

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

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Abstract

Reusing wastewater effluent is a promising approach to counter growing freshwater scarcity. However, adequate risk assessment and management measures are necessary to ensure that effluent reuse is safe. In this study, we assessed whether European Union and Dutch chemical substance regulations cover relevant organic substances found in Dutch municipal effluents. We combined a chemical analysis of Dutch effluents with a legal analysis of applicable EU and Dutch legislation. We show that a high percentage of organic substances with (potential) PMT/vPvM characteristics in Dutch effluents are not covered by applicable legislation, especially pesticides and pharmaceuticals, as well as their transformation products. Additionally, prohibited organic substance found in the general sewer system, indicate a lack of adherence to legal norms. Our findings highlight the need for stricter enforcement of existing legal norms as well as an expansion of organic substances covered by EU and/or Dutch legislation to specifically target risks during water reuse. Furthermore, our findings support calls for the 'one substance, one assessment' approach and grouping strategies in EU chemical substances legislation.

1. Background

In regions previously considered "water safe", which include much of the European Union (EU) and even the Netherlands, there is a growing demand for treated wastewater effluent reuse for freshwater provision. To match this need, EU laws such as the (recast) *Urban Wastewater Treatment Directive* (UWWTD) [1] and policies such as the *Circular Economy Action Plan* [2, 3] promote the reuse of treated wastewater effluent. At the most specific level, *Regulation 2020/741 on the minimum requirements for water reuse* creates a specific legal framework for the reuse of wastewater effluent for agricultural irrigation [4].

Numerous organic substances are not removed in conventional wastewater treatment and are emitted in the wastewater treatment plant effluent. These organic substances include pharmaceutical residues, personal care products, pesticides, and industrial chemicals such as per- and polyfluoroalkyl substances (PFASs). Some organic substances can leach to the groundwater, travel over long distances, and/or be taken up by crops [5–12]. Leaching to groundwaters and long travel distances have been documented for a number of organic substances at field scale, with far-reaching consequences for the quality of groundwaters [5–8]. Consequently, such substances pose risks to drinking water sources. While there are no generalized approaches to assess organic substance uptake by crops, recent studies exploring this risk did not identify any immediate human health concerns [9, 10]. However, low threshold organic substances, including endocrine disrupting chemicals which cause adverse effects at very low concentrations, have not been comprehensively assessed in existing studies. Other field studies, especially from regions with a long history of effluent reuse in agriculture, suggest increased human exposure to organic substances via affected crops [11, 12].

To facilitate safe water reuse practices, proper risk management is required. For pathogens, the primary health risk in water reuse is established in international guidance values and regulations [13]. In contrast, comprehensive guidance on organic substances in effluent intended for direct reuse is lacking. Advancing legislative action on organic substances is hampered by the fact that their fate in the environment and the associated potential health risks are still not fully understood [7, 9, 14, 15], and differing use cases will result in differing regulatory needs.

One regulatory avenue which may be promising for better organic substances regulation for water reuse is based on the the *Classification, Labelling and Packaging Regulation* [16, 17]. This Regulation introduces a new chemical hazard category: "PMT/vPvM" (Persistent, Mobile, and Toxic / very Persistent, very Mobile). These hazard categories can cover both parent compounds as well as the wide range of transformation products (TPs) from diverse transformation processes. Once PMT/vPvM substances are released into the water system, this is difficult to reverse, as they are hardly removed using conventional water treatment technologies, leading to exposure for both animals and humans.

Most organic substances registered under the European Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) are not classified under these new hazard classes, and it is unlikely that within a reasonable period, the totality of substances under REACH will obtain the data needed for classification. However, moving forward, chemical substances that enter the European market will have to include PMT/vPvM assessments during their registration procedure, which will increase the information available to regulators and the public on these substances.

Within the EU, Member States are individually responsible for setting quality standards for organic substances of concern in municipal effluents intended for water reuse, leading to a wide regulatory diversity among the EU Member States. Therefore, many (potential) PMT/vPvM substances fall through the regulatory cracks and may not be sufficiently regulated for safe effluent reuse across Europe.

Using data from Dutch wastewater effluent as a case study, we explore to what extent existing EU and Dutch regulation applicable to water reuse covers organic substances found in Dutch effluent streams from 2015–2025. Moreover, we identify regulatory gaps by scoping organic substances not covered by existing EU or Dutch regulation and propose solutions to close these gaps.

2. Materials and Methods

To identify gaps in the regulation of organic substances found in Dutch effluent, this study bridges methods from both the legal and chemical disciplines. The former was applied to scoping and compiling the applicable legal framework, and the latter to identifying organic substances of concern.

2.1. Regulatory framework

The applicable legal framework was identified by piecing together existing EU and Dutch regulations based on their relevance to organic substances in water. We collected all applicable EU and Dutch legislations that lay down threshold values for organic substances in municipal effluent and surface water; these are detailed in section 2.2 and applied in sections 4 and 5.

2.2. Compiling and categorising Dutch municipal effluent emissions

The Dutch emission registration database Watson [19] was used to compile the substances discharged by all the municipal wastewater treatment plants (WWTP) in the Netherlands from 1 January 2015 until 31 January 2025. The Watson database reports influent and effluent data from 24h composite samples used to measure targeted substances from 332 wastewater treatment plants in the Netherlands. The data were retrieved on 21 October 2025, after the latest database update on 10 October 2025. The Watson database applies a reporting threshold for substances in the emission registration system. If a chemical substance is detected but at a concentration falls below this threshold value, the discharge is set to 0 mg/day [19]. Only substances with registered discharge above the reporting thresholds are considered as detected.

These substances were then categorised twice; once on use category and once on whether they fall under EU and/or Dutch legislation. First, the substances were grouped per (consumer) use category present in the Watson database, with a few amendments: We added one additional category, ‘Plastic chemical & TPs’, and matched this with the list from Wiesinger et al. (2024) based on the Chemical Abstract Number (CAS) number, the unique identification number assigned for every chemical substance. This group was added as many group members are potential PMT/vPvM substances [21, 22]. We also removed the category ‘Metals & elements’ as these are not organic substances and therefore fall outside the scope of this study.

We then assigned the organic substances to four EU and four national regulatory categories as shown in the Watson database, namely: E-PRTR water [23], WFD specified compounds, WFD prioritized compounds [24, 25], WFD watchlist [26], contaminants of emerging concern, potential contaminant of emerging concern [27], endocrine disrupting substances, and PFASs [28]. More broadly, the substances were further categorized under ‘Only EU regulation’, ‘Only Dutch regulation’, ‘Both EU & Dutch regulation’ for those substances that fall in both categories, and ‘Not in analysed water regulation’ for those substances not included in any EU or national Dutch regulation analysed (see Table 1).

Table 1 Applied categories for grouping by use and regulatory categories				
Use categories	EU regulation	Dutch regulation	Both EU & Dutch regulation	Not in analysed regulation
Addictive substance & TPs	E-PRTR water	Contaminants of emerging concern	Substances falling in both regulatory categories: EU and Dutch	Substance not covered in any of the EU or Dutch regulations analysed *Excluding ground water and drinking water regulations
Biocide & TPs	WFD specified substances	Potential contaminants of emerging concern		
Industrial chemical & TPs	WFD prioritized substances	Endocrine disrupting substances		
Metal & elements	WFD watchlist	PFAS		
Personal care products & TPs				
Pesticide & TPs				
Pharmaceuticals & TPs				
Plastic chemical & TPs				
Veterinary pharmaceuticals & TPs				

We used the PMT/vPvM classification method by Arp & Hale (2022) [18] to identify if organic substances qualify as (potential) PMT/vPvM, as currently only a limited number of PMT/vPvM substances have been self-reported in REACH (criteria in Table 2). Arp & Hale (2022) only considered REACH registered substances, excluding pesticides and biocides. To close this gap, for pesticides and biocides, we used the European Food Safety Authority (EFSA) dossiers (2008 to present day) and the pesticide properties database (PPDB) of University of Hertfordshire [29]. In addition, for pesticides, we identified minimum reported sorption coefficients to organic carbon (K_{OC}) to assess risks related to mobility, by using the variability analysis of K_{OC} by EFSA obtained from the EFSA journal [30]. We removed sums of chemicals (e.g. sum 4,5 - methyl benzotriazole) from the PMT/vPvM classification as the classification was done substance-by-substance.

Table 2

PMT/vPvM criteria according to the Classification, Labelling and Packaging Regulation [16, 17], *for ionizable substances lowest log K_{oc} between pH 4–9.

Classification	Criteria
Persistent	A substance shall be considered to fulfil the persistence criterion (P) in any of the following situations: a) the degradation half-life in marine water is higher than 60 days; b) the degradation half-life in fresh or estuarine water is higher than 40 days; c) the degradation half-life in marine sediment is higher than 180 days; d) the degradation half-life in fresh or estuarine water sediment is higher than 120 days; e) the degradation half-life in soil is higher than 120 days
very Persistent	A substance shall be considered to fulfil the “very persistent” criterion (vP) in any of the following situations: a) the degradation half-life in marine, fresh or estuarine water is higher than 60 days; b) the degradation half-life in marine, fresh or estuarine water sediment is higher than 180 days; c) the degradation half-life in soil is higher than 180 days.
Mobile*	Log K_{oc} < 3
very Mobile*	Log K_{oc} < 2
Toxic	A substance shall be considered to fulfil the toxicity criterion (T) in any of the following situations: a) The long-term no-observed effect concentration (NOEC) or ECx (e.g. EC10) for marine or freshwater organisms is less than 0,01 mg/l; b) The substance meets the criteria for classification as carcinogenic (category 1A or 1B), germ cell mutagenic (category 1A or 1B), or toxic for reproduction (category 1A, 1B, or 2); c) There is other evidence of chronic toxicity, as identified by the substance meeting the criteria for classification as specific target organ toxicity after repeated exposure (STOT RE category 1 or 2); d) The substance meets the criteria for classification as endocrine disruptor (category 1) for human health or the environment.

We applied a chemical feature grouping strategy proposed by Chirsir et al. (2024) [31] to add persistent and mobile substances to our curated organic substances list. The following groups were selected: halogenated (Br, Cl, F), PFAS according to the OECD 2021 [32] definition “Any substance that contains at least one fully fluorinated methyl (CF₃-) or methylene (-CF₂-) carbon atom (without any H/Cl/Br/I attached to it)”, trifluoroacetic acid (TFA) precursors, triazine, triazole, aromatic amine, melamine, benzotriazole, benzidine, polychlorinated biphenyls (PCBs), and phthalate esters. The chemical structure of each organic substance was included in the form of canonical Simplified Molecular Input Line Entry System (SMILES) in OPSIN (open parser for systematic IUPAC - International Union of Pure and Applied Chemistry- nomenclature) [33]. The software package RDKit was used in Python to assign the organic substances to these groups using SMILES arbitrary target specification (SMARTS) (see Supplementary Information – SI - for more details). Python was used for data analysis and illustration, using large language model tools for assistance in coding. The collected data were harmonized into .csv sheets (see SI).

3. Results and Discussion

3.1 Existing organic substances regulations relevant to effluent reuse

3.1.1 European Union legal framework for organic substances

At EU level, the regulation of substances in treated wastewater effluent is mainly governed by the WFD and the *Environmental Quality Standards Directive* (EQSD) [24, 25] as most wastewater is discharged into surface waters. Also relevant are the *Regulation 166/2006 on the establishment of a European Pollutant Release and Transfer Register* and the REACH Regulation [23, 34]. The broader, still relevant, legal framework also includes the recast UWWTD [35]. Together, these legal instruments establish environmental quality objectives and technical requirements for wastewater treatment, as well as regulating (parts of) the division of responsibilities, reporting obligations, and key definitions. If the wastewater is intended to be reused for agricultural irrigation, *Regulation 2020/741 on the minimum requirements for water reuse* is also applicable [4]. Other regulations, such as the *Pesticides Directive*, the *Biocidal Products Regulation* and *Plastic Food Contact Materials Regulation*, and the *Industrial Emissions Directive* also form part of, albeit indirectly, the regulation of organic substances that may end up in wastewater [36–40].

The WFD provides the overarching regulatory framework for water protection within the EU. A defining feature of the WFD is its river basin approach, which organizes water management according to natural hydrological boundaries rather than traditional administrative borders. This enables a more integrated and ecosystem-based approach to pollution control. The central objective of the WFD is the achievement of “good ecological and chemical status” for all surface and groundwater bodies. To this end, the Directive introduces a two-pathway system to regulate substances. The EU-wide priority substances are defined and controlled under the EQSD which also lays down environmental quality standards for these and certain other substances. In parallel, the WFD places the obligation on Member States to assess and regulate river-basin specific substances. While the first refers to the chemical status of freshwater bodies, the second is part of the assessment of their ecological status, however both regulate pollutants from a water quality perspective. In addition, a 2013

amendment to the WFD led to the creation of the “watch list”, a monitoring mechanism for emerging substances in European waters which can then inform subsequent regulation. Updated every two years, the most recent watchlist was published in 2025 [26]. This amendment also led to a more targeted strategy for pharmaceuticals in order to balance environmental concerns from pharmaceutical substances entering the water system with safe pharmaceutical use for humans [41].

Complementing the WFD, the UWWTD focuses specifically on the collection and treatment of urban and certain industrial wastewaters. It obliges Member States to ensure that wastewater is subject to appropriate treatment prior to discharge, with treatment levels and quality requirements tailored to the sensitivity of the receiving waters. For instance, in areas vulnerable to eutrophication, more stringent removal of nutrients such as nitrogen and phosphorus is required. If wastewater is to be reused for agricultural irrigation, *Regulation (2020/741) on minimum requirements for water reuse* is applicable. Wastewater is first treated in accordance with the UWWTD and subsequently treated to meet the minimum water quality standards laid down in *Regulation 2020/741* plus any additional standards laid down by local operators in the Risk Management Plan and subsequently by the appointed competent authority in the mandatory permit [4]. Lastly, Regulation E-PRTR established the publicly accessible European Pollutant Release and Transfer Register in which key environmental data from industrial facilities in Europe are stored. Operators of industrial facilities in, *inter alia*, the waste and wastewater sectors, must inform their competent national authority on their pollutant releases on an annual basis.

The regulation of organic compounds is characterised by regulatory silos in which substances are assessed and controlled according to their specific use, rather than through an integrated assessment. This is evident in instruments such as the Pesticides Directive, the Biocidal Products Regulation, the Plastic Food Contact Materials Regulation, and the *Industrial Emissions Directive*. These regulations require different forms of information on the identity, properties, uses, emissions, and risks of regulated substances, but the resulting data are not necessarily consistent or interoperable across regulatory domains. Consequently, information on a compound may be available in one regulatory framework while remaining difficult to identify or access in another. This fragmentation can produce situations in which a compound is prohibited or restricted for one application but remains authorised for another. For example, restrictions on a substance's use as a pesticide do not necessarily preclude its use as a biocidal active substance, as a component of food-contact materials, or in an industrial process subject to the Industrial Emissions Directive. Such use-specific regulation can therefore create the situation in which a compound no longer permitted for one use may continue to be introduced into wastewater, surface water, or other water systems through a different, legally permitted use. While this may sometimes be necessary to balance differing needs across sectors, regulatory silos not only complicate the identification and assessment of chemical compounds across these silos but also overlook the broader question of how substances move through and persist in the environment.

This legal framework is not set in stone. Instead, recent developments in broader water policy and EU substance regulation specifically indicate two gradual but significant shifts. First, there is a growing move from the regulation of individual substances towards the regulation of groups or classes of substances, particularly in response to substances of emerging concern such as pharmaceutical substances, microplastics, and PFAS. While earlier legislation relied on the fixed lists of individual substances that had to be monitored and limited, recent revisions and newer legislation increasingly shift their attention to group-based standards and mixture considerations. This shift reflects growing scientific consensus that pollution in water systems often occurs in the form of mixtures rather than isolated substances. For example, Backhaus et al. (2025) [42] argue that ‘chemical cocktails’ should be incorporated in REACH. Similarly, PFAS are now widely understood as a class of substances sharing extreme persistence and potential toxicity that needs regulation, rather than focusing on discrete substances only. The European Chemicals Agency supports group-based regulation of these substances [43].

This shift toward group-based regulation offers several advantages, although some disadvantages should not be overlooked. On the one hand, it enhances regulatory efficiency and responsiveness as it avoids the need for time-intensive, substance-by-substance, risk assessments. It also reduces the risk of “regrettable substitution”, whereby banned substances are replaced with similar alternatives of comparable concern [44]. It also aligns more closely with scientific insights and actual water system pollution, thereby improving environmental protection. On the other hand, group-based approaches may raise questions of proportionality. It can be argued that broad regulation runs the risk of over-regulation by imposing restrictions on relatively low-risk substances. However, regulations such as the EU Chemical Strategy for Sustainability allow for derogations for essential uses of substances, even with group-based regulation. For example, a current proposal for a group-based PFAS restriction under the REACH Regulation includes 74 specific derogated uses where no safer alternatives currently exist [43].

A second development is the gradual shift away from fragmented chemical regulation that addressed pollution within distinct legislative silos. Traditionally, EU environmental governance separated substances regulation (such as REACH), product safety law, occupational health rules, waste legislation, water protection, and industrial emissions into distinct legal regimes, each with its own institutions, risk assessments, and regulatory logics. This compartmentalisation often allowed hazardous substances to be restricted in one domain while remaining permissible in another, creating gaps in environmental protection as such hazardous substances end up in the water system nonetheless. In response, recent initiatives associated with the European Green Deal and the Chemicals Strategy for Sustainability seek to promote what policymakers describe as a “one substance, one assessment” (OSOA) approach, whereby scientific evaluation and risk management are coordinated across different areas of EU law [45–48].

Andreassen et al. (2025) and van Dijk et al. (2021) [49, 50] show a great overlap of organic substances falling in multiple regulatory frameworks, indicating a high potential for the OSOA approach. Following a provisional agreement between the Council and the European Parliament in 2025, the OSOA legislative package [46–48], officially entered into force on 1 January 2026. The deal consists of creating a common data platform hosted by the European Chemical Agency (ECHA) providing access to all the chemical data generated or submitted for implementation of approximately 70 pieces of EU legislation. The OSOA package offers a “one-stop shop” for chemical data from EU agencies and the Commission, enabling knowledge sharing from one legislative area to another.

3.1.2 The Dutch legal framework on organic substances

In the Netherlands, EU legislation is implemented and further specified through national regulatory and policy instruments. The regulation of pollutants in wastewater in the Netherlands is structured under the Environment and Planning Act (*Omgevingswet*), which entered into force in 2024 and symbolises a major overhaul of Dutch environmental legislation [51]. Rather than providing detailed emission standards within the Act itself, the legal framework operates through a system of delegated legislation, primarily the Activities Decree (*Besluit Activiteiten Leefomgeving*) and the Quality Decree (*Besluit Kwaliteit Leefomgeving*) [52, 53]. Together, these instruments establish a layered regulatory approach combining general rules and permitting requirements at national level, with a heavy emphasis on decentralised implementation.

This decentralised governance system is a defining feature of Dutch pollutant regulation. Although the national government establishes the overarching rules through the Act, the Activities Decree and the Quality Decree [52, 53], implementation and enforcement are largely entrusted to regional and local authorities. Regional water authorities (*Waterschappen*) play a central role in regulating discharges into surface waters and managing wastewater treatment infrastructure. Municipalities are responsible for sewer systems and may regulate indirect discharges through local planning instruments. In certain cases, provinces or national agencies retain competence, particularly where discharges affect larger or strategically important water bodies such as the IJsselmeer. This multi-level governance system aims to maintain a baseline of coherent, national pollutant regulation, combined with local decision-making. At the core of the system lies the Activities Decree and Quality Decree.

The Activities Decree contains the substantive rules governing discharges of wastewater. These rules are generally directly applicable to operators and include emission limit values, technical requirements, and prescriptions regarding discharge routes (e.g. discharges in sewer systems, surface waters, or soil). The Activities Decree adopts an activity-based approach: specific industrial or commercial activities are linked to predefined regulatory pathways and pollutant regulations. In other words, there is no 'pollutant perspective' in which emission values for substances are applicable regardless of activity, thereby following the EU's siloed approach to chemical substance regulation. Chapter 4 of the Activities Decree is particularly significant as it sets out requirements for discharges including limits on substance concentrations and obligations to apply appropriate treatment techniques. In addition, Chap. 5 introduces stricter provisions for "substances of very high concern" (*zeer zorgwekkende stoffen*). The Activities Decree further incorporates a specific duty of care which functions as a general standard applicable to all regulated activities. This duty requires operators such as industry to prevent or minimise adverse impacts on the aquatic environment, even in situations where no explicit emission standard is provided. As such, it operates as a regulatory safety net, ensuring that substances of emerging concern that do not (yet) have specific limit values are still addressed within the legal framework.

The Quality Decree, besides transposing the WFD's water quality objectives into Dutch legislation, provides the normative framework for discharge permits and administrative decision-making. Certain activities that pose higher environmental risks are subject to a permit requirement, as determined in Chap. 3 of the Quality Decree. In these cases, competent authorities must assess permit applications against the criteria set out in the Quality Decree. These criteria include compliance with environmental quality standards, the application of best available techniques (BAT), and the protection of water bodies in line with broader ecological objectives. The Quality Decree therefore ensures some level of consistency and legal certainty for operators in the evaluation of specific discharges, while still allowing for local and context-sensitive decision-making.

3.2 Scoping (un)regulated organic substances in Dutch municipal treated effluents

Dutch regional water authorities regularly monitor a wide range of substances in effluents and compile these data into the Dutch effluent database "Watson" [19]. From 2015–2025, the Watson database contained entries for 768 substances, of which 554 unique substances were detected in Dutch WWTP treated effluents. Of these 554 substances, 325 were not covered by any of the analysed water specific regulations (Fig. 1A). A total of 508 organic substances were detected; the largest group of organic substances are 'Pesticides & TPs' (231). A total of 46 substances were 'metals & elements', of which 47.8% are 'Not in analysed water regulations' (Fig. 1B). 'Metals & elements' are not organic substances and are therefore not further discussed in this study.

Furthermore, 188 substances of 554 fall in multiple use categories (Fig. 2), of which 168 fall under two categories, 15 under three, 4 under four, and 1 under five categories (permethrin). Of the 231 substances in 'Pesticides & TPs', 76 fall under multiple use substances (mainly 'Plastic chemicals & TPs' and 'Biocides & TPs'). 'Plastic chemicals & TPs' contains many substances also categorized under other use categories: 74 of 125 falling under 'Industrial chemical & TPs' and 28 under 'Pesticides & TPs'.

Our analysis presents opportunities for improving regulation. For instance, in our study, 188 out of 554 substances fall in multiple use categories and their regulation could thus be eased by the OSOA approach. For example, pesticides are regulated under the *Plant Protection Product Regulation 1107/2009*, however, 60% of the detected pesticides in our dataset are currently not found in the analysed water regulations [40]. Regulation of "data dense" organic substances that already have in-depth fate and risk analyses such as pesticides could be translated across different regulatory regimes to decrease monetary and time investments for their assessment, i.e. via the OSOA approach.

All detected organic substances were compared with the new hazard category "PMT/vPvM" to assess the generic risks they may pose [54]. Of all detected organic substances in our dataset, 8.0% are PMT, 4.1% vPvM, 4.4% vPvM & PMT, 17.2% potential PMT/vPvM, 47.5% are not PMT/vPvM, and for 30.0% there is currently insufficient data available to assign them to a (non) PMT/vPvM category (Fig. 3). For the water-regulated organic substances, 52.3% are still missing categorization, and 26.9% are in the group 'not analysed water regulations'. The lack of (experimental) data for these organic substances limits their assignment to a (non)PMT/vPvM category. To fill this data gap, prioritization is needed to determine which substances should be experimentally tested first and in which order experimental data of organic substances should be collected. Prioritization may be based on production volumes, frequency of detection in effluents, or use category, as the availability of information for classification of PMT/vPvM differs greatly across use categories (Fig. 4).

For pesticides, the PMT/vPvM categorization is explicitly distinct from the *Plant Protection Products Regulation*. For approval of a new pesticide, the persistence, bioaccumulation, potential for long-range environmental transport, and toxicity need to be known. Only pesticides considered not to be persistent organic pollutant (POP), persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) are accepted for use.

Approved pesticides are tested for mobility in the environment according to the OECD 106 sorption test determining experimental K_{OC} ranges [40, 55]. The experimental K_{OC} can be used to classify whether a pesticide is mobile, very mobile, or not mobile based on PMT/vPvM criteria. Similarly persistence data and DT₅₀ half-lives are determined and reported for approved pesticides. Therefore, it is relatively easy to determine PMT/vPvM for pesticides based on existing data required in the *Plant Protection Products Regulation 1107/2009*. The same PMT/vPvM classification approach can be used for biocides. Biocides fall under the *Biocidal Products Regulation 528/2012* and, like pesticides, are tested within POP, PBT, and vPvB regulation and on long-range environmental transport [38]. We were able to assign 95–96% of the pesticides and biocides to a PMT/vPvM class using publicly available data. The remaining pesticides and biocides that we were unable to assign to a class, were either a TP or already banned for use in Europe.

Our analysis shows that there is currently insufficient data for hazard classification for approximately half of the organic substances in the detected 'Industrial chemical & TPs'. As of 1 November 2026, all data relating to the classification and labelling of PMT/vPvM must be reported for new substances that enter the EU market under REACH [56]. This means that for those chemical substances entering the EU market before this date, PMT/vPvM classification was not required. However, as new information on PMT/vPvM properties of these substances comes to light, the classification and labelling should be updated.

The 'Plastic chemicals & TPs' category falls under multiple regulatory frameworks due to the overlap with the category 'Pesticide & TPs' and "Industrial chemical & TPs" (Fig. 2). Plastic additives fall under various regulations, including *Plastic Food Contact Materials Regulation 10/2011*, REACH, and/or *Plant Product Regulation 1107/2009* [39, 40, 56]. Thus, the plastic use determines under which regulation a plastic additive falls. Sharing information across different legal frameworks and sectors will be necessary to support the classification of (non) PMT/vPvM for 'Plastic chemicals & TPs'.

The "Human pharmaceuticals & TPs" and "Veterinary pharmaceuticals & TPs" categories fall under the *Human Medicinal Products Directive 2001/83/EC* and the *Veterinary Medicinal Products Regulation 2019/6* thus a PMT/vPvM classification is not required for these products [57, 58]. However, medicinal products do need to give an indication of any potential risks present for the environment with PBT/vPvB classification [59, 60]. As many pharmaceuticals and pharmaceutical products are currently found in effluent, it would be advisable to additionally include a PMT/vPvM classification in the environmental risk assessment required by the European Medicines Agency [61, 62].

The restriction of use of PMT/vPvM substances and prioritization for safer substitution could lead to a reduction of 147 of the detected organic substance identified in Dutch effluent entering the Dutch WWTP systems. Potentially a larger number of organic substances could be substituted and prevented from being emitted if more mobility and persistence data became available for those substances where data is currently lacking.

3.3 Grouping strategies to fill additional regulatory gaps

Assessing the potential hazard profiles for new and unregulated substances is time and resource intensive. However, unregulated substances could be grouped with regulated substances within the REACH under certain conditions. Specifically, in REACH substances can be grouped based on any of the following features: (i) a common functional group; (ii) common parent compound (precursor) and/or common TP; or (iii) a constant pattern in the changing of potency of the properties [34]. This is illustrated with three examples for each type of grouping.

As an example of (i), a group-based approach is currently being developed for PFAS by the Committees for Risk Assessment (RAC) and for Socio-Economic Analysis (SEAC) following a restriction proposal by the national authorities of Germany, Denmark, the Netherlands, Norway and Sweden using the OECD definition of PFAS [32]:

Per- and polyfluoroalkyl substances (PFASs) defined as: Any substance that contains at least one fully fluorinated methyl (CF₃-) or methylene (-CF₂-) carbon atom (without any H/Cl/Br/I attached to it). [...]

This common functional group is the cause of PFAS's extreme persistence [63]. Grouping based on this functional group will make regulation more inclusive and can prevent regrettable substitution.

An example of (ii) are substances with a triazole ring in their chemical structure. These could, for example, be grouped due to their ability to form triazole as a TP. Triazole is persistent and more mobile than known parent substances [64]. Another example of a common TP is TFA; a PMT and vPvM substance accumulating in the environment [65, 66]. Grouping based on common TP would prevent the need for regulations for each new substance that forms a given TP of concern.

Polychlorinated biphenyls (PCBs) are an example of (iii). PCBs have a core structure consisting of a biphenyl backbone that is substituted by different degrees of chlorine. Due to the constant pattern of toxicity and bioaccumulation across those structures, the whole group of PCBs has been identified as toxic and persistent, resulting in the group classification as persistent organic pollutants regulated by the Stockholm convention in 2001 [67]. Chemicals of a similar constant pattern could also be grouped and regulated under REACH.

These grouping strategies can be applied to the organic substances found in Dutch effluents. Table 3 shows that among the detected substances with common functional groups according to (i), halogenated organic substances were most commonly found. Based on their functional group, 88 of these organic substances are PFASs and could be managed as a group.

For grouping strategy (ii), we looked for potential precursors of TFA. We identified 15 organic substances that could form TFA, of which 14 are pesticides/biocides and 1 a pharmaceutical. Of the 14 pesticides/biocides, 3 have expired approval for use under the Plant Protection Products Regulation. However, 2 of the 3 still have an exemption for use in the Netherlands while being approved for use in countries like Australia and United States [29, 66]. Joerss et al. (2024) [66] indicated that pesticides can be a substantial source of TFA in water sources. Currently, these pesticides are individually approved.

Grouping strategies would provide more comprehensive management approaches for precursors of TFA. Such an approach has recently been implemented in Denmark, which withdrew approvals for the use of 23 TFA-precursor pesticide products collectively [68].

Common precursors with an amine were also identified within our dataset. We found, in descending quantities, aromatic amines (93 organic substances), followed by triazine, then triazole, benzotriazole, and benzidine, with the smallest group being melamine. The organic substances with aromatic amine, triazine, and/or triazole groups will breakdown to common transformation products (a series of nitrogenous heterocyclic substances) with a higher polarity than the parent compound [64]. Thereby, organic substances with multiple features can appear in multiple categories (see Table 3). For example, the same parent substances can form benzotriazole as well as triazole but could be managed as a single group.

For grouping strategy (iii), six organic substances were found to be PCBs. These were all from the use category ‘Industrial chemical & TPs’ and ‘Plastic chemicals & TPs’. Even after global and EU restrictions, PCBs could still be found in the effluent due to their very persistent nature. In addition, eight organic substances were found to have phthalates esters which could also be grouped based on a similar principle. These were all from the use category ‘Industrial chemical & TPs’ and ‘Plastic chemicals & TPs’ and include Bis(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), diisobutyl phthalate (DIBP), and benzyl butyl phthalate (BBP) and, dipentyl phthalate (DPeP), which are regulated in multiple products such as toys and childcare articles, cosmetics, and food contact material [39, 69, 70]. However, they are still detected in Dutch effluent, probably deriving from industrial uses or old plastic items, as noted by Palandri et al. (2026) [71]. Moreover, DPeP is not regulated within the DEHP, DBP, DIBP and BBP restrictions [72, 73].

Overall, grouping strategies can simplify organic substance regulation for water reuse by departing from time- and resource-intensive substance-by-substance regulations. Grouping strategies could support more effective regulation and risks assessment for water reuse, however they will not resolve the presence of these organic substances in the water system. Therefore, in addition to group-based substance regulation for water reuse, stronger upstream regulation at the source is needed, including the restrictions on the production and use of certain organic substances. Consequently, wastewater reuse would become quicker, cheaper, and safer; as a reduction in the total number of organic substances entering the WWTP will reduce additional treatment costs and reduce exposure to humans and the environment.

Table 3
Number of organic substances per chemical feature for total and per use category

Use category	Halogenated			PFAS OECD		Precursor	Amine features							
	Br	Cl	F	CF ₂	CF ₃		Triazine	Triazole	Aromatic amine	Melamine	Benzotriazole	Benzidine	PCB	F
Total SMARTS hits	12	167	78	35	53	16	20	4	93	2	4	4	6	8
Biocide & TPs	1	16	5	1	2	1	3		4	1				
Industrial chemical & TPs	6	30	36	34	36	1	1	4	1	1	4		6	8
Personal care products & TPs	1													
Pesticide & TPs	6	115	33	2	18	15	17		58	1		4		
Pharmaceuticals & TPs		27	11		1	1	2		31					
Plastic chemical & TPs	5	46	3	3	3		5	2	5		2		6	8
Veterinary pharmaceuticals & TPs		10	4		1	1			9					

4. Conclusion

Most organic substances identified in Dutch wastewater effluent are not covered by directly applicable Dutch or EU (waste)water regulations. However, scientific knowledge on these organic substances indicates that, due to their hazard and generic risk profiles, they should be subject to regulation. These organic substances could and should be regulated based on information from other regulatory ‘silos’. For example, organic substances regulated under the pesticides and biocides silos could and should equally be regulated under the ‘industry’, ‘household product’, or ‘wastewater’ silos. This also applies to organic substances identified in the treated wastewater effluent (end-of-pipe) that fall under source regulation (e.g. REACH) as well as specific emission regulations (e.g. Industrial Emissions Directive). This highlights the regulatory and enforcement gaps found along a given chemical’s life cycle. Moving forwards, some of these gaps can be closed using group-based strategies and the OSOA approach, while monitoring and enforcement will be necessary to yield tangible positive outcomes.

The developments surrounding the EU’s OSOA approach respond to the significant overlap of substances across regulatory frameworks. The creation of a common data platform hosted by the ECHA intends to centralise chemical data across EU legislation. By facilitating assessment and data sharing across regulatory domains, the OSOA would make implementation easier, cheaper, and quicker. Practically, this would also be the case for relatively new and complex actions such as wastewater reuse, as these actions are at the crossroads of many legislative silos. OSOA could merge these silos, including the regulation of organic substances from first use to water quality requirements. In this study, 33% of the detected substances in Dutch effluent fall under

multiple use categories and 58% are not covered by analysed EU or national legislation, highlighting the positive impact implementing a OSOA approach could have for assessing and managing these chemicals for safe water reuse.

Ee showed that a large number of organic substances found in Dutch effluent are not covered by EU or national regulation and describe group-based approaches for substance regulation that could address this issue, at least in part, and thus support effective regulations for water reuse. Notable advantages of group-based regulation for human and ecosystem health include the fact that group-based regulation reflects real-world exposure to mixtures of substances. Instead of assessing and regulating substances in isolation, it enables the assessment and regulation of cumulative effects within a group of substances. It also reduces the risk of “regrettable substitution”, where one harmful substance is replaced by another with similar properties; as group-based regulation is based on a common component of the substance, other future chemical substances with this common component would automatically fall under this regulation. Therefore, group-based regulation anticipates the creation and market entry of chemical substances that would harm the environment or humans, without the need for additional regulatory efforts.

As we show in this study, while ‘narrow’ regulation reduces immediate exposure for a given silo, these same organic substances being allowed in other sectors means they still end up in the environment and water systems. Water quality regulation alone will be insufficient to prevent certain organic substances from contaminating the water system. Regulation of substance use earlier in the chemical life cycle across silos must be expanded and better enforced. OSOA based regulation can help tie together sector-specific chemical regulation in favour of broader protection goals. These developments are necessary from an environmental protection point of view, but also for the uptake of quicker, cheaper, and safer wastewater reuse practices which lie at the crossroads of multiple legislative pathways.

In the broader context of water security, this study indicates that OSOA and group-based chemical substance regulation, alongside stronger enforcement, could not only increase protection for human and ecosystem health, but also support more integrated water quality management. Aquatic environments are typically exposed to complex mixtures of organic substances, many of which remain unidentified or are insufficiently regulated. As OSOA enables better knowledge exchange and group-based regulation better reflects chemical realities, regulators and industry will be able – and mandated - to better maintain the chemical quality of effluents. This would safeguard surface and groundwaters and enable quicker, cheaper, and safer water reuse across sectors.

Abbreviations

BAT
Best available technique
CAS
Chemical Abstract Number
CBS
Statistics Netherlands
ECHA
European Chemicals Agency
EFSA
European Food Safety Authorities
ESQD
Environmental Quality Standards Directive
IUPAC
International union of pure and applied chemistry
OPSIN
Open parser for systematic IUPAC nomenclature
OSOA
One substance, one assessment
PBT
persistent, bioaccumulative, toxic
PCB
Polychlorinated biphenyls PFAS:Per – and polyfluoroalkyl substance
PMT/vPvM
Persistent, mobile, toxic/very persistent, very mobile
POP
Persistent organic pollutant
PPDB
Pesticide properties database
RAC
Committees for Risk Assessment
REACH
European Registration, Evaluation, Authorization and Restriction of Chemicals
RIVM
Netherlands National Institute for Public Health and Environment

SEAC
Committee for Socio-Economic Analysis
SMARTS
SMILES arbitrary target specification
SMILES
Simplified Molecular Input Line Entry System
TFA
Trifluoroacetic acid
TP
Transformation product
vPvB
very persistent, very bioaccumulative
WFD
Water Framework Directive
WUR
Wageningen University and Research
WWTP
Wastewater treatment plant
UWWTD
Urban Wastewater Treatment Directive

Declarations

Ethics approval and consent to participate

Not applicable

Consent for publication

Not applicable

Competing interests

The authors declare no competing interests

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Ethics Declarations

Author Contribution

J.A.R.S. and S.M. wrote the main manuscript text, J.A.R.S. created all the figures, G.S. guided the conceptualization and led the supervision. All authors reviewed the manuscript and provided feedback.

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Data Availability

All data generated or analysed during this study are included in this published article and its supplementary information files.

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Footnotes

1. Throughout this paper, the term 'organic substances' will be used whenever possible. When regulation is discussed, the comparable regulatory term is used – often 'pollutant'.

Figures

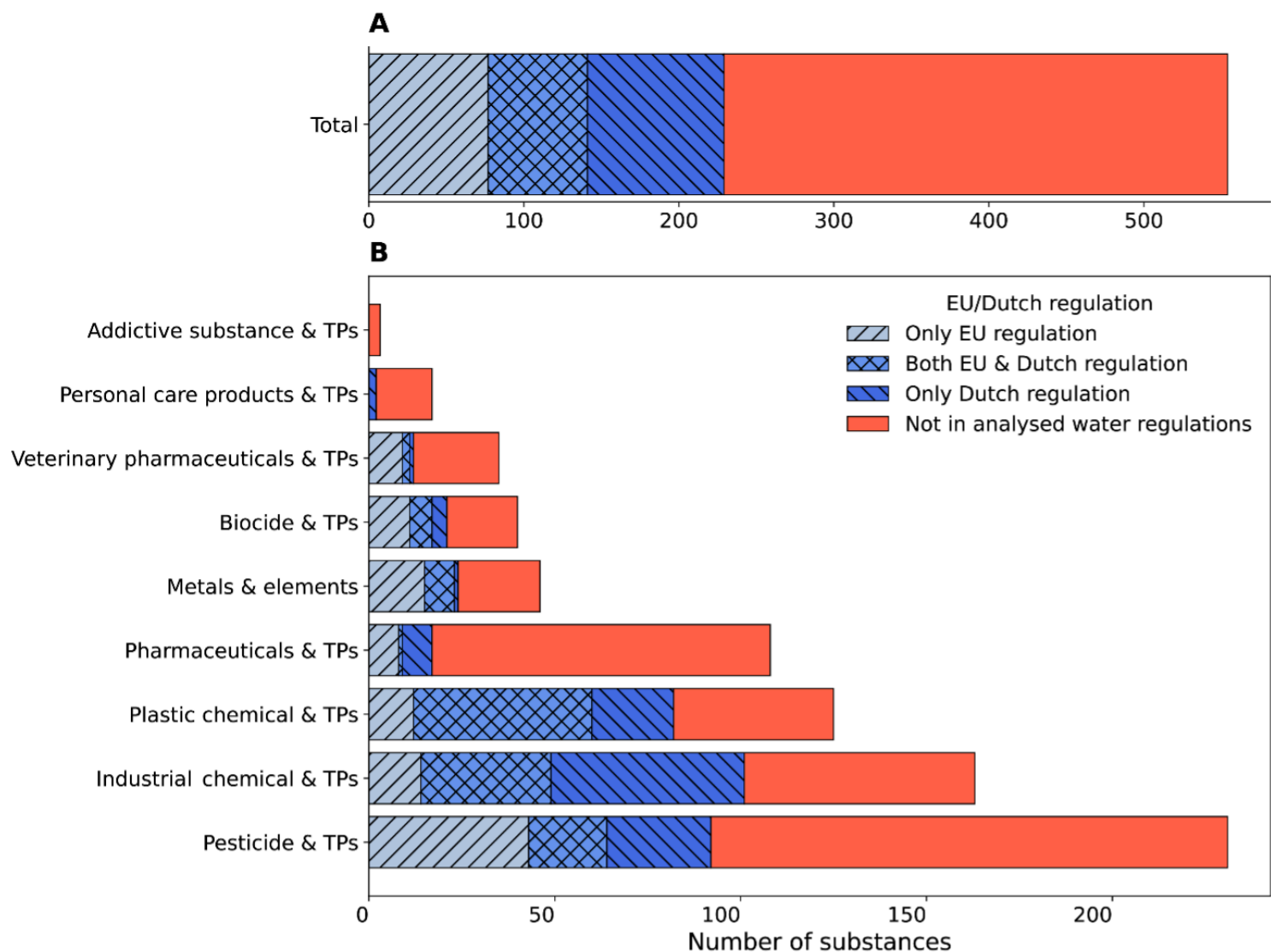


Figure 1

A: Division of all regulated and unregulated substances detected in Dutch effluent from 2015-2025, B: Regulated and unregulated substances detected in Dutch effluent from 2015-2025 per use category

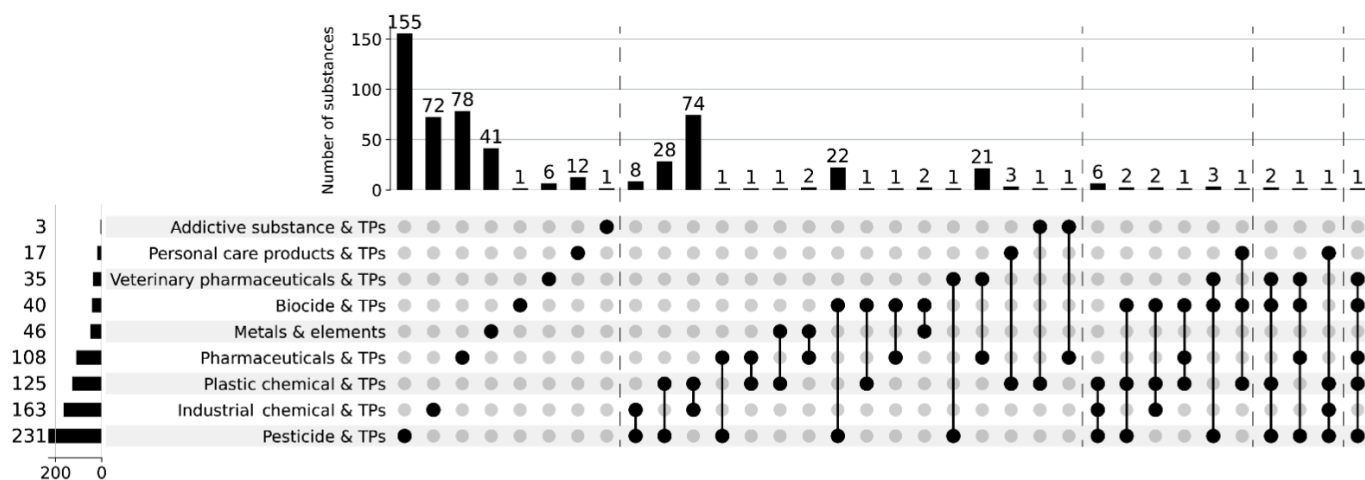


Figure 2

Overlap of substances between use categories, left side horizontal bar plots show the total number of substances per use category starting on top with the lowest number of substances use category to the highest number at the bottom, top vertical bar plots show the total number of substances per use category indicated with the black filled dot or combination of dots with substances in multiple categories

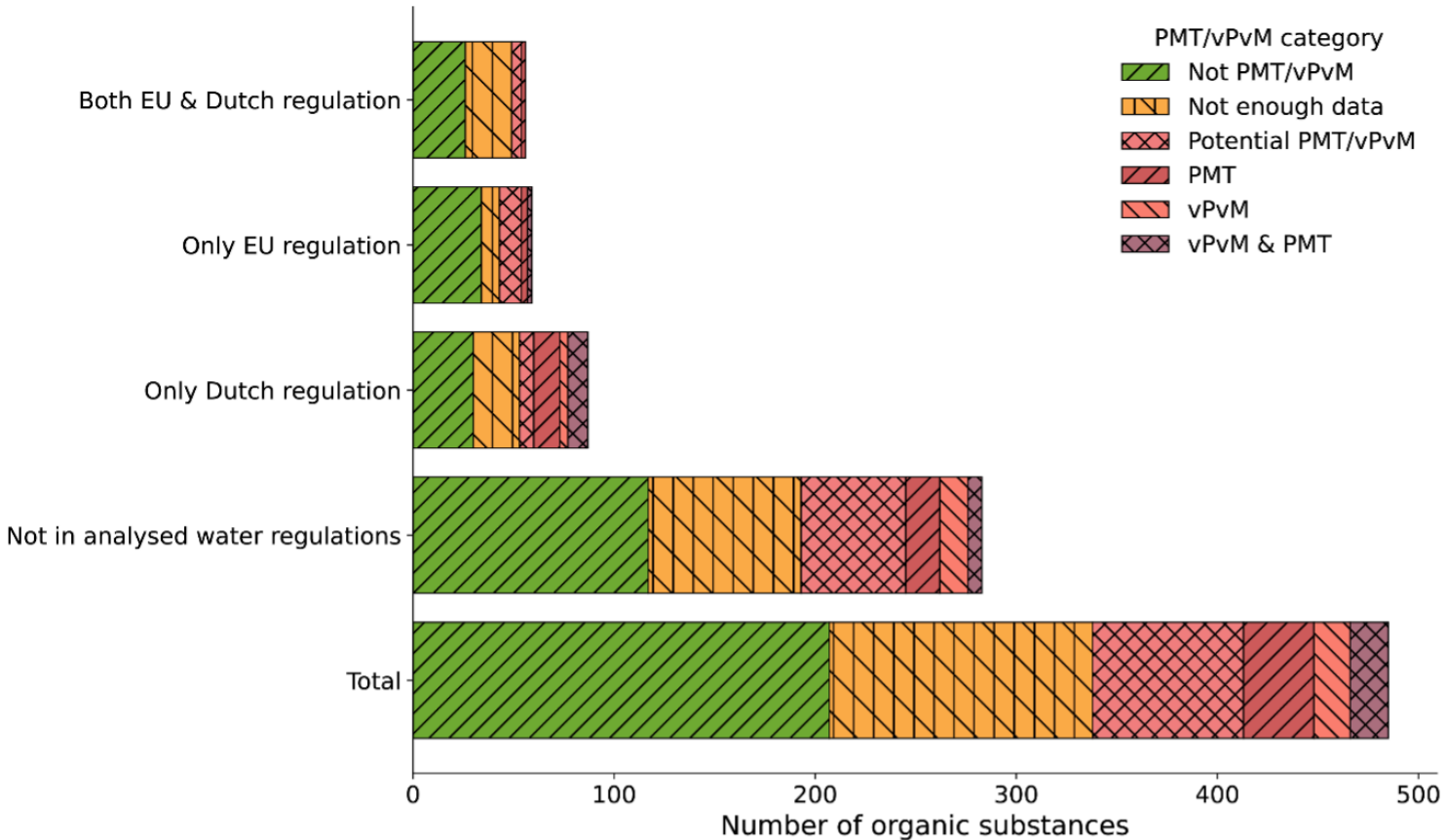


Figure 3
Detected organic substances with their respective PMT category per regulatory category. Database used for PMT/vPvM classification: [18], [29], as well as EFSA dossiers (2008 to present day).

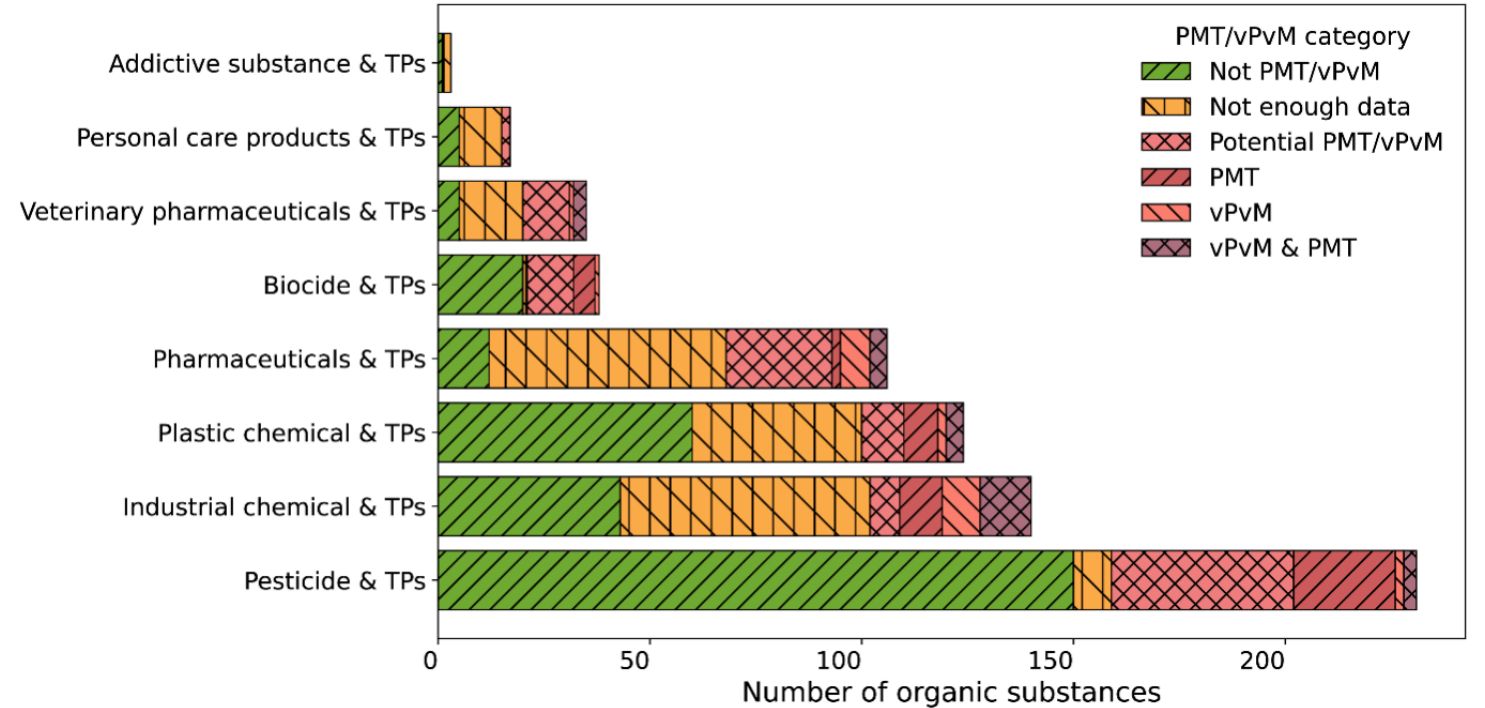


Figure 4

Regulated and unregulated organic substances per use category with their respective PMT/vPvM Category. Database used for PMT/vPvM classification: [18], [29], as well as EFSA dossiers (2008 to present day).

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- [S4SMARTS.txt](#)
- [S3Chemicalfeaturesgrouping.csv](#)
- [ReadmefileSIscoveringunregulatedorganicsub.pdf](#)
- [S1CuratedchemicalWatsondata.csv](#)
- [S2PMTvPvMclassification.csv](#)