate the score:
 - REACH App. XVII – restricted use list (1p)
 - REACH App XIV – authorization list (1p)
 - REACH Art. 59 – high concern list (1p)
 - CoRAP list – Evaluation list (0.5p)
 - SIN-list of substances of concern (0.3p)
- Scoring **cut-off = 0.7p** all compounds on the lists that qualify proceed to the next filter
- Of the 1528 - **195** compounds advanced to the next tier

The screenshot displays the ECHA CHEM website. At the top, a navigation bar titled "Find SIN List Chemicals In Your Industry" features five icons: a flask for "View all chemicals", a laptop for "Electronics", a shirt for "Textile", a roll of material for "Construction", and a food can for "Food contact materials". Below this, a green banner promotes "Find safer alternatives to hazardous chemicals on chemsec MARKETPLACE" with a "TRY IT NOW" button. The main header includes the ECHA CHEM logo and a notice about the transition from ECHA's public chemicals database. The central area welcomes users to ECHA CHEM, describing it as a public database for REACH, CLP, and POPs. A search bar is provided with the placeholder "Search for substances". On the left, a sidebar lists "Legal obligations" with links to "Restriction list" and "Candidate list", each with a "REACH" icon. On the right, a sidebar lists "Regulatory activities" with links to "Restriction process" and "Identification of substances of very high concern (SVHC)", each with a "REACH" icon.

FILTER 2: HAZARD PROFILE

Same lists scoring the 195 compounds which passed filter 1 relative to 27 different hazard criteria e.g.:

- Toxicity: H410; H411; H413 = 1p. each
- Cancer: H350 & H351 = 1p.
- Known CMR = 3p.
- EDC Cat 1 = 1p.
- EDC Cat 3b = 0.3p.
- On list but with no data at all = 3.5p.
- **Cut-off = 3p.** to advance to next filter
- **53** compounds advanced

Endocrine
Disruptor
Lists

<https://edlists.org/>



FILTER 3: EXPOSURE SCREENING

Substance

Cas no: 50-32-8

Name: BENZO[a]PYREN

EC no: 200-028-5

EXPOSURE

Country	Latest Year	Quantity (max: 5)	Use Index (UI, max: 5)						Range of Use (RoU, max: 5)	Article Index (AI, max: 3)
			Surface water	Air	Soil	Waste water	Consumer	Occu-pational		
DK	2018	1	2	2	3	3	3	4	2	3
NO	2018		3	3	3	4	5	4	2	3
SE	2018	4	2	3	3	2	5	4	2	3

norden

- **Article Index:** Gives indications if a substance may end up in the environment
- **Quantity Index:** Is based on the **amount** of annually consumed
- **Aggregate** exposure scores (0-18p)
- **10 exposure points → 4p = cut-off**
- **23 compounds** passed filter 3

Welcome to the SPIN website

SPIN is a database on the use of Substances in Products in the Nordic Countries. It is a public accessible database, which can be used free of charge.

You can find information on the chemicals that are used in the Nordic countries. The information includes quantities, industries in which it is used (NACE and national) and the function it is used for (USE Category).

START BROWSING AND SEARCHING THE DATABASE

DOWNLOAD OFFLINE DATABASE

The database is based on data from the Product Registries of [Norway](#), [Sweden](#), [Denmark](#) and [Finland](#).

The database is financed by the Nordic Council of Ministers Chemical Group.

Please send us an e-mail should you encounter any issues.

News

New report on dangerous substances

A new report on dangerous substances is now available at our website. The report is a follow-up on a previous work on trying to identify CAS numbers for generic groups of substances on the harmonized list in annex I to directive 67/548/EEC, now Annex VI to the CLP Regulation 1272/2008/EU. This was published in the form [...]

Posted in [News](#), [Uncategorized](#) | Comments Off on New report on dangerous substances

FILTER 4: TONNAGE

Total use

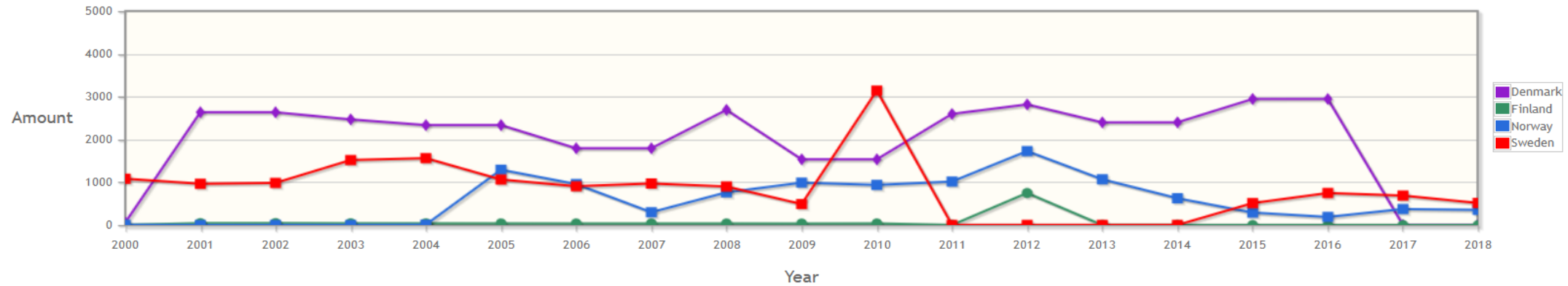
Index

Amount

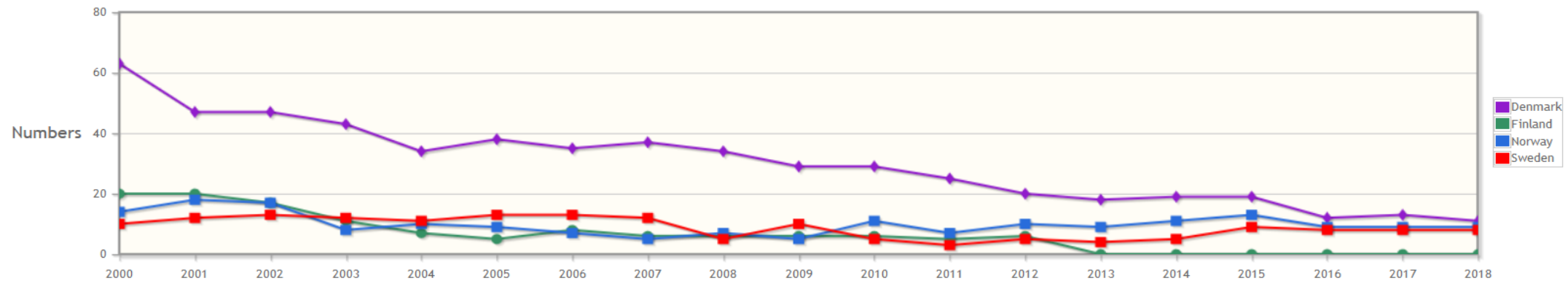
Number

Cas No: 50-32-8 & Name: BENZO[a]PYREN

Total amount of substance in tonnes



Total Number of preparations



SPIN
Substances in Preparations in Nordic Countries

Database | Resources | Download | Contact | Userguide

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News

New report on dangerous substances

A new report on dangerous substances is now available at our website. The report is a follow-up on a previous work on trying to identify CAS numbers for generic groups of substances on the harmonised list in areas in Annex II of REACH. The report is available in the form of a PDF document. The report is published in the form of a PDF document. The report is published in the form of a PDF document.



FILTER 5: MONITORING

- Reviewed the **23 compounds** which also passed the fourth filter if they appear in any **national monitoring** or have been reported in **WoS**:
 - Looked for within this decade (1p)
 - Looked for in this year (1p)
 - Looked for 2+ locations (1p)
 - More than 2 matrices (1p)
 - Looked for less than 50 times (3p)
 - No data at all (7p)
- **Cut-off = 3p**



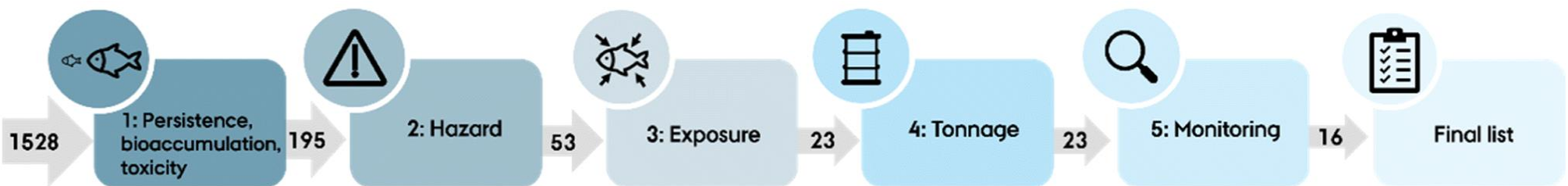


Table 13. Name, CAS and EC-number and total scoring points of 16 proposed chemical candidates for screening.

CAS Number	EC Number	Name	PBT	Total points Hazard (not weighted Haz- ard lists)	Total points Hazard (weighted Hazard lists)	Total points Exposure	Total points Quantity	Total points Environmental Monitoring	Final points - total sum
26471-62-5	247-722-4	m-tolylidene diisocyanate	0.7	6	3	7	6	7	23
2451-62-9	219-514-3	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	0.7	5.4	5.4	5	5	7	22.4
96-69-5	202-525-2	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	0.7	4.6	2.3	6	6	7	21.3
101-68-8	202-966-0	4,4'-Methylenediphenyl diisocyanate	0.7	5	5	7	6	2	20
75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	0.7	3.5	1.75	6	5	7	19.75
98-29-3	202-653-9	4-tert-butylpyrocatechol	0.7	3.2	1.6	6	5	7	19.6
628-96-6	211-063-0	Ethylene dinitrate	0.7	3	1.5	5	6	7	19.5
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	0.7	4.8	2.4	5	5	7	19.4
2814-77-9	220-562-2	Pigment Red 4	0.7	4.5	2.25	4	5	7	18.25
110-88-3	203-812-5	1,3,5-trioxane	0.7	3.9	1.95	5	3.5	7	17.45
693-21-0	211-745-8	Oxydiethylene dinitrate	0.7	4.3	2.15	4	3.5	7	16.65
2425-85-6	219-372-2	Pigment Red 3	0.7	4.5	2.25	6	5	3	16.25
127-18-4	204-825-9	Perchloroethylene; tetrachloroethylene	0.7	5.9	2.95	6	5	2	15.95
81-15-2	201-329-4	Musk Xylene	1	4	4	5	3.5	2	14.5
79-94-7	201-236-9	Tetrabromobisphenol A (TBBPA)	0.7	3.6	1.8	5	5	2	13.8
4979-32-2	225-625-8	N,N-dicyclohexylbenzothiazole-2-sulphenamide	0.7	4.1	2.05	4	3.5	2	11.55

≥100 000 tonnes per annum in EU – hydrolyses to TDA in water

Take Home: 62% - no measurements or monitoring in Nordic

Need to consider fate properties -
#1 – hydrolyses quickly
#2 does not

SUBSTANCE SELECTION (API)

RSC
Sustainability

PAPER

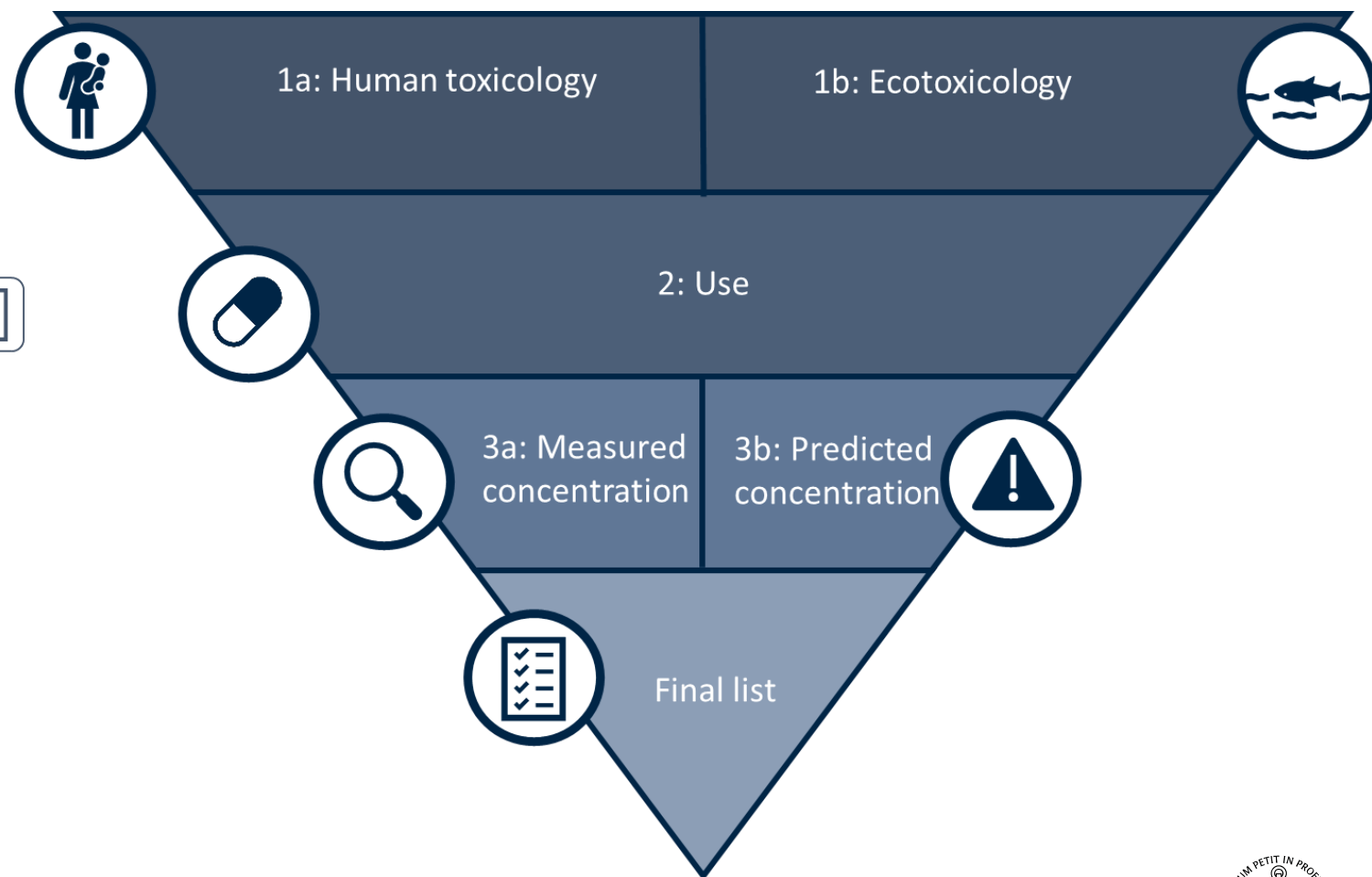
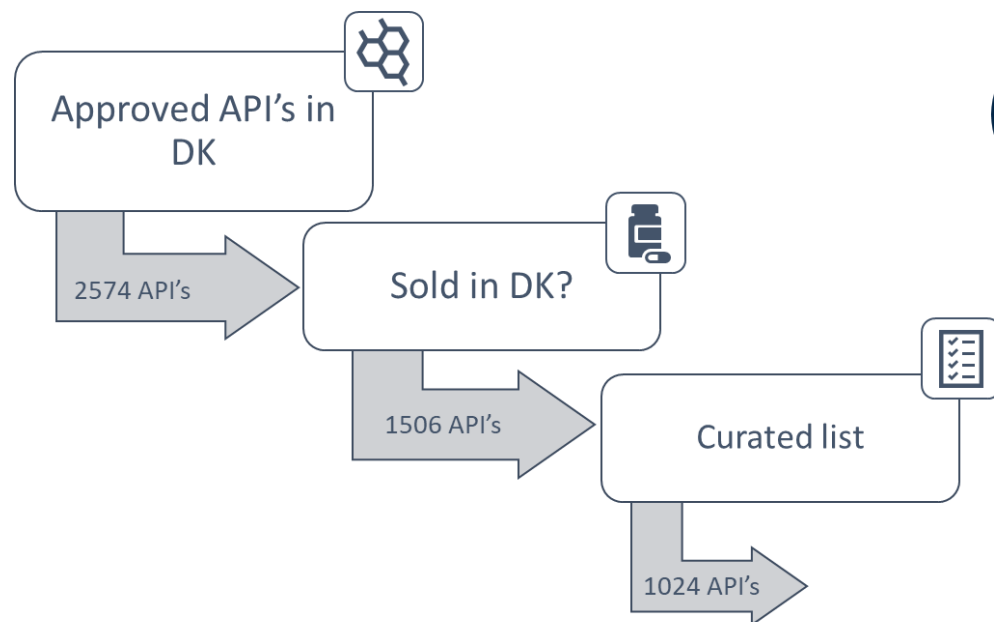
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Cite this: DOI: 10.1039/d5su00120j

Comprehensive prioritisation scheme for active pharmaceutical ingredients in Denmark

Hans Sanderson,¹* Linda Bengtström,² Patrik Fauser,³ Pedro N. Carvalho,⁴ Kai Bester,⁵ Martin Hansen,⁶ Mulatu Y. Nanusha⁷ and Pia Lassen⁸



TOP-15

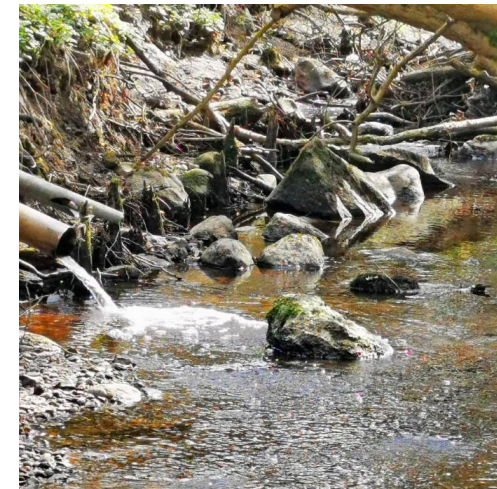
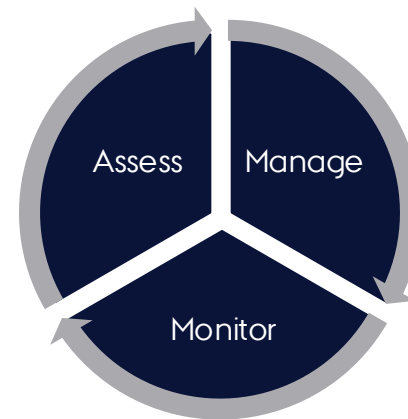
Take-homes:

- ❖ 50% of the top-six are on the EU list – never measured in DK
- ❖ >50% of top-15 - never measured in DK
- ❖ >80% of top-50 - never measured in DK

Preferred name	CAS Number	Therapeutic use	Comment - Therapeutic use	Total score	Analysed in DK?	On the EU watch list?
Metformin	657-24-9	Drugs Used In Diabetes	Antihyperglycemic (lowers blood sugar levels)	162,3	No	Yes
Estradiol	50-28-2	Sex Hormones And Modulators Of The Genital System	Female steroid hormone	150,0	Yes	No
Trimethoprim	738-70-5	Antibacterials For Systemic Use	Antibiotic	144,6	Yes	Yes
Carbamazepine	298-46-4	Antiepileptics	Anticonvulsant medication	144,2	Yes	No
Clindamycin	18323-44-9	Antibacterials For Systemic Use	Antibiotic	125,4	No	Yes
Miconazole	22916-47-8	Stomatological Preparations	Antifungal	124,3	No	Yes
Diclofenac	15307-86-5	Other Dermatological Preparations	Nonsteroidal anti-inflammatory drug (NSAID)	91,6	Yes	No
Amoxicillin	26787-78-0	Antibacterials For Systemic Use	Antibiotic	90,2	Yes	No
Warfarin	81-81-2	Antithrombotic Agents	Anticoagulant (blood thinner)	81,4	Yes	No
Tiotropium bromide	136310-93-5	Drugs For Obstructive Airway Diseases	Anti-asthmatic	80,6	No	No
Metoprolol	51384-51-1	Beta Blocking Agents	Treat high blood pressure (hypertension)	80,0	Yes	No
Diazepam	439-14-5	Psycholeptics	Benzodiazepine (anxiolytic)	79,6	No	No
Sertraline	79617-96-2	Psychoanaleptics	Anti-depressant (Selective serotonin reuptake inhibitor (SSRI))	79,4	Yes	No
Midazolam	59467-70-8	Psycholeptics	Benzodiazepine (anxiolytic)	78,0	No	No
Lisinopril	76547-98-3	Agents Acting On The Renin-Angiotensin System	Treat high blood pressure (hypertension)	75,8	No	No

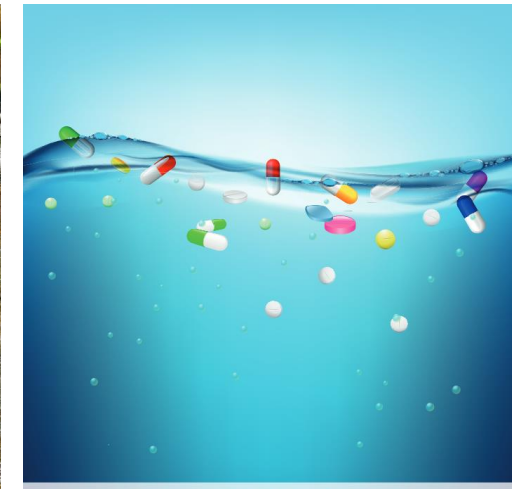
CONCLUSIONS

- ❖ Dose-makes –the-poison – exposure alone is not enough – need **risk-based approach** (DWD)
- ❖ Use of non-target screening – combine with High-Through-Put New Approach Methods (**NAMs**) and AI → **risk-based prioritization**
- ❖ Risk-based approach to the **0.1 µg/L** value on non-relevant **pesticide metabolite** value?
- ❖ New monitoring compounds; 17-Beta-estradiol and NPE and PFAS sum and PFAS total (DWD)
- ❖ Human health risk-approach – toxicological values (**EQS**)
- ❖ Treatment and cleaning of tap water (cost...)?



PRIORITIZATION OF EMERGING CONTAMINANTS FOR A NORDIC SCREENING STUDY

Scientific Report from DCE - Danish Centre for Environment and Energy No. 444 2021



RISK-BASED PRIORITIZATION OF ACTIVE PHARMACEUTICAL INGREDIENTS IN DANISH SURFACE WATERS FOR FUTURE MONITORING

Scientific Report from DCE - Danish Centre for Environment and Energy No. 401 2024

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Thank you for your attention

I wish to acknowledge my co-workers
as well as the NCM and DK-EPA for funding



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