

Supporting information underlying the publication: Scoping (un)regulated organic micropollutants in aqueous effluents for circular water use: a Dutch case study

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Related publication:

Scoping (un)regulated organic substances in aqueous effluents for circular water use: a Dutch case study

Description:

CSV files and txt file of the supporting information underlying the publication: Scoping (un)regulated organic micropollutants in aqueous effluents for circular water use - a Dutch case study. Containing data to identify the regulatory gaps in the regulation of organic substances found in Dutch effluent, this study bridges methods from both the chemical and legal disciplines by, on the one hand, identifying organic substances of concern, and, on the other, by scoping and compiling the applicable legal framework. The Materials & Methods description describes how the collected data was gathered.

Keywords:

effluent, organic micropollutants, water reuse, EU regulation, Dutch regulation, 'one substance, one assessment', grouping strategies EU chemicals legislation

Spatial coverage:

The Netherlands

Temporal coverage:

From 1 January 2015 until 31 January 2025.

This dataset contains the following files:

S1_Curated_chemical_Watson_data	Curated list of all the chemical substances above reporting threshold found in Dutch municipal effluent between 2015-2025 originating from the Watson Database (1), with regulatory framework and use categorisation
S2_PMT_vPvM_classification	Assigned PMT/vPvM classification to organic substances (2,3,4)
S3_Chemical_features_grouping	Chemical feature grouping based on SMILES OSPIN (5) with the use of SMARTS
S4_SMARTS.txt	RDkit identification of chemical features via SMILES in txt format

(1) Watson Database. Available from: <https://www.emissieregistratie.nl/data/watson-rwzi-emissiedata/watson-database>

(2) Hans Peter H. Arp and Sarah E. Hale ACS Environmental Au 2022 2 (6), 482-509 DOI: 10.1021/acsenvironau.2c00024

(3) EFSA Journals. Available from: <https://efsa.onlinelibrary.wiley.com/journal/18314732>

(4) University of Hertfordshire, PPDB: Pesticide Properties Database. Available from: <https://sitem.herts.ac.uk/aeru/ppdb/en/>

(5) Lowe DM, Corbett PT, Murray-Rust P, Glen RC (2011) Chemical Name to Structure: OPSIN, an Open Source Solution. J Chem Inf Model 51:739–753. <https://doi.org/10.1021/CI100384D>

Explanation of variables:

Column name	Explanation
PARAMETERCODE	Code given to substance in Watson data base
CAS_NUMBER	The unique identification number assigned by the Chemical Abstract Number (CAS) for every chemical substance
SUBSTANCE NAME	Name of chemical substance
MIN	Minimum reported concentration of chemical substance in Watson database
MED	Median reported concentration of chemical substance in Watson database
AVG	Average reported concentration of chemical substance in Watson database

PERC90	P90
MAX	Maximum reported concentration of chemical substance in Watson database
UNIT	Concentration unit in mg/day
NUMBER > RT	Total times concentrations found above reporting threshold
TOTAAL	Total number of times looked for chemical substance
Use category	Assigned (consumer) use category
Regulatory category	Assigned regulatory category
EU_Dutch regulation	Under what regulation is the chemical falling EU, Dutch or Not in analysed water regulations
PMT/vPvM conc. EC Arp & Hale	PMT/vPvM classification information per chemical according to publication Hans Peter H. Arp and Sarah E. Hale ACS Environmental Au 2022 2 (6), 482-509 DOI: 10.1021/acsenvironau.2c00024
PMT_Category	In between assigning PMT/vPvM classification
LogKoc	Lowest logkoc values for pesticides and biocides that are missing this information EFSA Journals. Available from: https://efsa.onlinelibrary.wiley.com/journal/18314732 , University of Hertfordshire, PPDB: Pesticide Properties Database. Available from: https://sitem.herts.ac.uk/aeru/ppdb/en/
M/vM	Assigned M, vM or not M to LogKoc values based on PMT/vPvM classification
Soil DT50	Half time in soils
P/vP	Assigned P, vP or not P to soil DT50 values based on PMT/vPvM classification
PMT/vPvM_updated	Updated PMT/vPvM classification
SMILES	Canonical Simplified Molecular Input Line Entry System (SMILES) from OPSIN
Structure	Chemical structure code RDkit
Br_groups	Number Br groups found based on SMILES
Cl_groups	Number Cl groups found based on SMILES
F_groups	Number F groups found based on SMILES
CF2_groups	Number CF2 (PFAS) groups found based on SMILES
CF3_groups	Number CF3 (PFAS) groups found based on SMILES
triazine_groups	Number triazine groups found based on SMILES
triazole_groups	Number triazole groups found based on SMILES
aromatic_amine_groups	Number aromatic amine groups found based on SMILES
melamine_groups	Number melamine groups found based on SMILES
benzotriazole_groups	Number benzotriazole groups found based on SMILES
phthalate_groups	Number phthalate groups found based on SMILES
benzidine_groups	Number benzidine groups found based on SMILES
TFA_precursor	Number of potential precursor of TFA

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