



***NORMAN Databases workshop***

# **The NORMAN databases in support of European environmental policies**

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# Network of reference laboratories, research centers and related organisations for monitoring of emerging environmental substances



## Mission:

- **Exchange information** on emerging substances
- Improve **data quality**
- Promote **synergies** among research teams and **more efficient transfer** of research findings to **policy-makers**



**Network of reference laboratories,  
research centers and related organisations  
for monitoring of  
emerging environmental substances**



## **Working Groups**

**1) Prioritisation**

**2) Bioassays**

**3) Effect-Directed Analysis**

**4) Engineered Nanoparticles**

**5) Wastewater reuse**

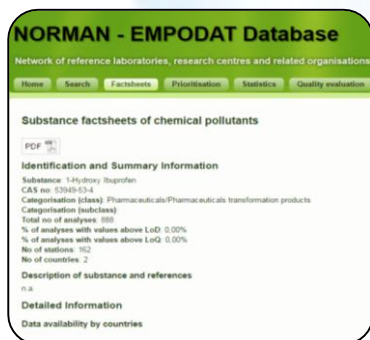
**6) Indoor environment**

**+ 2 Cross-WG: Passive sampling and NT screening**



# Information and data exchange

## EMPODAT Chemical module



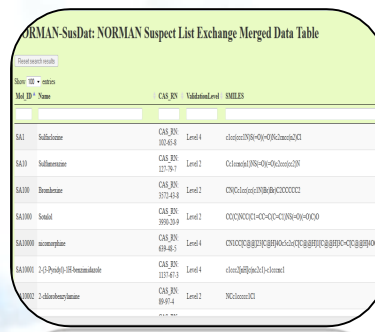
A database of more than 9 million geo-referenced monitoring data on emerging substances

## EMPODAT Ecotox module



A platform for systematic collection and evaluation of ecotoxicity studies for harmonised derivation of

## NORMAN SusDat module



The screenshot shows the NORMAN-SusDat: NORMAN Suspect List Exchange Merged Data Table interface. It features a table with columns for CAS RN, Validated, SMILES, and Name. The table lists several substances, including Substances, Substances, Substances, Substances, and Substances.

CAS RN	Validated	SMILES	Name
100-46-4	Level 1	Clc1ccc2c(c1)ccccc2	Substances
121-76-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances
317-43-1	Level 1	Clc1ccc2c(c1)ccccc2	Substances

An open-access database of substances, accompanied by information for mass-spectral

## NORMAN MassBank database



An open-access database of mass spectra for more than 1,000 environmental contaminants

And more modules are in the pipeline: Digital Sample Freezing Platform (DSFP), Passive Sampling, Bioassays, ARB/ARG.....

# 1st edition of NORMAN databases workshop – Berlin, 2011

NORMAN Position paper “Towards a harmonised approach for collection and interpretation of data on emerging substances in support of European environmental policies”

- Environmental monitoring data are not systematically collected at the EU level.
- Need for a better integrated approach to collection, management and assessment of data on emerging substances with adequate metadata.
- Need to continue the NORMAN data collection effort.
- All EU-funded research projects should provide all data on emerging substances generated within their scope to a central open access database.
- A harmonised data reporting format should be adopted both at the national and European level.

## 2017, 2<sup>nd</sup> Database Workshop

### The progress made

- IPCHEM has been created
  - Recognition by the Commission of the need to develop and maintain a permanent platform for collection and sharing of monitoring data (all compartments, not only environmental data..)
  - Decision of the Commission to add a clause in all EU-funded projects: all research monitoring data will be stored in IPCHEM



## 2017 Status and progress made

- NORMAN has contributed to the EU effort for systematic data collection and analysis
  - In 2014 NORMAN recommendations for the definition of the 1st EU Watch List
  - In 2015 NORMAN datasets have been shared with JRC to support the review of the list of the WFD PS
  - In 2017 agreement with DG ENV to integrate EMPODAT in IPCHEM
  - Dynamic link with IPCHEM possible as a next step
    - possibility for NORMAN to retrieve the raw data in EMPODAT and use them for prioritisation activities?

# Perspectives : our vision

- NORMAN databases are the basis for prioritisation
- Trend is now from hundreds, to tens of thousands substances
  - prioritisation of relevant compounds >> identification of compounds on which to put higher effort for actions

## Delete / hide

### 38 compounds :

WFD PS (diuron, dichlorvos, dicofol, heptachlor, PCBs, BDE -47, BDE-153, BDE-154, HBCDD, PAHs, PFOS, etc.)  
Microcystines  
Well known Industrial Chem. (aniline, styrene, toluene, xylenes, etc.)

## Former emerging substance

### • 72 compounds :

- Phthalates
- Organotins
- Nitro musks
- Organo-lead
- 8 well known PFASs
- 23 herbicides / insecticides, banned in EU and /or not frequently detected / quantif
- 10 surfactants (NPEOs, LAS)

## Keep on NORMAN List

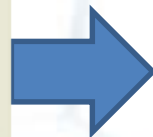
### • 527 compounds

- 8 Plasticisers
- 73 PPP
- 20 PPP / biocides or biocides
- 209 Pharmas
- 60 Pers care prod.
- 16 Flame retard.
- 44 Ind. Chemicals
- 8 PFASs, ....etc.
- **61 DBP (only drinking water)**

## NEW: Add to NORMAN List

### • 253 compounds :

- 67 flame ret. (used as alternatives to banned products)
- 10 PPP most frequently detected, highest conc. or chronic EQS exceeded in recent studies
- 118 PPP/biocides & biocides in use or under review
- 50 PFASs in use
- 8 Pharmas, etc.



**NORMAN-SusDat: NORMAN Suspect List Exchange Merged Data Table**

Reset search results

Show 100 entries

Mol_ID	Name	CAS_RN	ValidationLevel	SMILES
SA1	Sulfaclozine	CAS_RN: 102-65-8	Level 4	<chem>c1cc(ccc1N)S(=O)(=O)Nc2ccc(n2)Cl</chem>
SA10	Sulfamerazine	CAS_RN: 127-79-7	Level 2	<chem>Cc1ccc(n1)NS(=O)(=O)c2ccc(cc2)N</chem>
SA100	Bromhexine	CAS_RN: 3572-43-8	Level 2	<chem>CN(Cc1cc(ccc1N)Br)BrC2CCCCC2</chem>
SA1000	Sotalol	CAS_RN: 3930-20-9	Level 2	<chem>CC(C)NCC(C1=CC=C(C=C1)NS(=O)(=O)C)O</chem>
SA10000	nicomorphine	CAS_RN: 639-48-5	Level 4	<chem>CN1CC[C@]23[C@H]4O[C@@H]5C2[C@@H]1[C@]3(C)[C@@H]4[C@@H]5C=C[C@]2(C)[C@@H]4OC</chem>
SA10001	2-(3-Pyridyl)-1H-benzimidazole	CAS_RN: 1137-67-3	Level 4	<chem>c1ccc2[nH]c(nc2c1)-c1cccnc1</chem>
SA10002	2-chlorobenzyamine	CAS_RN: 89-97-4	Level 2	<chem>NC1CCCC1Cl</chem>

**NORMAN prioritisation list:** 860+ subst.

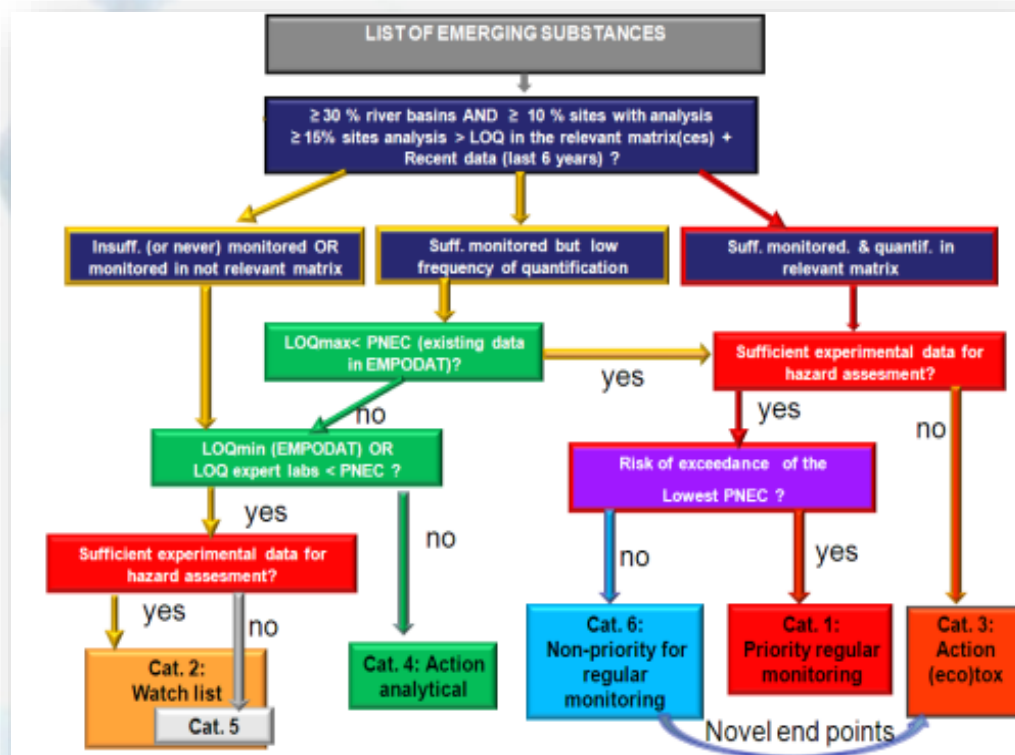
**NORMAN SusDat:** 20000+

<http://www.norman-network.com/?q=node/236>



# NORMAN prioritisation concept – current scheme

- Categorisation and prioritisation of a list of candidate compounds: 6 actions categories
- HOW to extend this scheme to a much larger « Universe of chemicals »?



## Actions needed

- We need to put more effort in data collection for tens thousands of compounds:
  - NOT ONLY monitoring data BUT also:
    - Info on substance properties (physico-chemical properties, hazardous properties, ..)
    - Info to support identification of unknowns in HRMS spectra
    - PNEC values (experimental or predicted values)
    - Exposure indices: indicators derived from tonnage, use pattern, literature PEC, etc. to prioritise compounds for which NO monitoring data is available
    - Indicators derived from NTS data (frequency of appearance of signal, etc.)

From hundreds, to tens  
of thousands candidate  
substances

GO TO NORMAN TARGET PRIORITISATION

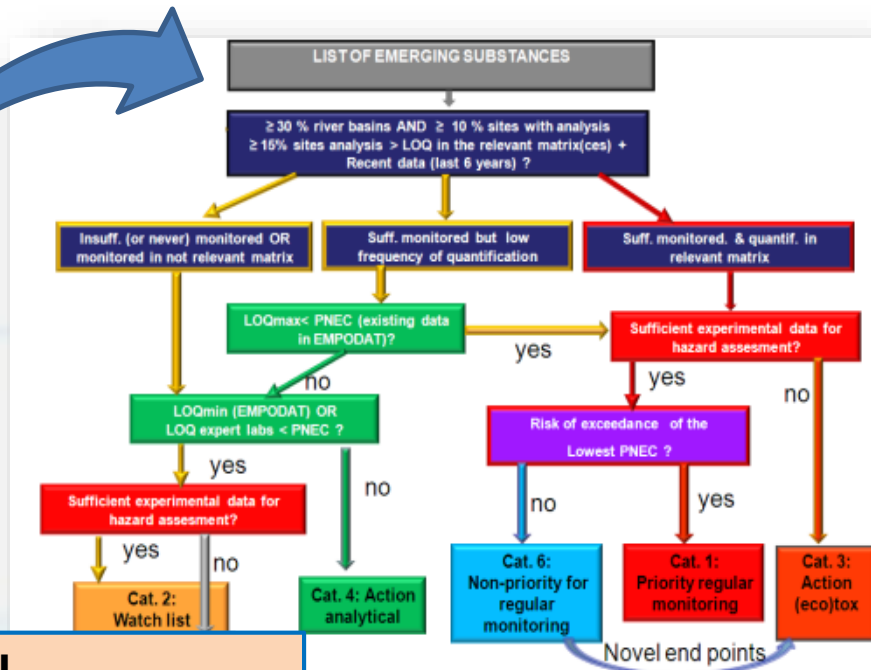
NT CATEGORY 1 - FoA\* + EoE + FoE (0-3)

NT CATEGORY 2A - FoA\* + EoE + FoE (semiquantitative info available)  
NT CATEGORY 2B - FoA\* (0-1; semiquantitative info NOT available)

NT CATEGORY 3 - FoA\*

NT CATEGORY 4 - FoA\*

\* Cut-off: 4 countries, 100 sites detected



Non-target  
screening  
**prioritisation**

## To discuss in this workshop

- Revision of the structure, new modules of the NORMAN database system to better support the new prioritisation vision
- Links with IPCHEM
- Links with other platforms, databases (US EPA Dashboard, FOR-IDENT, etc.): how to organise sustainable info sharing in the long-term
- Further development of the NTS tools / modules (NORMAN Massbank, SusDat, DSFP)



# Thank you



# Wishing you a fruitful workshop !