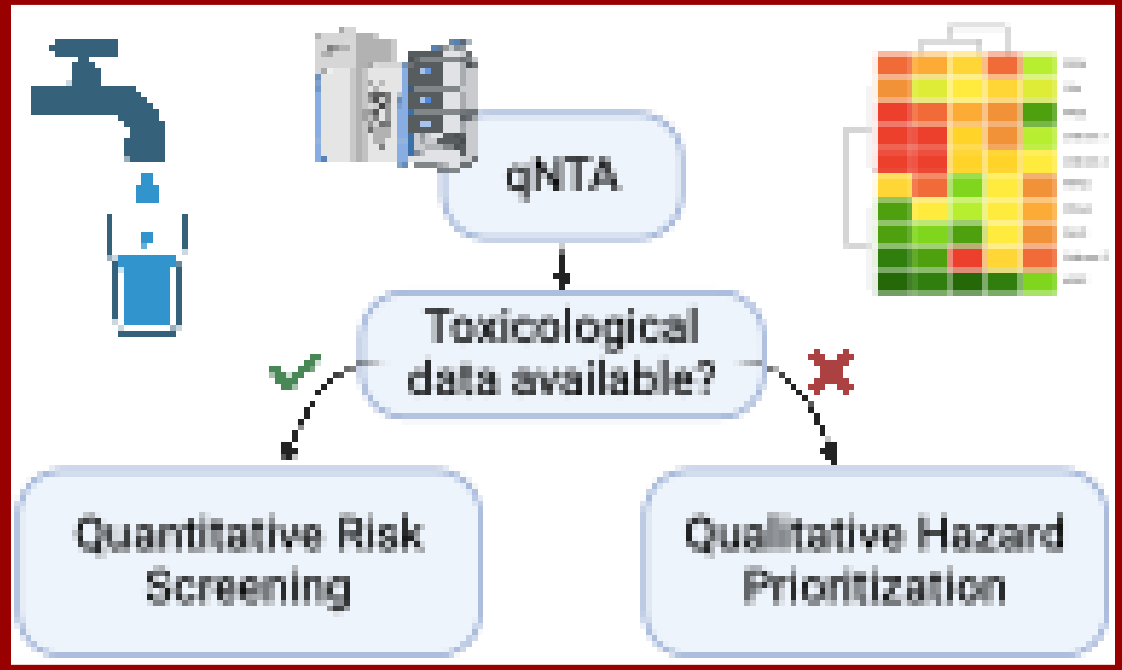
Hvad gemmer sig i vandet?

Non-target analyse af drikkevand og hvordan fund kan prioriteres



Martin Hansen

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Department of Environmental and Resource Engineering
Section of Environmental Contamination and Chemicals
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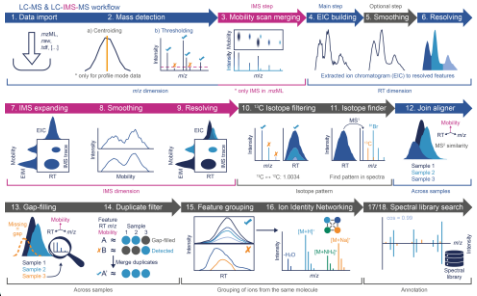
marthan@dtu.dk

qNTA: Drinking water

Quantitative!



High resolution mass spectrometry

InSa-Drikkevand

18 waterworks

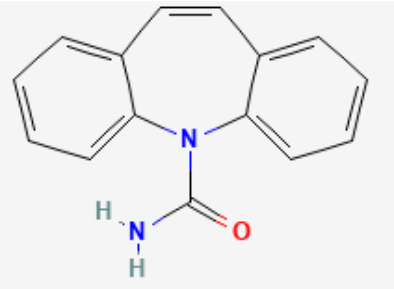
Total number of features	50,573
Total number of features after blank filtration	19,049
Number of features annotated from spectral libraries	1,314
Mass filtering Δm ±2 ppm	576
Filtering false positive (peak shape, duplicates)	404
Annotated compounds	278

Level 1: **40**
Level 2: 15
Level 3: 223

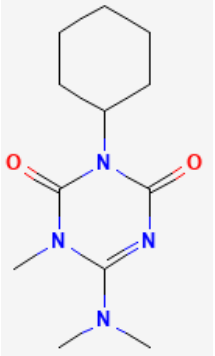
Nanusha et al. ES&T Water (2025)

278 Substances in drinking water

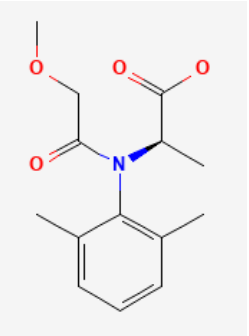
Compound (ng/L)	1	2	3	4	5	6	7	8	9	10
Desphenyl Chloridazon	6.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.10	1487.16
Methyl-desphenylchloridazon	1.41	1.16	0.33	0.02	0.00	0.00	0.00	0.00	0.42	202.25
(R)-2-((2,6-Dimethyl-phenyl)-(2-met	0.00	0.00	0.00	39.36	0.00	0.00	0.00	0.00	0.00	0.00
N-(2,6-dimethylphenyl)-N-(methoxy	0.00	0.00	0.00	27.03	0.00	0.00	0.00	0.00	0.00	0.00
2,6-dichlorbenzamid	2.72	4.50	0.53	0.55	0.58	3.95	0.17	0.05	4.77	0.26
Hexazinone	1.98	0.18	0.12	0.00	0.00	0.01	0.00	0.00	0.03	0.00
N,N-Dimethyl-N'-phenylsulfamide	0.01	1.67	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00
N,N-diethyl-m-toluamid	0.14	1.47	0.11	0.11	0.11	0.24	0.12	0.00	0.00	0.00
4-Methyl-1H-benzotriazole	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Alloxydim	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08
Carbamazepine	0.50	0.11	0.04	0.00	0.00	0.14	0.00	0.00	0.00	0.00
5-Methyl-1H-benzotriazole	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00



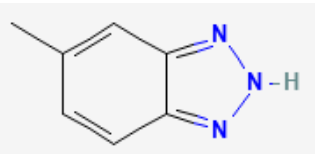
Carbamazepine
(treatment of epilepsy)



Hexazinone
(herbicide)



(R)-2-((2,6-Dimethyl-phenyl)-(2-methoxy-acetyl)-amino)-propionic acid
(Metalaxyl TP2)



5-Methyl-1H-benzotriazole

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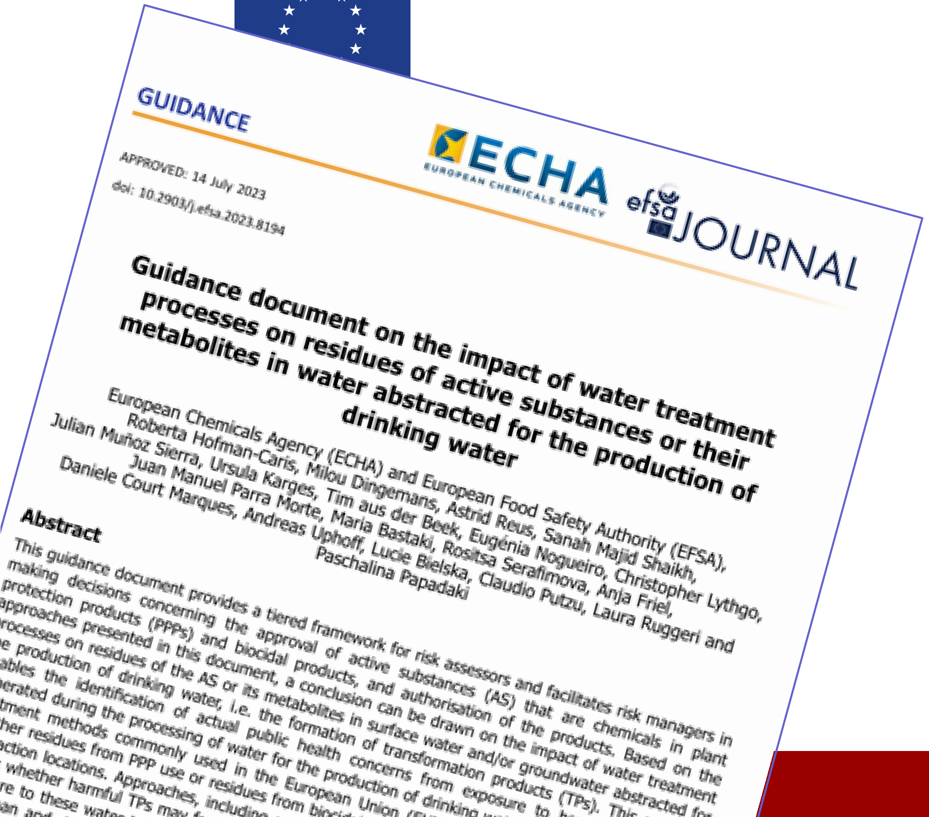
Health risk screening of contaminants in drinking water


GUIDANCE

ECHA EUROPEAN CHEMICALS AGENCY

efsa JOURNAL

APPROVED: 14 July 2023

doi: 10.2903/j.efsa.2023.8194

Guidance document on the impact of water treatment processes on residues of active substances or their metabolites in water abstracted for the production of drinking water

European Chemicals Agency (ECHA) and European Food Safety Authority (EFSA), Roberta Hofman-Caris, Milou Dingemans, Astrid Reus, Sanah Majid Shaikh, Julian Muñoz Sierra, Ursula Karges, Tim aus der Beek, Eugénia Nogueiro, Christopher Lythgo, Juan Manuel Parra Morte, Maria Bastaki, Rositsa Serafimova, Anja Friel, Daniele Court Marques, Andreas Uphoff, Lucie Bielska, Claudio Putzu, Laura Ruggeri and Paschalina Papadaki

Abstract

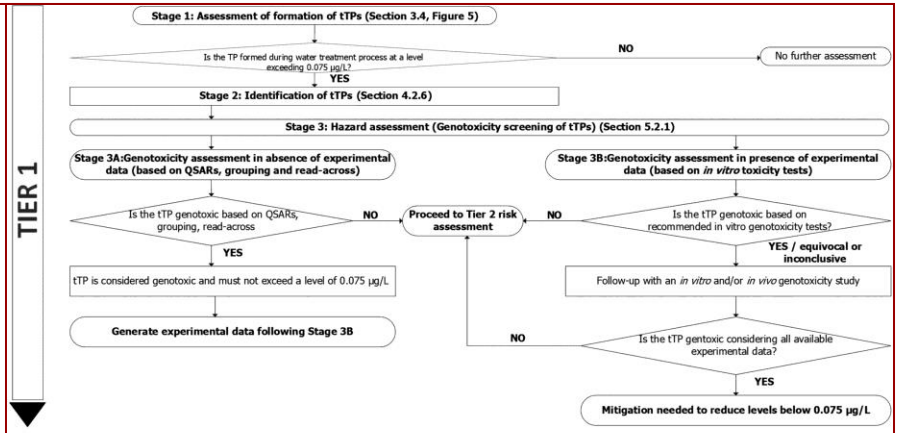
This guidance document provides a tiered framework for risk assessors and facilitates risk managers in making decisions concerning the approval of active substances (AS) that are chemicals in plant protection products (PPPs) and biocidal products, and authorisation of the products. Based on the approaches presented in this document, a conclusion can be drawn on the impact of water treatment processes on residues of the AS or its metabolites in surface water and/or groundwater abstracted for the production of drinking water, i.e. the formation of transformation products (TPs). This ...

*"…This guidance enables the **identification of actual public health concerns** from **exposure to harmful compounds** generated during … the production of **drinking water**…"*

*"The guidance presents the **method to address potential harm to human health** through the consumption of TP via drinking water."*

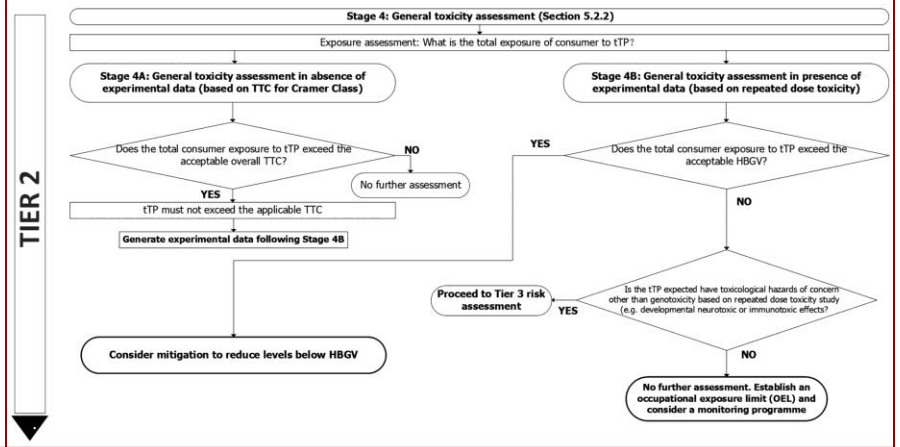
EFSA Guidance document

Genotoxicity screening



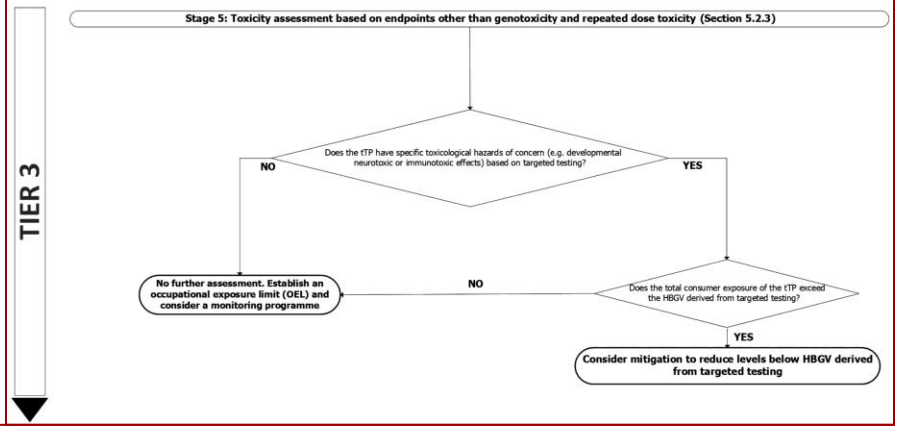
General toxicity assessment

In absence of experimental toxicological data -> Threshold of Toxicological Concern (TTC)



Refine risk assessment

Toxicity assessment based on other endpoints (e.g. developmental neurotoxicity, immunotoxic and reproductive effects). In vitro -> in vivo -> not 3R! / $$$!



Tier 1: Genotoxicity screening

TIER 1

Stage 3: Hazard assessment (Genotoxicity screening of tTPs) (Section 5.2.1)

Stage 3A:Genotoxicity assessment in absence of experimental data (based on QSARs, grouping and read-across)

Is the tTP genotoxic based on QSARs, grouping, read-across

NO → **Proceed to Tier 2 risk assessment**

YES

tTP is considered genotoxic and must not exceed a level of 0.075 µg/L

Generate experimental data following Stage 3B

Stage 3B:Genotoxicity assessment in presence of experimental data (based on *in vitro* toxicity tests)

Is the tTP genotoxic based on recommended in vitro genotoxicity tests?

NO → **Proceed to Tier 2 risk assessment**

YES / equivocal or inconclusive

Follow-up with an *in vitro* and/or *in vivo* genotoxicity study

Is the tTP gentoxic considering all available experimental data?

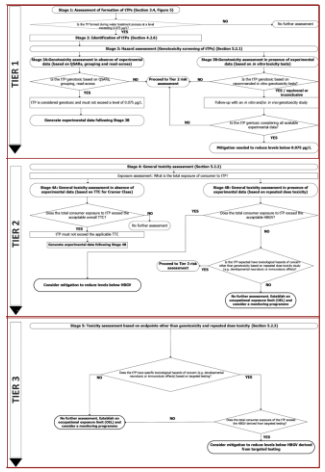
NO → **Proceed to Tier 2 risk assessment**

YES

Mitigation needed to reduce levels below 0.075 µg/L

"Non-identified substances [...] exceeding 0.075 µg/L in drinking water, should be considered genotoxic (worst-case) unless demonstrated otherwise. Consequently, mitigation would be needed to ensure levels would be below 0.075 µg/L...". (In DK this value is even lower: 7.5 ng/L)

Risk Screening Workflow (PharmaRisk)



Quantitative Nontarget Analysis

Substance

Toxicological data available?

Yes

No

Point of Departure (POD)

Acceptable/Tolerable daily intake (ADI/TDI)

Hazard Scoring

TTC value derived

No TTC value derived

Calculate Margin of Exposure (MoE)

Calculate Risk Quotient (RQ)

Threshold of Toxicological Concern (TTC)

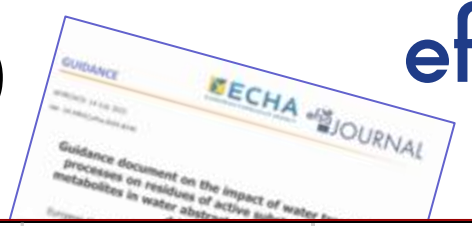
Quantitative Risk Screening

Qualitative Hazard Prioritization

https://insa-drikkevand.dk/insa-drikkevand/vidensbank/igangvaerende-projekter/pharmarisk-vaerktoej-til-workshop-oktober-2025

Nanusha et al. ES&T Water (2025)

Risk Quotient (RQ) and Margin of Exposure (MoE)



Typical for pesticides and pharmaceuticals

$$RQ_{substance} = \frac{C_{substance}}{DWEL_{substance}}$$

$$Drinking\ Water\ Equivalent\ Level\ (DWEL)\ \left(\frac{ng}{L}\right) = \frac{\mathbf{0.2} \times \boldsymbol{ADI} \times BW}{DWI}$$

ADI, acceptable daily intake (mg/kg/day); BW, body weight (kg) ; DWI, drinking water intake (L/day)

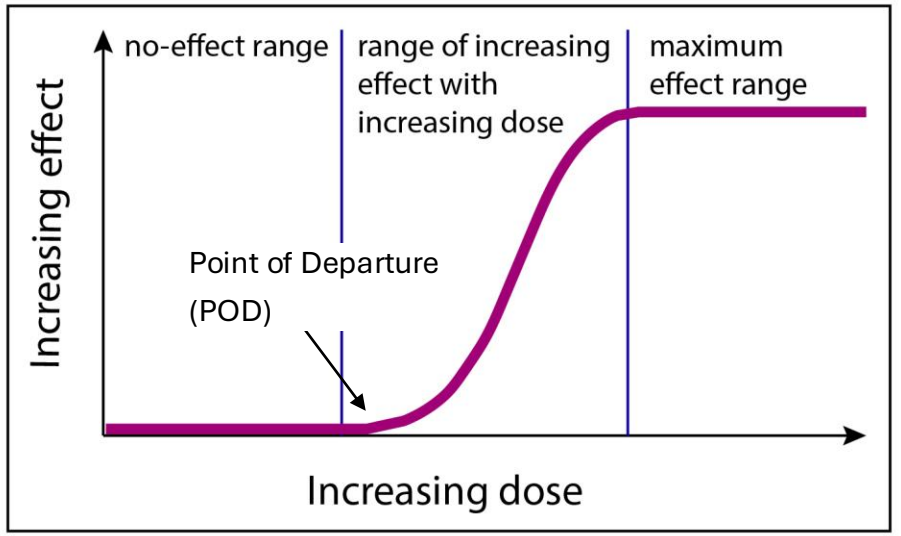
Age Groups	Body weight (kg)	DWI (L/day)
0-6 months	5.75	0.19
6-12 months	8.8	1
1-3 yrs	11.9	1.3
3-10 yrs	23.1	1.6
10-14yrs	43.4	2
14-18 yrs	61.3	2.25
Adults(>18 years)	70	2.25

Other substances with toxicological data

$$Margin\ of\ Exposure\ (MoE) = \mathbf{0.2}\frac{POD}{ADD}$$

$$Average\ daily\ dose\ (ADD) = \frac{C_{substance} \times DWI}{BW}$$

An MoE of below 100 for the general population and 1000 for the sensitive population is unacceptable and generally warrants further toxicological investigation.



Threshold of Toxicological Concern (TTC) – pragmatic screening tool for substances without toxicological data

Classification	TTC value in µg/person per day	TTC value in µg/kg bw per day[(a)]
Potential DNA-reactive mutagens and/or carcinogens	0.15	0.0025
Organophosphates and carbamates	18	0.3
Cramer Class III	90	1.5
Cramer Class II	540	9.0
Cramer Class I	1,800	30

1-20% pollutant load is accepted from drinking water.

Denmark

A 10% pollutant load is accepted from drinking water, i.e. the TTC value for carcinogens /genotoxicants are corrected from 0.15 to 0.015 µg/person/day (i.e. 15 ng/person/day).

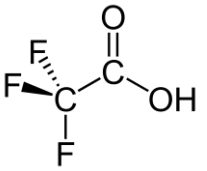
i.e. for a 2.25 L drinking water consumption:

The drinking water limit is 6.7 ng/L for **SUM** carcinogens / genotoxicants!

Table 1: Structural classes for chemicals proposed in the Cramer scheme (Cramer et al., 1978)

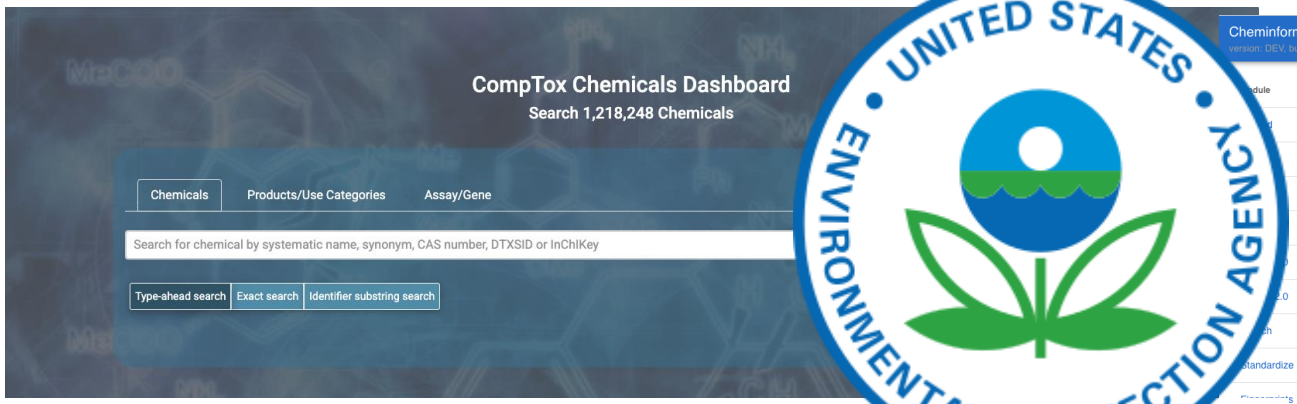
Class I	Substances with simple chemical structures and for which efficient modes of metabolism exist, suggesting a low order of oral toxicity. This class would include normal constituents of the body (excluding hormones); simply-branched, acyclic aliphatic hydrocarbons; common carbohydrates; common terpenes; substances that are sulfonate or sulfamate salts, without any free primary amines
Class II	Substances which possess structures that are less innocuous than Class I substances, but do not contain structural features suggestive of toxicity like those substances in Class III. This class would include common components of food; substances containing no functional groups other than alcohol, aldehyde, side-chain ketone, acid, ester, or sodium, potassium or calcium sulfonate or sulfamate, or acyclic acetal or ketal and are either a monocycloalkanone or a bicyclic substance with or without a ring ketone
Class III	Substances with chemical structures that permit no strong initial presumption of safety or may even suggest significant toxicity or have reactive functional groups. This class would include structures that contain elements other than carbon, hydrogen, oxygen, nitrogen or divalent sulfur; certain benzene derivatives; certain heterocyclic substances; aliphatic substances containing more than three types of functional groups

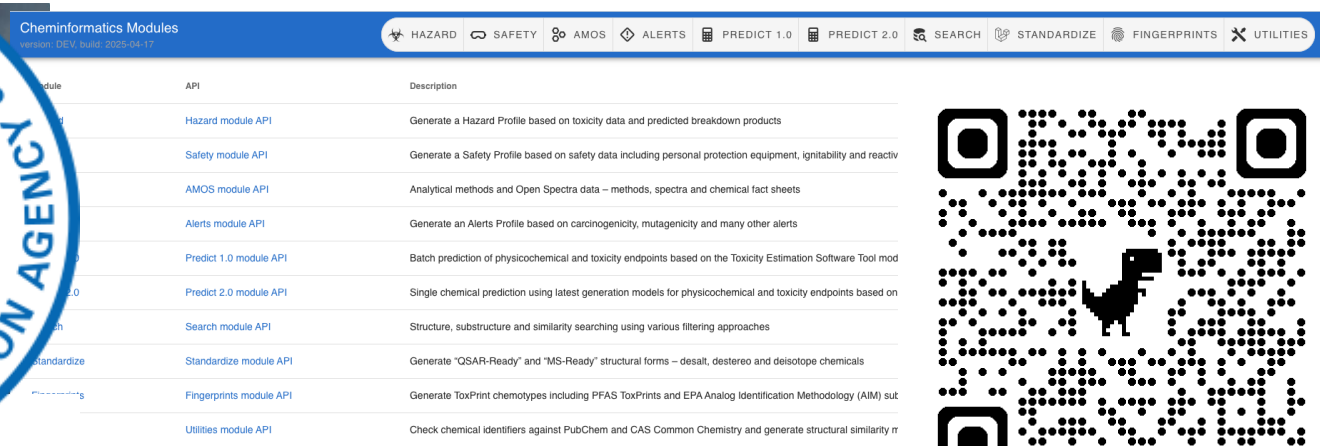
US EPA databases look-up



TFA, trifluoroacetic acid

SMILES: FC(F)(F)C(=O)O





Authoritative sources

- European Chemicals Agency (ECHA) Classification Labeling and Packaging (CLP)
- EPA mid-Atlantic Region Human Health Risk-Based Concentrations
- Germany Permanent Senate Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area
- World Health Organization International Agency for Research on Cancer (IARC) Monographs on the Evaluation of Carcinogenic Risks to Humans
- Integrated Risk Information System (IRIS)

Screening Sources

- Safe Work Australia Hazardous Chemical Information System (HCIS)
- Canada CNESST Workplace Hazardous Materials Information System (WHMIS)
- Environment and Climate Change Canada Domestic Substance List (DSL)
- Health Canada Priority Substances Lists (2006) (Carcinogenicity)
- Health Canada Priority Substances Lists (2006) (Reproductive Toxicity)

https://www.epa.gov/comptox-tools/cheminformatics-analysis-modules-resource-hub

Nanusha et al. ES&T Water (2025)

Hazard scores, grading and rankings

Chemicals: 467

Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable *Authority:* **Authoritative** Screening *QSAR Model*

Skipped (0)
Unlikely (0)
Filters (0)
Sorting (0)
Structure

CAS / Name	Human Health Effects															Ecotoxicity		Fate		
	Acute Mammalian Toxicity							Neurotoxicity		Systemic Toxicity										
	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
79-06-1 AIGBTMS Acrylamide	**H**	**M**	**M**	**VH**	**VH**	*L*	**M**	**H**	H	H	**H**	H	**H**	**H**	**H**	**M**	**M**	*M*	L	*H*
35400-43-2 GBT Sulprofos	H	I	H	**L**	L	*L*	L	L	H	H			L	L	L	**H**	**VH**		*M*	*L*

$$Combined\ Hazard\ Score = \frac{\sum Hazard\ score\ values}{number\ of\ available\ sources}$$

VH=4, H=3, M=2, L=1

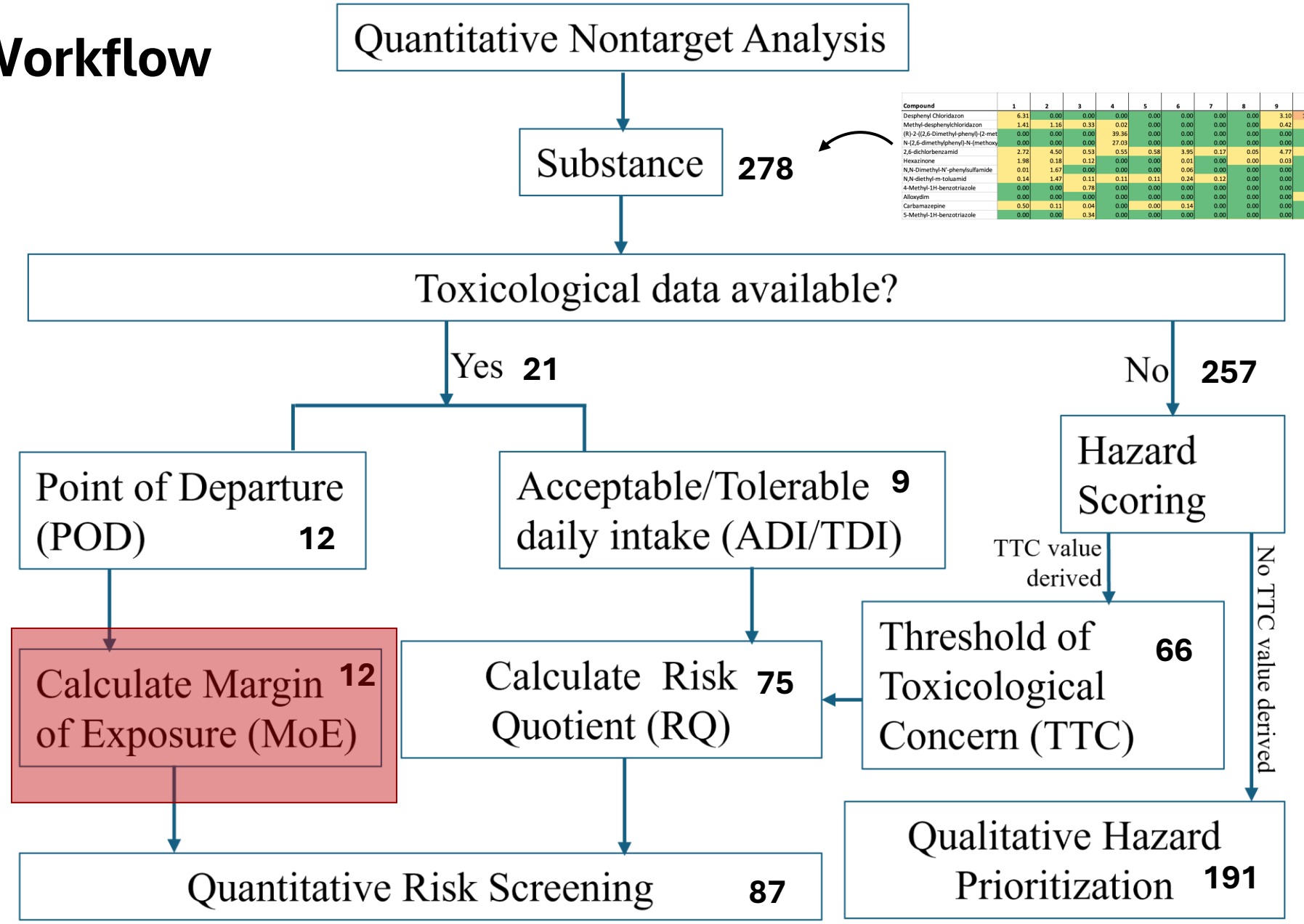
Authoritative = 3, Screening = 2, Predicted =1

$$Combined\ Quality\ Score = \frac{\sum Authority\ values}{number\ of\ available\ sources}$$

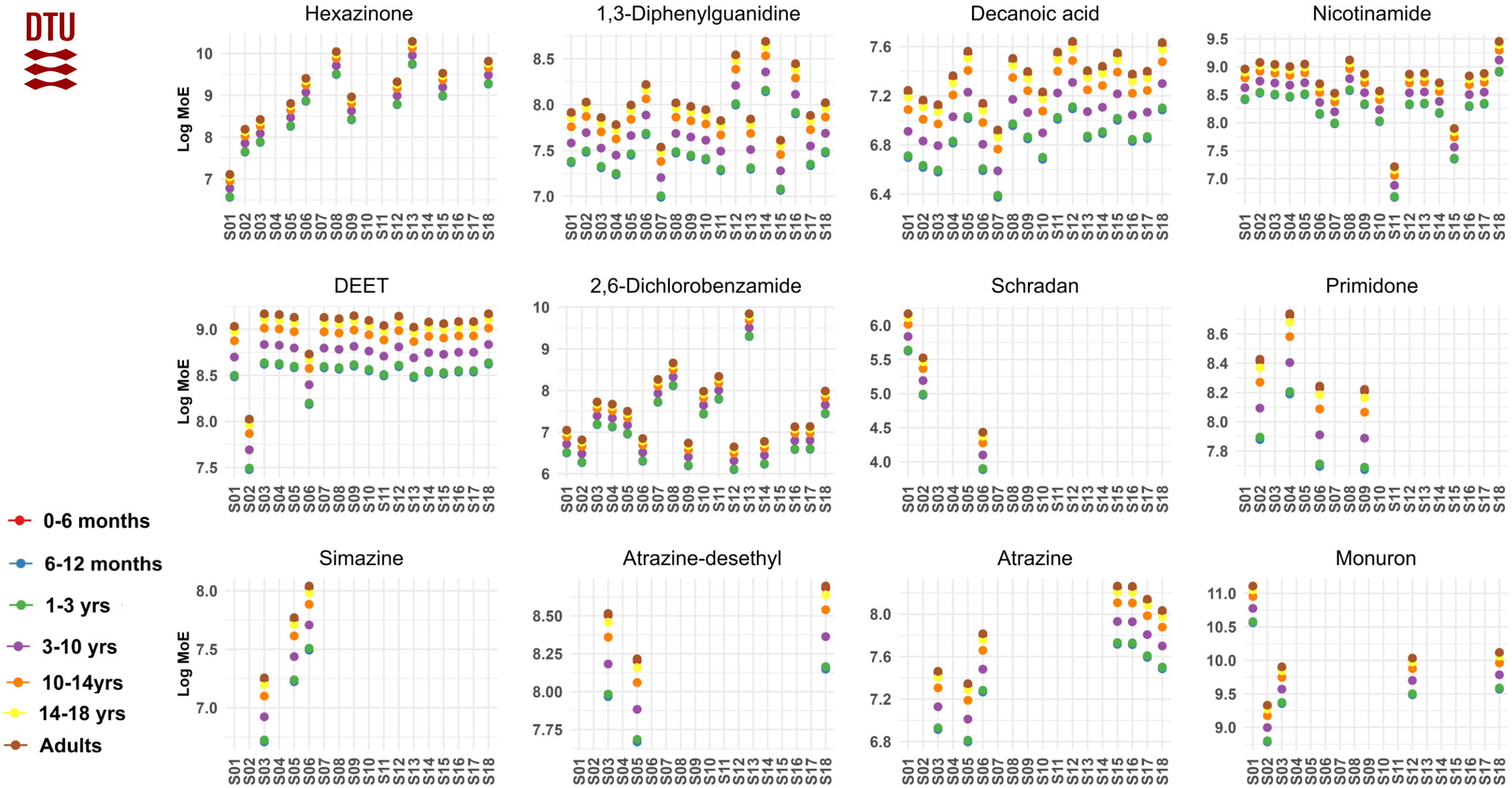
$$Completeness\ Score = \frac{number\ of\ available\ sources}{number\ of\ end\ points\ selected}$$

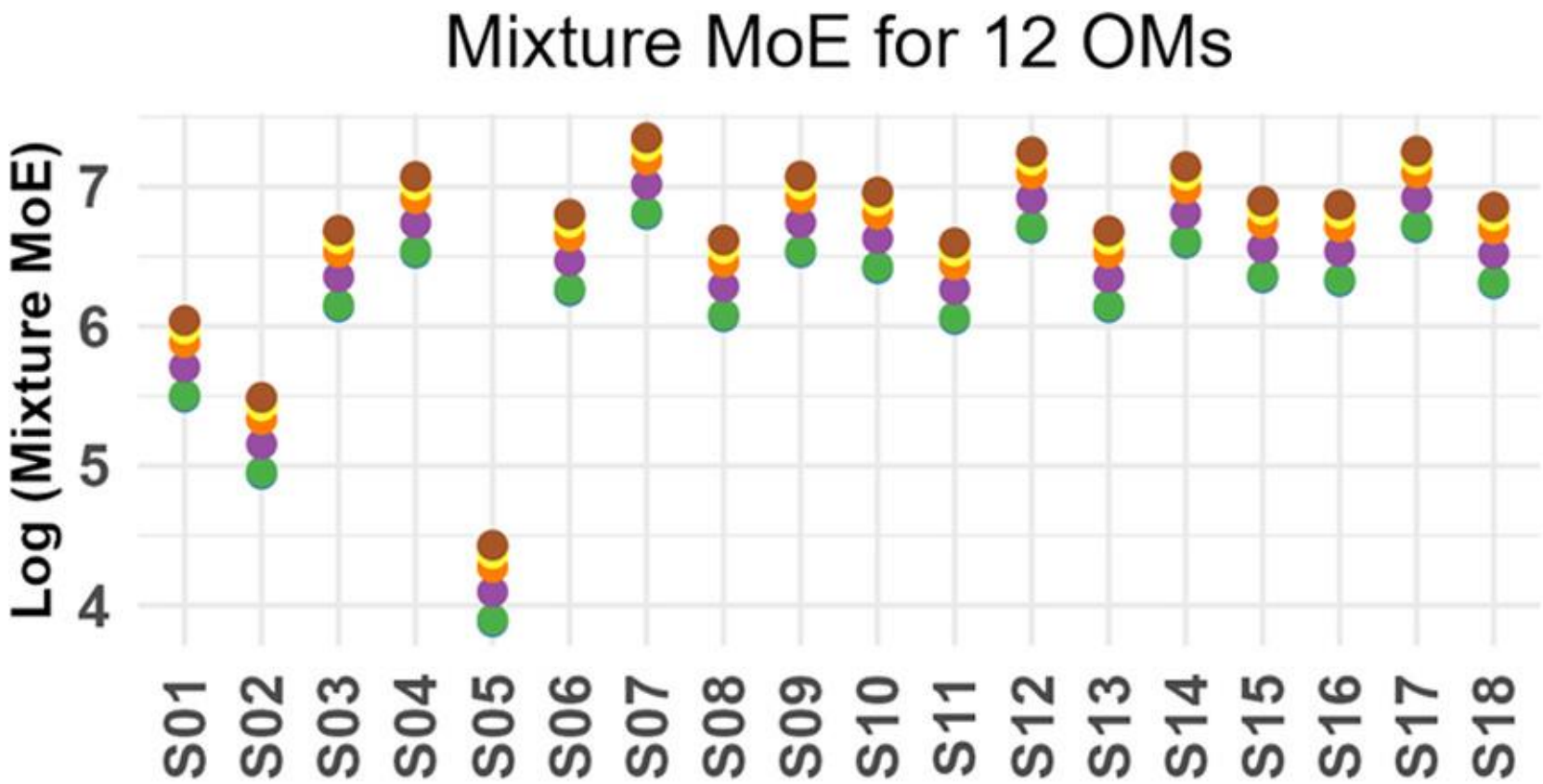
Nanusha et al. ES&T Water (2025)

Risk Screening Workflow



Nanusha et al. ES&T Water (2025)


Hexazinone
1,3-Diphenylguanidine
Decanoic acid
Nicotinamide
DEET
2,6-Dichlorobenzamide
Schradan
Primidone
Simazine
Atrazine-desethyl
Atrazine
Monuron
Log MoE
S01 S02 S03 S04 S05 S06 S07 S08 S09 S10 S11 S12 S13 S14 S15 S16 S17 S18
0-6 months
6-12 months
1-3 yrs
3-10 yrs
10-14yrs
14-18 yrs
Adults

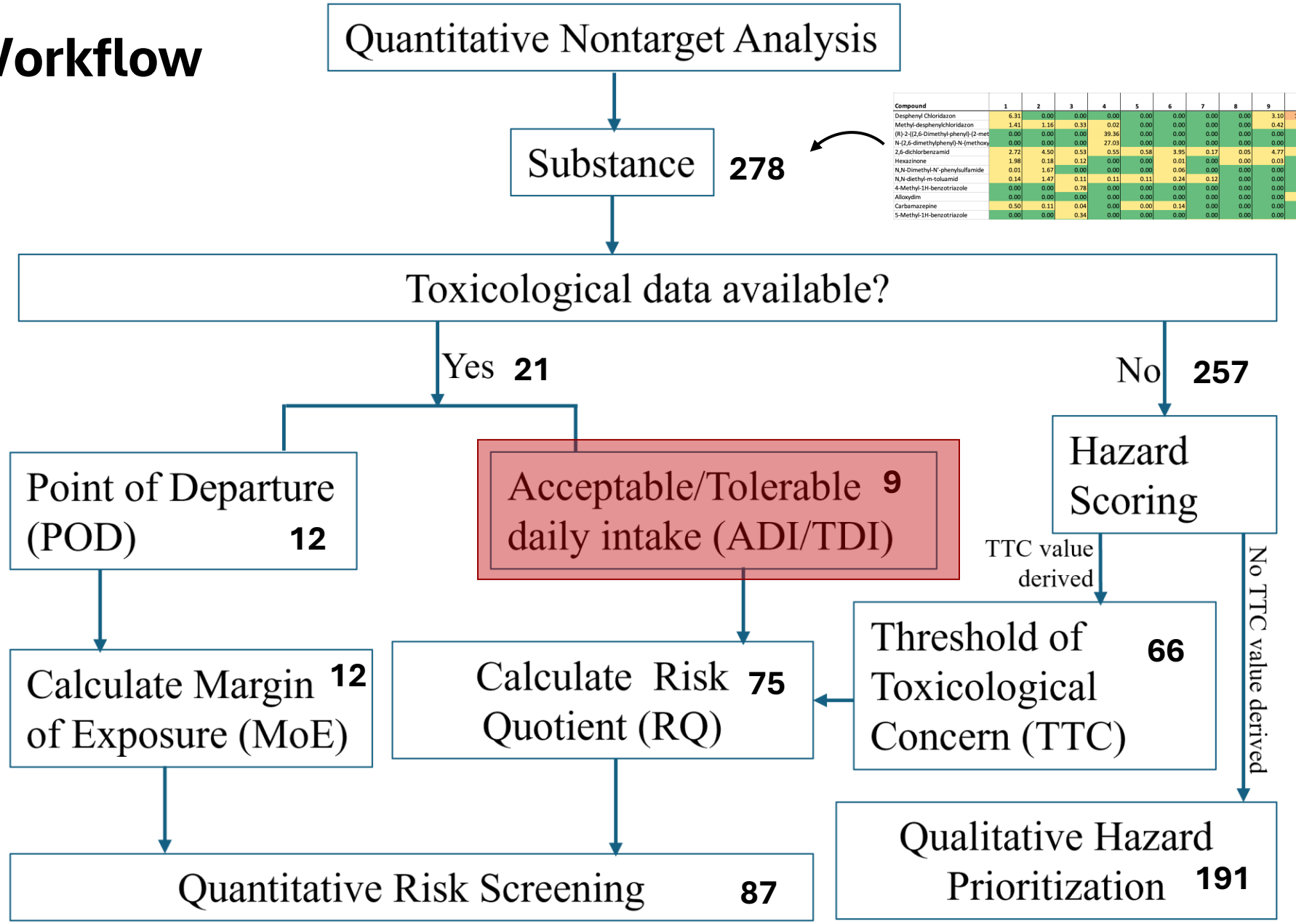


$$\mathrm{MoE}_{\mathrm{mixture}} = \left(\sum_{i=1}^{n} \frac{1}{\mathrm{MoE}_i} \right)^{-1}$$

0-6 months 6-12 months 1-3 yrs 3-10 yrs 10-14yrs 14-18 yrs Adults(>18 years)

Nanusha et al. ES&T Water (2025)

Risk Screening Workflow



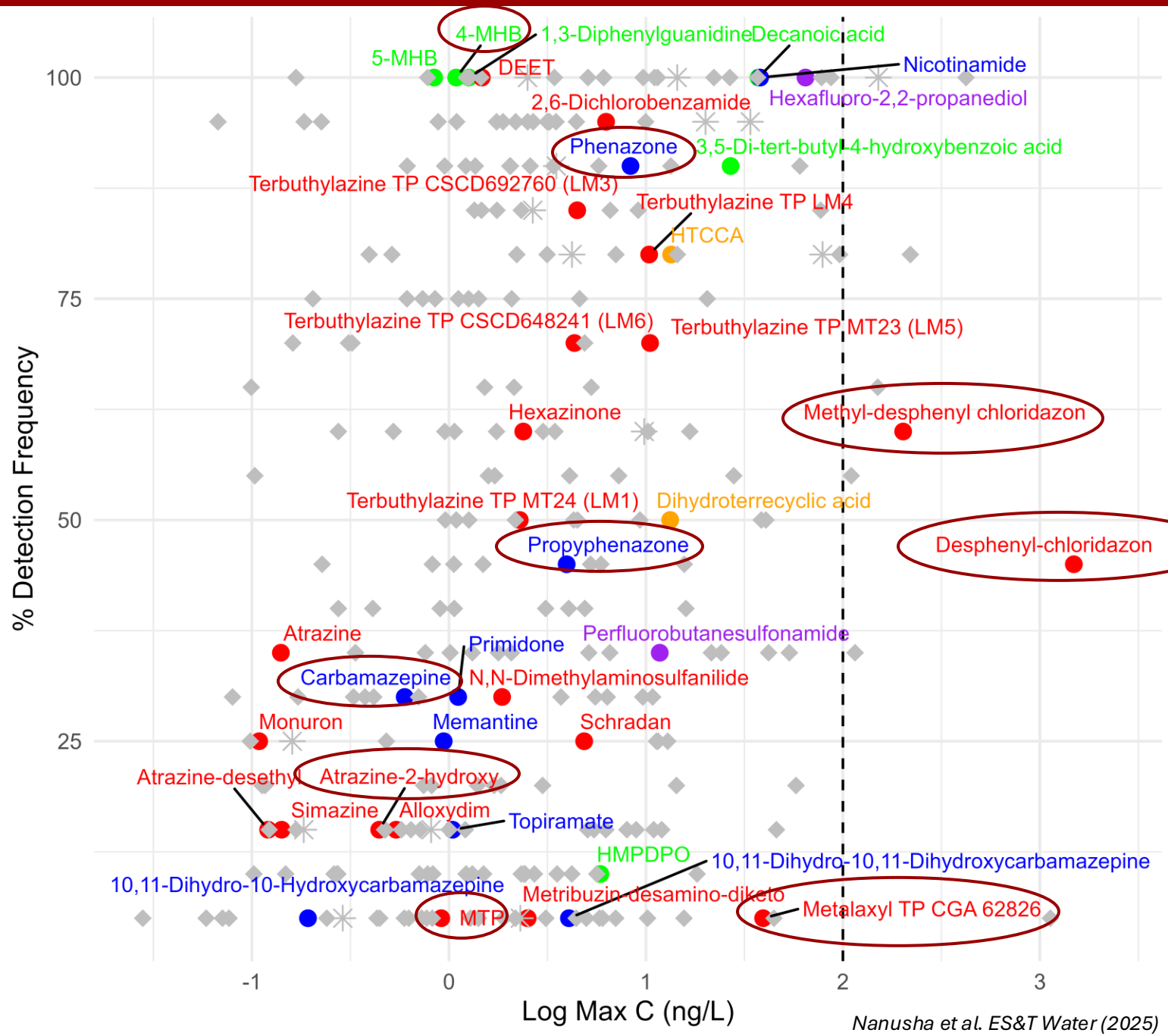
Compound	1	2	3	4	5	6	7	8	9
Desphenyl Chloridazon	6.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.10
Methyl-desphenylchloridazon	1.41	1.16	0.33	0.02	0.00	0.00	0.00	0.00	0.42
(R)-2-(2,6-Dimethyl-phenyl)-[2-met	0.00	0.00	0.00	39.36	0.00	0.00	0.00	0.00	0.00
N-(2,6-dimethylphenyl)-N-(methoxy	0.00	0.00	0.00	27.03	0.00	0.00	0.00	0.00	0.00
2,6-dichlorbenzamid	2.72	4.50	0.53	0.55	0.58	3.95	0.17	0.05	4.77
Hexazinone	1.98	0.18	0.12	0.00	0.00	0.01	0.00	0.00	0.03
N,N-Dimethyl-N'-phenylsulfamide	0.01	1.67	0.00	0.00	0.00	0.06	0.00	0.00	0.00
N,N-diethyl-m-toluamid	0.14	1.47	0.11	0.11	0.11	0.24	0.12	0.00	0.00
4-Methyl-1H-benzotriazole	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.00	0.00
Alloxydim	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbamazepine	0.50	0.11	0.04	0.00	0.00	0.14	0.00	0.00	0.00
5-Methyl-1H-benzotriazole	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00

Nanusha et al. ES&T Water (2025)

Acceptable daily intake (ADI)

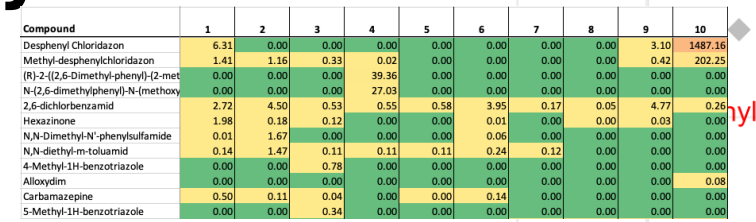
Substance	mg/kg bw/day
Carbamazepine	0.00034
4-Methyl-1H-benzotriazole	0.0067
Methyl-desphenyl chloridazon	0.01
Desphenyl-chloridazon	0.015
Propyphenazone	0.021
Phenazone	0.036
Atrazine-2-hydroxy	0.04
Metalaxyl TP CGA 62826	0.08
Metalaxyl TP CGA 108906	0.08

Values from literature, WHO, PPDB

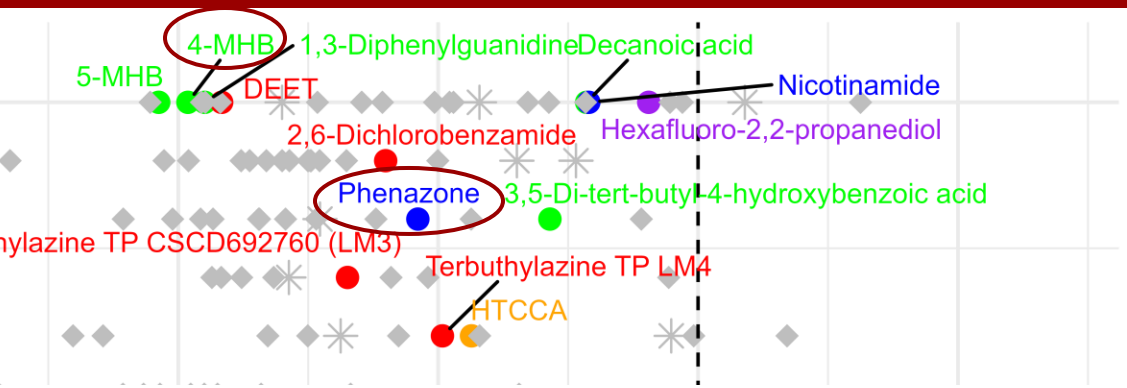


Nanusha et al. ES&T Water (2025)

Acceptable daily intake (ADI)

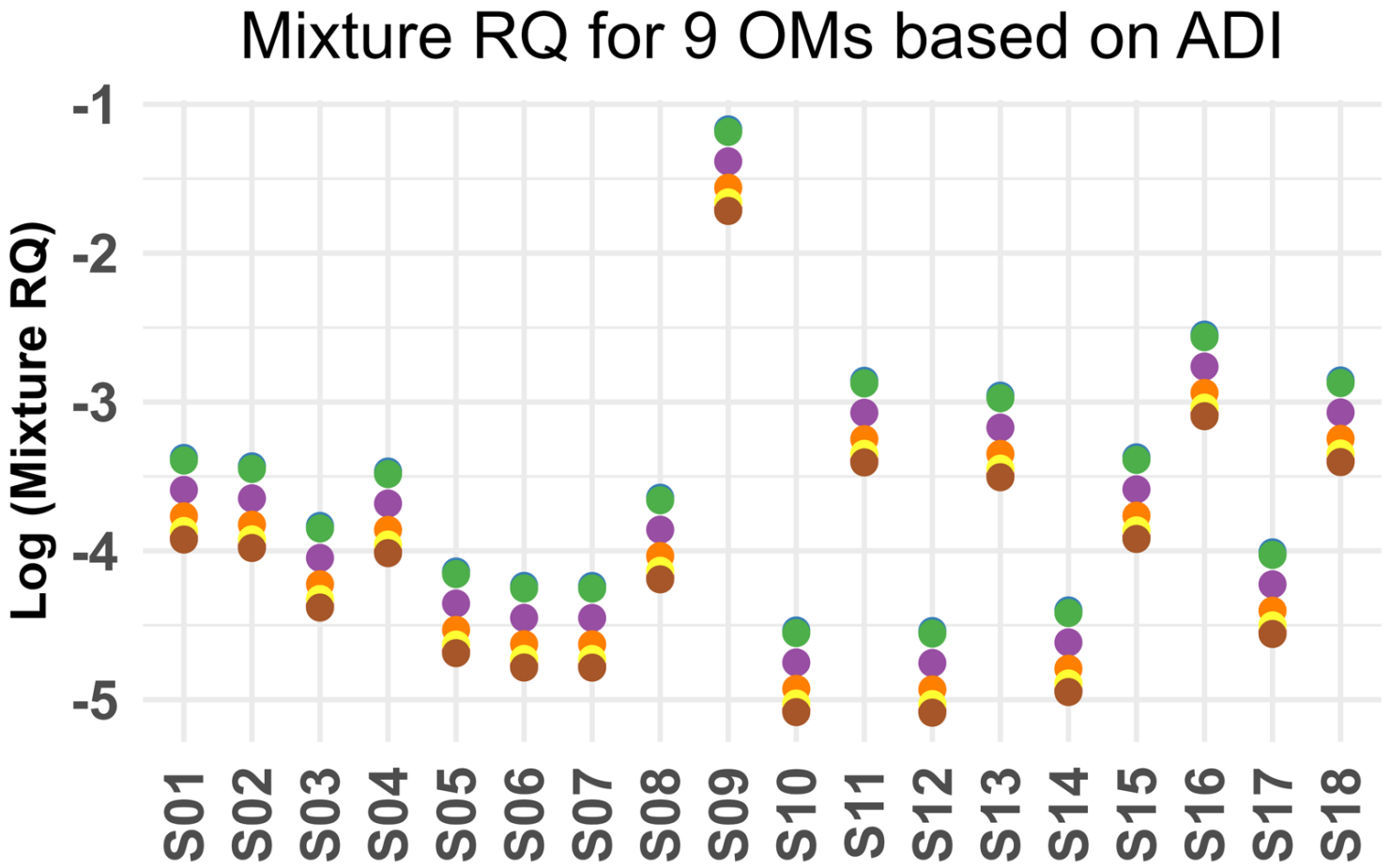


Compound	1	2	3	4	5	6	7	8	9	10
Desphenyl Chloridazon	6.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.10	1487.16
Methyl-desphenylchloridazon	1.41	1.16	0.33	0.02	0.00	0.00	0.00	0.00	0.42	202.25
(R)-2-((2,6-Dimethyl-phenyl)-(2-met	0.00	0.00	0.00	39.36	0.00	0.00	0.00	0.00	0.00	0.00
N-(2,6-dimethylphenyl)-N-(methoxy	0.00	0.00	0.00	27.03	0.00	0.00	0.00	0.00	0.00	0.00
2,6-dichlorbenzamid	2.72	4.50	0.53	0.55	0.58	3.95	0.17	0.05	4.77	0.26
Hexazinone	1.98	0.18	0.12	0.00	0.00	0.01	0.00	0.00	0.03	0.00
N,N-Dimethyl-N'-phenylsulfamide	0.01	1.67	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00
N,N-diethyl-m-toluamid	0.14	1.47	0.11	0.11	0.11	0.24	0.12	0.00	0.00	0.00
4-Methyl-1H-benzotriazole	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Alloxydim	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08
Carbamazepine	0.50	0.11	0.04	0.00	0.00	0.14	0.00	0.00	0.00	0.00
5-Methyl-1H-benzotriazole	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00



Substance	mg/kg bw/day
Carbamazepine	0.00034
4-Methyl-1H-benzotriazole	0.0067
Methyl-desphenyl chloridazon	0.01
Desphenyl-chloridazon	0.015
Propyphenazone	0.021
Phenazone	0.036
Atrazine-2-hydroxy	0.04
Metalaxyl TP CGA 62826	0.08
Metalaxyl TP CGA 108906	0.08

Values from literature, WHO, PPDB



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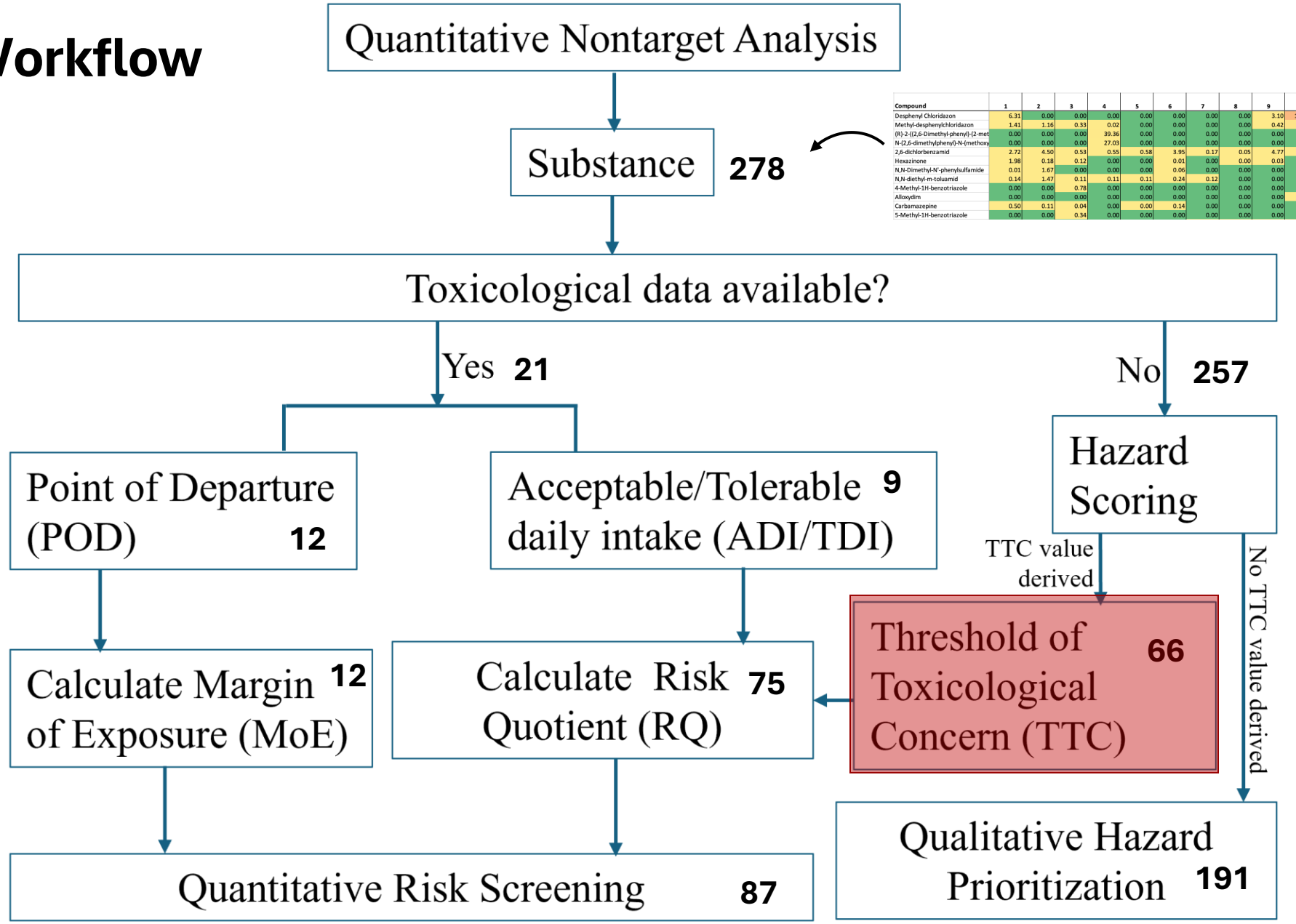
Risk Screening Workflow



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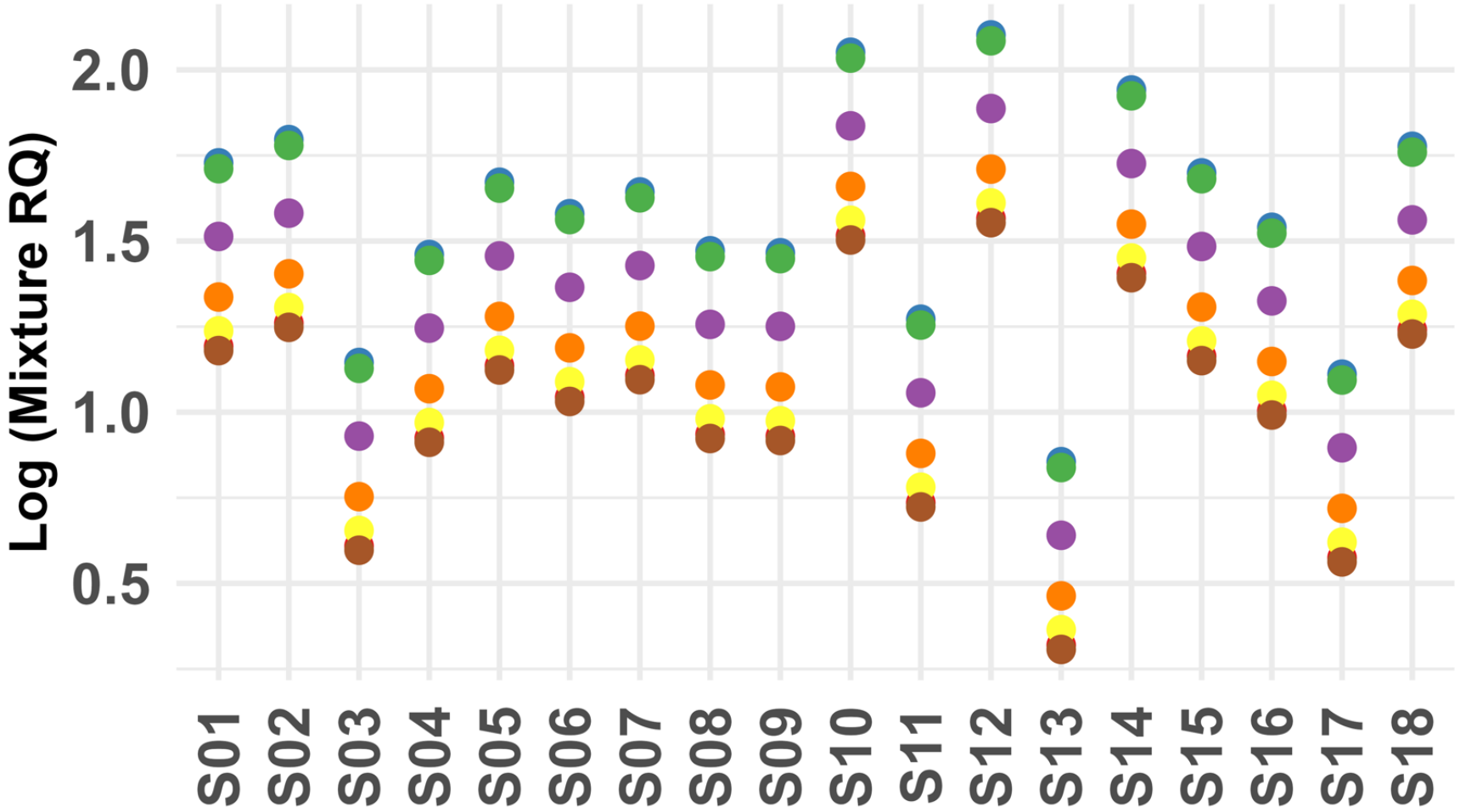
Compound name for annotation databases (compounds names marked in **yellow** are whose risk assessment was evaluated quantitatively)	DTXSID	CAS	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure
Pilocarpine	DTXSID1021162	92-13-7	VH	VH	VH		VH	L		H	
3,3'-Dimethoxybenzidine	DTXSID3025091	119-90-4	M			VH	VH				
Arsenic acid	DTXSID1034341	7778-39-4	VH	VH	M	VH	M		H	H	
5-Methyl-1H-benzotriazole	DTXSID1038743	136-85-6	M				VH				
4-Anilinophenol	DTXSID5037739	122-37-2	M				VH				
honokiol	DTXSID30188845	35354-74-6	H				H	H		H	
Maculosin	DTXSID30196526	4549-02-4	M				VH	H		H	
Rilmenidine	DTXSID3045194	54187-04-1					H			H	
Ethyl 2,4-dimethylthiazole-5-carboxylate	DTXSID70345334	7210-77-7					H	H		H	
Meprobamate	DTXSID3023261	57-53-4	M				H	L	M	H	
Alprostadil	DTXSID9022578	745-65-3	H				VH		M		
6-[1-Hydroxy-1-(3-methyl-5-oxotetrahydro-2-furanyl)ethyl]-4-methoxy-3-me			H				H	H		H	
N-[5-(2,5-Dioxo-1-pyrrolidinyl)pentyl]-N-hydroxyacetamide							H	H		H	
8-methoxy-2,6-dimethyl-8-(2-phenylethc	DTXSID30915719	94291-84-6	M				H	H		H	
1-amino-4-(methylamino)anthracene-9,1	DTXSID8051621	1220-94-6	L			H	VH			H	
Amorfrutin 2	DTXSID901166040	80489-91-4	M				H	H		H	
Tris((dimethylamino)methyl)phenol	DTXSID80181043	26444-72-4	M				H	H		H	
1-Isopropyl-1H-benzimidazole-5-carboxy	DTXSID30405746	284673-16-1	M				H	H		H	
4,4'-Propane-2,2-diylbis(2-aminophenol	DTXSID00278969	1220-78-6	M				H	H		H	
N-(4-Nitrophenyl)prolinamide	DTXSID30994549	7369-91-7	VH				H	L		H	
Pimonidazole	DTXSID50867867	70132-50-2	M				H	H		H	
5,6-Diamino-1,3-dimethyluracil	DTXSID8063886	5440-00-6	M				VH	L		H	

15 ng/person/day

Nanusha et al. ES&T Water (2025)

Mixture RQ for 66 OMs based on TTC



Compound	1	2	3	4	5	6	7	8	9
Desphenyl Chloridazon	6.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.10
Methyl-desphenylchloridazon	1.41	1.16	0.33	0.02	0.00	0.00	0.00	0.00	0.42
(R)-2-(2,6-Dimethyl-phenyl)-(2-met	0.00	0.00	0.00	39.36	0.00	0.00	0.00	0.00	0.00
N-(2,6-dimethylphenyl)-N-(methoxy	0.00	0.00	0.00	27.03	0.00	0.00	0.00	0.00	0.00
2,6-dichlorbenzamid	2.72	4.50	0.53	0.55	0.58	3.95	0.17	0.05	4.77
Hexazinone	1.98	0.18	0.12	0.00	0.00	0.01	0.00	0.00	0.03
N,N-Dimethyl-N'-phenylsulfamide	0.01	1.67	0.00	0.00	0.00	0.06	0.00	0.00	0.00
N,N-diethyl-m-toluamid	0.14	1.47	0.11	0.11	0.11	0.24	0.12	0.00	0.00
4-Methyl-1H-benzotriazole	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.00	0.00
Alloxydim	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbamazepine	0.50	0.11	0.04	0.00	0.00	0.14	0.00	0.00	0.00
5-Methyl-1H-benzotriazole	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00

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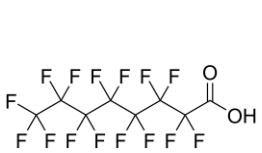
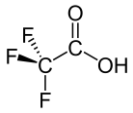
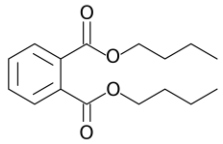
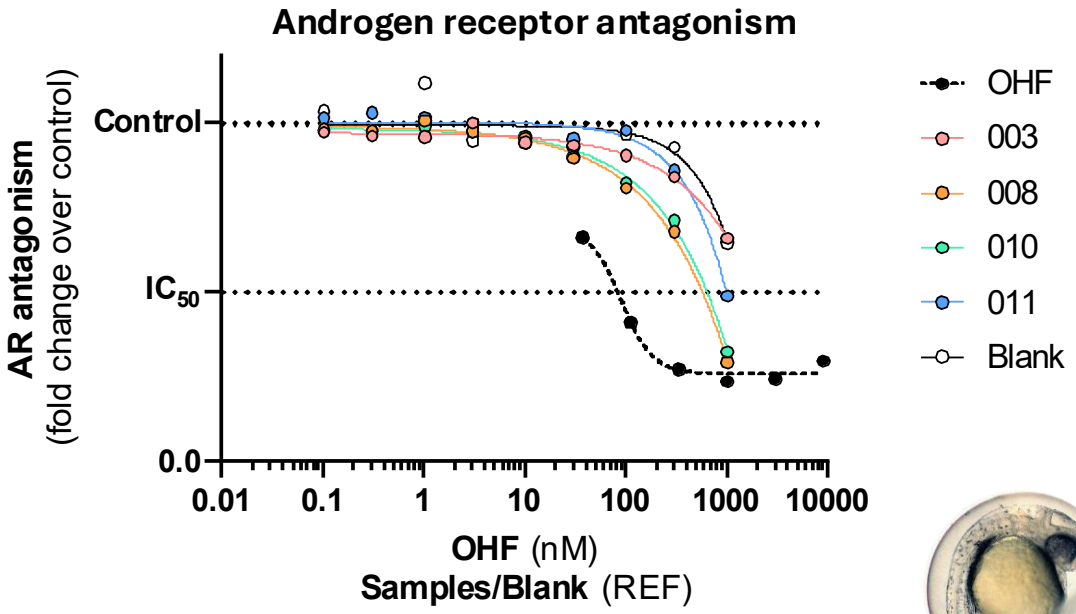
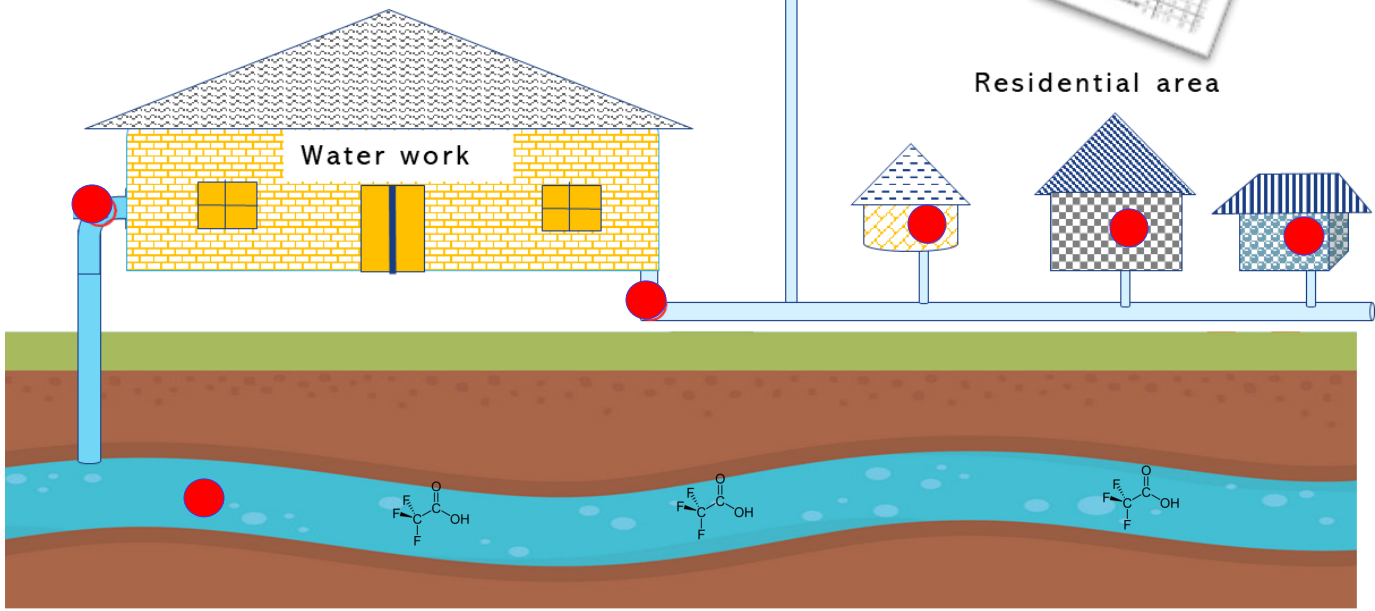
Effect-directed analysis

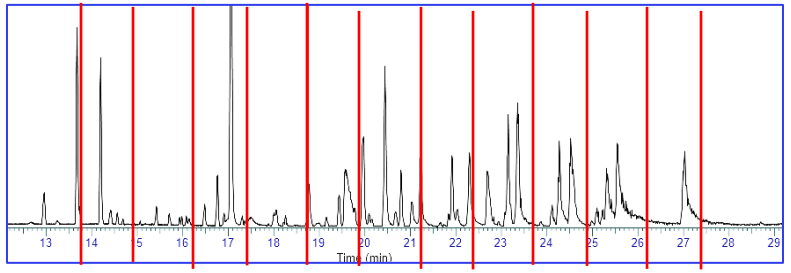


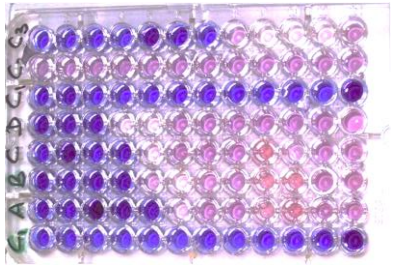


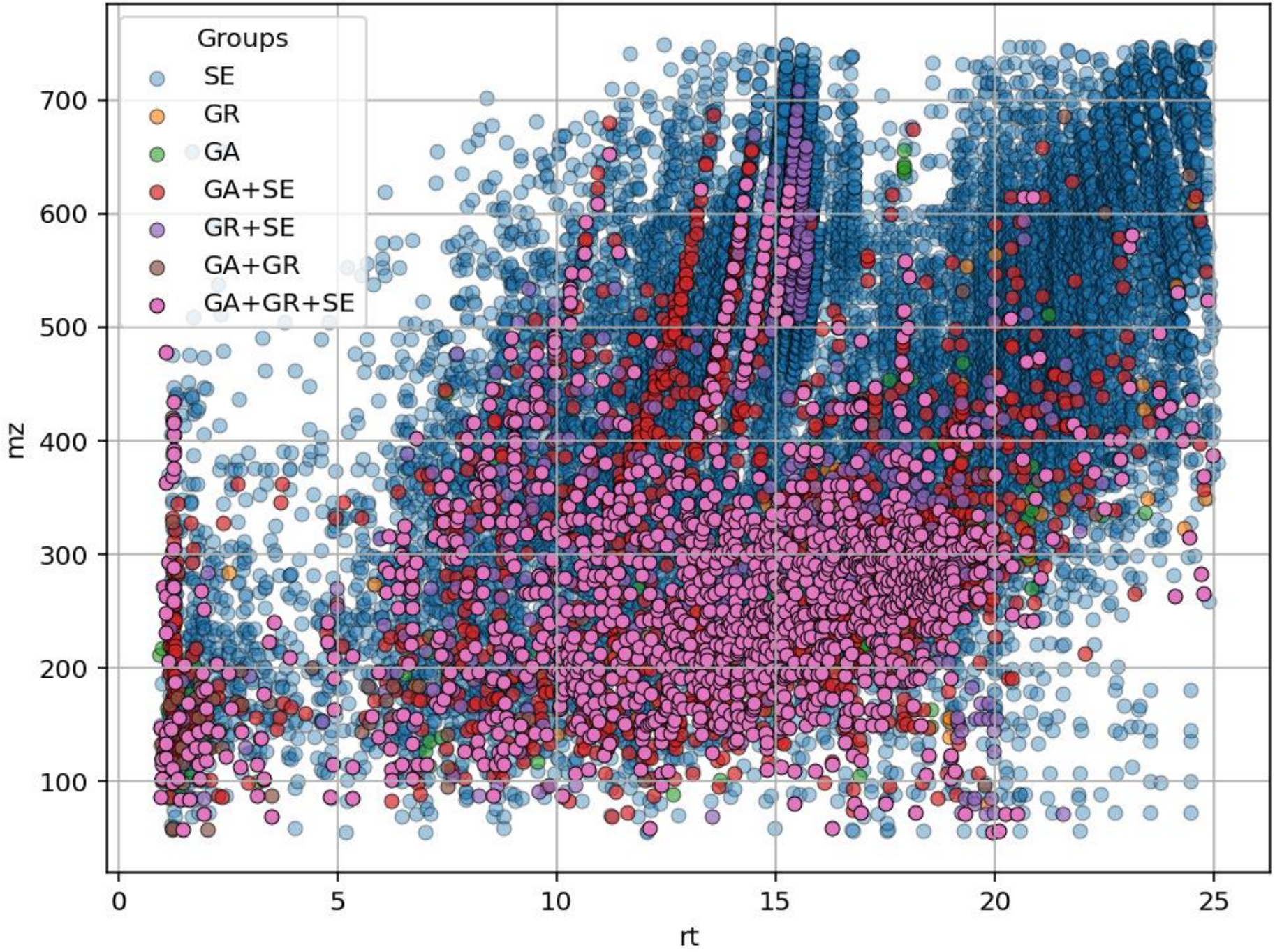











Groups
SE
GR
GA
GA+SE
GR+SE
GA+GR
GA+GR+SE
700
600
500
400
300
200
100
mz
0
5
10
15
20
25
rt


DTU

- Risk screening approach
- PMTs (Persistent, Mobile, Toxic)
  - Tiny PFAS
  - Inorganic “PFAS”
- Nitrate !
- Organophosphates
- Carbamazepine (and its metabolites)
- Benzotriazoles (5-Methyl-1H-benzotriazole)
- Triazine herbicides and their metabolites
- Diphenylguarnidine

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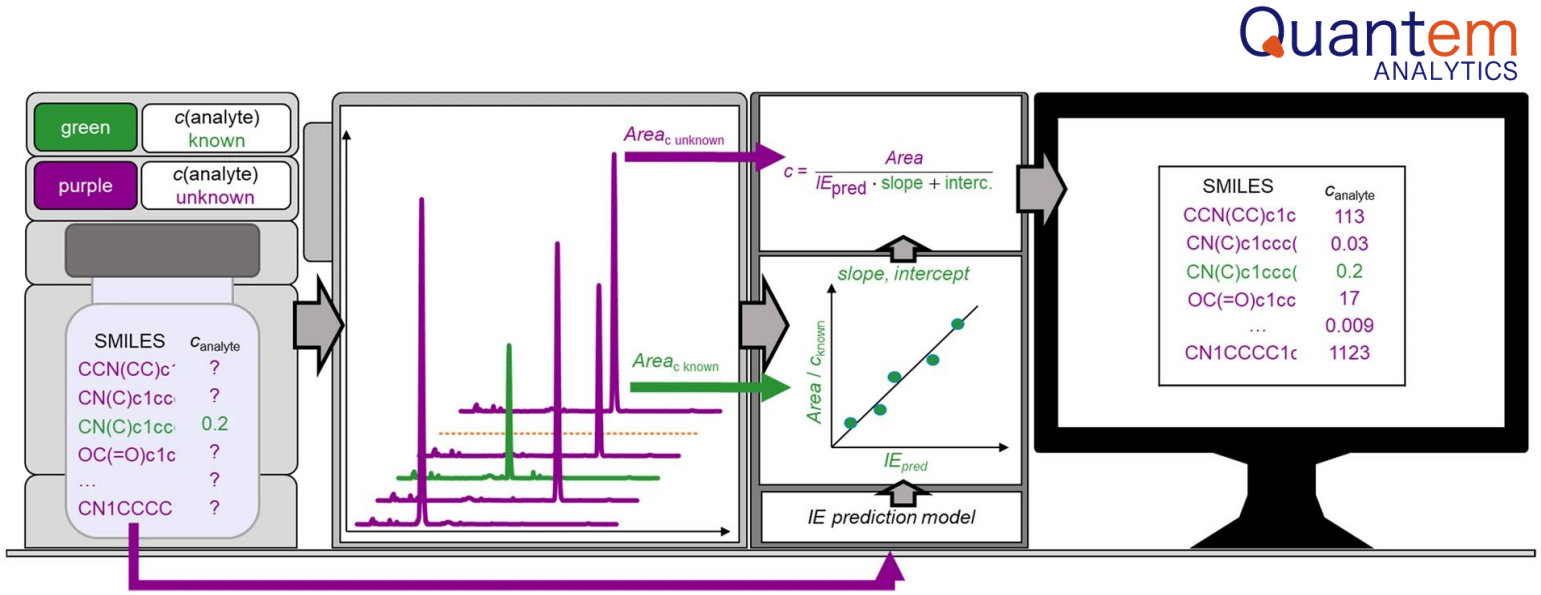
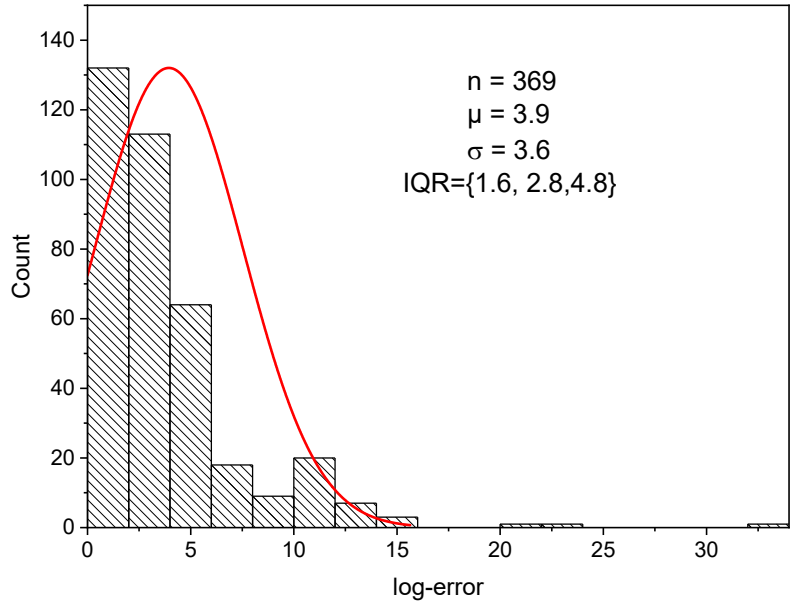
Semi-quantitation evaluation

A	E	J	K	L	M	N	O	P	Q	R	S	T	U	V
Method	Compound	Z001	Z002	Z003	Z004	Z005	Z006	Z007	Z008	Z009	Z010	Z011	Z012	Z013
Calibration	2,6-Dichlorobenzamide (BAM)	2.46	4.22	1.50	4.45	3.62	4.92	2.90	3.02	4.51	3.22	3.83		
Semiquant	2,6-Dichlorobenzamide (BAM)	11.08	22.71	5.73	22.23	18.06	24.52	14.49	13.97	26.03	15.33	18.18		
Calibration	Acesulfame K	4.87	3.56	17.81	6.44	4.59	2.74	12.32	17.52	15.92	19.96	12.61		
Semiquant	Acesulfame K	18.17	14.77	79.30	24.94	16.22	7.76	55.71	77.19	79.89	108.80	60.34		
Calibration	Alachlor ESA													
Semiquant	Alachlor ESA													

- 21 substances
- 114 samples

$$\text{log-Error} = 10^{\left|\log_{10}\frac{\bar{c}_{pred}}{c}\right|}$$





Liigand, J., Wang, T., Kellogg, J. *et al.* Quantification for non-targeted LC/MS screening without standard substances. *Sci Rep* 10, 5808 (2020). https://doi.org/10.1038/s41598-020-62573-z

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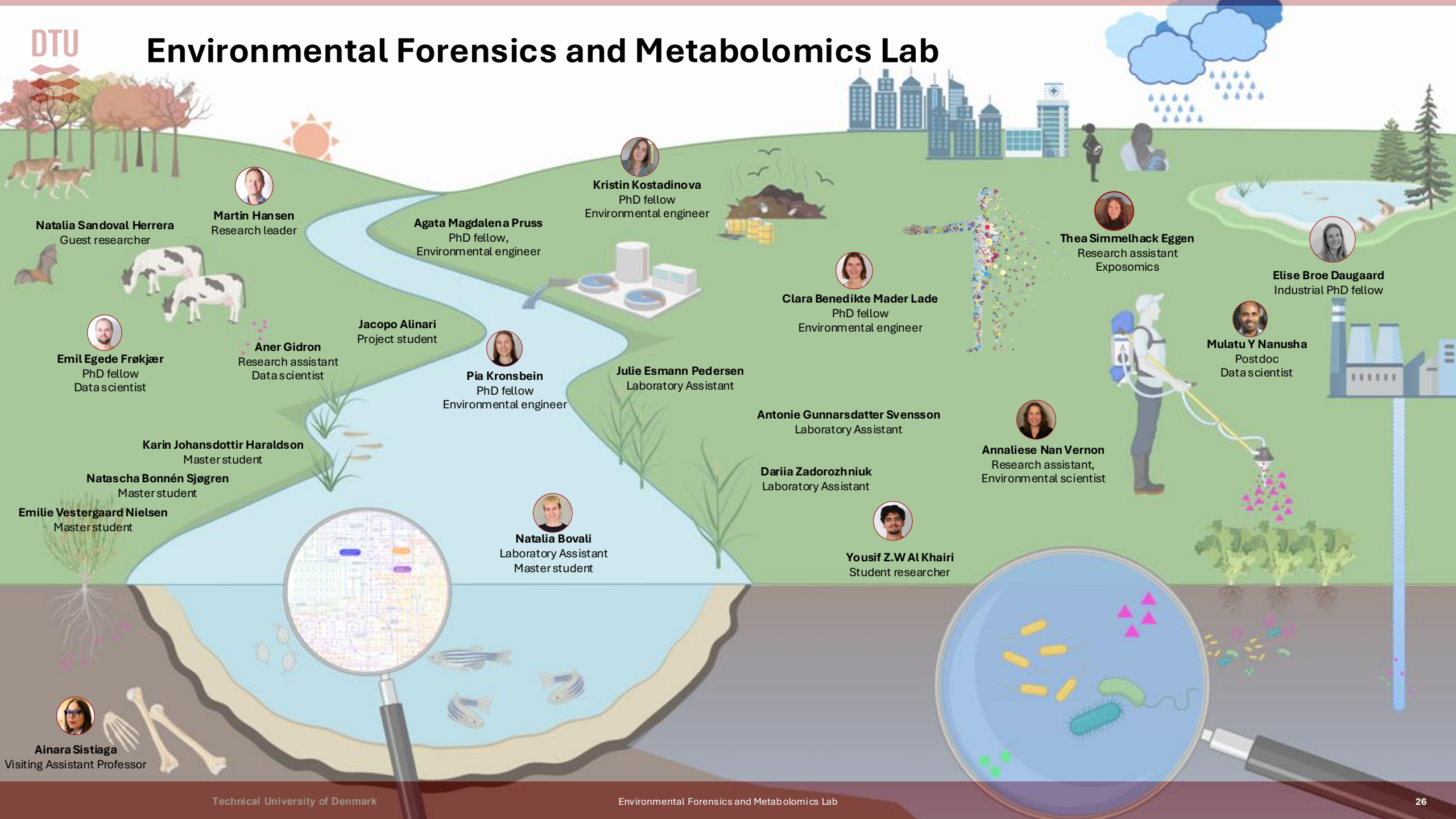

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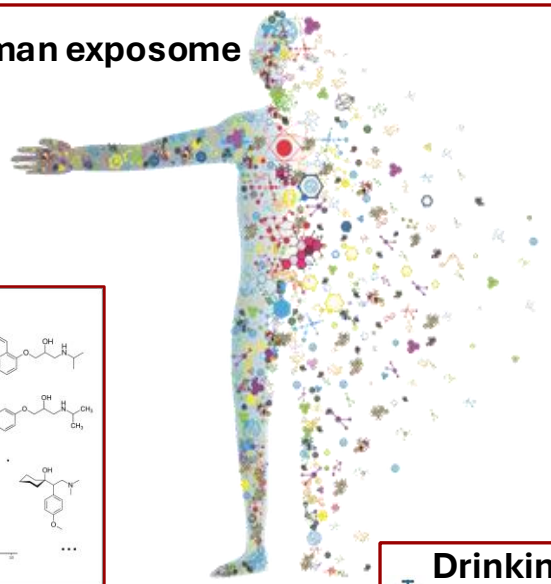
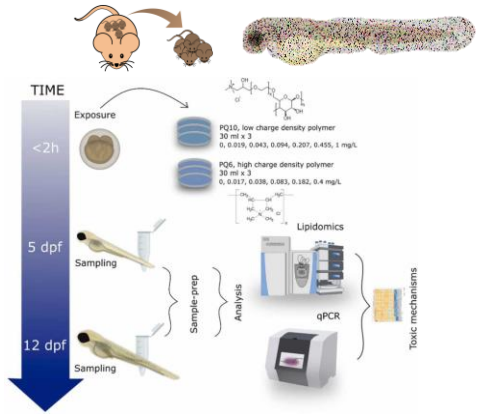
Environmental Forensics and Metabolomics Lab

PFAS Center

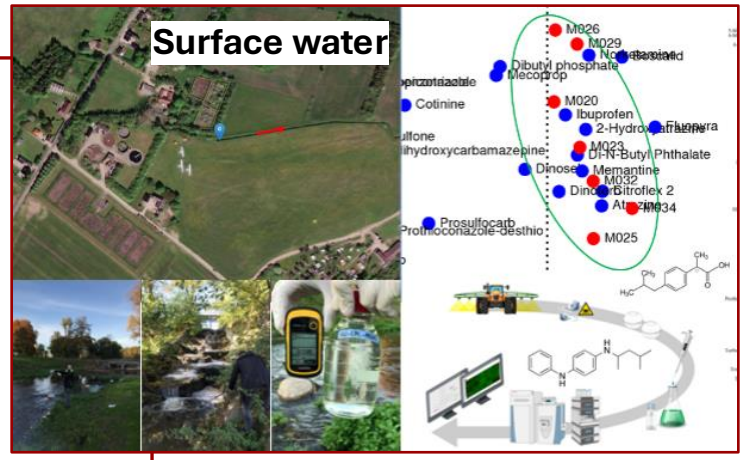
Human exposome



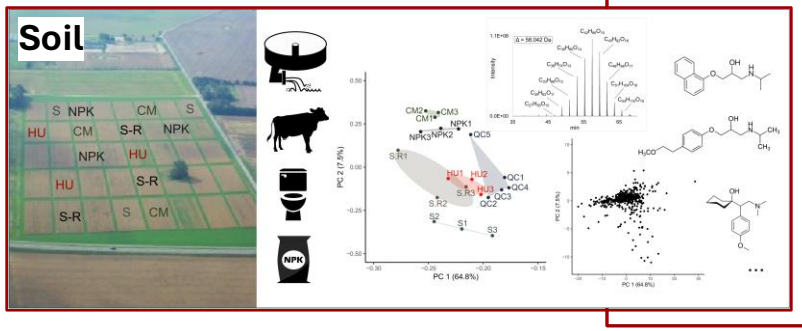
Toxicometabolomics



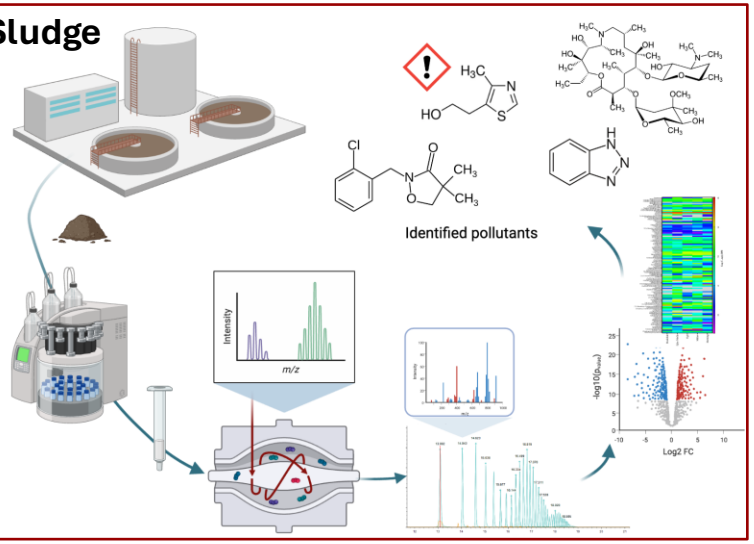
Surface water



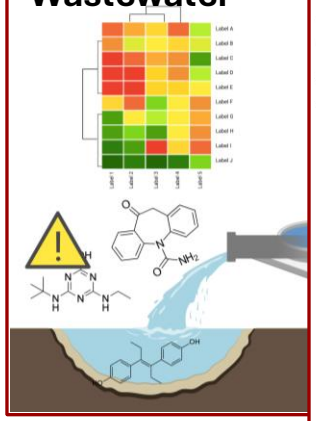
Soil



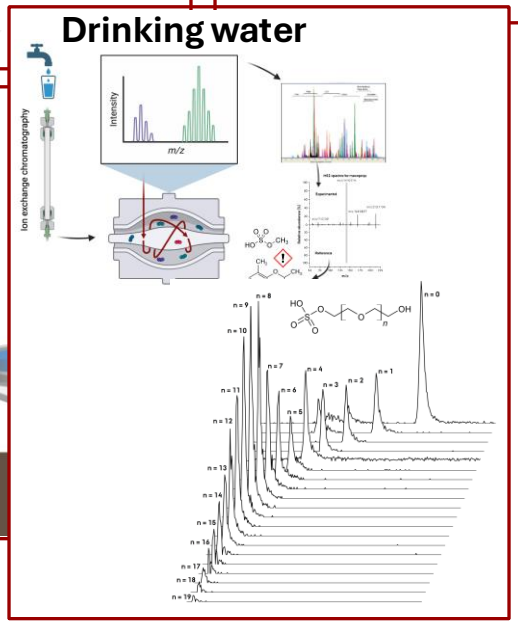
Sludge



Wastewater



Drinking water



Groundwater