



**Universiteit  
Leiden**  
The Netherlands

## **Harmonizing ecotoxicological data reporting: a guide for toxicologists and chemists**

Balraadjsing, S.; Kropf, P.; Boeije, A.G.; Barmentlo, S.H; Peijnenburg, W.J.G.M.; Vijver, M.G.

### **Citation**

Balraadjsing, S., Kropf, P., Boeije, A. G., Barmentlo, S. H., Peijnenburg, W. J. G. M., & Vijver, M. G. (2026). Harmonizing ecotoxicological data reporting: a guide for toxicologists and chemists. *Environmental Toxicology And Chemistry*. doi:10.1093/etjnl/vgag061

Version: Publisher's Version

License: [Creative Commons CC BY 4.0 license](https://creativecommons.org/licenses/by/4.0/)

Downloaded from:

**Note:** To cite this publication please use the final published version (if applicable).



# Harmonizing ecotoxicological data reporting: A guide for toxicologists and chemists

Surendra Balraadsing<sup>1,\*</sup>, Philipp Kropf<sup>1</sup>, Annetrude Boeije<sup>1</sup>, S. Henrik Barmantlo<sup>1</sup>, Willie J.G.M Peijnenburg<sup>1,2</sup>, and Martina G. Vijver<sup>1</sup>

<sup>1</sup>Institute of Environmental Sciences (CML), Leiden University, Leiden, RA, The Netherlands

<sup>2</sup>Centre for Safety of Substances and Products, National Institute of Public Health and the Environment (RIVM), Bilthoven, BA, The Netherlands

\*Corresponding author: Surendra Balraadsing, Email: [s.balraadsing@cml.leidenuniv.nl](mailto:s.balraadsing@cml.leidenuniv.nl)

## Abstract

Concerns have been raised regarding the findings and reproducibility of scientific research, including ecotoxicological studies. In environmental risk assessment, controlled laboratory or field-based exposure experiments are conducted to evaluate the effects of substances towards individual species or ecosystems. Exposure experiments generate crucial data but the process of collecting such data is both time-consuming and costly, with limited emphasis on ensuring reproducibility. The value of experimental data is immense and can have multiple applications or can be made fit for secondary scientific and regulatory use. Effective reuse of ecotoxicological experimental data is often hindered by (unintended) suboptimal reporting practices such as poorly described methodologies or inconsistent reporting of units or data. The purpose of this study is to highlight the issue of insufficient reporting in ecotoxicology through examples from publications as well as to provide solutions, focusing on how the data or metadata itself are reported rather than which variables are reported from experiments. Published data and metadata on nanomaterials, neonicotinoids, and per- and polyfluoroalkyl substances were analyzed to gain insight into the extent to which insufficiently reported data are present across the literature.

**Keywords** data reporting, data quality, standardization, reproducibility, harmonization

## Introduction

Empirical studies generate valuable data and metadata and contribute to the general knowledge of scientific fields (Hillebrand & Gurevitch, 2013). Although at first glance, studies seem rich with information, a large proportion of them are irreproducible (Baker, 2016; Hitchcock et al., 2018). Indeed, concerns have been raised regarding the findings of scientific research: chemistry and biology studies were deemed the least reproducible quantitative disciplines (Baker, 2016; Hanson et al., 2017; Jacobs et al., 2024). The poor reproducibility of scientific studies has been broadly attributed to flawed experimental design, insufficient reporting, and an inaccessibility of data and metadata (Hillebrand & Gurevitch, 2013; Percie Du Sert et al., 2020).

Data generated by empirical studies can form part of subsequent studies (e.g., modeling or meta-analyses) and help gain new insights. Reusing data is an essential part of the findable, accessible, interoperable, and reusable (FAIR) principles (Wilkinson et al., 2016). The FAIR principles put emphasis on data sharing and management to ensure easy findability, accessibility, interoperability, and reusability for both humans and machines (Groenewold et al., 2024; Jeliaskova et al., 2021). Although good data sharing and management practices are

crucial to the reuse of data, it is only one aspect of a larger process (Furxhi et al., 2023). Another aspect of reusing data involves the quality of the data itself (Groenewold et al., 2024). Data quality is important because poor quality data adversely affects modeling efforts, meta-analyses (Ajisafe et al., 2025; Chen et al., 2015; Furxhi et al., 2023; Hartung & Kleinstreuer, 2025; Przybylak et al., 2012), and regulatory decision-making (Ågerstrand et al., 2018). Studies cannot be reproduced or compared with another when insufficient information is reported, thereby diminishing their scientific value as well as contributing to resource waste (Hanson et al., 2017; Mebane et al., 2019; Samuel et al., 2016).

**Textbox 1** Empirical studies generate valuable data from direct observations and contain scientifically valuable data in the form of their metadata (or data about data; Drobne, 2021; Papadiamantis et al., 2020). Data from direct observations include experimental measurements of chemicals/materials (e.g., concentrations, physicochemical properties), exposure conditions (e.g., pH, temperature) and toxicity endpoints (e.g., EC50 values). Examples of important metadata include the metadata about methods (e.g., which used protocol), instruments (e.g., models and parameters), and bibliographic data (e.g., authors or publication date).

**Received:** October 2, 2024. **Revised:** February 23, 2026. **Accepted:** March 3, 2026

© The Author(s) 2026. Published by Oxford University Press on behalf of the Society of Environmental Toxicology and Chemistry. This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<https://creativecommons.org/licenses/by/4.0/>), which permits unrestricted reuse, distribution, and reproduction in any medium, provided the original work is properly cited.

Data quality concerns the completeness and reliability of the data or metadata itself. The quality is determined by the robustness of the methods used, reproducibility of the results and adequate description of the study (Shao et al., 2023).

In ecotoxicological studies, researchers perform exposure experiments in a laboratory or field setting (Comandella et al., 2020) and publish their finding in scientific journals or reports. Despite the availability of standardized guidelines (e.g., Organisation for Economic Co-operation and Development [OECD] 202, [2004]), the quality of ecotoxicological data and metadata is frequently insufficient (Aurisano & Fantke, 2022; Hanson et al., 2017; Karcher et al., 2018; Olker et al., 2022). Specifically, methodological information and statistical and experimental outcomes are underreported and/or inconsistent within publications (Bosker et al., 2013; Erickson & Rattner, 2020; Furxhi et al., 2024; Henke et al., 2024). As a result, it has been acknowledged that curated databases based on published data are currently not suitable for *in silico* modeling (Jeliazkova et al., 2021; Z. Ji et al., 2021). Inadequate data quality has been widely recognized across ecotoxicological research involving a wide range of substances: nanomaterials (Comandella et al., 2020; Fernández-Cruz et al., 2018; Karcher et al., 2018; Plata & Janković, 2021), micro- and nanoplastics (Askham et al., 2023; Jenkins et al., 2022; Kokalj et al., 2024; Nyadjro et al., 2023; Pang et al., 2023), and soluble chemicals (Ankley et al., 2021; Olker et al., 2022; Przybylak et al., 2018; Schür et al., 2023). These issues also extend across various experimental approaches such as “omics” (Henke et al., 2024; Saarimäki et al., 2022), *in vitro* (Krebs et al. 2020), *in vivo* (Balraadsing et al., 2024; Schür et al., 2023), and field studies (Hanson et al., 2017).

It has become increasingly common for ecotoxicological modeling, meta-analyses, and regulatory studies to highlight data quality insufficiencies and inadequate reporting. However, relatively few studies have attempted to quantify the extent of these issues across the ecotoxicological literature. In the past, Bosker et al. (2013) and Erickson and Rattner (2020) discussed reporting insufficiencies within the toxicological literature but focused only on statistical information. However, inadequate reporting in ecotoxicology goes beyond statistical information. Therefore, the aim of this article is twofold: (1) to identify, quantify, and discuss common data reporting issues prevalent in ecotoxicological literature and (2) provide suggestions on how to mitigate reporting issues. Common shortcomings are highlighted and discussed, followed by an analysis of published scientific ecotoxicology data for three groups of compounds: nanomaterials, per- and polyfluoroalkyl substances (PFAS), and neonicotinoid insecticides. As little consensus exists between researchers regarding which variables are important to report (Exner et al., 2023), the focal point of this article will be mainly how data and metadata are reported in the literature rather than which variables are reported. Improved and transparent reporting procedures can improve the quality and reproducibility of ecotoxicological studies and is beneficial to all across the discipline (Ågerstrand et al., 2018; Hutson, 2022; Nian et al., 2025). This would result in fewer repeated experiments and save time, money, animals, and resources (Hanson et al., 2017).

## Common reporting shortcomings

Inadequate reporting practices in ecotoxicology literature can be broadly categorized as heterogenous and incompletely reported data or metadata. This section is not intended as an exhaustive list of shortcomings but to highlight common data reporting mistakes in publications. Examples were chosen at random and used only to exemplify common shortcomings rather than criticize individual publications.

**Textbox 2** Data completeness is defined here as the extent to which key ecotoxicological variables were reported within publications (European Food Safety Authority [EFSA] et al. 2025). Incomplete reporting signifies the lack of reported data (underreporting or data gaps; Ågerstrand et al., 2018).

Data heterogeneity is defined here as the diversity of data formats and levels of detail used to report data. This refers to unstandardized, unharmonized, or inconsistent data reporting between studies. Data heterogeneity as described here is analogous to the European Food Safety Authority (EFSA) definition for data consistency (EFSA et al., 2025).

## Incomplete reporting

### Methodologies

Publications generally describe experimental setups and conditions but vary considerably in the level of detail they provide (Ågerstrand et al., 2014; Plata & Janković, 2021). Studies commonly cite only standardized test guidelines when describing experimental methodologies, which is not always sufficient (Ågerstrand et al., 2014; Przybylak et al., 2012). Citing only experimental guidelines, without providing exact conditions or measurements, lacks the necessary detail to reproduce experiments or reuse data. To use such data in meta-analyses and models, assumptions must be made to address ambiguously described parameters that introduce uncertainty into analyses.

Standardized protocols provide structured guidance but do not always describe the exact conditions necessary to conduct experiments (Pulido-Reyes et al., 2024). To elaborate, Annunziato et al. (2019) utilized OECD 212 (OECD, 1998) which allows researchers autonomy to use alternative media as needed as long as it adheres to annex 5 of the guideline. Although the authors reported the standardized guideline as their methodology, they provided limited information about the media (composition) or water quality parameters. Water quality parameters greatly influence the fate of chemicals (Verschoor et al., 2011) or (nano)materials (Xiao et al., 2016), and subsequent toxic responses can differ in relation to for example, pH or dissolved organic carbon levels with similar chemical doses.

Standardized protocols allow for parameters to be within specified ranges rather than providing exact fixed values. The *Daphnia* sp. acute immobilization test, OECD 202 (OECD, 2004), states that media pH must “remain stable and be between 6 to 9” in addition to recommending water hardness levels “between 140 and 250 mg/L CaCO<sub>3</sub>, but lower is also acceptable”. The guideline provides ambiguous direction to researchers, giving

them the autonomy to use alternative media as needed. However, the flexible guidelines become problematic when authors fail to report exact experimental conditions, thereby preventing others from knowing or reproducing this data. This can be observed in [Barmiento et al. \(2015\)](#), where water quality parameters were reported as being “within the requirements” of the guideline, but exact measurements per tested concentration were not given (concentrations were reported as ranges of all measurements). Additionally, [Barmiento et al. \(2015\)](#) reported the water hardness as “exceeding the recommended value of < 250 mg/L”.

Inaccessible and erroneously reported experimental guidelines also create additional barriers for the reuse of data and reproducibility of experiments. For example, [Valerio-García et al. \(2021\)](#) exposed zebrafish to nanomaterials using “OECD (guide 21,02,013)”. However, such a guideline does not exist and insufficient details were provided to deduct the correct guideline.

### Statistical information

Deficiencies in statistical reporting are widely recognized in the ecotoxicological literature ([Bosker et al., 2013](#); [Comandella et al., 2020](#); [Erickson & Rattner, 2020](#); [Sumpter et al., 2021](#); [Wheeler & Lower, 2021](#)). Statistical information gives crucial insight into experimental outcomes and is necessary to compare studies in meta-analyses ([Hitchcock et al., 2018](#)). Statistical reporting deficiencies include a failure to report *p*-values, degrees of freedom, effect sizes, and statistical power, which have been extensively reported on in [Bosker et al. \(2013\)](#) and [Erickson and Rattner \(2020\)](#).

Furthermore, researchers commonly summarize data ranges into point estimates using descriptive statistics (e.g., mean, median). However, reporting descriptive statistics without measures of statistical dispersion or uncertainty (e.g., *SD*) results in the loss of information regarding the underlying data. [Faria et al. \(2018\)](#) illustrated this by considering the size of nanomaterials with uniform distributions ranging from 100–900 nm versus particles ranging from 495–505 nm. Both size distributions have a mean of 500 nm and thus, reporting only their descriptive statistics without statistical dispersion means essential information about the size distribution is lost.

Not reporting the underlying (raw) data used to calculate descriptive statistics can also be problematic. Raw data can be particularly crucial in studies where zeros are not treated equally, such as chromatographic or spectrometric measurements ([Sumpter et al., 2021](#)). In such measurements, concentrations labelled as “not detected” are not standardized and may either be included, replaced, or disregarded entirely in descriptive statistics ([Barr et al., 2006](#); [Chik et al., 2018](#)). Measurement data with limits of detections are a form of censored data and their handling in analyses is not straightforward ([George et al., 2021](#); [Sumpter et al., 2021](#)).

### Graphical results

Publications may occasionally report data solely within graphs without providing the underlying data elsewhere in the main text or online [supplementary material](#). This is exemplified in [Yung et al. \(2017\)](#), where the zeta-potential, hydrodynamic size, and particle dissolution were measured over time, but the corresponding data were only presented in graphical form. Similarly,

[Li et al. \(2010\)](#) reported median effect concentration (EC50) data exclusively in bar graphs and discussing only a portion of the displayed data within the main text. To reuse this data, the exact values must be estimated or extracted with alternative tools, thereby introducing uncertainty in analyses.

### Reused data

Researchers may reuse previously published data across multiple publications as part of subsequent (but related) experiments. However, authors may occasionally fail to explicitly state the reuse of previously published data within publications. Not explicitly declaring the reuse of data between publications can be seen in [Fazelian et al. \(2020\)](#): the EC50 and EC90 toxicity values for CuO nanomaterials are identical to those provided in the authors’ previous publication ([Fazelian et al., 2019](#)) using the same materials. Such reporting oversights may not be problematic in itself, and are insignificant towards reproducing experiments or the quest for harmonized data and metadata. However, such reused data may end up within databases where they would result in duplicated entries that go undetected if not examined carefully.

### Positive and negative results

Although positive results have a propensity to be published, negative findings are reported less frequently ([Ågerstrand et al., 2014](#); [Martin et al., 2019](#)). “Negative findings” here denotes results that show no (significant) effects. Building models using only positive findings will inadvertently lead to biased outcomes ([Hartung & Kleinstreuer, 2025](#)). Reporting negative findings would also avoid the need for repeating experiments and complete the overall picture of investigated substances ([Krug, 2018](#)). Nevertheless, negative outcomes are frequently omitted from publications even when they form part of the same experimental scheme. For example, in gas chromatography–mass spectrometry analyses, studies commonly report data pertaining only to compounds detected above a certain threshold, such as [Eulaers et al. \(2013\)](#), which only included chemicals detected in more than 50% of samples.

## Heterogeneous reporting

### Reporting formats

Researchers may report experimentally measured variables as either continuous (numerical) or categorical data. However, heterogeneous reported data formats are common for experimentally measured variables across ecotoxicological studies ([Furxhi et al., 2023](#)). Heterogeneous reporting formats hinder data reuse and complicate comparisons between publications.

Continuous variables can be reported numerically, as numerical ranges or by using qualifiers (e.g., <, >; [Aggarwal et al., 2024](#); [Saouter et al., 2019](#)). Reporting continuous variables using numerical ranges or qualifiers creates problematic censored data. For example, authors primarily report EC50 values as the mean effect of multiple measurements, although some studies may report them as numerical ranges instead (the minimum and maximum effect concentration; [Schür et al., 2023](#)). Likewise, researchers may report the same variable as either categorical or continuous values across studies, as is the case

with data on nanomaterial crystallinity. Crystallinity is regularly reported qualitatively, as the dominant crystal state of a material (e.g., anatase, rutile, “anatase with some rutile present,” etc.). However, studies may also express crystallinity quantitatively as proportions (e.g., “10% anatase and 90% rutile”).

### Experimental measurements

Substance concentrations may be reported ambiguously in studies by researchers as nominal or actual concentrations, with the former being more commonly reported (Lead et al., 2018; Mancardi et al., 2023; Saouter et al., 2019). Differences between nominal and actual measured concentrations may be considerable as highlighted by Pulido-Reyes et al. (2024). The authors report an overestimation of median lethal concentration values based on nominal concentrations compared with actual concentrations.

Ambiguity in the reporting of experimental data also extends to the timepoints at which researchers measure parameters. Chemical concentrations are typically measured at the start and/or end of exposure (OECD, 2004). However, concentrations often fluctuate nonlinearly throughout the exposure duration due to chemical processes such as degradation and metabolization (Barmiento et al., 2019). Similarly, the behavior and bioavailability of nanomaterials may change due to transformation processes (e.g., dissolution or aggregation; Lead et al., 2018). Such dynamic processes affect the exposure of substances towards organisms, and it is therefore crucial to report the timepoint at which parameters were measured.

Researchers may measure an organism’s weight as either dry or wet weight, but this is not always clearly stated within publications (Askham et al., 2023). For instance, Schanzer et al. (2022) reported measurements involving bat livers but the reported data did not indicate whether this was the wet or dry weight.

Comparing experimental measurements between studies is difficult when different approaches are used to express parameters such as substance concentrations or weights. This also applies to measurements done at diverse timepoints or media.

### Units

Scientific literature has frequently cited the use of inconsistent units across publications as reporting insufficiency (Alves et al., 2021; Askham et al., 2023; Krug, 2022; Pang et al., 2023; Scharmüller et al., 2020). Although the majority of units in datasets can be easily converted and harmonized, there remain particular cases where this is not straightforward (Furxhi et al., 2024). Nam et al. (2015) expressed toxicity as the number of particles/ml, which is a valid unit for expressing nanotoxicity. However, particles/ml is not always easily convertible into mass (e.g., mg/L) or molar-based units (e.g., mol/L), which are more commonly used across ecotoxicology. This requires information on the size and either the mass or volume of the nanomaterial (Wheeler & Lower, 2021), which can be difficult to estimate when the particle shape is irregular.

Instances of inadequate or erroneous unit reporting can also be found in literature. Oukarroum et al. (2013) reported the ionic strength as a unitless parameter, whereas Bernot and Brandenburg (2013) reported conductivity as “51–70 mg/L CaCO<sub>3</sub>”. The latter was likely a mislabeling and the reported property should have been water hardness instead. Although

reporting errors are unintentional, they may go unnoticed and affect how studies are assessed (Ingre-Khans et al., 2019).

### Toxicological outcomes

Ecotoxicological outcomes are generally reported as EC<sub>x</sub> values, with *x* commonly being equal to 50. Effect concentrations may occasionally also be expressed as EC<sub>x</sub> values other than EC<sub>50</sub>s such as EC<sub>10</sub>s or EC<sub>90</sub>s. Due to its widespread use, EC<sub>50</sub>s are easily comparable between studies in relation to other EC<sub>x</sub> values. Comparability between studies is particularly hindered when studies report various levels of EC<sub>x</sub> values or when the parameters of fitted dose-response curves are not reported.

### Terminology

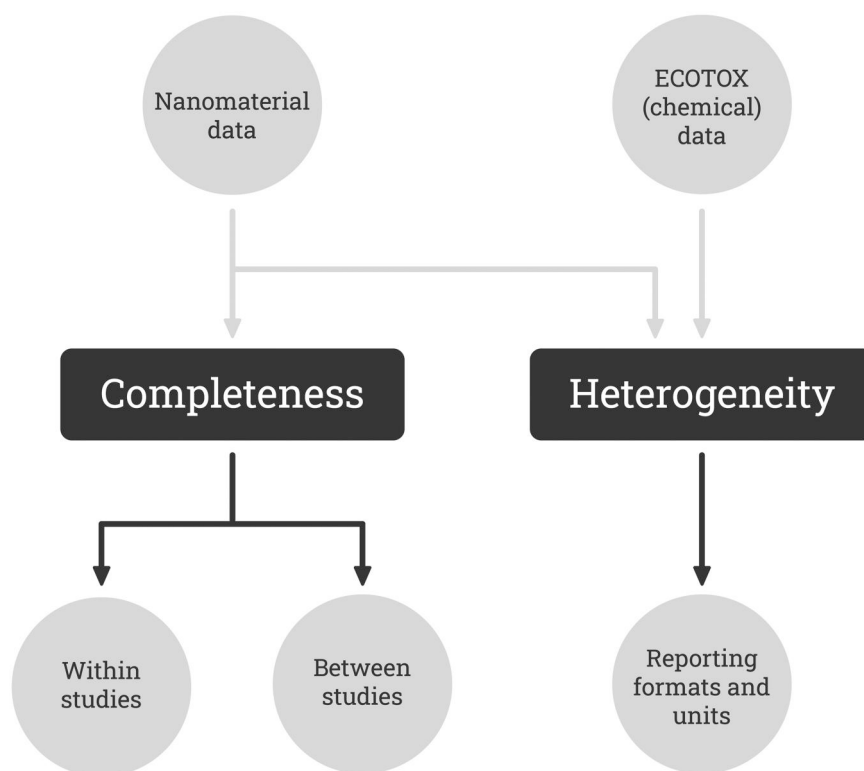
Ecotoxicology studies commonly use heterogeneous terminology, using different terms for analogous concepts or identical terms for different concepts (Hartung et al., 2019; Karcher et al., 2018). Unharmonized terminology causes confusion and creates barriers for the reuse and integration of data from multiple sources (Furxhi et al., 2020; Shao et al., 2023; X. Yan et al., 2023). Moreover, unharmonized terminology also limits machine readability and text mining efforts (X. Yan et al., 2023). In nanomaterial literature, the terms “agglomeration,” “aggregation,” and “hydrodynamic size” are often used interchangeably, despite being subtly different processes (e.g., Aruoja et al. [2015] uses “agglomerates”, N. Yan et al. [2019] uses “aggregates” to refer to the same process). Likewise, within the context of the acute *Daphnia* sp. toxicity test (OECD, 2004), “immobilization” and “mortality” are used interchangeably (immobilization is a proxy to measure mortality). Nevertheless, studies may at times report immobilization and mortality as two distinct endpoints, which can be seen in Cui et al. (2017). Such distinctions and deviations from already established definitions give misleading measurements and errors in meta-analyses.

## Reporting trends in the literature

### Materials and methods

We investigated data and metadata from the literature to illustrate and quantify reporting insufficiencies (Figure 1). Two datasets were analyzed to demonstrate that reporting insufficiencies are independent from the type of compounds studied: (1) a curated nanomaterial dataset from Balraadsing et al. (2026) and (2) organic chemical (neonicotinoids and PFAS) data from the U.S. Environmental Protection Agency (USEPA) Ecotoxicology (ECOTOX) Knowledgebase (<https://cfpub.epa.gov/ecotox>). Both datasets contain ecotoxicity data and metadata on acute in vivo endpoints for laboratory-based experiments using aquatic species.

Data and metadata were assessed based on their completeness and heterogeneity. The completeness was assessed as the proportion information reported in studies based on two approaches: per data point (gives indication of reporting within studies) and per variable (gives indication of reporting between studies). The criteria for assessing completeness was solely whether studies reported any information regarding a



**Figure 1** Diagram of the analysis conducted in this study to investigate the level of data completeness and heterogeneity within ecotoxicological studies.

variable (the level of detail was not considered). Furthermore, completeness was only assessed for the nanomaterial dataset as the ECOTOX Knowledgebase does not accurately reflect the completeness of ecotoxicity studies. Data or metadata may be present within publications but are not included in the database entries of the ECOTOX Knowledgebase. For example, the entries for [Ashauer et al. \(2010\)](#) and [Pestana et al. \(2010\)](#) were mostly empty within the downloaded dataset (see [online supplementary material ecotox\\_data.xlsx](#)). However, data for empty entries within the dataset could be found within the articles or their [online supplementary materials](#).

Data heterogeneity was analyzed by summing the amount of distinct formats and units used to report numeric data within variables across studies. The quality of reporting could be assessed on a range of variables but there is no agreement amongst researchers on which variables are important to include in studies ([Exner et al., 2023](#)). Therefore, we assessed the completeness and heterogeneity based on variables that are deemed crucial to the reproducibility of ecotoxicological experiments as well as those required by standardized guidelines to be measured and reported. These variables include the physicochemical information (nanomaterial dataset only), experimental conditions and toxicity outcome.

Additional details regarding the datasets and variables assessed can be found in the [supplementary materials](#) (see [online supplementary material S1 and S2](#)). The analysis was conducted using R 4.3.3 ([R Core Team, 2024](#)) and the script can be found attached as [supplementary material](#) (see [online supplementary material analysis.R](#)).

## Results and discussion

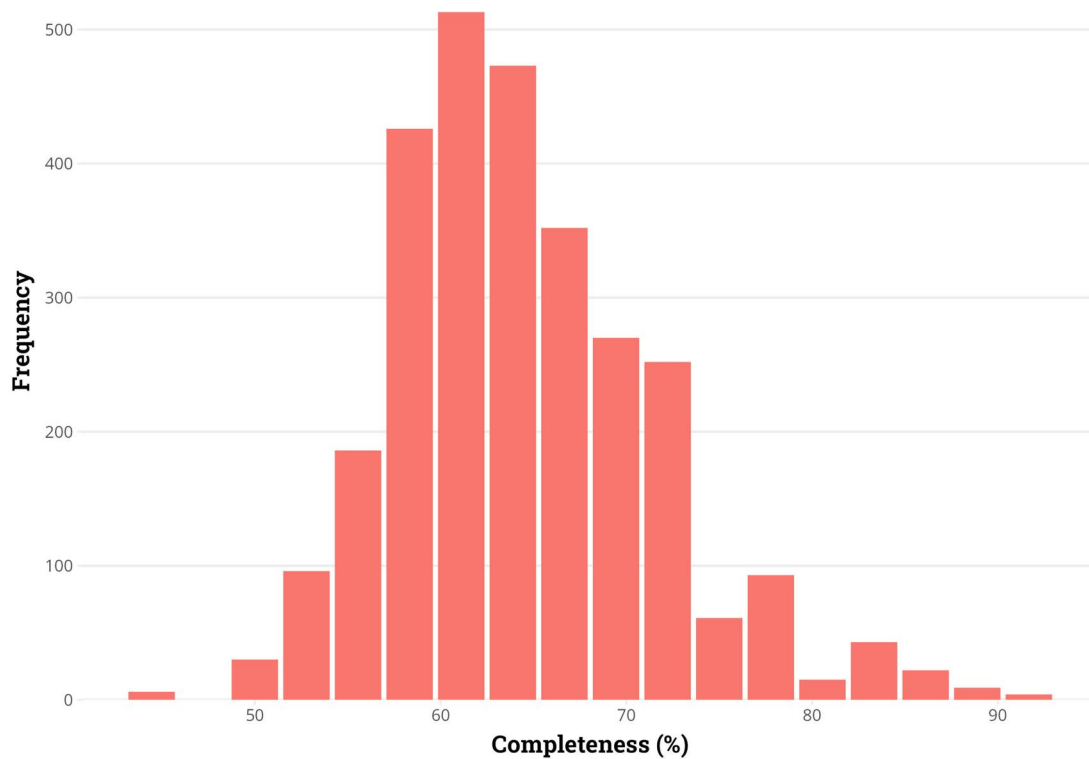
### Nanomaterials

The majority of nanotoxicity studies generally reported acute ecotoxicity data and metadata with a completion rate between 55% and 75% ([Figure 2](#)). Notably, no nanotoxicity study had a completion rate below 45%, whereas few achieved completion rates higher than 80%.

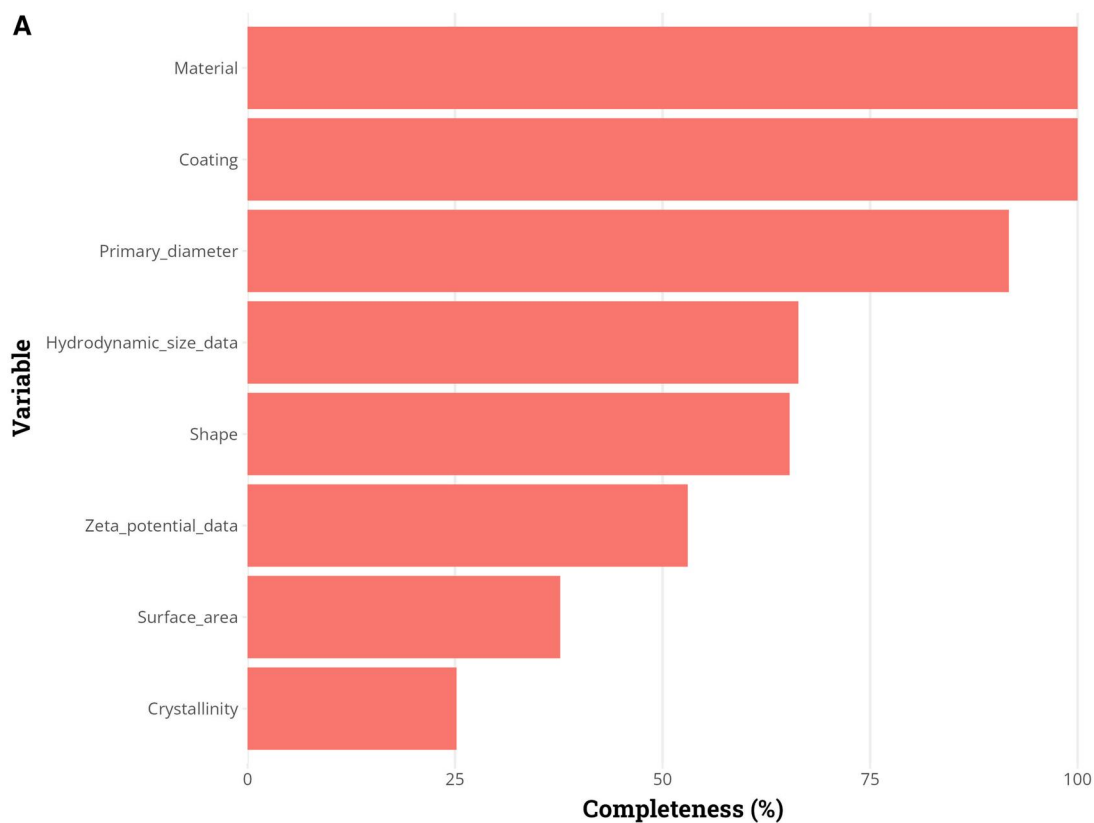
Furthermore, results highlighted the varying levels at which nanomaterial physicochemical property and experimental condition data were reported across studies ([Figures 3A and B](#)). The most commonly reported physicochemical properties ([Figure 3A](#)) included size information (primary diameter and hydrodynamic size), coating, material composition, and shape. In contrast, information on the zeta-potential, surface area, and crystallinity of nanomaterials was reported the least across studies.

Authors frequently report variables related to the experimental conditions of nanotoxicological experiments ([Figure 3B](#)). A 100% completion was observed for the majority of variables, with the exception of the following: endpoint value, test media, temperature, illumination conditions, pH, dispersion method, salinity, ionic strength/conductivity, alkalinity/water hardness, and dissolved oxygen. It should be noted that 100% completion was observed for specific variables due to assumptions made in the assembly of the [Balraadsing et al. \(2026\)](#) nanomaterial dataset, which applies to the following variables: particle coating, UV radiation, suspension aging, and the use of pre-illumination.

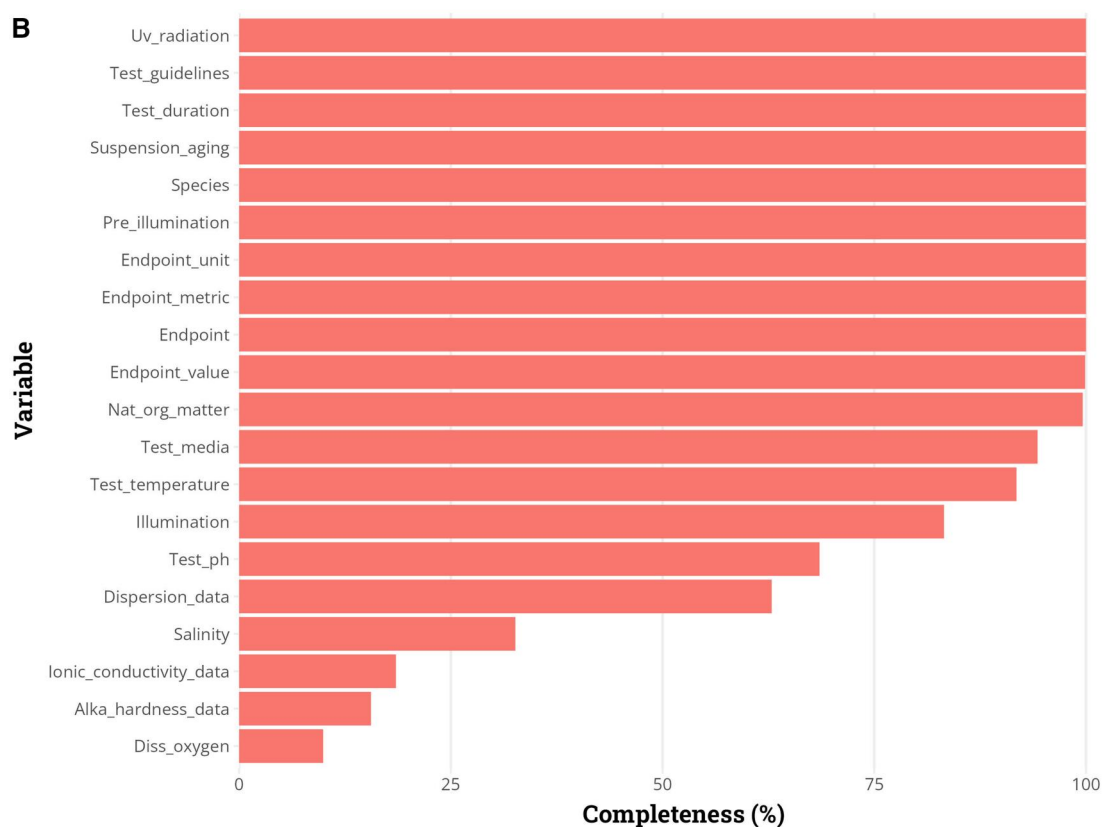
Analysis into the heterogeneity of reported nanotoxicity data and metadata revealed a range of approaches used to report numerical values such as point estimates (e.g., mean), ranges, or



**Figure 2** Histogram showing the overall completeness of variable reporting in nanotoxicology literature. The x-axis displays the percentage completeness for each data point in the dataset, the y-axis displays the frequency (amount of datapoints) corresponding to the percentage completeness.



**Figure 3A** Percentage of completeness of each variable between studies related to the physicochemical properties of nanomaterials. The x-axis displays the percentage completeness for each variable in the dataset, the y-axis displays the variable names.



**Figure 3B** Percentage of completeness of each variable between studies related to the experimental conditions of nanotoxicity experiments. The x-axis displays the percentage completeness for each variable in the dataset, the y-axis displays the variable names.

**Table 1** Reporting of numeric variables using qualifiers, point estimates (means) or numerical ranges in nanotoxicity literature.

Variable	Qualifiers	Point estimates	Ranges	Other
Surface area	18	896	160	0
Primary diameter	297	1,900	418	0
Test duration	0	2,847	4	0
Salinity	0	865	38	27
Dissolved oxygen	39	165	79	0
Water hardness	0	279	113	0
Alkalinity	0	85	58	0
Ionic strength	0	78	8	39
Conductivity	0	338	97	0
pH	4	1,330	620	0
Temperature	0	2,491	107	19
Endpoint value	591	2,244	13	0

Note. Other = other method of data reporting or the data was not extracted in raw dataset, but data was available.

qualifiers (Table 1). Across all numerical variables, point estimates were the most frequently used reporting format, followed by numerical ranges (except for endpoint values). Only the surface area, primary size, dissolved oxygen, and endpoint values contained entries reported using qualifiers.

Moreover, the diversity of units used across studies displayed notable variability. Conductivity (Table 2), surface area (Table 3), and endpoint value (Table 4) were chosen as examples here. Results showed that conductivity was reported using nine distinct units, surface area with three, and endpoint value with 14. Despite this variability, the majority of units could be easily

converted into a preferred (standardized) unit: most units for conductivity were expressed as a form of electrical conductance per distance (97%; typically mS/cm), whereas the majority of endpoint values were a form of mass per volume (94%; typically mg/L), molarity (3%; typically mol/L), or parts per million/billion (3%). Although the surface area was expressed using three distinct units, the vast majority was expressed in m<sup>2</sup>/g (99%).

Each assessed variable also included instances that were more challenging to convert. For conductivity, four data points were expressed as mS/cm<sup>2</sup>, which differs from the more commonly used electrical conductance per distance format.

**Table 2** Variance in units used to express the conductivity of nanomaterials.

Unit	Count
mS/cm	94
mS/cm <sup>2</sup>	4
mS/m	6
mg CaCO <sub>3</sub> /L	2
mho/cm	12
μS/cm	258
μM/cm	6
μS	31
μmho(s)/cm	22

Note. Count = amount of data points where each unit was used to express the parameter.

**Table 3** Variance in units used to express the surface area of nanomaterials.

Unit	Count
m <sup>2</sup> /cm <sup>3</sup>	3
m <sup>2</sup> /g	1,067
nm <sup>2</sup> /particle	4

Note. Count = amount of data points where each unit was used to express the parameter.

**Table 4** Variance in units used to express the endpoint of nanotoxicity experiments.

Unit	Count
g/L	7
mg/L	2,247
mg/mL	5
mmol/L	5
mol/L (M)	3
nM	20
ng/ml	11
particles/ml	11
ppb	6
ppm	76
μM	48
μg/g	2
μg/L	366
μg/ml	44

Note. Count = amount of data points where each unit was used to express the parameter. The measured endpoints consisted of acute in vivo toxicity for aquatic species.

Similarly, the surface area was expressed as m<sup>2</sup>/cm<sup>3</sup> or nm<sup>2</sup>/particle in seven instances, which deviates from the more commonly used m<sup>2</sup>/g. Finally, particles/ml were used to express the toxicological outcome of 11 datapoints, which deviates from the generally used mass per volume format.

Altogether, these findings indicate that the majority of studies report crucial experimental details to a certain degree for nanomaterials. Our results indicate a general underreporting of water chemistry parameters and specific physicochemical features. Physicochemical features such as particle crystallinity and surface

area are required for registration under Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) regulation and are thus considered crucial properties for reporting (Comandella et al., 2020). However, crystallinity and surface area of nanomaterials were amongst the least reported features in studies. Although the reporting of physicochemical features has improved over time (Saarimäki et al., 2021; Siivola et al., 2022), underreporting remains an issue as evidenced in our results.

Analysis into the heterogeneity of reporting indicated a preference for reporting numerical data as point estimates in addition to using numerical ranges and qualifiers. Furthermore, units varied widely across studies, but the majority could be readily harmonized into preferred units. Instances were present in which the harmonization was not straightforward and additional information is needed.

These conclusions are in line with nanotoxicology literature that frequently highlights the considerable data gaps and quality of data (Comandella et al., 2020; Elberskirch et al., 2022; Karcher et al., 2018; Lead et al., 2018; Scott-Fordsmand & Amorim, 2023). The eNanomapper database was analyzed by Comandella et al. (2020), who concluded that nanoparticles were poorly characterized within the database and that studies had poor completeness scores overall. Incomplete reporting in nanotoxicity studies stems from the use of different (unstandardized) protocols and a lack of physicochemical characterization (Afantitis et al., 2020; Comandella et al., 2020; Elberskirch et al., 2022; Pulido-Reyes et al., 2024). As a result, nanotoxicity data is currently inadequate for modeling and substantial curation or gap filling is necessary to reuse such data (Basei et al., 2019; Jeliazkova et al., 2021). Although only acute ecotoxicity data were analyzed here, these trends have also been highlighted for other nanotoxicity subdisciplines, such as in vivo studies on mutagenicity and inhalation (Krug, 2018) and cytotoxicity studies (Furxhi et al., 2023, 2024; Mirzaei et al., 2021).

## Organic chemicals

Patterns of heterogeneous reporting were also observed for organic chemicals and were consistent with those observed in the nanomaterial dataset. Reporting formats for numerical variables in the organic chemical dataset varied from point estimates to ranges and qualifiers (Tables 5 and 6). Studies most frequently reported data using point estimates, followed by data ranges (chemical purity reporting for PFAS was an exception). Additionally, the use of qualifiers was limited solely to chemical purity, organism age, dissolved oxygen, and duration of experiments. Further observations include the use of multiple reporting formats within the same study (e.g., data reported as both ranges and point estimates).

The organic chemical dataset displayed considerable heterogeneity in the units used to express experimental data (Table 7). The conductivity was reported using seven distinct units, but the vast majority (neonicotinoids = 98%, PFAS = 100%) could be readily converted into a (standardized) unit of preference. The sole exception were three neonicotinoid instances reported as μS/cm<sup>3</sup>, which require additional information for conversion. Only conductivity is provided here as example, as the remaining units were already largely harmonized across the ECOTOX Knowledgebase. This applies to units of temperature, water hardness, alkalinity, and salinity (data not shown here).

These findings suggest that organic chemical ecotoxicity data and metadata are reported heterogeneously across studies, similar

**Table 5** Reporting of numeric variables using qualifiers, point estimates (means) or numerical ranges in per- and polyfluoroalkyl substance literature.

Variable	Qualifiers	Point estimates	Ranges	Multiple
Chemical purity	269	418	4	0
Organism age	112	337	173	0
Organism initial length	0	10	25	0
Organism initial weight	0	24	4	0
Observed duration	0	751	68	0
Exposure duration	0	799	19	0
Temperature	0	562	70	132
Water hardness	0	184	88	0
Alkalinity	0	138	67	0
Dissolved oxygen	10	92	123	98
pH	0	186	233	148
Salinity	0	9	14	12
Conductivity	0	194	68	24

Note. Multiple = data was reported using multiple of the listed methods;  $n = 821$ .

**Table 6** Reporting of numeric variables using qualifiers, point estimates (means) or numerical ranges in neonicotinoid literature.

Variable	Qualifiers	Point estimates	Ranges	Multiple
Chemical purity	15	260	102	0
Organism age	92	99	168	0
Organism initial length	0	4	21	0
Organism initial weight	0	5	1	0
Observed duration	1	435	1	0
Exposure duration	0	427	0	0
Temperature	0	342	25	33
Water hardness	0	29	74	91
Alkalinity	0	41	72	91
Dissolved oxygen	23	23	176	30
pH	0	47	154	59
Salinity	0	0	1	3
Conductivity	0	27	104	82

Note. Multiple = data was reported using multiple of the listed methods;  $n = 437$ .

**Table 7** Variance in units used to express the conductivity of organic chemicals (amount of data points where each unit was used to express the parameter for each chemical group).

Unit	Neonicotinoids	PFAS
S/cm	8	0
mS/cm	72	24
$\mu\text{S/cm}$	130	162
$\mu\text{S/cm}^3$	3	0
$\mu\text{S}$	0	63
$\mu\text{S/m}$	0	4
$\mu\text{mhos/cm}$	0	33

Note: PFAS = per- and polyfluoroalkyl substances.

to the nanomaterial dataset. Because both chemical groups displayed similar heterogeneity, these results indicate that patterns of heterogeneous reporting prevail irrespective of the chemical assessed. Issues regarding unharmonized chemical toxicity data have also been recognized in the literature. [Ankley et al. \(2021\)](#)

discusses the underreporting of test concentrations and water quality parameters in PFAS studies. Additionally, [Wang et al. \(2024\)](#) concluded that relatively few PFAS studies could be considered reliable or of high quality. No study has yet evaluated the quality of neonicotinoid data, to the best of our knowledge. However, the similarities observed between reporting insufficiencies in PFAS and neonicotinoid data suggest that comparable results can be expected for neonicotinoids. In the broader toxicology literature, [Langan et al. \(2025\)](#) also reports on the insufficient reporting of basic experimental information for transcriptomics studies such as the lighting conditions, feeding, and water quality parameters for a range of chemicals. [Harris and Sumpter \(2015\)](#) evaluated studies published in 2013 across three journals and concluded that reporting was generally poor based on the assessed criteria. The ECOTOX Knowledgebase relies on author-reported details and thus contains data gaps due to insufficient reporting, thereby hindering the reuse of data ([Hrovat et al., 2009](#); [Olker et al., 2022](#)). Such issues of insufficient and heterogeneous reporting are not limited to the ECOTOX Knowledgebase but have also been reported elsewhere, such as the REACH database ([Saouter et al., 2019](#)).

## Suggestions

Heterogeneous and detailed reporting are imperative for the reuse, reproducibility, and comparability of studies. Based on the identified shortcomings in the ecotoxicological literature, we present suggestions below to improve the quality of studies and promote harmonized reporting. Table 8 gives an overview of reporting shortcomings and suggestions for improvement. This table serves as a checklist for authors preparing new manuscripts.

## Complete reporting

### Methodologies

Researchers should describe methodologies with detailed accounts of experimental procedures, species used, and the necessary information needed to reproduce the study (Faria et al., 2018; Hanson et al., 2017; Krebs et al. 2020). Numerous templates (e.g., Investigation/Study/Assay tab-delimited [ISATAB] format [Sansone et al., 2012], NanoReg [Totaro et al., 2017]), checklists (e.g., Nano Criteria for Reporting and Evaluating Ecotoxicity Data (nanoCRED; Hartmann et al., 2017; C. T. A. Moermond et al., 2016), Animal Research Reporting of In Vivo Experiments (ARRIVE; <https://arriveguidelines.org/>), and guidelines (e.g., OECD 202; OECD, 2004), USEPA 821-R-02-012 (USEPA, 2002), Society of Environmental Toxicology and Chemistry (SETAC) minimum reporting information (SETAC, 2019), recommendations for soil micro- and nanoplastic (Kokalj et al., 2024) exist to aid with experimental elements that should be reported (Hartung et al., 2019). The Enhancing the Quality and Transparency of Health Research (EQUATOR) Network (<https://www.equator-network.org>) also acts as a hub that links to reporting guidelines. Electronic lab notebooks have also been suggested for data reporting and management (Exner et al., 2023; Papadiamantis et al., 2020). Comandella et al. (2020) and Ågerstrand (2020) discuss the effectiveness of reporting templates and checklists, highlighting increased quality and completeness for studies where they were utilized. When experimental details cannot be placed in the main text (e.g., due to journal restrictions), this information should be published in the online supplementary material (Ågerstrand et al., 2014), as was done in Kadlec et al. (2024), for instance.

Authors citing experimental guidelines should also specify the exact conditions (and timepoints) applied during exposure even when using the previously mentioned templates, checklists, or guidelines. This also extends to the use of nonstandardized media, which should be clearly described in terms of water quality parameters and elemental composition (Hanson et al., 2017). Similarly, citing (nonstandardized) methodologies found elsewhere in the literature should be accompanied by brief descriptions of the procedure. For example, G. Ji et al. (2022) cited the experimental guideline used but also provided a brief procedural overview within their study. This is beneficial, as other (older) publications may be inaccessible or also suffer from insufficient reporting (Przybylak et al., 2012).

### Statistical information

Researchers should report information relating to statistical analyses as thoroughly as possible (Faria et al., 2018). This includes the reporting of  $p$ -values, degrees of freedom, effect

sizes, and statistical power (Bosker et al., 2013; Erickson & Rattner, 2020). Furthermore, descriptive statistics used to summarize parameters should be accompanied by measures of dispersion, such as the  $SD/SE$  or confidence interval (Aurisano & Fantke, 2022; Hanson et al., 2017) and sample size. In this context, Mebane et al. (2019) also suggests the reporting of extreme percentiles (e.g., the 10th to 90th percentile) instead of numerical ranges. Misinterpretations and ambiguity can be avoided by explicitly stating which data were used for descriptive statistical calculations or by reporting the raw data.

### Graphical results

Researchers should place the underlying values used in graphical representations either within the figures (without overburdening them; Hartung et al., 2019), in the main text, a table, or the online supplementary material. Alternatively, raw data can be shared through databases or repositories (e.g., Zenodo; Jenkins et al., 2022; Martin et al., 2019).

### Reused data

Data reused from prior work must be clearly and prominently disclosed within publications. This disclosure includes a direct citation of the source and a specification of the reused data. To avoid the creation of reference chains that hinder data traceability, authors should cite the original data source rather than secondary publications that mention the same data (e.g., using digital object identifiers).

### Positive and negative results

Negative findings should be reported because they give crucial context for understanding experiments and help mitigate biases in models (Hanson et al., 2017; Martin et al., 2019). Nevertheless, we recognize that (traditional) journals accept manuscripts less frequently when they report only negative results (Krug, 2018). Alternative journals are therefore available for the peer review and publication of negative findings (e.g., *PlosONE*, *Journal of Pharmaceutical Negative Results*, *F1000Research*) and must be utilized more often within ecotoxicology. Importantly, reporting negative results must be held to the same scientific standards as positive findings: rigorous peer review, well-formulated research questions, appropriate statistical power analyses, and proper data reporting practices.

## Harmonized reporting

### Reporting formats

Researchers should report numerical data using point estimates whenever possible. Ranges or qualifiers should be discouraged unless no alternative is available. We recognize that this is not always feasible and is dependent on the type of experiments conducted. However, we strongly encourage the use of point estimates together with statistical measures of dispersion (as previously discussed in the *Statistical information* section) to promote harmonized data that can be readily reused in meta-analyses or modeling studies. Additionally, consistent categories or grouping schemes should be used when reporting categorical data. Efforts have been made, for example, to standardize nano-material shape nomenclature (Muñoz-Mármol et al., 2015).

**Table 8** Summary of data reporting shortcomings within ecotoxicological publications and suggestions for improved data reporting.

Data reporting shortcoming	Suggestions to improve
Level of detail in materials and methods sections of publications are inconsistent and lack detailed experimental information (Ågerstrand et al., 2014; Hanson et al., 2017; Henke et al., 2024; Hund-Rinke et al., 2018; Olker et al., 2022).	<ul style="list-style-type: none"> <li>· Be detailed in describing the methodology used by giving detailed accounts of the experimental procedures, species used and remaining information required to reproduce the study (Hanson et al., 2017). This includes specifying the exact conditions and water quality parameters used during exposure and the time points at which measurements were taken. Citing guidelines alone is not sufficient because they may not always provide the exact conditions for exposure.</li> <li>· Utilize existing templates (e.g., ISA-TAB), checklists (e.g., (nano)CRED, ARRIVE), or guidelines (e.g., OECD, ISO, USEPA) as guidance on which variables to report from toxicological experiments. If detailed information about experimental procedures or results cannot be placed in the main text, report them within the <a href="#">supplementary materials</a> (Ågerstrand et al., 2014). Briefly describe experimental procedures when citing (unstandardized) methods from other publications (publications are not always easily accessible).</li> </ul>
Insufficient reporting of statistical information ( <i>p</i> -values, degrees of freedom, effect sizes, statistical power etc.). The reporting of descriptive statistics without measurements of dispersion or uncertainty and refraining from reporting the underlying (raw) data used in calculations (Bosker et al., 2013; Erickson & Rattner, 2020).	<ul style="list-style-type: none"> <li>· Report statistical information such as <i>p</i>-values, degrees of freedom, effect sizes, and statistical power as thoroughly as possible (Bosker et al., 2013; Erickson &amp; Rattner, 2020).</li> <li>· Report descriptive statistics (mean, median etc.) along with standard errors or deviations, confidence intervals and/or sample sizes (Hanson et al., 2017).</li> <li>· Avoid misinterpretations and ambiguity by explicitly stating which data were used to calculate descriptive statistics or report the underlying (raw) data.</li> </ul>
Reporting of results only within graphs without providing the underlying values elsewhere in the article or supplementary information.	<ul style="list-style-type: none"> <li>· Place the underlying values displayed on the graphs within the graph itself (without overburdening it; Hartung et al., 2019), the main text, a table, or the <a href="#">supplementary material</a>.</li> <li>· Share raw data using databases or repositories (e.g., Zenodo; Jenkins et al., 2022; Martin et al., 2019).</li> </ul>
Reuse of data from previous publications without making this explicit in the article.	<ul style="list-style-type: none"> <li>· Clearly state what data is reused and cite the publication using persistent identifiers (e.g., DOI).</li> </ul>
Only reporting the positive (significant) results.	<ul style="list-style-type: none"> <li>· Report negative findings (e.g., when chemicals showed no effects or were not detected; Hanson et al., 2017; Martin et al., 2019) in journals that accept such data (e.g., PlosONE, F1000Research).</li> </ul>
Inconsistent reporting formats used to report numerical and categorical data between studies.	<ul style="list-style-type: none"> <li>· Use point estimates when possible for numerical data along with statistical measures of dispersion. Numerical ranges or qualifiers should only be used when necessary, as re-using this type of data complicates modeling or meta-analyses.</li> <li>· Categorical data should be reported consistently between studies through the use of available grouping schemes such as Muñoz-Mármol et al. (2015) for nanomaterial shapes for example.</li> </ul>
Researchers report experimental measurements ambiguously between studies. This includes substance concentrations which are reported as nominal or actual measurements, and organism weight measurements which may be reported as dry or wet weights. Measurements are also done at diverse timepoints or using different media than used during exposure within studies.	<ul style="list-style-type: none"> <li>· Clearly state whether experimental measurements to limit ambiguity. Substance concentrations must clearly state whether they are nominal or actual measurements (ideally, both they actual and nominal concentrations should be reported). Similarly, measurements of organism weights must clearly disclose whether this was based on dry or wet weights.</li> <li>· Conduct measurements at consistent and fixed time points, within the same media used for exposure. Use standardized operating procedures and good laboratory practices standards for consistent and standardized experiments and reporting (Ankley et al., 2021; Martin et al., 2019; C. Moermond et al., 2017). When using standardized operating procedures, be detailed and include the exact conditions used as previously stated.</li> </ul>
Units used to express parameters are inconsistent across articles (Alves et al., 2021; Askham et al., 2023; Krug, 2022; Nyadjro et al., 2023).	<ul style="list-style-type: none"> <li>· Use consistent (and commonly accepted) units to express parameters such as SI units.</li> <li>· Provide the necessary information to convert data into commonly used units when alternative or unconventional units are used.</li> </ul>

(continued)

Table 8 (continued)

Data reporting shortcoming	Suggestions to improve
Inconsistent reporting of ecotoxicological outcomes (as EC <sub>x</sub> values, with x often being equal 50 but occasionally also other values such as 10 or 90).	· Report the obtained dose-response equation with its parameters so the effective concentration can be calculated at any desired percentage of its maximal effect.
Use of unstandardized terminology or vocabulary between studies (Hartung et al., 2019; Papadiamantis et al., 2020; Plata & Janković, 2021).	· Use standardized terminology by utilizing existing tools and frameworks, or compare against them (e.g., eNanomapper ontology, Bioportal ontology). The IUPAC glossary of terms used in ecotoxicology (Nordberg et al., 2009) or ISO vocabulary standards (e.g., Water Quality—Vocabulary [ISO Standard No. 6107:2021; 2021]) can be conducted to aid in standardized terminology.

## Experimental measurements

Studies should clearly state whether reported concentrations are nominal or actual measurements. As nominal concentration may not accurately reflect exposure concentrations (Pulido-Reyes et al., 2024), the actual concentration should be reported in addition to the nominal concentration. Similarly, documentation of dry or wet measurements should be adequately detailed. Although either could be reported, it is important to clearly disclose this within studies for harmonization and transparency across literature (Askham et al., 2023).

The lack of comparability among studies due to differences in methodologies can be remedied through the use of standardized operating procedures and adherence to good laboratory practices (GLPs). Standardized operation procedures (together with our suggestions from the “methodologies” section) and GLP facilitates rigorous and standardized reporting (Martin et al., 2019; C. Moermond et al., 2017). However, it is impractical to conduct every experiment using standardized tests or species. Therefore, we wish to emphasize that our suggestion here means that experimental measurements should be done “in the spirit of GLP,” taking rigorous experimental design and harmonized reporting into account (Ankley et al., 2021).

## Units

Uniform (and commonly accepted) units should be used to express parameters (e.g., internationally standardized SI units). If authors opt to express parameters in unconventional units, the necessary information required for accurate conversion should be provided. For instance, Park et al. (2014) expressed surface area in nm<sup>2</sup>/particle, but included detailed particle information (Table 1 of Park et al. [2014]), enabling conversion into the more generally used m<sup>2</sup>/g.

## Toxicological outcomes

Researchers reporting ecotoxicological outcomes as EC<sub>x</sub> values should also provide the mathematical equation of the fitted dose-response curve. Reporting the parameters of the dose-response curve enables the calculation and interpolation of any desired EC<sub>x</sub> value (beyond the published EC<sub>x</sub> values). For example, Gomes et al. (2024) reported the parameters of the fitted dose-response curve together with the toxicological outcomes of their experiments. The dose-response data can thus be easily reused and compared between studies in addition to permitting

modeling studies that predict complete dose-response curves (e.g., Bunmahotama et al. [2022]).

## Terminology

Standardized terminology is strongly encouraged to promote clarity and consistency. However, we recognize that implementing such standardization is difficult and requires collective commitment from researchers (Groenewold et al., 2024). Adopting common vocabulary is especially challenging in multidisciplinary fields where identical terms are used to describe different concepts.

Any action taken towards standardization will result in partial effectiveness due to the breadth of the article published, number of authors involved, and natural variation in language use (Hartung et al., 2019). Tools and frameworks for standardized vocabularies/ontology exist (e.g., eNanomapper ontology, BioPortal ontology, International Union of Pure and Applied Chemistry [IUPAC] glossary of term used in ecotoxicology [Nordberg et al., 2009] or ISO standards such as Water Quality—Vocabulary [ISO Standard No. 6107:2021; 2021]), but are underutilized. The challenges and opportunities associated with vocabulary standardization and ontology have been explored extensively elsewhere (e.g., Papadiamantis et al. [2020], Thessen et al. [2022] and Kosnik et al. [2022]).

## Critical perspective

Recent years have seen a transition from animal experiments towards more molecular, in vitro, and in silico based hazard assessment (so called “new approach methodologies”; Alves et al., 2021; Henke et al., 2024). This shift towards in silico approaches also requires the availability of high-quality data and metadata (Afantitis et al., 2020). Tremendous efforts are made in ecotoxicology to improve published data through the FAIR principles, data stewardship, and standardized reporting templates (Exner et al., 2023; Papadiamantis et al., 2020). Data stewards or shepherds have been suggested to oversee the management and reporting of data and metadata (EFSA et al., 2025; Furxhi, 2022; Papadiamantis et al., 2020), but it should be acknowledged that such concepts (including FAIR) require time to mature and be implemented across the community (Exner et al., 2023). Instead, more short-term and pragmatic solutions are necessary to rapidly improve data reporting practices in ecotoxicology. Otherwise, it is probable that the current “status quo” of inadequate reporting will continue into the foreseeable future, gradually creating more unnecessary data gaps.



- to increase the scientific basis for regulatory decision-making: Improve reporting of research studies for regulatory decision-making. *Journal of Applied Toxicology*, 38, 783–785. <https://doi.org/10.1002/jat.3578>
- Ågerstrand, M., Edvardsson, L., & Rudén, C. (2014). Bad reporting or bad science? Systematic data evaluation as a means to improve the use of peer-reviewed studies in risk assessments of chemicals. *Human and Ecological Risk Assessment*, 20, 1427–1445. <https://doi.org/10.1080/10807039.2013.854139>
- Aggarwal, R., Holmquist, H., Arvidsson, R., Reppas-Chrysovtisinos, E., & Peters, G. (2024). Influence of data selection on aquatic ecotoxicity characterization factors for selected persistent and mobile substances. *International Journal of Life Cycle Assessment*, 29, 344–354. <https://doi.org/10.1007/s11367-023-02263-w>
- Ajisafe, O. M., Adekunle, Y. A., Egbon, E., Ogbonna, C. E., & Olawade, D. B. (2025). The role of machine learning in predictive toxicology: A review of current trends and future perspectives. *Life Sciences*, 378, 123821. <https://doi.org/10.1016/j.lfs.2025.123821>
- Alves, V. M., Auerbach, S. S., Kleinstreuer, N., Rooney, J. P., Muratov, E. N., Rusyn, I., Tropsha, A., & Schmitt, C. (2021). Curated data in-trustworthy in silico models out: The impact of data quality on the reliability of artificial intelligence models as alternatives to animal testing. *Alternatives to Laboratory Animals: ATLA*, 49, 73–82. <https://doi.org/10.1177/02611929211029635>
- Ankley, G. T., Cureton, P., Hoke, R. A., Houde, M., Kumar, A., Kurias, J., Lanno, R., McCarthy, C., Newsted, J., Salice, C. J., Sample, B. E., Sepúlveda, M. S., Steevens, J., & Valsecchi, S. (2021). Assessing the ecological risks of per- and polyfluoroalkyl substances: Current state-of-the science and a proposed path forward. *Environmental Toxicology and Chemistry*, 40, 564–605. <https://doi.org/10.1002/etc.4869>
- Annuziato, K. M., Jantzen, C. E., Gronski, M. C., & Cooper, K. R. (2019). Subtle morphometric, behavioral and gene expression effects in larval zebrafish exposed to PFHxA, PFHxS and 6:2 FTOH. *Aquatic Toxicology*, 208, 126–137. <https://doi.org/10.1016/j.aquatox.2019.01.009>
- Aruoja, V., Pokhrel, S., Sihtmäe, M., Mortimer, M., Mädler, L., & Kahru, A. (2015). Toxicity of 12 metal-based nanoparticles to algae, bacteria and protozoa. *Environmental Science: Nano*, 2, 630–644. <https://doi.org/10.1039/C5EN00057B>
- Ashauer, R., Caravatti, I., Hintermeister, A., & Escher, B. I. (2010). Bioaccumulation kinetics of organic xenobiotic pollutants in the freshwater invertebrate *Gammarus pulex* modeled with prediction intervals. *Environmental Toxicology and Chemistry*, 29, 1625–1636. <https://doi.org/10.1002/etc.175>
- Askham, C., Pauna, V. H., Boulay, A.-M., Fantke, P., Jolliet, O., Lavoie, J., Booth, A. M., Coutris, C., Verones, F., Weber, M., Vijver, M. G., Lusher, A., & Hajjar, C. (2023). Generating environmental sampling and testing data for micro- and nano-plastics for use in life cycle impact assessment. *Science of the Total Environment*, 859, 160038. <https://doi.org/10.1016/j.scitotenv.2022.160038>
- Aurisano, N., & Fantke, P. (2022). Semi-automated harmonization and selection of chemical data for risk and impact assessment. *Chemosphere*, 302, 134886. <https://doi.org/10.1016/j.chemosphere.2022.134886>
- Baker, M. (2016). 1,500 scientists lift the lid on reproducibility. *Nature*, 533, 452–454. <https://doi.org/10.1038/533452a>
- Balraadsing, S. J. G. M., Peijnenburg, W., & Vijver, M. G. (2024). Building species trait-specific nano-QSARs: Model stacking, navigating model uncertainties and limitations, and the effect of dataset size. *Environment International*, 188, 108764. <https://doi.org/10.1016/j.envint.2024.108764>
- Balraadsing, S., Peijnenburg, W. J. G. M., & Vijver, M. G. (2026). A curated dataset on the acute in vivo ecotoxicity of metallic nanomaterials from published literature. *Data*, 11, 22. <https://doi.org/10.3390/data11010022>
- Barmntlo, S. H., Schrama, M., Van Bodegom, P. M., De Snoo, G. R., Musters, C. J. M., & Vijver, M. G. (2019). Neonicotinoids and fertilizers jointly structure naturally assembled freshwater macroinvertebrate communities. *Science of the Total Environment*, 691, 36–44. <https://doi.org/10.1016/j.scitotenv.2019.07.110>
- Barmntlo, S. H., Stel, J. M., Van Doorn, M., Eschauzier, C., De Voogt, P., & Kraak, M. H. S. (2015). Acute and chronic toxicity of short chained perfluoroalkyl substances to *Daphnia magna*. *Environmental Pollution*, 198, 47–53. <https://doi.org/10.1016/j.envpol.2014.12.025>
- Barr, D. B., Landsittel, D., Nishioka, M., Thomas, K., Curwin, B., Raymer, J., Donnelly, K. C., McCauley, L., & Ryan, P. B. (2006). A survey of laboratory and statistical issues related to farm-worker exposure studies. *Environmental Health Perspectives*, 114, 961–968. <https://doi.org/10.1289/ehp.8528>
- Basei, G., Hristozov, D., Lamon, L., Zabeo, A., Jeliakova, N., Tsiliki, G., Marcomini, A., & Torsello, A. (2019). Making use of available and emerging data to predict the hazards of engineered nanomaterials by means of in silico tools: A critical review. *NanoImpact*, 13, 76–99. <https://doi.org/10.1016/j.impact.2019.01.003>
- Baskaran, S., Chirsir, P., Joudan, S., Wolf, R., Bolton, E. E., Thiessen, P. A., & Schymanski, E. L. (2025). Reporting chemical data in the environmental sciences. *ACS Environmental Au*, 5, 444–456. <https://doi.org/10.1021/acsenvironau.5c00034>
- Bernot, R. J., & Brandenburg, M. (2013). Freshwater snail vital rates affected by non-lethal concentrations of silver nanoparticles. *Hydrobiologia*, 714, 25–34. <https://doi.org/10.1007/s10750-013-1509-6>
- Beronius, A., Molander, L., Rudén, C., & Hanberg, A. (2014). Facilitating the use of non-standard in vivo studies in health risk assessment of chemicals: A proposal to improve evaluation criteria and reporting: Evaluation and reporting of non-standard in vivo studies. *Journal of Applied Toxicology*, 34, 607–617. <https://doi.org/10.1002/jat.2991>
- Bosker, T., Mudge, J. F., & Munkittrick, K. R. (2013). Statistical reporting deficiencies in environmental toxicology. *Environmental Toxicology and Chemistry*, 32, 1737–1739. <https://doi.org/10.1002/etc.2226>
- Bunmahotama, W., Vijver, M. G., & Peijnenburg, W. (2022). Development of a quasi-quantitative structure-activity relationship model for prediction of the immobilization response of *Daphnia magna* exposed to metal-based nanomaterials. *Environmental Toxicology and Chemistry*, 41, 1439–1450. <https://doi.org/10.1002/etc.5322>
- Chen, G., Vijver, M. G., & Peijnenburg, W. J. G. M. (2015). Summary and analysis of the currently existing literature data

- on metal-based nanoparticles published for selected aquatic organisms: Applicability for toxicity prediction by (Q)SARs. *Alternatives to Laboratory Animals*, 43, 221–240. <https://doi.org/10.1177/026119291504300404>
- Chik, A. H. S., Schmidt, P. J., & Emelko, M. B. (2018). Learning something from nothing: the critical importance of rethinking microbial non-detects. *Frontiers in Microbiology*, 9, 2304. <https://doi.org/10.3389/fmicb.2018.02304>
- Comandella, D., Gottardo, S., Rio-Echevarria, I. M., & Rauscher, H. (2020). Quality of physicochemical data on nanomaterials: An assessment of data completeness and variability. *Nanoscale*, 12, 4695–4708. <https://doi.org/10.1039/C9NR08323E>
- Cui, R., Chae, Y., & An, Y.-J. (2017). Dimension-dependent toxicity of silver nanomaterials on the cladocerans *Daphnia magna* and *Daphnia galeata*. *Chemosphere*, 185, 205–212. <https://doi.org/10.1016/j.chemosphere.2017.07.011>
- Drobne, D. (2021). Adding toxicological context to nanotoxicity study reporting using the NanoTox metadata list. *Small*, 17, e2005622. <https://doi.org/10.1002/smll.202005622>
- Dumit, V. I., Ammar, A., Bakker, M. I., Bañares, M. A., Bossa, C., Costa, A., Cowie, H., Drobne, D., Exner, T. E., Farcial, L., Friedrichs, S., Furxhi, I., Grafström, R., Haase, A., Himly, M., Jeliaskova, N., Lynch, I., Maier, D., Noorlander, C. W., ... Nymark, P. (2023). From principles to reality. FAIR implementation in the nanosafety community. *Nano Today*, 51, 101923. <https://doi.org/10.1016/j.nantod.2023.101923>
- Elberskirch, L., Binder, K., Riefler, N., Sofranko, A., Liebing, J., Minella, C. B., Mädler, L., Razum, M., van Thriel, C., Unfried, K., Schins, R. P. F., & Kraegeloh, A. (2022). Digital research data: From analysis of existing standards to a scientific foundation for a modular metadata schema in nanosafety. *Particle and Fibre Toxicology*, 19, 1. <https://doi.org/10.1186/s12989-021-00442-x>
- Erickson, R. A., & Rattner, B. A. (2020). Moving beyond  $p < 0.05$  in ecotoxicology: A guide for practitioners. *Environmental Toxicology and Chemistry*, 39, 1657–1669. <https://doi.org/10.1002/etc.4800>
- Eulaers, I., Jaspers, V. L. B., Bustnes, J. O., Covaci, A., Johnsen, T. V., Halley, D. J., Moum, T., Ims, R. A., Hanssen, S. A., Erikstad, K. E., Herzke, D., Sonne, C., Ballesteros, M., Pinxten, R., & Eens, M. (2013). Ecological and spatial factors drive intra- and interspecific variation in exposure of subarctic predatory bird nestlings to persistent organic pollutants. *Environment International*, 57–58, 25–33. <https://doi.org/10.1016/j.envint.2013.03.009>
- Charles, S., Focks, A., Haselman, J. T., Carnesecchi, E., Gibin, D., Ippolito, A., Linguadoca, A., & Teodorović, I.; European Food Safety Authority (EFSA). (2025). EFSA statement on the interpretation of FAIR principles for mechanistic effect models in the regulatory environmental risk assessment of pesticides. *EFSA Journal*, 23, e9741. <https://doi.org/10.2903/j.efsa.2025.9741>
- Exner, T. E., Papadiamantis, A. G., Melagraki, G., Amos, J. D., Bossa, N., Gakis, G. P., Charitidis, C. A., Cornelis, G., Costa, A. L., Doganis, P., Farcial, L., Friedrichs, S., Furxhi, I., Klaessig, F. C., Lobaskin, V., Maier, D., Rumble, J., Sarimveis, H., Suarez-Merino, B., ... Lynch, I. (2023). Metadata stewardship in nanosafety research: Learning from the past, preparing for an “on-the-fly” FAIR future. *Frontiers in Physics*, 11, 1233879. <https://doi.org/10.3389/fphy.2023.1233879>
- Faria, M., Björnalm, M., Thurecht, K. J., Kent, S. J., Parton, R. G., Kavallaris, M., Johnston, A. P. R., Gooding, J. J., Corrie, S. R., Boyd, B. J., Thordarson, P., Whittaker, A. K., Stevens, M. M., Prestidge, C. A., Porter, C. J. H., Parak, W. J., Davis, T. P., Crampin, E. J., & Caruso, F. (2018). Minimum information reporting in bio-nano experimental literature. *Nature Nanotechnology*, 13, 777–785. <https://doi.org/10.1038/s41565-018-0246-4>
- Fazelian, N., Movafeghi, A., Yousefzadi, M., & Rahimzadeh, M. (2019). Cytotoxic impacts of CuO nanoparticles on the marine microalga *Nannochloropsis oculata*. *Environmental Science and Pollution Research International*, 26, 17499–17511. <https://doi.org/10.1007/s11356-019-05130-0>
- Fazelian, N., Yousefzadi, M., & Movafeghi, A. (2020). Algal response to metal oxide nanoparticles: Analysis of growth, protein content, and fatty acid composition. *BioEnergy Research*, 13, 944–954. <https://doi.org/10.1007/s12155-020-10099-7>
- Fernández-Cruz, M. L., Hernández-Moreno, D., Catalán, J., Cross, R. K., Stockmann-Juvala, H., Cabellos, J., Lopes, V. R., Matzke, M., Ferraz, N., Izquierdo, J. J., Navas, J. M., Park, M., Svendsen, C., & Janer, G. (2018). Quality evaluation of human and environmental toxicity studies performed with nanomaterials—the GUIDEnano approach. *Environmental Science: Nano*, 5, 381–397. <https://doi.org/10.1039/C7EN00716G>
- Furxhi, I. (2022). Health and environmental safety of nanomaterials: O data, where art thou? *NanoImpact*, 25, 100378. <https://doi.org/10.1016/j.impact.2021.100378>
- Furxhi, I., Faccani, L., Zanoni, I., Briigliadori, A., Vespignani, M., & Costa, A. L. (2024). Design rules applied to silver nanoparticles synthesis: A practical example of machine learning application. *Computational and Structural Biotechnology Journal*, 25, 20–33. <https://doi.org/10.1016/j.csbj.2024.02.010>
- Furxhi, I., Murphy, F., Mullins, M., Arvanitis, A., & Poland, C. A. (2020). Nanotoxicology data for in silico tools: A literature review. *Nanotoxicology*, 14, 612–637. <https://doi.org/10.1080/17435390.2020.1729439>
- Furxhi, I., Willighagen, E., Evelo, C., Costa, A., Gardini, D., & Ammar, A. (2023). A data reusability assessment in the nanosafety domain based on the NSDRA framework followed by an exploratory quantitative structure activity relationships (QSAR) modeling targeting cellular viability. *NanoImpact*, 31, 100475. <https://doi.org/10.1016/j.impact.2023.100475>
- George, B. J., Gains-Germain, L., Broms, K., Black, K., Furman, M., Hays, M. D., Thomas, K. W., & Simmons, J. E. (2021). Censoring trace-level environmental data: Statistical analysis considerations to limit bias. *Environmental Science & Technology*, 55, 3786–3795. <https://doi.org/10.1021/acs.est.0c02256>
- Gomes, S. I. L., Zanoni, I., Blosi, M., Costa, A. L., Hristozov, D., Scott-Fordsmand, J. J., & Amorim, M. J. B. (2024). Safe and sustainable by design Ag nanomaterials: A case study to evaluate the bio-reactivity in the environment using a soil model invertebrate. *Science of the Total Environment*, 927, 171860. <https://doi.org/10.1016/j.scitotenv.2024.171860>
- Groenewold, M., Bleeker, E. A. J., Noorlander, C. W., Sips, A. J. A. M., van der Zee, M., Aitken, R. J., Baker, J. H., Bakker, M. I., Bouman, E. A., Doak, S. H., Drobne, D., Dumit, V. I., Florin, M.-

- V., Fransman, W., Gonzalez, M. M., Heunisch, E., Isigonis, P., Jeliaskova, N., Jensen, K. A., ... Scott-Fordsmand, J. J. (2024). Governance of advanced materials: Shaping a safe and sustainable future. *NanoImpact*, 35, 100513. <https://doi.org/10.1016/j.impact.2024.100513>
- Hanson, M. L., Wolff, B. A., Green, J. W., Kivi, M., Panter, G. H., Warne, M., St, J., Ågerstrand, M., & Sumpter, J. P. (2017). How we can make ecotoxicology more valuable to environmental protection. *Science of the Total Environment*, 578, 228–235. <https://doi.org/10.1016/j.scitotenv.2016.07.160>
- Harris, C. A., & Sumpter, J. P. (2015). Could the quality of published ecotoxicological research be better? *Environmental Science & Technology*, 49, 9495–9496. <https://doi.org/10.1021/acs.est.5b01465>
- Hartmann, N. B., Ågerstrand, M., Lützhøft, H.-C. H., & Baun, A. (2017). NanoCRED: A transparent framework to assess the regulatory adequacy of ecotoxicity data for nanomaterials – Relevance and reliability revisited. *NanoImpact*, 6, 81–89. <https://doi.org/10.1016/j.impact.2017.03.004>
- Hartung, T., De Vries, R., Hoffmann, S., Hogberg, H. T., Smirnova, L., Tsaïoun, K., Whaley, P., & Leist, M. (2019). Toward good in vitro reporting standards. *ALTEX*, 36, 3–17. <https://doi.org/10.14573/altex.1812191>
- Hartung, T., & Kleinstreuer, N. (2025). Challenges and opportunities for validation of AI-based new approach methods. *ALTEX*, 42, 3–21. <https://doi.org/10.14573/altex.2412291>
- Henke, A. N., Chilukuri, S., Langan, L. M., & Brooks, B. W. (2024). Reporting and reproducibility: Proteomics of fish models in environmental toxicology and ecotoxicology. *Science of the Total Environment*, 912, 168455. <https://doi.org/10.1016/j.scitotenv.2023.168455>
- Hillebrand, H., & Gurevitch, J. (2013). Reporting standards in experimental studies. *Ecology Letters*, 16, 1419–1420. <https://doi.org/10.1111/ele.12190>
- Hitchcock, D. J., Andersen, T., Varpe, Ø., & Borgå, K. (2018). Improving data reporting in ecotoxicological studies. *Environmental Science & Technology*, 52, 8061–8062. <https://doi.org/10.1021/acs.est.8b03324>
- Hrovat, M., Segner, H., & Jeram, S. (2009). Variability of in vivo fish acute toxicity data. *Regulatory Toxicology and Pharmacology*, 54, 294–300. <https://doi.org/10.1016/j.yrtph.2009.05.013>
- Hund-Rinke, K., Schlich, K., Kühnel, D., Hellack, B., Kaminski, H., & Nickel, C. (2018). Grouping concept for metal and metal oxide nanomaterials with regard to their ecotoxicological effects on algae, daphnids and fish embryos. *NanoImpact*, 9, 52–60. <https://doi.org/10.1016/j.impact.2017.10.003>
- Hutson, M. (2022). Taking the pain out of data sharing. *Nature*, 610, 220–221. <https://doi.org/10.1038/d41586-022-03133-5>
- Ingre-Khans, E., Ågerstrand, M., Beronius, A., & Rudén, C. (2019). Toxicity studies used in registration, evaluation, authorisation and restriction of chemicals (REACH): How accurately are they reported? *Integrated Environmental Assessment and Management*, 15, 458–469. <https://doi.org/10.1002/ieam.4123>
- International Organization for Standardization (ISO). (2021). *Water quality—Vocabulary (ISO Standard No. 6107:2021)*. International Organization for Standardization.
- Jacobs, M. N., Hoffmann, S., Hollnagel, H. M., Kern, P., Kolle, S. N., Natsch, A., & Landsiedel, R. (2024). Avoiding a reproducibility crisis in regulatory toxicology—On the fundamental role of ring trials. *Archives of Toxicology*, 98, 2047–2063. <https://doi.org/10.1007/s00204-024-03736-z>
- Jeliaskova, N., Apostolova, M. D., Andreoli, C., Barone, F., Barrick, A., Battistelli, C., Bossa, C., Botea-Petcu, A., Châtel, A., De Angelis, I., Dusinska, M., El Yamani, N., Gheorghe, D., Giusti, A., Gómez-Fernández, P., Grafström, R., Gromelski, M., Jacobsen, N. R., Jeliaskov, V., ... Nymark, P. (2021). Towards FAIR nanosafety data. *Nature Nanotechnology*, 16, 644–654. <https://doi.org/10.1038/s41565-021-00911-6><https://doi.org/10/gj4vw4>
- Jenkins, T., Persaud, B. D., Cowger, W., Szigeti, K., Roche, D. G., Clary, E., Slowinski, S., Lei, B., Abeynayaka, A., Nyadjro, E. S., Maes, T., Thornton Hampton, L., Bergmann, M., Aherne, J., Mason, S. A., Honek, J. F., Rezanezhad, F., Lusher, A. L., Booth, A. M., ... Van Cappellen, P. (2022). Current state of microplastic pollution research data: Trends in availability and sources of open data. *Frontiers in Environmental Science*, 10, 912107. <https://doi.org/10.3389/fenvs.2022.912107>
- Ji, G., Gu, J., Guo, M., Zhou, L., Wang, Z., Shi, L., & Gu, A. (2022). A systematic comparison of the developmental vascular toxicity of bisphenol A and its alternatives in vivo and in vitro. *Chemosphere*, 291, 132936. <https://doi.org/10.1016/j.chemosphere.2021.132936>
- Ji, Z., Guo, W., Sakkiah, S., Liu, J., Patterson, T., & Hong, H. (2021). Nanomaterial databases: Data sources for promoting design and risk assessment of nanomaterials. *Nanomaterials*, 11, 1599. <https://doi.org/10.3390/nano11061599><https://doi.org/10/gkq3p3>
- Kadlec, S. M., Backe, W. J., Erickson, R. J., Hockett, J. R., Howe, S. E., Mundy, I. D., Piasecki, E., Sluka, H., Votava, L. K., & Mount, D. R. (2024). Sublethal toxicity of 17 per- and polyfluoroalkyl substances with diverse structures to *Ceriodaphnia dubia*, *Hyalella azteca*, and *Chironomus dilutus*. *Environmental Toxicology and Chemistry*, 43, 359–373. <https://doi.org/10.1002/etc.5784>
- Karcher, S., Willighagen, E. L., Rumble, J., Ehrhart, F., Evelo, C. T., Fritts, M., Gaheen, S., Harper, S. L., Hoover, M. D., Jeliaskova, N., Lewinski, N., Marchese Robinson, R. L., Mills, K. C., Mustad, A. P., Thomas, D. G., Tsiliki, G., & Hendren, C. O. (2018). Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations. *NanoImpact*, 9, 85–101. <https://doi.org/10.1016/j.impact.2017.11.002>
- Kokalj, A. J., Kalčíková, G., Selonen, S., Bosker, T., Drobne, D., Dvořáková, D., Hofman, J., Hurley, R., Kernchen, S., Laforsch, C., Löder, M. G. J., Van Loon, S., Redondo-Hasselerharm, P. E., Saartama, V., Šmídová, K., Tsagkaris, A. S., Zantis, L. J., Nizzetto, L., & Van Gestel, C. A. M. (2024). Strategy towards producing relevant and reliable data for the hazard assessment of micro- and nanoplastics in agricultural soils. *Trends in Analytical Chemistry*, 172, 117567. <https://doi.org/10.1016/j.trac.2024.117567>
- Kosnik, M. B., Kephelopoulou, S., Muñoz, A., Aurisano, N., Cusinato, A., Dimitroulopoulou, S., Slobodnik, J., De Mello, J., Zare Jeddi, M., Cascio, C., Ahrens, A., Bruinen De Bruin, Y., Lieck, L., & Fantke, P. (2022). Advancing exposure data analytics and repositories as part of the European Exposure Science

- Strategy 2020–2030. *Environment International*, 170, 107610. <https://doi.org/10.1016/j.envint.2022.107610>
- Krebs, A., Waldmann, T., Wilks, M. F., Van Vugt-Lussenburg, B. M. A., Van der Burg, B., Terron, A., Steger-Hartmann, T., Ruegg, J., Rovida, C., Pedersen, E., Pallocca, G., Luijten, M., Leite, S. B., Kustermann, S., Kamp, H., Hoeng, J., Hewitt, P., Herzler, M., Hengstler, J. G., ... Leist, M. (2020). Template for the description of cell-based toxicological test methods to allow evaluation and regulatory use of the data. *ALTEX*, 37, 164–699. <https://doi.org/10.14573/altex.1909271>
- Krug, H. F. (2018). The uncertainty with nanosafety: Validity and reliability of published data. *Colloids and Surfaces. B, Biointerfaces*, 172, 113–117. <https://doi.org/10.1016/j.colsurfb.2018.08.036>
- Krug, H. F. (2022). Collection of controlled nanosafety data—The CoCoN-database, a tool to assess nanomaterial hazard. *Nanomaterials*, 12, 441. <https://doi.org/10.3390/nano12030441>
- Langan, L. M., Baettig, C. G., Cole, A. R., Lovin, L., Scarlett, K., Wronski, A. R., O'Brien, M. E., Shmaitelly, Y., & Brooks, B. W. (2025). Experimental reporting of fish transcriptomic responses in environmental toxicology and ecotoxicology. *Environmental Toxicology and Chemistry*, 44, 2580–2598. <https://doi.org/10.1093/etoxnl/vgae077>
- Lead, J. R., Batley, G. E., Alvarez, P. J. J., Croteau, M.-N., Handy, R. D., McLaughlin, M. J., Judy, J. D., & Schirmer, K. (2018). Nanomaterials in the environment: Behavior, fate, bioavailability, and effects—An updated review: Nanomaterials in the environment. *Environmental Toxicology and Chemistry*, 37, 2029–2063. <https://doi.org/10.1002/etc.4147>
- Li, T., Albee, B., Alemayehu, M., Diaz, R., Ingham, L., Kamal, S., Rodriguez, M., & Whaley Bishnoi, S. (2010). Comparative toxicity study of Ag, Au, and Ag–Au bimetallic nanoparticles on *Daphnia magna*. *Analytical and Bioanalytical Chemistry*, 398, 689–700. <https://doi.org/10.1007/s00216-010-3915-1>
- Mancardi, G., Mikolajczyk, A., Annapoorani, V. K., Bahl, A., Blekos, K., Burk, J., Çetin, Y. A., Chairetakis, K., Dutta, S., Escorihuela, L., Jagiello, K., Singhal, A., van der Pol, R., Bañares, M. A., Buchete, N.-V., Calatayud, M., Dumit, V. I., Gardini, D., Jeliaskova, N., ... Chiavazzo, E. (2023). A computational view on nanomaterial intrinsic and extrinsic features for nanosafety and sustainability. *Materials Today*, 67, 344–370. <https://doi.org/10.1016/j.mattod.2023.05.029>
- Martin, O. V., Adams, J., Beasley, A., Belanger, S., Breton, R. L., Brock, T. C. M., Buonsante, V. A., Galay Burgos, M., Green, J., Guiney, P. D., Hall, T., Hanson, M., Harris, M. J., Henry, T. R., Huggett, D., Junghans, M., Laskowski, R., Maack, G., Moermond, C. T. A., ... Ågerstrand, M. (2019). Improving environmental risk assessments of chemicals: Steps towards evidence-based ecotoxicology. *Environment International*, 128, 210–217. <https://doi.org/10.1016/j.envint.2019.04.053>
- Mebane, C. A., Sumpster, J. P., Fairbrother, A., Augspurger, T. P., Canfield, T. J., Goodfellow, W. L., Guiney, P. D., LeHuray, A., Maltby, L., Mayfield, D. B., McLaughlin, M. J., Ortego, L. S., Schlekat, T., Scroggins, R. P., & Verslycke, T. A. (2019). Scientific integrity issues in environmental toxicology and chemistry: Improving research reproducibility, credibility, and transparency. *Integrated Environmental Assessment and Management*, 15, 320–344. <https://doi.org/10.1002/ieam.4119>
- Mirzaei, M., Furxhi, I., Murphy, F., & Mullins, M. (2021). A machine learning tool to predict the antibacterial capacity of nanoparticles. *Nanomaterials*, 11, 1774. <https://doi.org/10.3390/nano11071774>
- Moermond, C., Beasley, A., Breton, R., Junghans, M., Laskowski, R., Solomon, K., & Zahner, H. (2017). Assessing the reliability of ecotoxicological studies: An overview of current needs and approaches. *Integrated Environmental Assessment and Management*, 13, 640–651. <https://doi.org/10.1002/ieam.1870>
- Moermond, C. T. A., Kase, R., Korkaric, M., & Ågerstrand, M. (2016). CRED: Criteria for reporting and evaluating ecotoxicity data. *Environmental Toxicology and Chemistry*, 35, 1297–1309. <https://doi.org/10.1002/etc.3259>
- Muñoz-Mármol, M., Crespo, J., Fritts, M. J., & Maojo, V. (2015). Towards the taxonomic categorization and recognition of nanoparticle shapes. *Nanomedicine: Nanotechnology, Biology, and Medicine*, 11, 457–465. <https://doi.org/10.1016/j.nano.2014.07.006>
- Nam, S.-H., Shin, Y.-J., Lee, W.-M., Kim, S. W., Kwak, J. I., Yoon, S.-J., & An, Y.-J. (2015). Conducting a battery of bioassays for gold nanoparticles to derive guideline value for the protection of aquatic ecosystems. *Nanotoxicology*, 9, 326–335. <https://doi.org/10.3109/17435390.2014.930531>
- Nian, M., Chen, X., & Fang, M. (2025). Addressing pitfalls of metabolomics for toxicology: A call for standardization, reproducibility and data sharing. *Chemical Research in Toxicology*, 38, 1150–1156. <https://doi.org/10.1021/acs.chemrestox.4c00555>
- Nordberg, M., Templeton, D. M., Andersen, O., & Duffus, J. H. (2009). Glossary of terms used in ecotoxicology (IUPAC Recommendations 2009). *Pure and Applied Chemistry*, 81, 829–970. <https://doi.org/10.1351/PAC-REC-08-07-09>
- Nyadjro, E. S., Webster, J. A. B., Boyer, T. P., Cebrian, J., Collazo, L., Kaltenberger, G., Larsen, K., Lau, Y. H., Mickle, P., Toft, T., & Wang, Z. (2023). The NOAA NCEI marine microplastics database. *Scientific Data*, 10, 726. <https://doi.org/10.1038/s41597-023-02632-y>
- Olker, J. H., Elonen, C. M., Pilli, A., Anderson, A., Kinziger, B., Erickson, S., Skopinski, M., Pomplun, A., LaLone, C. A., Russom, C. L., & Hoff, D. (2022). The ECOTOXicology Knowledgebase: A curated database of ecologically relevant toxicity tests to support environmental research and risk assessment. *Environmental Toxicology and Chemistry*, 41, 1520–1539. <https://doi.org/10.1002/etc.5324>
- Organisation for Economic Co-operation and Development (OECD). (1998). *Test No. 212: Fish, Short-term Toxicity Test on Embryo and Sac-Fry Stages*. OECD. <https://doi.org/10.1787/9789264070141-en>
- Organisation for Economic Co-operation and Development (OECD). (2004). *Test No. 202: Daphnia sp. Acute Immobilisation Test*. OECD. <https://doi.org/10.1787/9789264069947-en>
- Oukarroum, A., Barhoumi, L., Pirastru, L., & Dewez, D. (2013). Silver nanoparticle toxicity effect on growth and cellular viability of the aquatic plant *Lemna gibba*. *Environmental Toxicology and Chemistry*, 32, 902–907. <https://doi.org/10.1002/etc.2131>
- Pang, L., Lin, Q., Zhao, S., Zheng, H., Li, C., Zhang, J., Sun, C., Chen, L., & Li, F. (2023). Data quality assessment for studies investigating microplastics and nanoplastics in food products:

- Are current data reliable? *Frontiers of Environmental Science & Engineering*, 17, 94. <https://doi.org/10.1007/s11783-023-1694-0>
- Papadiamantis, A. G., Klaessig, F. C., Exner, T. E., Hofer, S., Hofstaetter, N., Himly, M., Williams, M. A., Doganis, P., Hoover, M. D., Afantitis, A., Melagraki, G., Nolan, T. S., Rumble, J., Maier, D., & Lynch, I. (2020). Metadata stewardship in nanosafety research: Community-driven organisation of metadata schemas to support FAIR nanoscience data. *Nanomaterials*, 10, 2033. <https://doi.org/10.3390/nano10102033><https://doi.org/10/gjxq3m>
- Park, J.-W., Oh, J.-H., Kim, W.-K., & Lee, S.-K. (2014). Toxicity of citrate-coated silver nanoparticles differs according to method of suspension preparation. *Bulletin of Environmental Contamination and Toxicology*, 93, 53–59. <https://doi.org/10.1007/s00128-014-1296-4>
- Percie Du Sert, N., Hurst, V., Ahluwalia, A., Alam, S., Avey, M. T., Baker, M., Browne, W. J., Clark, A., Cuthill, I. C., Dirnagl, U., Emerson, M., Garner, P., Holgate, S. T., Howells, D. W., Karp, N. A., Lazic, S. E., Lidster, K., MacCallum, C. J., Macleod, M., ... Würbel, H. (2020). The ARRIVE guidelines 2.0: Updated guidelines for reporting animal research. *Journal of Cerebral Blood Flow and Metabolism*, 40, 1769–1777. <https://doi.org/10.1177/0271678X20943823>
- Pestana, J. L. T., Loureiro, S., Baird, D. J., & Soares, A. M. V. M. (2010). Pesticide exposure and inducible antipredator responses in the zooplankton grazer, *Daphnia magna* Straus. *Chemosphere*, 78, 241–248. <https://doi.org/10.1016/j.chemosphere.2009.10.066>
- Plata, D. L., & Janković, N. Z. (2021). Achieving sustainable nanomaterial design through strategic cultivation of big data. *Nature Nanotechnology*, 16, 612–614. <https://doi.org/10.1038/s41565-021-00902-7><https://doi.org/10/gj2m9c>
- Przybylak, K. R., Madden, J. C., Covey-Crump, E., Gibson, L., Barber, C., Patel, M., & Cronin, M. T. D. (2018). Characterisation of data resources for in silico modeling: Benchmark datasets for ADME properties. *Expert Opinion on Drug Metabolism & Toxicology*, 14, 169–181. <https://doi.org/10.1080/17425255.2017.1316449>
- Przybylak, K. R., Madden, J. C., Cronin, M. T. D., & Hewitt, M. (2012). Assessing toxicological data quality: Basic principles, existing schemes and current limitations. *SAR and QSAR in Environmental Research*, 23, 435–459. <https://doi.org/10.1080/1062936X.2012.664825>
- Pulido-Reyes, G., Moreno-Martín, G., Gómez-Gómez, B., Navas, J. M., Madrid, Y., & Fernández-Cruz, M. L. (2024). Fish acute toxicity of nine nanomaterials: Need of pre-tests to ensure comparability and reuse of data. *Environmental Research*, 245, 118072. <https://doi.org/10.1016/j.envres.2023.118072>
- R Core Team. (2024). *R: A language and environment for statistical computing* (Version 4.3.3) [Computer software]. R Foundation for Statistical Computing. <https://www.R-project.org/>
- Saarimäki, L. A., Federico, A., Lynch, I., Papadiamantis, A. G., Tsoumanis, A., Melagraki, G., Afantitis, A., Serra, A., & Greco, D. (2021). Manually curated transcriptomics data collection for toxicogenomic assessment of engineered nanomaterials. *Scientific Data*, 8, 49. <https://doi.org/10.1038/s41597-021-00808-y>
- Saarimäki, L. A., Melagraki, G., Afantitis, A., Lynch, I., & Greco, D. (2022). Prospects and challenges for FAIR toxicogenomics data. *Nature Nanotechnology*, 17, 17–18. <https://doi.org/10.1038/s41565-021-01049-1>
- Samuel, G. O., Hoffmann, S., Wright, R. A., Lalu, M. M., Patlewicz, G., Becker, R. A., DeGeorge, G. L., Fergusson, D., Hartung, T., Lewis, R. J., & Stephens, M. L. (2016). Guidance on assessing the methodological and reporting quality of toxicologically relevant studies: A scoping review. *Environment International*, 92–93, 630–646. <https://doi.org/10.1016/j.envint.2016.03.010>
- Sansone, S.-A., Rocca-Serra, P., Field, D., Maguire, E., Taylor, C., Hofmann, O., Fang, H., Neumann, S., Tong, W., Amaral-Zettler, L., Begley, K., Booth, T., Bougueleret, L., Burns, G., Chapman, B., Clark, T., Coleman, L.-A., Copeland, J., Das, S., ... Hide, W. (2012). Toward interoperable bioscience data. *Nature Genetics*, 44, 121–126. <https://doi.org/10.1038/ng.1054>
- Saouter, E., Biganzoli, F., Pant, R., Sala, S., & Versteeg, D. (2019). Using REACH for the EU environmental footprint: Building a usable ecotoxicity database, Part I. *Integrated Environmental Assessment and Management*, 15, 783–795. <https://doi.org/10.1002/ieam.4168>
- Schanzer, S., Koch, M., Kiefer, A., Jentke, T., Veith, M., Bracher, F., Bracher, J., & Müller, C. (2022). Analysis of pesticide and persistent organic pollutant residues in German bats. *Chemosphere*, 305, 135342. <https://doi.org/10.1016/j.chemosphere.2022.135342>
- Scharmüller, A., Schreiner, V. C., & Schäfer, R. B. (2020). Standartox: Standardizing toxicity data. *Data*, 5, 46. <https://doi.org/10.3390/data5020046>
- Schür, C., Gasser, L., Perez-Cruz, F., Schirmer, K., & Baity-Jesi, M. (2023). A benchmark dataset for machine learning in ecotoxicology. *Scientific Data*, 10, 718. <https://doi.org/10.1038/s41597-023-02612-2>
- Scott-Fordsmand, J. J., & Amorim, M. J. B. (2023). Using machine learning to make nanomaterials sustainable. *Science of the Total Environment*, 859, 160303. <https://doi.org/10.1016/j.scitotenv.2022.160303>
- Shao, G., Beronius, A., & Nymark, P. (2023). SciRAPnano: A pragmatic and harmonized approach for quality evaluation of in vitro toxicity data to support risk assessment of nanomaterials. *Frontiers in Toxicology*, 5, 1319985. <https://doi.org/10.3389/ftox.2023.1319985>
- Siivola, K. M., Burgum, M. J., Suárez-Merino, B., Clift, M. J. D., Doak, S. H., & Catalán, J. (2022). A systematic quality evaluation and review of nanomaterial genotoxicity studies: A regulatory perspective. *Particle and Fibre Toxicology*, 19, 59. <https://doi.org/10.1186/s12989-022-00499-2>
- Society of Environmental Toxicology and Chemistry (SETAC). (2019). Technical issue paper: Recommended minimum reporting information for environmental toxicity studies. Society of Environmental Toxicology and Chemistry.
- Sumpter, J. P., Runnalls, T. J., Donnachie, R. L., & Owen, S. F. (2021). A comprehensive aquatic risk assessment of the beta-blocker propranolol, based on the results of over 600 research papers. *Science of the Total Environment*, 793, 148617. <https://doi.org/10.1016/j.scitotenv.2021.148617>
- Thessen, A. E., Marvel, S., Achenbach, J. C., Fischer, S., Haendel, M. A., Hayward, K., Klüver, N., Könemann, S., Legradi, J., Lein, P., Leong, C., Mylroie, J. E., Padilla, S., Perone, D., Planchart,

- A., Prieto, R. M., Muriana, A., Quevedo, C., Reif, D., ... Hamm, J. (2022). Implementation of zebrafish ontologies for toxicology screening. *Frontiers in Toxicology*, 4, 817999. <https://doi.org/10.3389/ftox.2022.817999>
- Totaro, S., Crutzen, H., & Riego Sintes, J. (2017). *NANoREG data logging templates for the environmental, health and safety assessment of nanomaterials*. Publications Office. <https://data.europa.eu/doi/10.2787/505397>
- U. S. Environmental Protection Agency (USEPA). (2002). *Methods for measuring the acute toxicity of effluents and receiving waters to freshwater and marine organisms* (5th ed.). U. S. Environmental Protection Agency. [https://www.epa.gov/sites/default/files/2015-08/documents/acute-freshwater-and-marine-wet-manual\\_2002.pdf](https://www.epa.gov/sites/default/files/2015-08/documents/acute-freshwater-and-marine-wet-manual_2002.pdf)
- Valerio-García, R. C., Medina-Ramírez, I. E., Arzate-Cardenas, M. A., & Carbajal-Hernández, A. L. (2021). Evaluation of the environmental impact of magnetic nanostructured materials at different trophic levels. *Nanotoxicology*, 15, 257–275. <https://doi.org/10.1080/17435390.2020.1862335>
- Verschoor, A. J., Vink, J. P. M., De Snoo, G. R., & Vijver, M. G. (2011). Spatial and temporal variation of watertype-specific no-effect concentrations and risks of Cu, Ni, and Zn. *Environmental Science & Technology*, 45, 6049–6056. <https://doi.org/10.1021/es2007963>
- Wang, L., Yang, T., Liu, X., Liu, J., & Liu, W. (2024). Critical evaluation and meta-analysis of ecotoxicological data on per- and polyfluoroalkyl substances (PFAS) in freshwater species. *Environmental Science & Technology*, 58, 17555–17566. <https://doi.org/10.1021/acs.est.4c04818>
- Wheeler, R. M., & Lower, S. K. (2021). A meta-analysis framework to assess the role of units in describing nanoparticle toxicity. *NanoImpact*, 21, 100277. <https://doi.org/10.1016/j.impact.2020.100277><https://doi.org/10/gnsx85>
- Wilkinson, M. D., Dumontier, M., Aalbersberg, I. J. J., Appleton, G., Axton, M., Baak, A., Blomberg, N., Boiten, J.-W., da Silva Santos, L. B., Bourne, P. E., Bouwman, J., Brookes, A. J., Clark, T., Crosas, M., Dillo, I., Dumon, O., Edmunds, S., Evelo, C. T., Finkers, R., ... Mons, B. (2016). The FAIR guiding principles for scientific data management and stewardship. *Scientific Data*, 3, 160018. <https://doi.org/10.1038/sdata.2016.18>
- Xiao, Y., Peijnenburg, W. J. G. M., Chen, G., & Vijver, M. G. (2016). Toxicity of copper nanoparticles to *Daphnia magna* under different exposure conditions. *Science of the Total Environment*, 563-564, 81–88. <https://doi.org/10.1016/j.scitotenv.2016.04.104>
- Yan, N., He, X., Tang, B. Z., & Wang, W.-X. (2019). Differentiating silver nanoparticles and ions in medaka larvae by coupling two aggregation-induced emission fluorophores. *Environmental Science & Technology*, 53, 5895–5905. <https://doi.org/10.1021/acs.est.9b01156>
- Yan, X., Yue, T., Winkler, D. A., Yin, Y., Zhu, H., Jiang, G., & Yan, B. (2023). Converting nanotoxicity data to information using artificial intelligence and simulation. *Chemical Reviews*, 123, 8575–8637. <https://doi.org/10.1021/acs.chemrev.3c00070>
- Yung, M. M. N., Kwok, K. W. H., Djurišić, A. B., Giesy, J. P., & Leung, K. M. Y. (2017). Influences of temperature and salinity on physicochemical properties and toxicity of zinc oxide nanoparticles to the marine diatom *Thalassiosira pseudonana*. *Scientific Reports*, 7, 3662. <https://doi.org/10.1038/s41598-017-03889-1>