Supporting Information S2

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Deep Dive into Plastic Monomers, Additives, and Processing aids

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LIST OF ABBREVIATIONS

Abbr.	Meaning
ABS	Acrylonitrile butadiene styrene (polymer)
AqTox	Chronic aquatic toxicity (hazard classification)
B	Bioaccumulative (hazard classification)
B&C	Building and construction (industrial sector)
C	Carcinogenic (hazard classification)
C&L	Classification and Labelling (regulation)
CAS	Chemical Abstract Service (organization)
CASRN	Chemical Abstract Service Registry Numbers (identifier)
CDR	Chemical Data Reporting (regional chemical inventory)
CLP	Classification, Labelling and Packaging of substances and mixtures (regulation)
CMR	Carcinogenicity, mutagenicity, reproductive toxicity (hazard classification)
CPCat	Chemicals in product categories database by the USEPA (database)
CPPdb	Chemicals associated with Plastic Packaging database by Groh et al (2019) (database)
ECHA	European Chemicals Agency (organization)
ED / EDC	Endocrine disrupting / endocrine disrupting chemical (hazard classification)
EEE	Electrical and electronic equipment (industrial sector)
EPA	Environmental Protection Agency (organization)
EPS	Expanded polystyrene (polymer)
EU	European Union (country or region)
FCM	Food-contact material (industrial sector)
FDA	Food and Drug Administration (organization)
GADSL	Global Automotive Declarable Substance List
GHS	Globally harmonized system of classification and labelling of chemicals
GRAS	Generally Recognized As Safe (regulation)
HDPE	High-density polyethylene (polymer)
HIPS	High-impact polystyrene (polymer)
HPV / HPVC	High production volume / high production volume chemical. Production volume > 1000 t/yr
KEMI	Swedish Chemicals Agency (organization)
LDPE	Low-density polyethylene (polymer)
M	Mutagenic (hazard classification)
OECD	Organisation for Economic Co-operation and Development (country or region)
P	Persistent (hazard classification)
PA	Polyamides (polymer)
PBT	Persistent, bioaccumulative and toxic (hazard classification)
PC	Polycarbonates (polymer)
PE	Polyethylene (polymer)
PET	Polyethylene terephthalate (polymer)
PP	Polypropylene (polymer)
PS	Polystyrene (polymer)
PUR	Polyurethanes (polymer)
PVC	Polyvinylchloride (polymer)
R	Toxic for reproduction (hazard classification)

REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (regulation)
RespSens	Respiratory sensitization (hazard classification)
SMILES	Simplified Molecular-Input Line-Entry System (identifier)
SPIN	Substances in Preparations in Nordic Countries (regional chemical inventory)
STOT-RE	Specific target organ toxicity upon repeated exposure (hazard classification)
t/yr	Metric tonnes per year (unit)
US	United States (country or region)
UVCB	Substances of unknown or variable composition, complex reaction products or biological materials (in the substance category for this study also simple mixtures and polymers are included)
vB	Very bioaccumulative (hazard classification)
vP	Very persistent (hazard classification)
vPvB	Very persistent and very bioaccumulative (hazard classification)

S1 METHOD DETAILS

S1.1 Identification of relevant data sources

In total, 186 plastic-related sources were identified; the full list can be found in the accompanying excel file, categorized according to information content (Sheet S1 in Supporting Information S1). The majority of them were scientific sources (73 %), followed by regulatory sources (16%), industrial sources (8%), and sources compiled by civil society organizations (3%). In this study, only 63 of these sources that provided readily accessible information were further processed and analysed. Most of the industry and regulatory sources identified substances by their assigned Chemical Abstract Service Registry Numbers (CASRNs) and could thus be used for the analysis, whereas only a quarter of scientific sources did so. The regulatory sources exclusively came from European countries, Canada or the United States of America (US).

Table S1: Major data sources for the identification of plastic monomers, additives and processing aids and their information content. Either a footnote with the URL or a reference is provided for each source. Details on the retrieval of these and all remaining sources are described in detail in Sheet S1 in Supporting Information S1, relevant entries can be linked via “id”.

Type	id	Source name	CASRNs	Information content			
				Function	Polymer type	Industrial Sector	Further information
Scientific	13	CPPdb [1]	4237	☑	☑	☑	• Hazard data • Legal status
	57	Sheftel_2000 [2]	1211	☑			• Hazard data
	67	Ullmann_2003[3]	793	☑	☑	☑	• Hazard data
	23	Maier_Schiller_2016 [4]	596	☑	☑	☑	• Trade names
	282	Kirk_Othmer_2000 [5]	504	☑	☑		• Phys.-chem. properties
Regulatory	36	REACH_plastics [6]	3362	☑		☑	• Regional use • Production Volume
	12	CPCat_plastics[a]	2934	☑		☑	• Regional use • Production Volume
	142	Comptox_Plastic[b]	2669				• Regional use • Production Volume
	50	SPIN_plastic[c]	2018	☑		☑	• Regional use • Production Volume
	45	CDR_2012[d]	1547	☑		☑	• Regional use • Production Volume
	84	EPA_CD_plastic[e]	934	☑		☑	• Regional use • Production Volume
	146	EC_FCM_UnionList [7]	729	☑	☑	☑	• Regional use • Legal Status
Industry	66	SpecialChemSelector_2019[f]	2664	☑	☑	☑	• Phys.-chem. properties • Trade names
	114	GADSL[g]	958	☑	☑	☑	

[a] https://actor.epa.gov/cpcat/faces/home.xhtml
[b] https://comptox.epa.gov/dashboard/consumer_products/chemicals?cp_cat_term=plastics
[c] http://www.spin2000.net/
[d] https://www.epa.gov/chemical-data-reporting
[e] https://comptox.epa.gov/dashboard/downloads
[f] https://polymer-additives.specialchem.com/
[g] https://www.gadsl.org/

The 63 sources typically contained between 100 and 1000 relevant substances, with the Chemicals associated with Plastic Packaging database (CPPdb) having reported most.[1] Among all the sources, regulatory sources reported most substances per source (Figure S1).

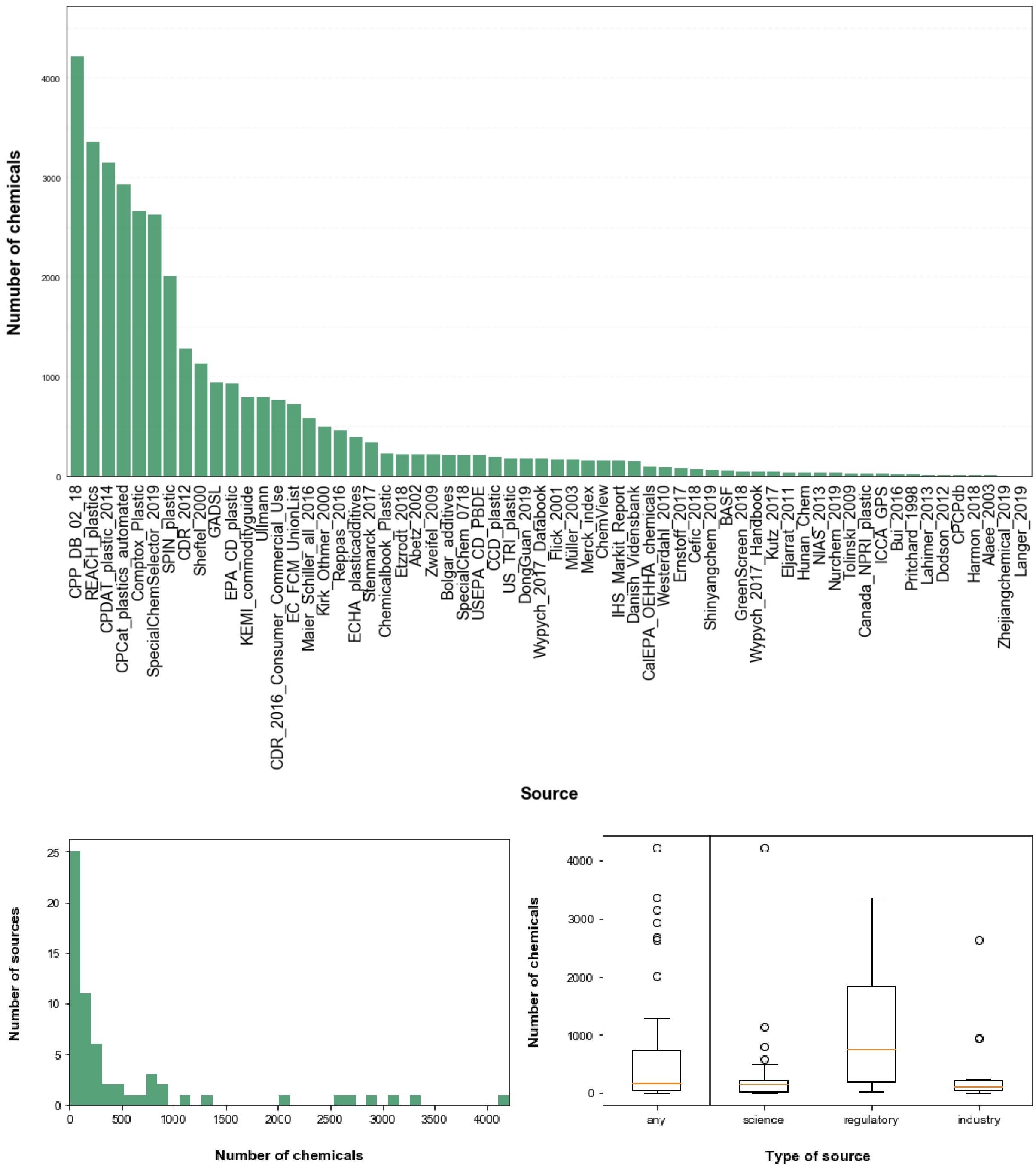

Figure S1: Numbers of plastic monomers, additives and processing aids identified per information source, as a bar chart (top). The corresponding distributions of individual sources with regard to the numbers of substances identified therein are presented as a histogram (bottom left) and boxplot (bottom right). Differences among source types are also visualized in the box plot (bottom right).

S1.2 Inclusion of individual substances and associated information

S1.2.1 Identification of relevant substances

Details on information extraction for each source can be found in the accompanying excel file (Sheet S1 – Column "preparation"). All plastic-related keywords used for identifying relevant substances can be found in Table S2 under "Identification method". Antioxidants were considered generic functions due to their wide use in the food, drug and fuel industries.[8] When no structured information was available, CASRNs were extracted from unstructured text by using automated search for the regular expression "[0-9]*-[0-9][0-9]-[0-9]".

S1.2.2 CASRN verification

All CASRNs retrieved were subsequently verified using the check-digit method.[9] For a specific entry, if the check digit did not equal the shown calculation (Equation S1) and no blunders (e.g. misread input) could be identified, it was excluded.

Structure of a CASRN	$N_i \ldots N_4\, N_3 - N_2\, N_1 - R$
Position	i … 4 3 2 1 check digit
Check-digit method	$R = mod10\left(\sum_{pos=1}^{i} N_{pos} * pos\right)$

Equation S1: The check-digit-method set by the Chemical Abstract Service, using the last digit in a CASRN as the "check digit".

Furthermore, the verified CASRNs were searched in SciFinder to retrieve their related CASRNs (deleted or alternate), standard names and molecular formula.[10] All information was downloaded in the form of ".tsv"-files. Only standard/active CASRNs were further used as the unique identifiers for individual substances, whereas all related CASRNs (i.e. alternative and deleted ones) were used to search for and include substance-related information such as use patterns and hazard classifications to ensure maximum coverage (for more details, see S1.2.4 below).

S1.2.3 Confidence assignment

Confidence assignment was conducted for the sources as described in Section 2.2 in the main text, and more specifically, following the criteria described in Table S2. The resulting confidence scores for individual sources can be found in the accompanying excel file (Sheet S1), with their distribution illustrated in Figure S3. Scientific sources have generally lower confidence scores than regulatory and industrial sources (Figure S3 – bottom left), mostly because regulatory and industrial sources more frequently report first-hand information. The sources reporting a large number of chemicals show similar confidence as those reporting fewer chemicals (Figure S3 – bottom right).

Substance confidence scores were assigned primarily based on the scores of their sources (Sheet S1 in Supporting Information S1). For substances that were included in multiple sources, the highest score was considered. For substances that were reported by multiple first-hand information sources, a combined confidence score was calculated according to Equation S2, i.e., assignment method A: The main idea behind this calculation is that all first-hand information sources need to "fail" to report correct information in order to lead to a false positive report. The failure rate of reporting can be imagined as reverse of the confidence scores assigned to each source (for implementation, see Figure S2). The failure rate of first-hand information sources reporting the same information was assumed to be independent, leading to an overall error frequency as product of the individual error frequencies. Thus, the confidence score for individual substances that were reported by several first-hand-information sources is calculated using Equation S2.

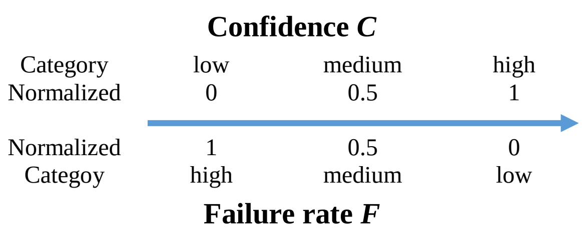

Figure S2: Relationship between confidence (C) and assumed failure rate (F) on different scales ("Category" and "Normalized")

$$C_{tot,norm} = 1 - \prod_{\substack{i=relevant \\ first-hand \\ sources}} F_i$$

Equation S2: Total normalized confidence score ($C_{tot,norm}$) of a substance that is reported by several first-hand information sources. Error frequencies of reporting by different sources are assumed to be independent.

Robustness of the confidence score assignment for different chemicals was tested by using two additional assignment methods: assignment method B: All substances inherit the confidence score from their highest-scored source; and assignment method C: All substances inherit the confidence score from their highest-scored source, and additionally a bonus point (+1) was assigned for substances with multiple first-hand information sources.

Table S2: Pedigree matrix for assessing the confidence scores of individual sources with three data quality levels and four indicators.

	Criterion	Weight	High 66-100%	Medium 33-66%	Low 0-33%
Source	Information origin	40%	First-hand use information	Second-hand or compiled use information	Information of unknown origin
	Outlet control	20%	Independent (peer-) review process	Very basic review and plausibility check	No or unknown control of outlet
Processing	Identification method	20%	Clear evidence of use in plastics. *i.e. "plastics" / "polymer" directly in relevant field (e.g. "use in...")*	Likely used in plastics. • *"plastic"/"polymer" in closely associated field (e.g. "use by … industry")* • *plastic specific functions (i.e. "monomer", "plasticizer", "flame-retardant")*	Potentially used in plastics. *e.g. generic functions (i.e. "antioxidants", "biocides", "lubricants")*
	Processing needs	20%	No further processing *e.g. digital structured data*	Automatic extraction of semi-structured data *(e.g. entry by entry extraction)* or manual extraction *(e.g. text in natural language, pictures, analog sources)*	Automatic extraction of unstructured data

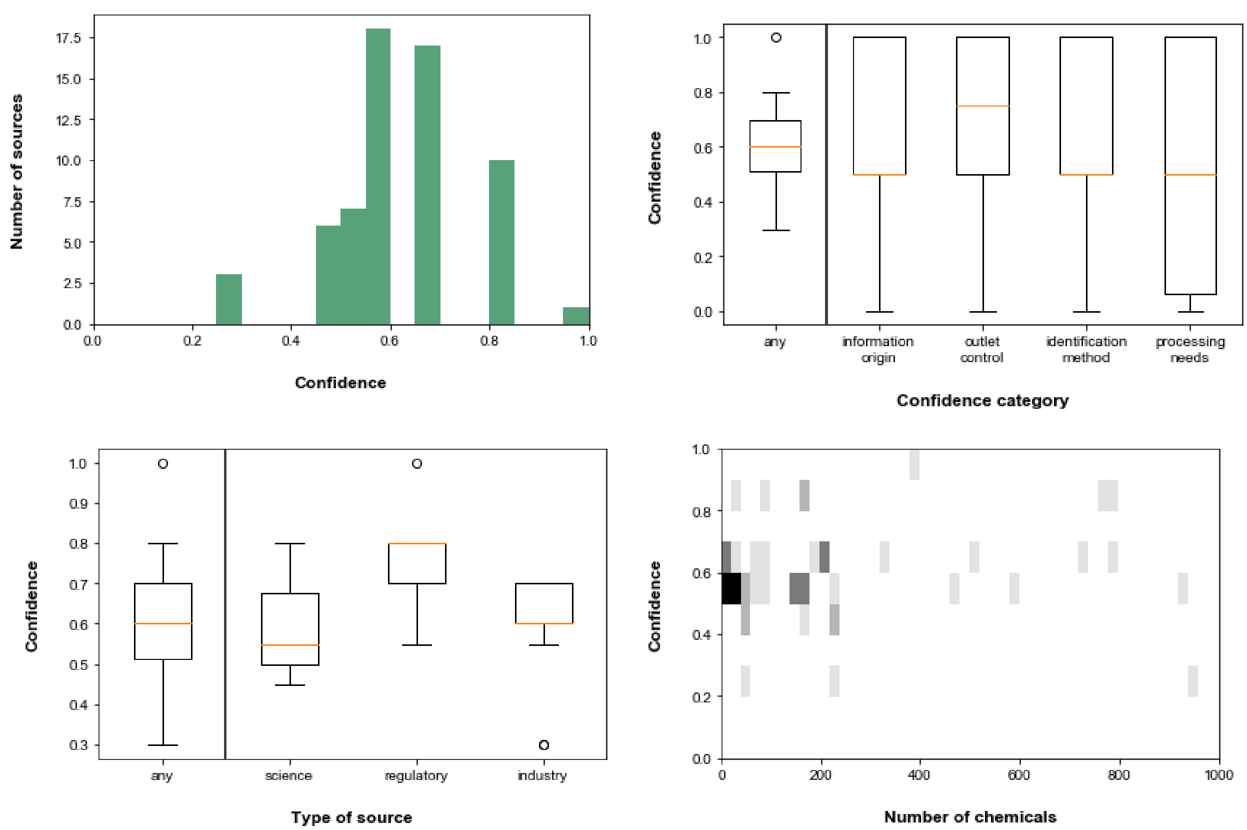

Figure S3: Distribution of confidence scores of individual sources. Source confidence score distribution as a histogram (top left) and boxplot for the different confidence criteria (top right). Source confidence scores are based on source type (bottom right) and the number of plastic-related chemicals described by the source (bottom left).

Comparing the different assignment methods shows that confidence assignment method A is fairly robust, as independent sources are only relevant for the substances that come from sources with already high confidence scores (Figure S4).

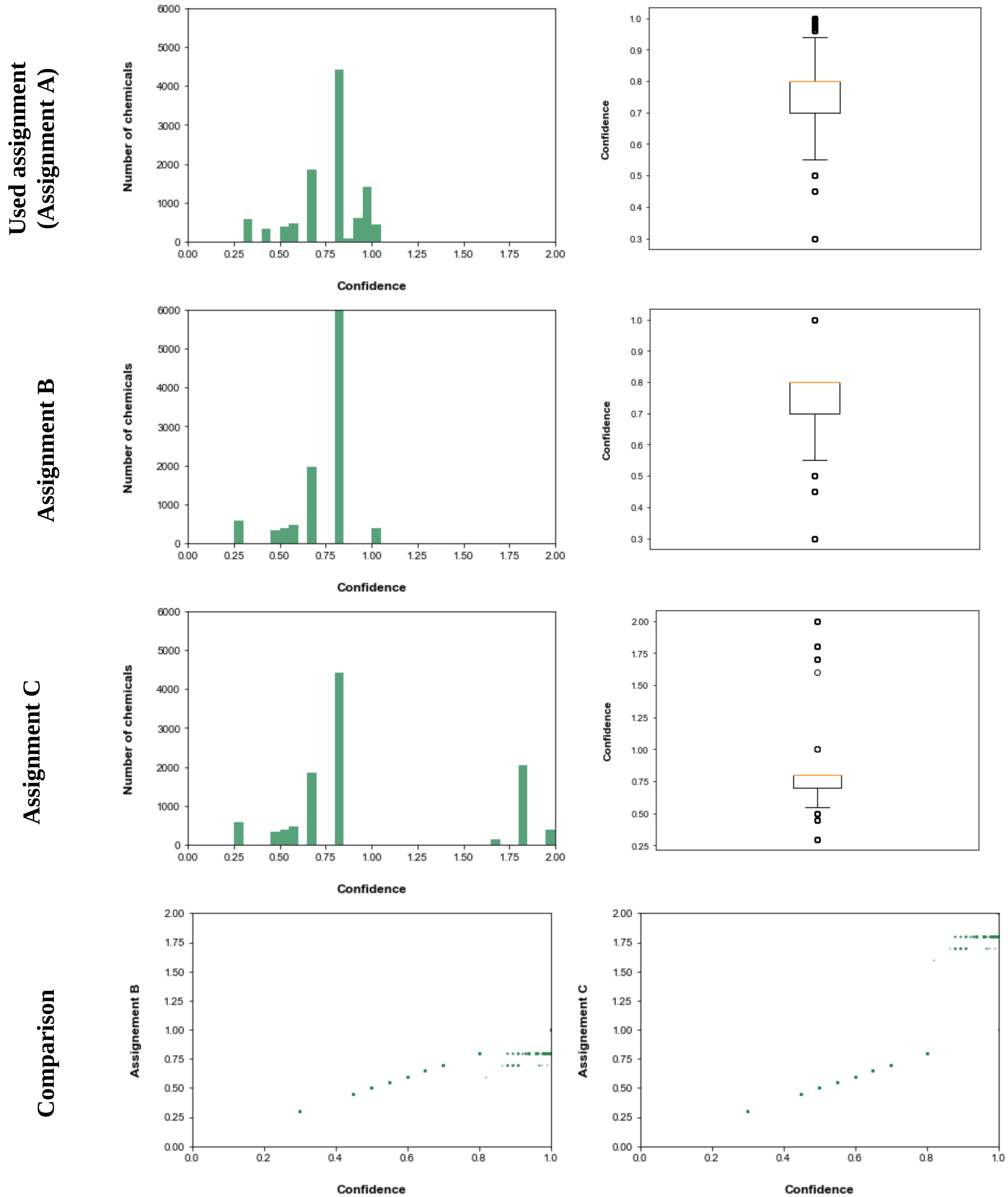

Figure S4: Robustness check of substance confidence assignment using different assignment methods. Distribution of the total confidence of individual substances presented as a histogram (left) and a boxplot (right) for the different assignments (top three rows). Direct comparison of confidence with assignment method A with B and C as a scatter plot (bottom row).

S1.2.4 Inclusion of further information

Details on the sources and respective retrieval procedures for further information can be found in the accompanying excel file (Sheet S2 in Supporting Information S1).

The regional use status was assessed by checking the official chemical inventories from different countries and regions; their geographical coverage and information scope are depicted in Figure S5. Using the income classification by the World Bank[11], regional chemical inventories were mostly provided by high and upper-middle-income countries, only 3 lower-middle-income countries (Vietnam, Philippines, India) and no low-income countries provided inventories. Lacking regional coverage regarding production, use or import of chemicals hinders assessing the global relevance/market relevance of plastic monomers, additives and processing aids identified. Furthermore, information on production volumes and industrial uses of chemicals (Figure S5 – red filled) were only provided by the US, the EU und and the Nordic Countries (Norway, Sweden, Finland, Denmark), further limiting assessment of global relevance and overall production volumes of individual chemicals.

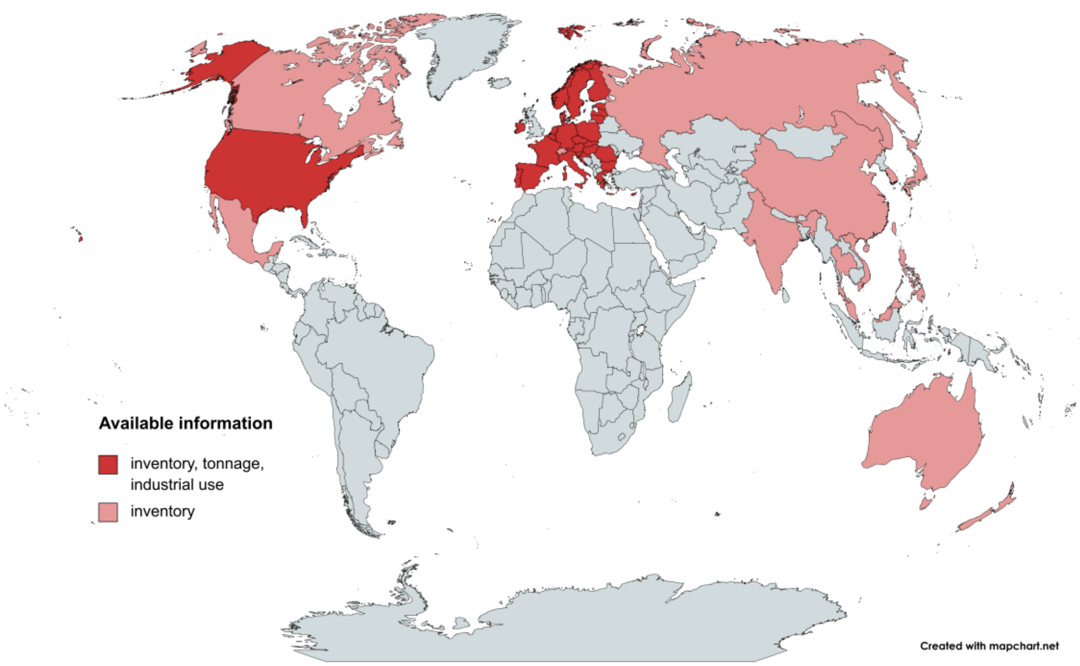

Figure S5: Coverage of the national and regional inventories used for production volume and regional use status in this study.

For individual hazard properties considered in this study, the consistency of hazard data was investigated by checking which substances were reported by which source (Figure S6).

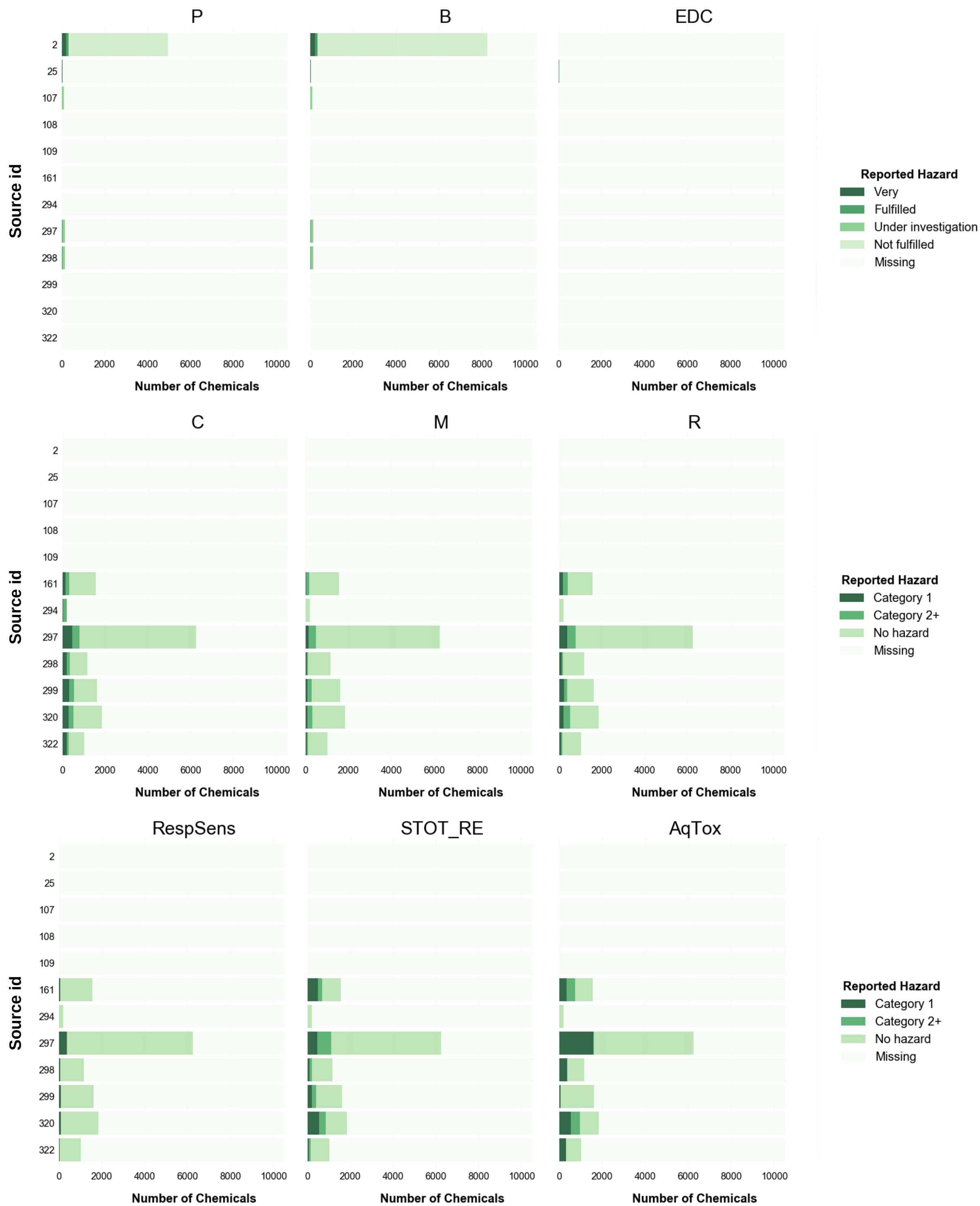

Figure S6: Overview of hazard data reported by different sources. Sources are referred to by their id (for details see Sheet S2 in Supporting Information S1). The following hazard properties are considered: P=persistent, B=bioaccumulation potential, EDC=endocrine disrupting chemical, C=carcinogenicity, M=mutagenicity, R=reproductive toxicity, RespSens=respiratory sensitization, STOT_RE=specific target organ toxicity upon repeated exposure, AqTox=chronic aquatic toxicity. For persistence and bioaccumulation (first row), substances may also be reported as "very persistent" or "very bioaccumulative", respectively, which is highlighted using the dark green category.

The regulatory status of individual substances was assessed using several international and regional regulatory lists. For international regulatory lists, the latest amendments, as of the time when this study was prepared (August 2020), were used; their geographical coverage varied not only among the conventions/protocols, but also by amendments (i.e. some countries automatically ratify all amendments, whereas others need to ratify each new amendment). Regional regulatory lists were retrieved from the US, Japan, Republic of Korea and the EU (depicted in Figure S7).

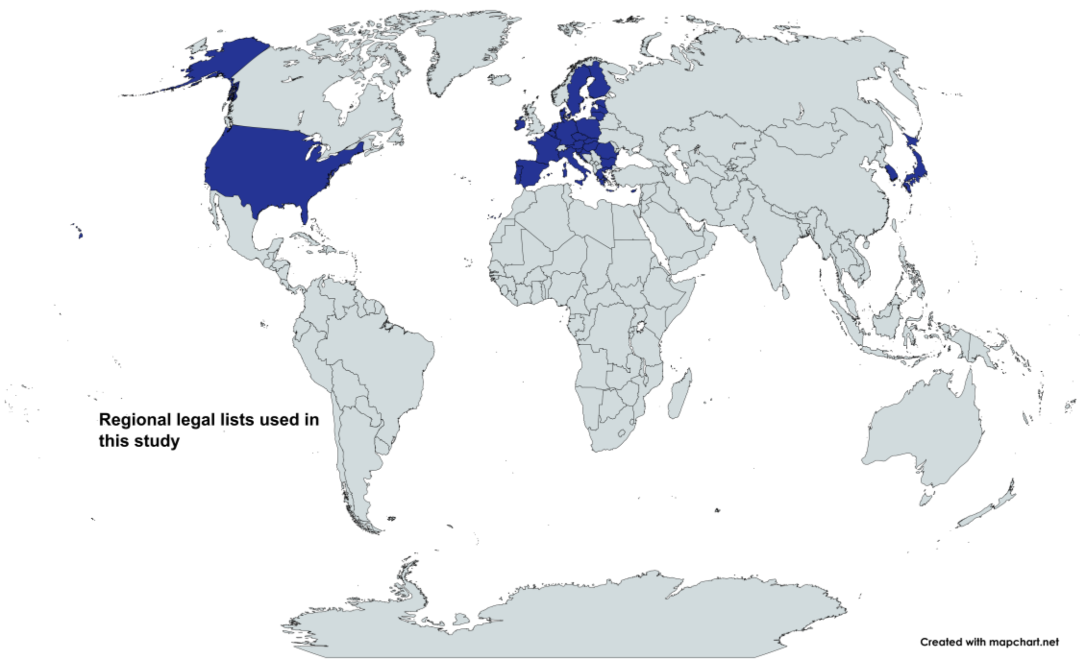

Figure S7: Geographical coverage of the regional regulatory lists used in assessing the regulatory status of chemicals.

S1.3 Categorization of substance types and use patterns

S1.3.1 Detailed workflow

Use descriptions in the original sources were used to categorize the functions, compatible polymer types and industrial sectors of use of individual substances. Regarding functions and industrial sectors, around 40000 separate use descriptions were available and analyzed, covering 91% (for functions) and 84% (for industrial sector) of all of the substances identified, respectively. Regarding polymer compatibility, both the total number of descriptions available and the substance coverage were significantly lower, with a total of 8120 descriptions covering 45% of all of the substances identified.

Chemical identifiers (such as standardized names, molecular formulas and SMILES) were used to categorize substance types. The latter were retrieved from SciFinder [10] (only these standardized identifiers were used to determine the substance type of a chemical, whereas identifiers mentioned in other sources were stored but not further processed). 32548 data points are available for chemical names, molecular formulas and SMILES, covering all of the identified substances.

The categorization was conducted using the categories and keywords in the accompanying excel file (Sheets S3–S6 in Supporting Information S1). The raw text from the descriptions and names, and the final categorization, are visualized as wordclouds in Figure S8 (the larger a word, the more frequently it occurs). The text was preprocessed by removing already defined keywords and language-specific irrelevant terms (e.g. "a", "the", "and") before visualization. The substance type of each substance was determined based on chemical elements present in the substance according to Table S3.

Table S3: Assignment of substance types based on elements present

Substance Type	Presence	Absence	Example
Inorganics		Organic carbon	Titanium(IV) chloride ($TiCl_4$, CASRN 7550-45-0)
Metalorganics/ Organometallics / organic metal salts	Organic carbon, metals or metalloids		Zirconocene dichloride (Cp_2ZrCl_2, CASRN 1291-32-3)
Organosilicon[1]	Organic carbon, silicon	Metals, metalloids	Ethenyltrimethoxysilane ($C_5H_{12}O_3Si$, CASRN 2768-02-7)
Organophosphorus[1]	Organic carbon, phosphorus	Metals, metalloids, silicon	Tris(1,3-dichloro-2-propyl) phosphate ($C_9H_{15}Cl_6O_4P$, CASRN 13674-87-8)
Organosulfurs[1]	Organic carbon, sulfur	Metals, metalloids, silicon, phosphorous	Bisphenol S ($C_{12}H_{10}O_4S$, CASRN 80-09-1)
Organohalogens[1]	Organic carbon, halogen	Metals, metalloids, silicon, phosphorus, sulfur	Hexabromocyclododecane ($C_{12}H_{18}Br_6$, CASRN 3194-55-6)
Other aromatics[1]	Aromatic carbon	Metals, metalloids, silicon, phosphorus, sulfur, halogens	Bis(2-ethylhexyl) phthalate ($C_{24}H_{38}O_4$, CASRN 117-81-7)
Other organics[1]	Organic carbon	Metals, metalloids, silicon, phosphorus, sulfur, halogens, aromatic carbon	Octadecanoic acid ($C_{18}H_{36}O_2$, CASRN 57-11-4)

[1] excluding metal and metalloid salts

Iterative manual checking and correction of search terms was performed to avoid unforeseen mistakes. That means after each categorization run, a random selection of the assigned categories was manually checked for errors; for the encountered errors, the corresponding search terms were deleted, corrected or inserted. These checks can be found in the accompanying excel file (Sheet S7 in Supporting Information S1). Error checking was repeated until each occurring search term yielded less than 10% errors (typically unavoidable ones based on the context or the ambiguous semantics of the terms). In total, 1100 substance type assignments, 5333 function assignments, 1457 compatible polymer assignments, and 3240 industrial sector assignments were manually checked. The correct hits and error frequency of each keyword during manual check can be found in Figure S9.

S1.3.2 Confidence assignment

After the final categorization, a confidence score was assigned to each categorization, based on information origin and outlet control of individual sources (in line with the source confidence score assignment in Table S2), processing needs to get the final description text, nature of the keywords (i.e. synonym, hyponym, hypernym), and observed error frequency (Table S4).

Table S4: Pedigree matrix used for assessing the confidence of individual category assignments with three data quality levels and five data quality indicators.

	Criterion	**Weight**	**High** **66-100%**	**Medium** **33-66%**	**Low** **0-33%**
Source	Information origin	50%	First-hand use information	Second-hand or compiled use information	Information of unknown origin
	Outlet control	10%	Independent (peer-) review process	Basic review and plausibility check	No or unknown control of outlet
Processing	Processing Needs	20%	No further processing *e.g. digital structured data*	Automatic extraction of semi-structured data *(e.g. entry by entry extraction)* or manual extraction *(e.g. text in natural language, pictures, analog sources)*	Automatic extraction of unstructured data
	Nature of keyword	10%	Synonyms *e.g. "Polyvinylchloride" for "PVC"*	Hyponyms *e.g. "Milk bottle" for "Food Packaging"*	Hypernym *e.g. "Packaging for Food Packaging*
	Error frequency	10%	<3.3 % errors	3.3-6.6 % errors	>6.6 % errors

S1.3.3 Single-use vs. durable applications

A preliminary analysis was conducted to assess differences in plastic monomers, additives and processing aids used in "single-use" and "durable" applications in different industrial sectors. For this purpose, packaging was considered "single-use", while other industrial sectors were considered “durable”. However, significant uncertainties remain due to substantial data gaps in understanding the industrial sector of use of individual substances and potential bias caused by inclusion of several major sources specifically dealing with “packaging”. The results can be found in Section S2.2.2 below.

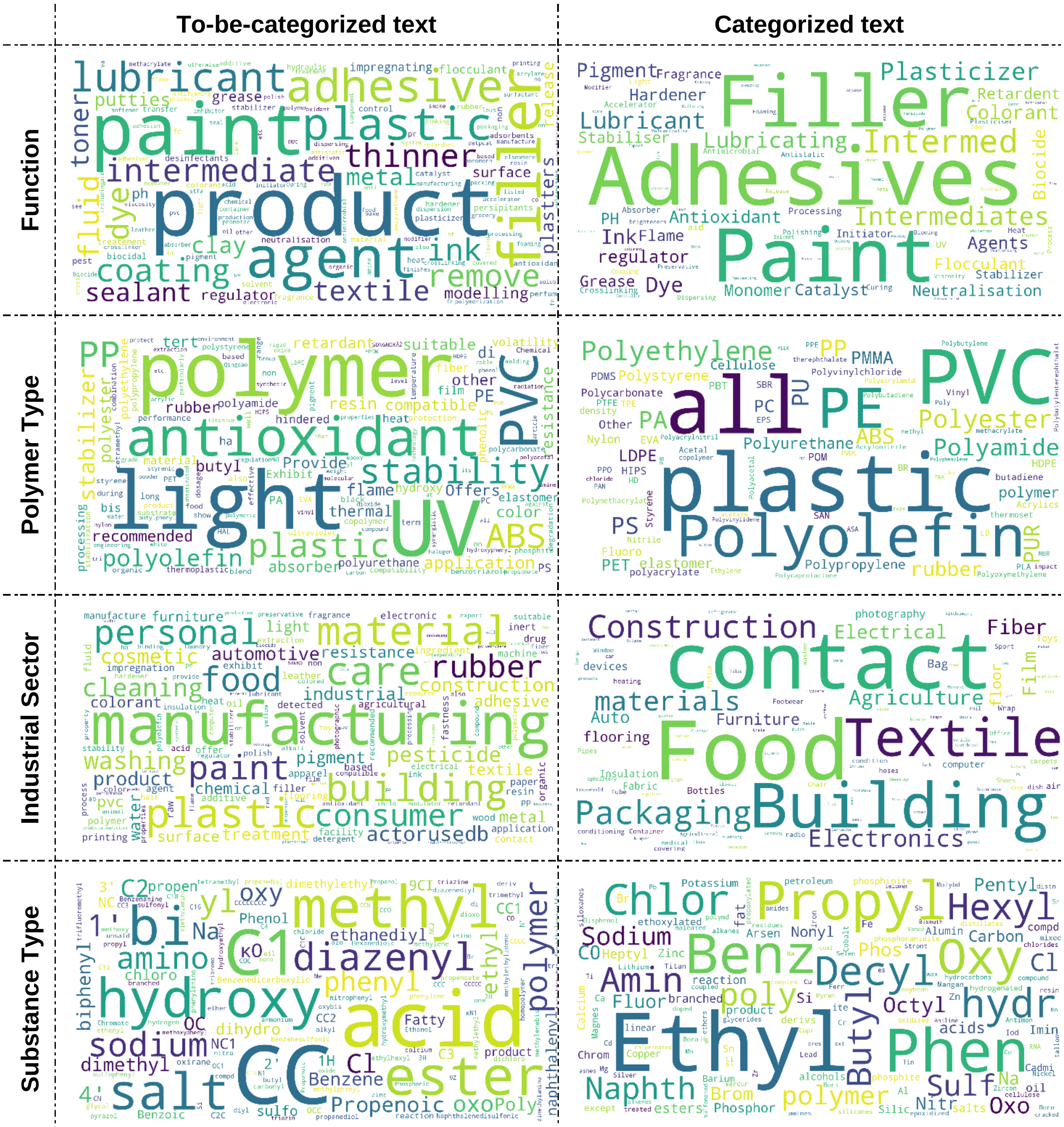

Figure S8: Text visualization of all reported information before categorization (left) and final categorization (right) with regard to function (top row), polymer type (second row), industrial sector (third row) and substance type (bottom row). The size of a word corresponds to its frequency in the text, and common words (e.g. a, the, and) are excluded.

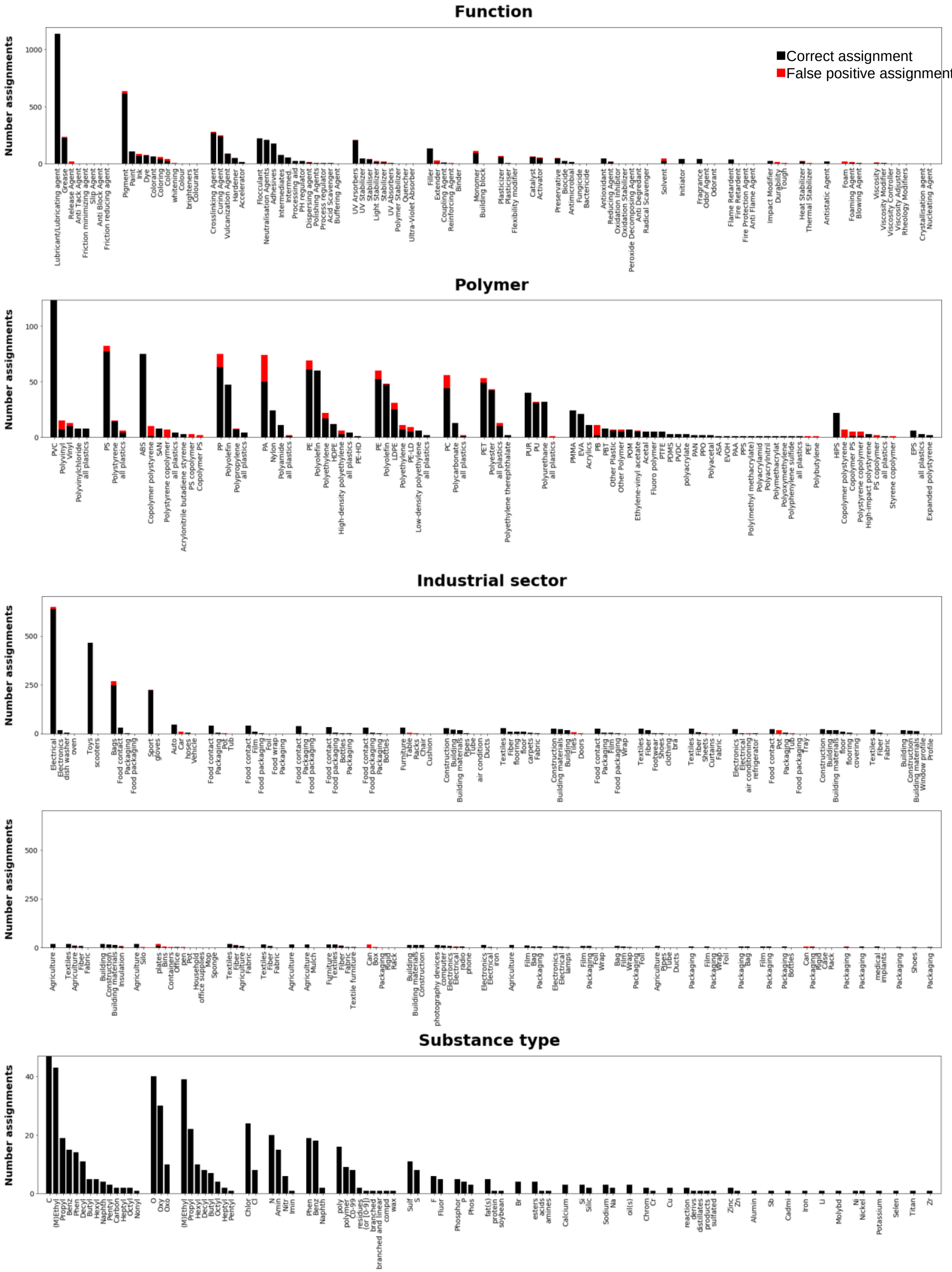

Figure S9: Correct (black) and false positive (red) assignments of keywords during manual error checks. Regarding industrial sector, two rows of figures are presented due to the large number of keywords used.

S1.4 Identification of substances of potential concern

To determine substances of potential concern, hazard criteria concerning Article 57 on substances of very high concern and ANNEX XIII on persistent, bioaccumulative and toxic substances under REACH were used (for details on individual criteria and implementation in this study, see Table S5). Regarding persistence, bioaccumulation, and endocrine disruption, only regulator-harmonized hazard data were considered in this study because (1) properties relevant for persistence and bioaccumulation were not readily extractable from company-reported hazard data sources and (2) endocrine disruption does not yet have its own hazard classification category.[12] Carcinogenicity, mutagenicity, reproductive toxicity, specific target organ toxicity upon repeated exposure, and chronic aquatic toxicity were often only identified using data from the REACH and CLP registration dossiers and data from eChemPortal.

Table S5: Criteria used for identifying substances of potential concern and their implementation in this study. ID numbers in the implementation refer to the respective data sources (Sheet S2 in Supporting Information S1).

<table>
<tr><th></th><th>Criteria according to REACH (Article 57 or ANNEX XIII)</th><th>Implementation in this study[1]</th></tr>
<tr><td>High production volume chemical</td><td>-</td><td>On the OECD HPVC list (ID = 158), or the sum production volumes of US + EU (or SPIN) above 1000 tonnes/year.</td></tr>
<tr><td>Persistent</td><td>A substance fulfills the persistence criterion (P) in any of the following situations:
a) the degradation half-life in marine water is higher than 60 days;
b) the degradation half-life in fresh or estuarine water is higher than 40 days;
c) the degradation half-life in marine sediment is higher than 180 days;
d) the degradation half-life in fresh or estuarine water sediment is higher than 120 days;
e) the degradation half-life in soil is higher than 120 days.

A substance fulfills the ‘very persistent’ criterion (vP) in any of the following situations:
a) the degradation half-life in marine, fresh or estuarine water is higher than 60 days;
b) the degradation half-life in marine, fresh or estuarine water sediment is higher than 180 days;
c) the degradation half-life in soil is higher than 180 days.</td><td>• REACH_PBT List (ID = 107)
<table><tr><th>Outcome</th><th>P</th><th>vP</th><th>B</th><th>vB</th></tr><tr><td>PBT</td><td>1</td><td>0</td><td>1</td><td>0</td></tr><tr><td>vPvB</td><td>1</td><td>1</td><td>1</td><td>1</td></tr><tr><td>not PBT/vPvB</td><td>0</td><td>0</td><td>0</td><td>0</td></tr><tr><td>under development / pending / postponed</td><td>0.5</td><td>0.5</td><td>0.5</td><td>0.5</td></tr></table>• REACH_hazard (ID = 297, 298)
<table><tr><th>Assessment</th><th>P</th><th>vP</th><th>B</th><th>vB</th></tr><tr><td>Recognized/ Broad agreement</td><td>1</td><td>-</td><td>1</td><td>-</td></tr><tr><td>Minority position / Under assessment</td><td>0.5</td><td>-</td><td>0.5</td><td>-</td></tr></table></td></tr>
</table>

<table>
<tr><td>Bioaccumulative</td><td>A substance fulfills the bioaccumulation criterion (B) when the bioconcentration factor in aquatic species is higher than 2000.

A substance fulfills the ‘very bioaccumulative’ criterion (vB) when the bioconcentration factor in aquatic species is higher than 5000.</td><td>• Legal lists (ID=25, 108)<table><tr><th>Reason for inclusion</th><th>P</th><th>vP</th><th>B</th><th>vB</th></tr><tr><td>PBT</td><td>1</td><td>0</td><td>1</td><td>0</td></tr><tr><td>vPvB</td><td>1</td><td>1</td><td>1</td><td>1</td></tr></table></td></tr>
<tr><td>Toxic</td><td>Any of the following hazards</td><td></td></tr>
<tr><td>Chronic aquatic toxicity</td><td>The long-term no-observed effect concentration (NOEC) or EC10 for marine or freshwater organisms is less than 0,01 mg/l;</td><td><table><tr><th>GHS Hazard Codes</th><th>AqTox</th></tr><tr><td>H400</td><td>1</td></tr><tr><td>H401, H402</td><td>0.5</td></tr></table></td></tr>
<tr><td>Specific organ toxicity upon repeated exposure</td><td>A substance meets the criteria for specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No 1272/2008.</td><td><table><tr><th>GHS Hazard Codes</th><th>STOT_RE</th></tr><tr><td>H372</td><td>1</td></tr><tr><td>H373</td><td>0.5</td></tr></table></td></tr>
<tr><td>Carcinogen, mutagen or reproductive toxicant (CMR)</td><td>A substance meets the criteria for classification as carcinogenic (category 1A or 1B), germ cell mutagenic (category 1A or 1B), or toxic for reproduction (category 1A, 1B, or 2) according to Regulation EC No 1272/2008;</td><td><table><tr><th>GHS Hazard Codes</th><th>C</th><th>M</th><th>R</th></tr><tr><td>H350</td><td>1</td><td>-</td><td>-</td></tr><tr><td>H351</td><td>0.5</td><td>-</td><td>-</td></tr><tr><td>H340</td><td>-</td><td>1</td><td>-</td></tr><tr><td>H341</td><td>-</td><td>0.5</td><td>-</td></tr><tr><td>H360, H362</td><td>-</td><td>-</td><td>1</td></tr><tr><td>H361</td><td>-</td><td>-</td><td>0.5</td></tr></table></td></tr>
<tr><td>Endocrine disruption</td><td>A substance has endocrine-disrupting properties according to Regulations EU No 528/20121 and EC No 1107/2009</td><td>• REACH_EDC List (ID = 109)<table><tr><th>Outcome</th><th>EDC</th></tr><tr><td>EDC</td><td>1</td></tr><tr><td>not EDC</td><td>0</td></tr><tr><td>under development / postponed</td><td>0.5</td></tr></table>• REACH_hazard (ID = 297, 298)<table><tr><th>Assessment</th><th>EDC</th></tr><tr><td>Recognized</td><td>1</td></tr><tr><td>Under assessment</td><td>0.5</td></tr></table>• Other Lists (ID=25, 108)<table><tr><th>Reason for inclusion</th><th>EDC</th></tr><tr><td>endocrine</td><td>1</td></tr></table></td></tr>
</table>

[1] Details on the mentioned sources can be found on Sheet S2 in Supporting Information S1 under the corresponding IDs

S2 ADDITIONAL RESULTS

S2.1 Substance types

Chemical elements occurring in each plastic monomer, additive or processing aid were investigated. The majority of the substances contain carbon, oxygen and hydrogen (Figure S10). Around 80% were found to contain some organic moiety: alkylated substances (e.g. containing -methyl, -ethyl, or -propyl moieties) were most common, followed by substances containing aromatic moieties (e.g. phenyl, benzyl, naphthalene groups). Furthermore, halogens and metals were frequently identified, in 20% and 25% of the substances, respectively (Figure S17). Chlorine was the most frequent halogen atom, and the most frequent metals and metalloids were sodium (8%), silicon (4%), zinc (2%), arsenic (1%), tin (1%) and chromium (1%).

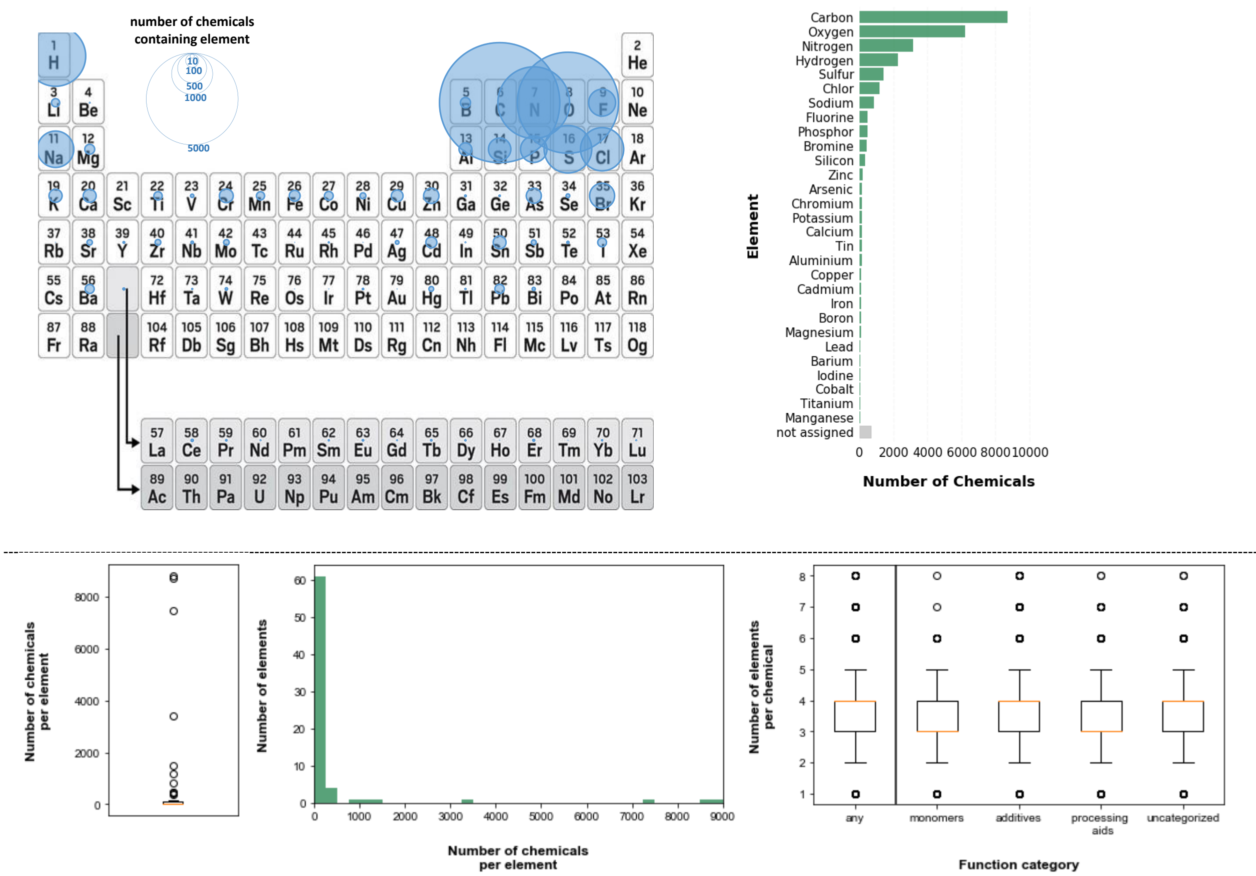

Figure S10: Occurrence of chemical elements in individual plastic monomers, additives and processing aids. Top: Number of chemicals containing individual elements in the periodic table (left) and bar chart (right). Bottom–Left: Number of chemicals per chemical element as a boxplot. Bottom–Middle: Number of chemicals per element as a histogram. Bottom–Right: Number of elements contained per chemical for different function categories.

S2.2 Use patterns

The following figures provide an additional overview of the substances identified, in terms of functions (Figure S11), compatible polymer types (Figure S13), industrial sectors of use (Figure S14), regional use status (Figure S15), production volumes (Figure S12), and numbers of related scientific references in SciFinder (Figure S16).

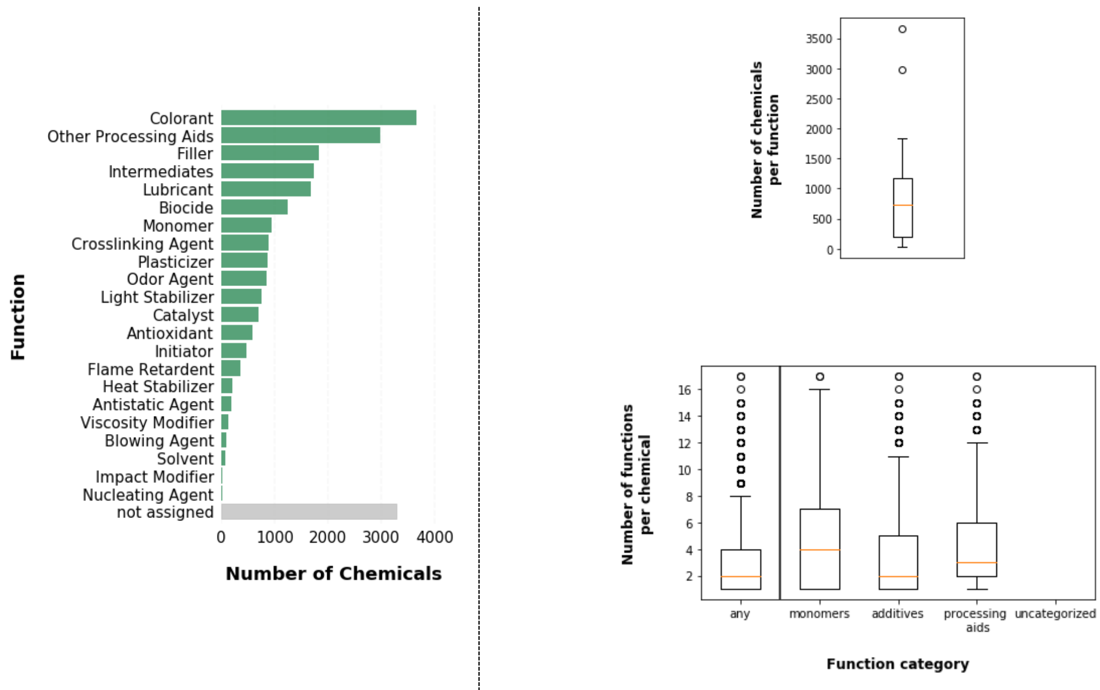

Figure S11: Functions of the substances identified. Left: Number of chemicals fulfilling individual functions. Right–Top: Number of chemicals per function as a boxplot. Right–Bottom: Number of functions per chemical as a boxplot for different function categories.

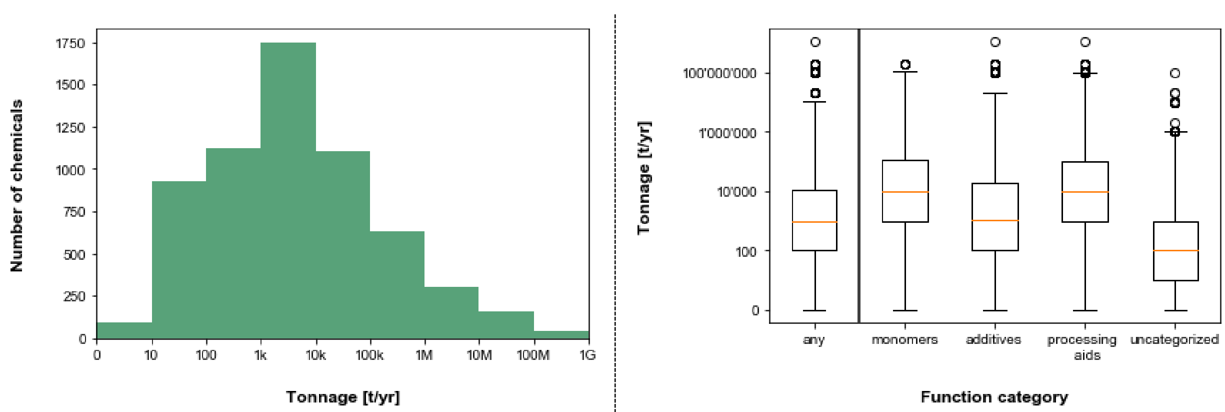

Figure S12: Reported production volumes of the substances identified in the US and EU(or SPIN) combined. Left: Distribution of tonnage data as a histogram. Right: Distribution as a boxplot for different function categories.

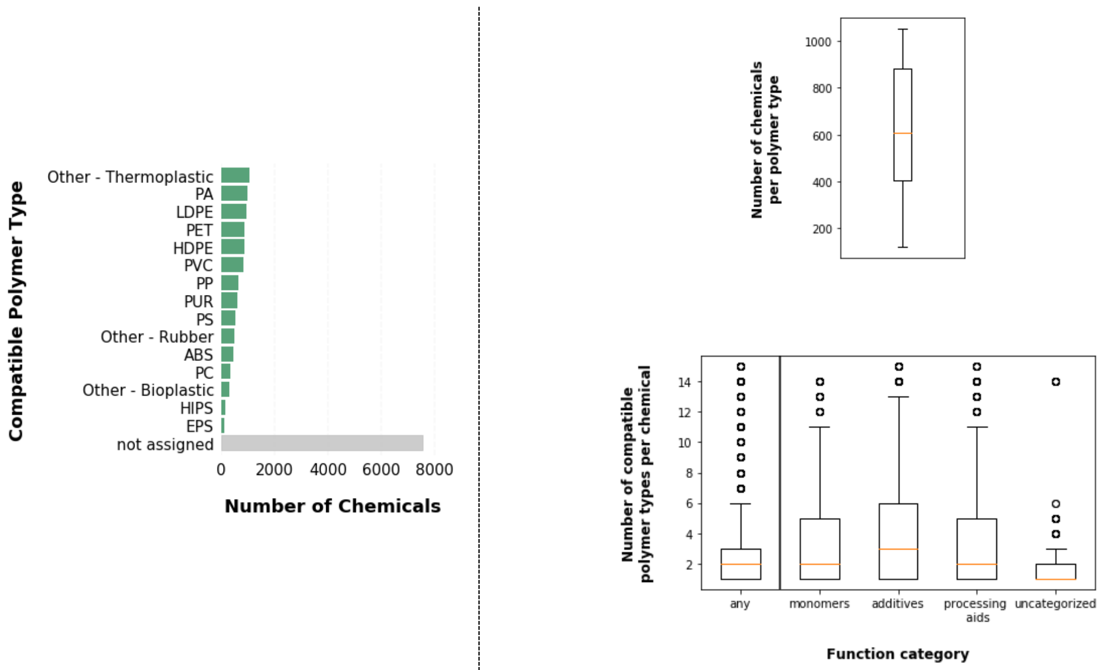

Figure S13: Polymer type compatibility of the substances identified. Left: Number of chemicals compatible with individual polymer types. Right–Top: Number of compatible chemicals per polymer type as a boxplot. Right–Bottom: Number of compatible polymer types per chemical as a boxplot for different function categories. PA = Polyamides, LDPE = Low-density polyethylene, PET = Poly(ethylene terephthalate), HDPE = High-density polyethylene, PVC = Polyvinylchloride, PP = Polypropylene, PUR = Polyurethanes, PS = Polystyrene, ABS = Acrylonitrile butadiene styrene, PC = Polycarbonates, HIPS = High-impact polystyrene, EPS = Expanded polystyrene

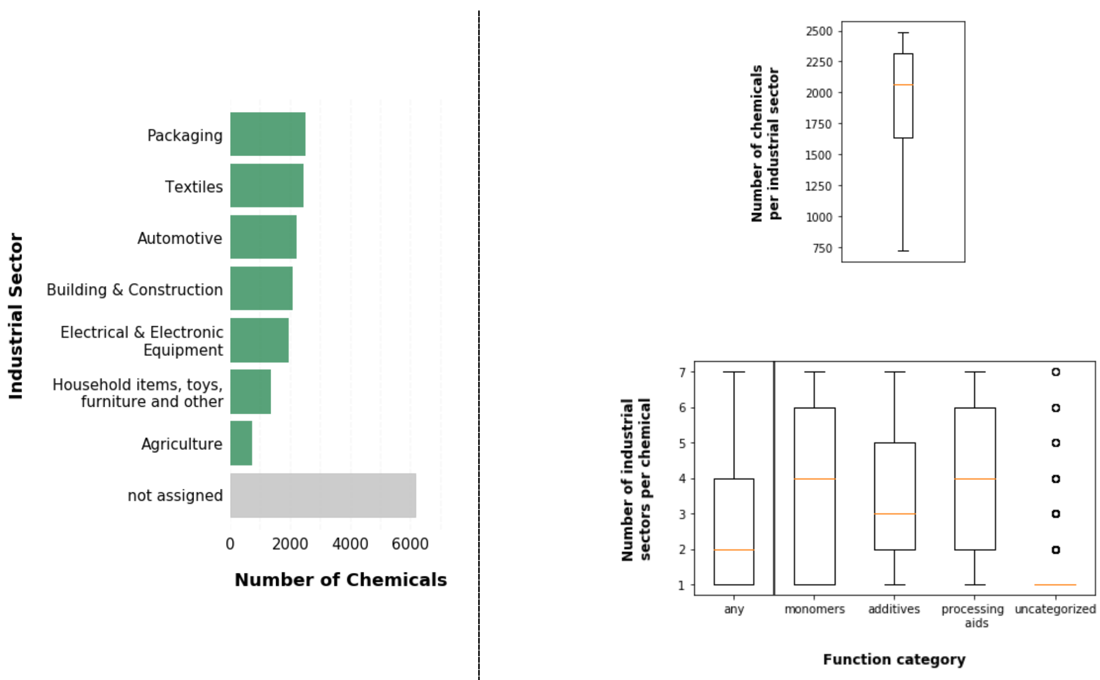

Figure S14: Industrial sectors of use of the substances identified. Left: Number of chemicals used in each industrial sector. Right–Top: Number of chemicals per industrial sector as a boxplot. Right–Bottom: Number of industrial sectors per chemical as a boxplot for different function categories.

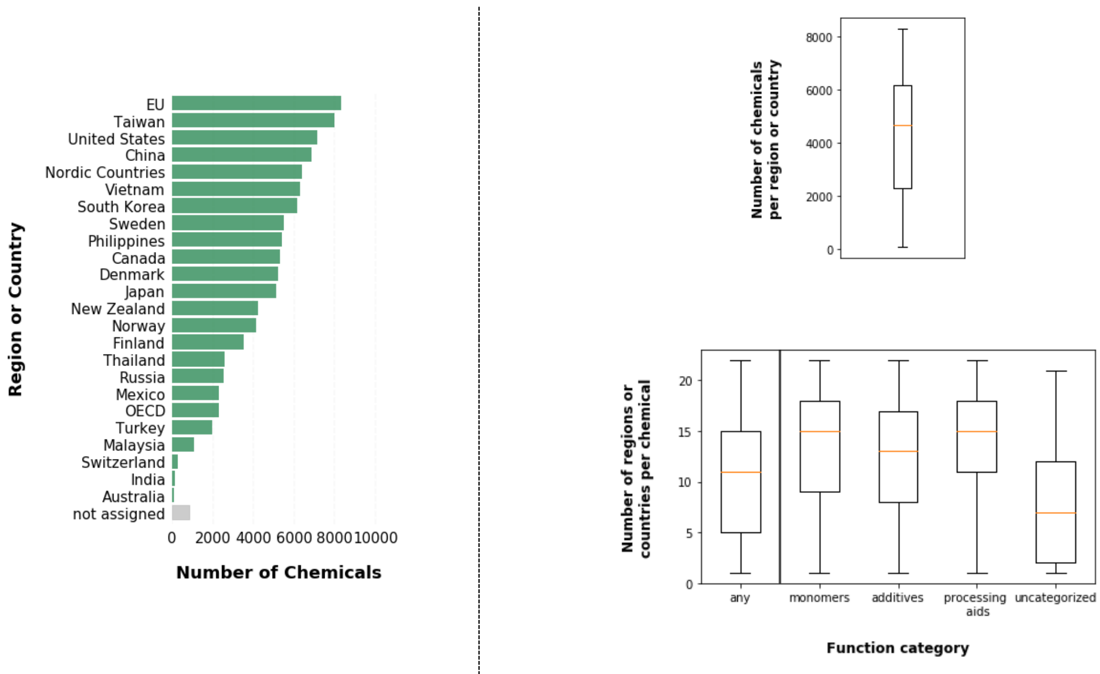

Figure S15: Regions or countries of use of the substances identified. The Nordic countries (Denmark, Finland, Norway, Sweden) are also participating within the EU; however, they report substances used within their jurisdictions directly. The "OECD" row comprises only the substances produced in high volumes (>1000 t/yr) by the OECD member states. Left: Number of chemicals per region or country. Right–Top: Number of chemicals per region or country as a boxplot. Right–Bottom: Number of regions or countries per chemical as a boxplot for different function categories.

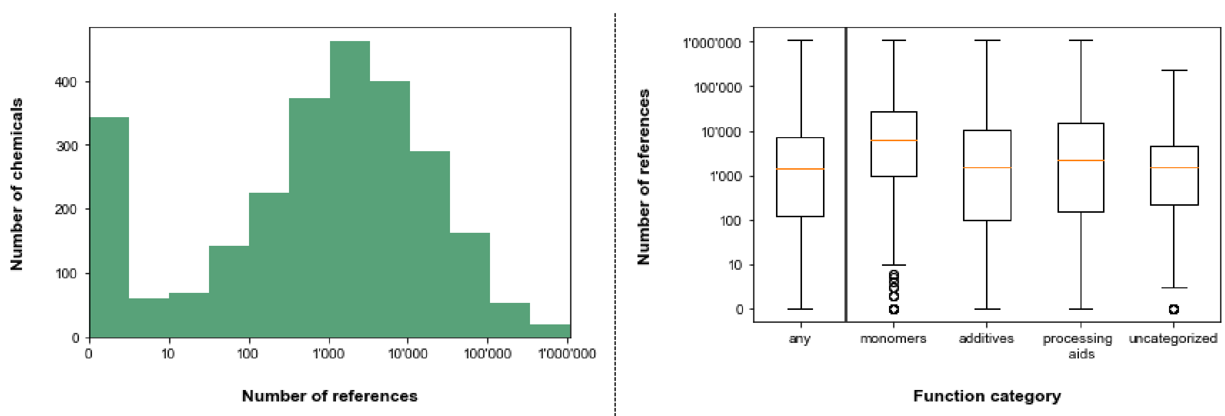

Figure S16: Numbers of scientific references relating to the substances reported in SciFinder. Left: Distribution of the number of references as a histogram. Right: Distribution as a boxplot for different function categories.

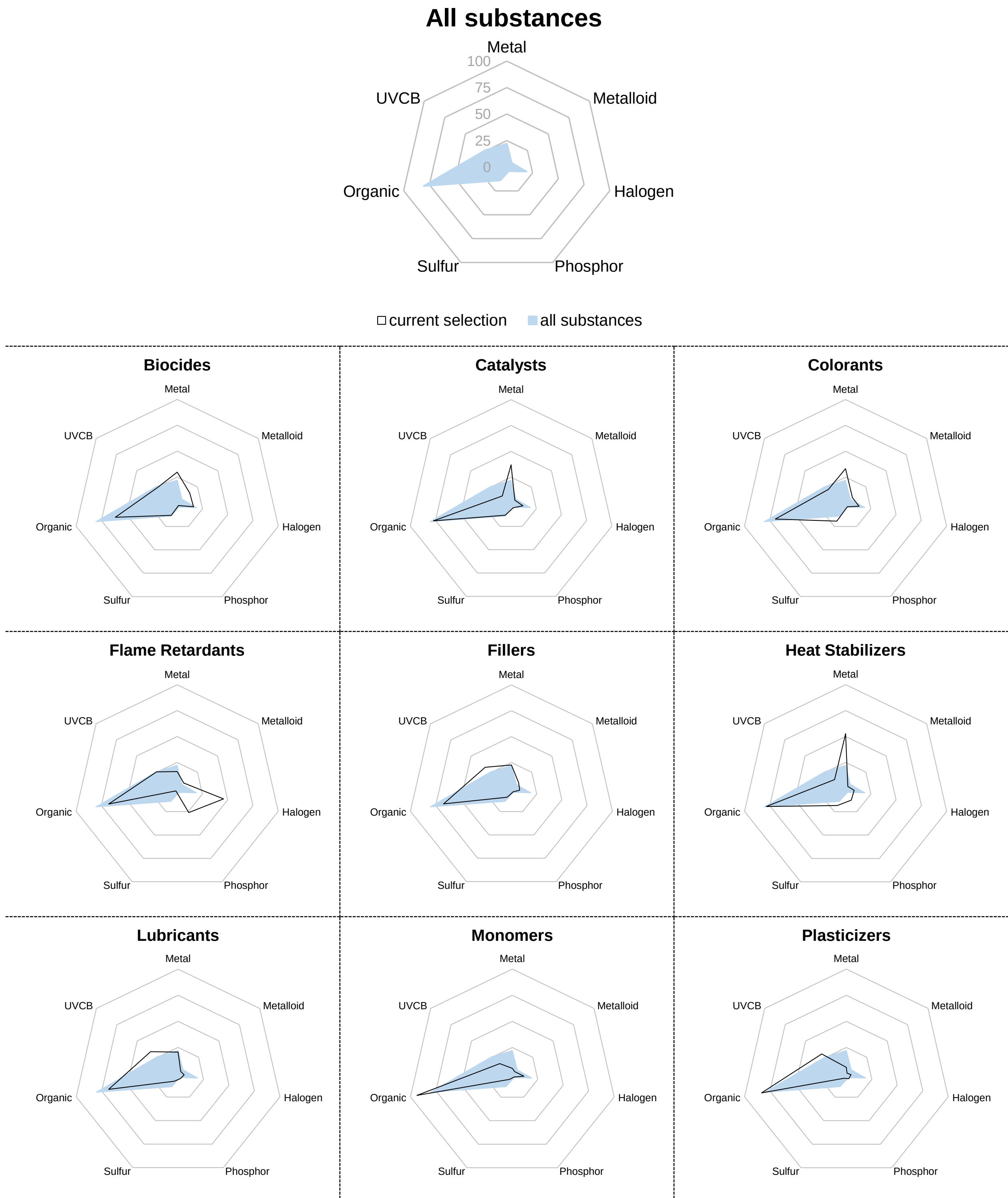

Figure S17: Substance type profiles as radar charts for selected functions. Each axis shows the percentage of the substances containing the respective elements or belonging to the respective group. UVCB = Substances of unknown or variable composition, complex reaction products, or biological materials (for this graphic, UVCBs also contain simple mixtures and polymers)

S2.2.1 Use patterns

Polymer compatibility and industrial sector of use can be dependent on the function a substance fulfills in the plastic. However, due to large data gaps and many uncategorizable substances (functions: 31%, compatible polymer types: 72%, industrial sectors of use: 58%), only a few patterns are observed and need to be interpreted with caution. Plasticizers are more frequently assigned to PVC than to other polymer types. Blowing agents are reported more often in polyurethane (PUR) than in other polymer types.

Substance type profiles vary considerably across individual functions (Figure S17). Notably, catalysts more frequently contain metals than other functions. A large number of flame-retardants contain halogens or phosphorous. All of these patterns were expected based on existing literature, e.g. the common use of metal catalysts, or brominated or phosphor flame-retardants. Substances without information on their functions typically also lack information on their compatible polymer types or industrial sectors of use.

S2.2.2 Single-use vs. durable applications

From 4382 CASRNs that were categorized according to industrial use, 843 CASRNs were only assigned to single-use applications, 1893 to only durable applications, and 1646 CASRNs may be used in both. Some interesting differences between single-use and durable applications can be observed, but due to the data gaps and potential bias from source selection (many focused on packaging) these need to be interpreted with caution: (1) Halogens are more common in durable applications, (2) colorants and biocides are more often used in durable applications, (3) tonnages and regional registrations are less well known for durable applications, and (4) proportionally more substances of concern are used in durable applications (Figure S18).

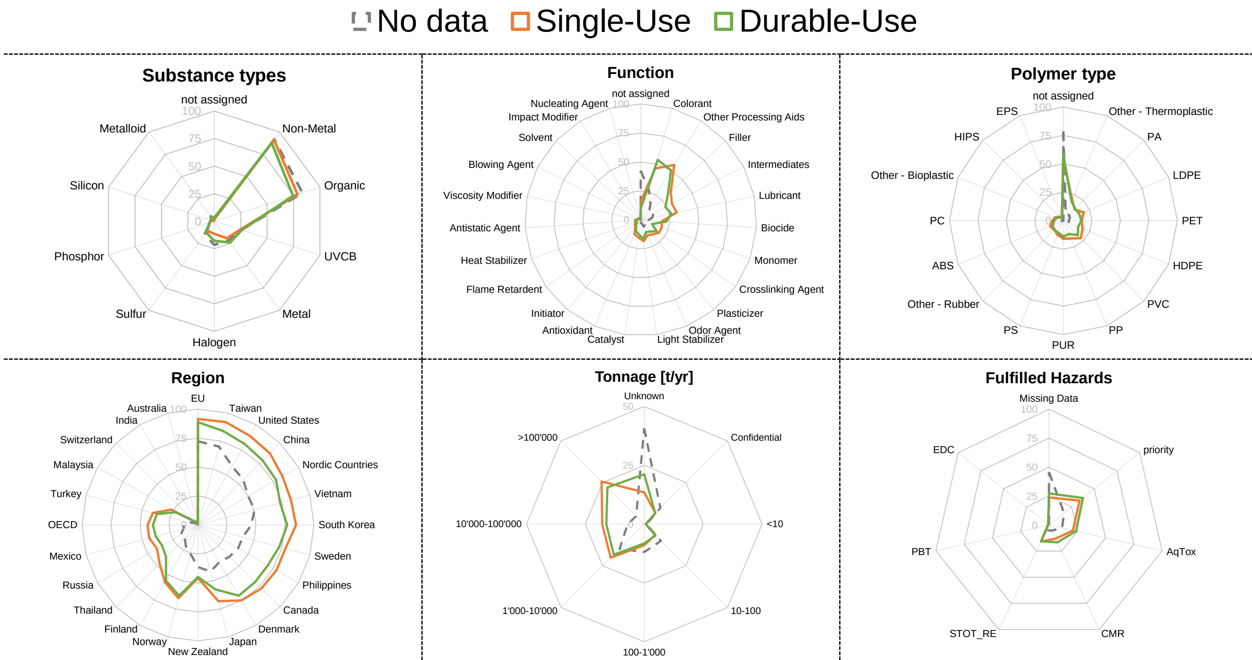

Figure S18: Comparisons of single-use and durable applications regarding their substance type, use and hazard profiles of relevant plastic monomers, additives and processing aids. Each axis shows the percentage of substances belonging to the respective group. UVCB = Substances of unknown or variable composition, complex reaction products or biological materials (for this graphic UVCBs also contain regular mixtures and polymers), PA = Polyamides, LDPE = Low-density polyethylene, PET = Polyethylene terephthalate, HDPE = High-density polyethylene, PVC = Polyvinylchloride, PP = Polypropylene, PUR = Polyurethanes, PS = Polystyrene, ABS = Acrylonitrile butadiene styrene, PC = Polycarbonates, HIPS = High-impact polystyrene, EPS = Expanded polystyrene, OECD = Organisation for Economic Cooperation and Development, AqTox = chronic aquatic toxicity, CMR = carcinogenicity, mutagenicity or reproductive toxicity, STOT_RE = specific organ toxicity upon repeated exposure, PBT = persistence, bioaccumulation and toxicity, EDC = endocrine-disrupting chemicals.

S2.3 Substances of potential concern and regulated substances

More than half of the substances of potential concern were identified using regulator-harmonized hazard classifications (51% for any considered hazard, 63% for CMR substances, 33% for substances causing chronic aquatic toxicity, 69% for substances causing specific target organ toxicity upon repeated exposure), while the rest were identified using company-reported hazard classifications.

When comparing all plastic monomers, additives and processing aids to subgroups of substances of potential concern (Figure S22, Figure S21), the following observations can be made:

- 15% of UVCBs, polymers and mixtures were identified as substances of potential concern, which is lower than the average when all substances are considered (24%). This is most likely due to the substantial data gaps of hazardous properties for UVCBs, polymers and mixtures.
- In general, use patterns of the substances of potential concern are better characterized than those of the other plastic monomers, additives and processing aids.
- Generally, substances of potential concern are more frequently registered in each region except New Zealand than the rest substances. A possible explanation might be that New Zealand's chemical inventory focuses on hazardous substances, with limited substances with low level of concern registered there.

When comparing among substances of potential concern, it is noted that a larger fraction of the substances identified using regulator-harmonized hazard data are HPVCs, or regulated, than the substances identified using all available hazard data (Table S6). This observation is likely based on the fact that HPVCs are often subject to greater regulatory scrutiny (e.g. under REACH, HPVCs had to be registered earlier than other substances with more comprehensive data requirements), which leads to greater availability of regulator-harmonized hazard data and to the subsequent addition to regulatory lists.

Table S6: Substances of potential concern used as plastic monomers, additives or processing aids identified using different investigated hazard data sources. Company-reported classifications were taken from the EU REACH and CLP registration dossiers (id=297) and the OECD eChemPortal (id=320), while regulator-harmonized hazard classifications were retrieved from all other hazard data relevant sources (Sheet S2 in Supporting Information S1). Company-reported hazard data excludes PBT and EDC classification as these are not reported by these sources or are not extractable.

	Hazard Type[a]	Total	HPVC[b]		Not regulated[c]		Without scientific references[d]	
		#	#	%	#	%	#	%
All Hazard Data	PBT	57	26	45.6	10	17.5	10	17.5
	CMR	951	501	52.7	350	36.8	91	9.6
	EDC	30	17	56.7	3	10.0	3	10.0
	AqTox	1646	754	45.8	897	54.5	188	11.4
	STOT_RE	891	562	63.1	331	37.1	57	6.4
	Total	2486	1254	50.4	1327	53.4	266	10.7
Regulator-harmonized Hazard Data	PBT	57	26	45.6	10	17.5	10	17.5
	CMR	603	311	51.6	143	23.7	68	11.3
	EDC	30	17	56.7	3	10.0	3	10.0
	AqTox	554	318	57.4	216	39.0	18	3.2
	STOT_RE	617	387	62.7	175	28.4	23	3.7
	Total	1260	739	58.7	461	36.6	90	7.1
Company-Reported Hazard Data	PBT	-	-	-	-	-	-	-
	CMR	856	480	56.1	321	37.5	82	9.6
	EDC	-	-	-	-	-	-	-
	AqTox	1640	751	45.8	893	54.5	187	11.4
	STOT_RE	783	509	65.0	298	38.1	46	5.9
	Total	2360	1218	51.6	1281	54.3	256	10.8

[a] PBT = persistence, bioaccumulation and toxicity, CMR = carcinogenicity, mutagenicity or reproductive toxicity, EDC = endocrine-disrupting chemicals, AqTox = chronic aquatic toxicity, STOT_RE = specific organ toxicity upon repeated exposure
[b] production volumes with more than 1000 t/yr
[c] regulated by any of the regulations considered in this study
[d] any scientific references according to SciFinder
[e] specific organ toxicity after repeated exposure or chronic aquatic toxicity

Highest score in column & hazard data group
Above-average of column & hazard data group

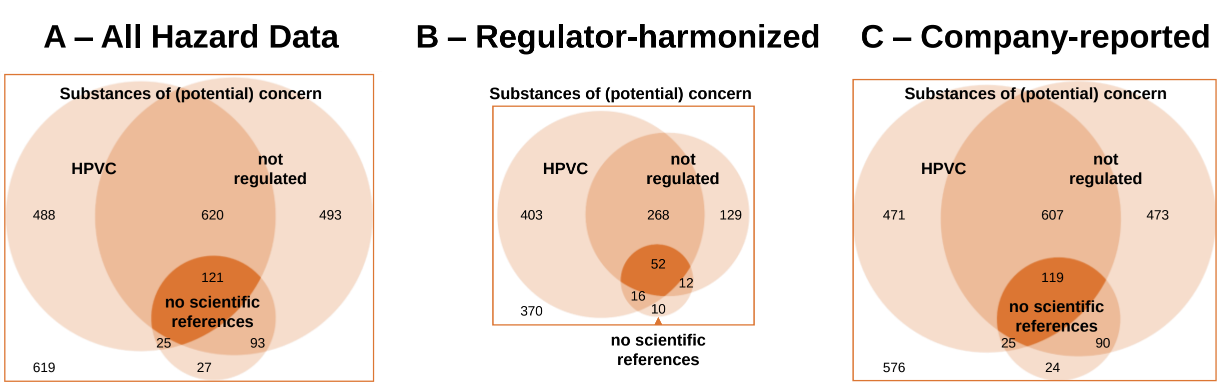

Figure S19: Overview of substances of potential concern for different hazard data sources investigated as a Venn diagram.

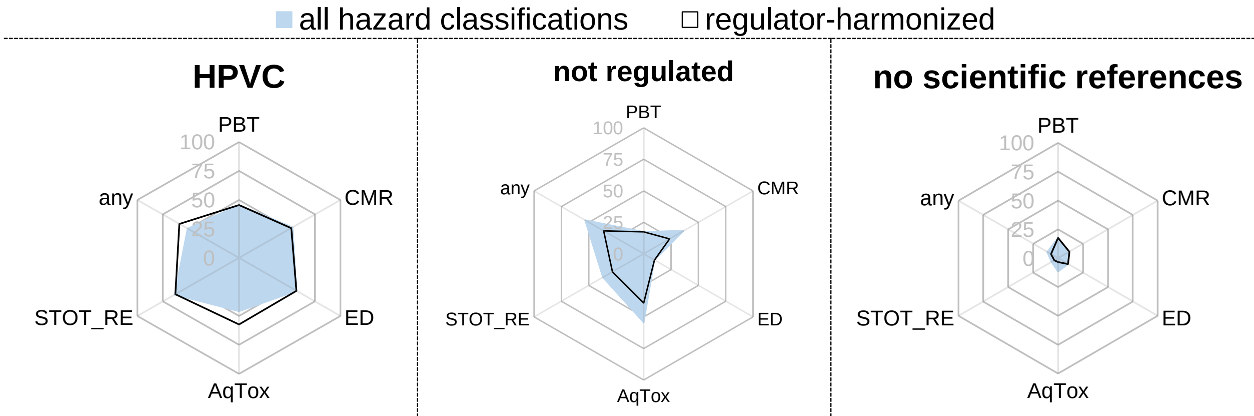

Figure S20: Overview of fractions of the substances of potential concern that are HPVC (right), regulated (middle) or researched according to SciFinder (left) in relation to hazards. PBT = persistence, bioaccumulation and toxicity, CMR = carcinogenicity, mutagenicity or reproductive toxicity, ED = endocrine-disrupting chemicals, AqTox = chronic aquatic toxicity, STOT_RE = specific organ toxicity upon repeated exposure

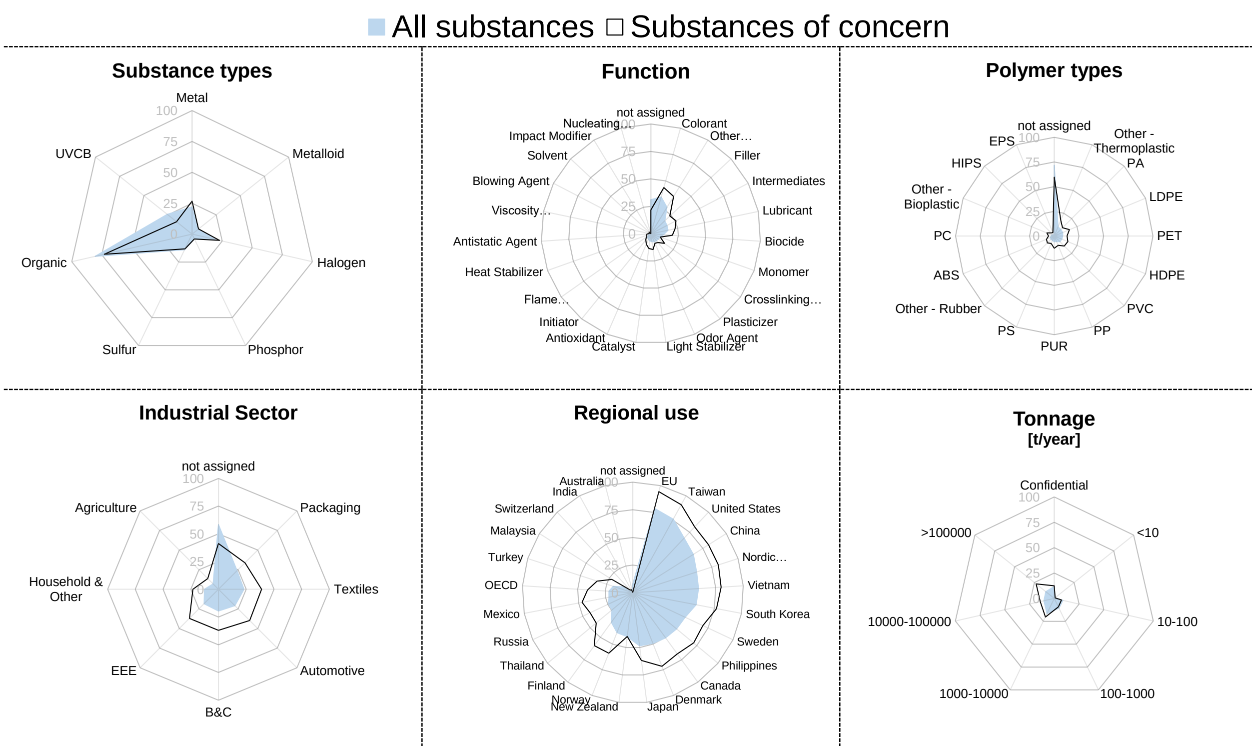

Figure S21: The use and substance type profiles of all plastic monomers, additives and processing aids identified in comparison to the identified substances of potential concern as radar charts. Each axis shows the percentage of the substances belonging to the respective group. UVCB = Substances of unknown or variable composition, complex reaction products or biological materials (for this graphic UVCBs also contain regular mixtures and polymers), PA = Polyamides, LDPE = Low-density polyethylene, PET = Polyethylene terephthalate, HDPE = High-density polyethylene, PVC = Polyvinylchloride, PP = Polypropylene, PUR = Polyurethanes, PS = Polystyrene, ABS = Acrylonitrile butadiene styrene, PC = Polycarbonates, HIPS = High-impact polystyrene, EPS = Expanded polystyrene, B&C = Building and construction, EEE = Electrical and electronic equipment,OECD = Organisation for Economic Cooperation and Development

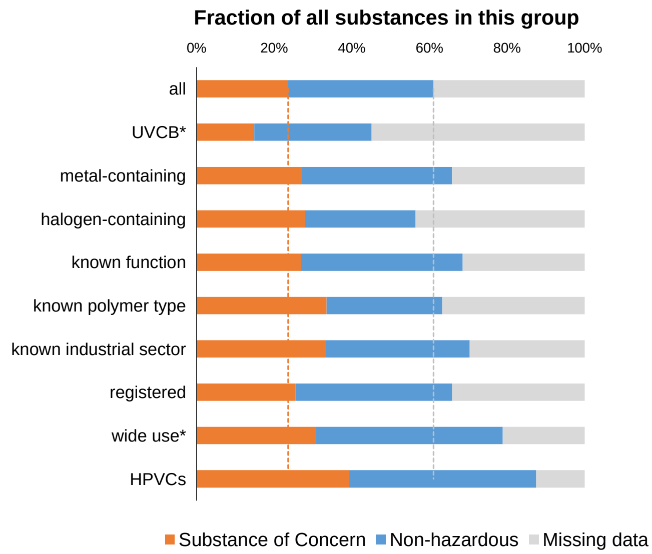

Figure S22: Comparison of numbers of substances of potential concern and substances with available hazard data for different substance groups. *UVCB = Substances of unknown or variable composition, complex reaction products or biological materials (UVCBs), simple mixtures and polymers; *wide use = use in more than 5 investigated regions

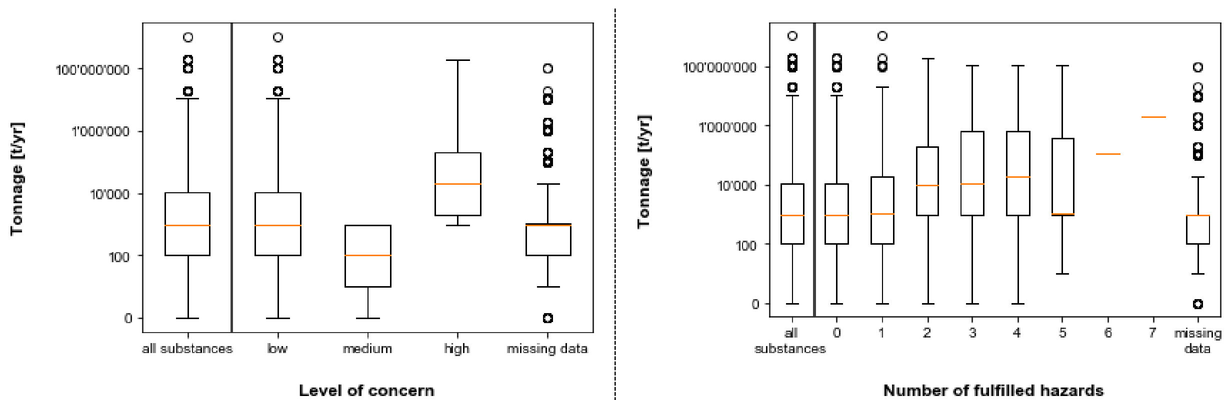

Figure S23: Tonnage comparison of plastic monomers, additives and processing aids depending on levels of concern (left) and numbers of hazards fulfilled (right).

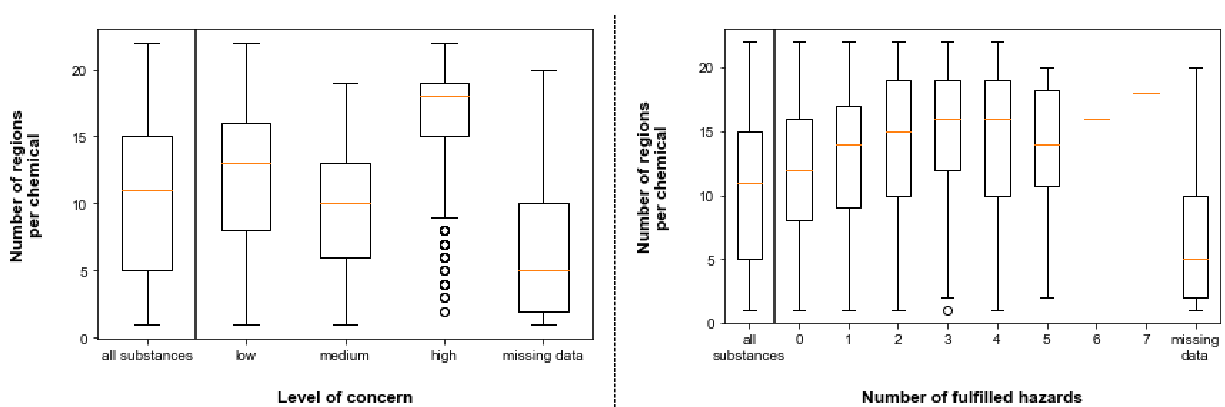

Figure S24: Regional use comparison of all plastic monomers, additives and processing depending on levels of concern (left) and numbers of hazards fulfilled (right).

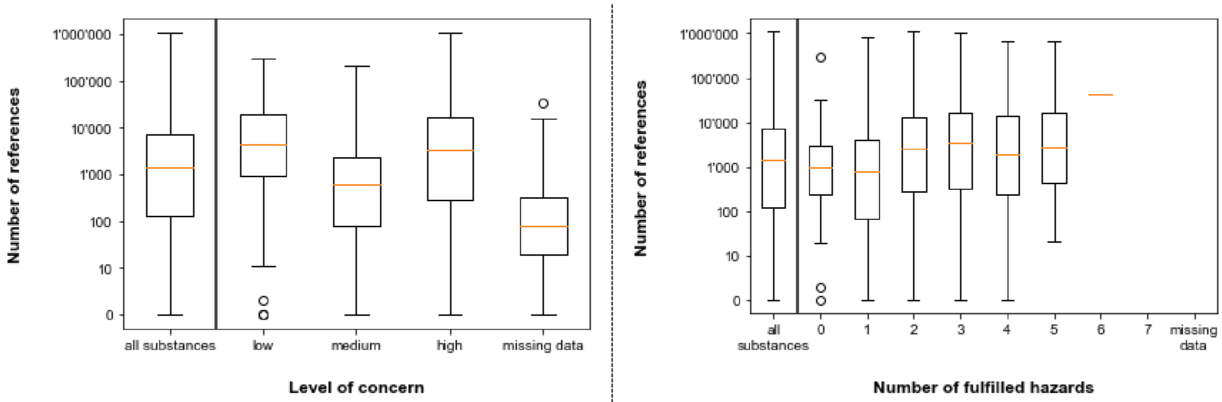

Figure S25: Scientific references comparison of all plastic monomers, additives and processing depending on level of concern (left) and numbers of hazards fulfilled (right).

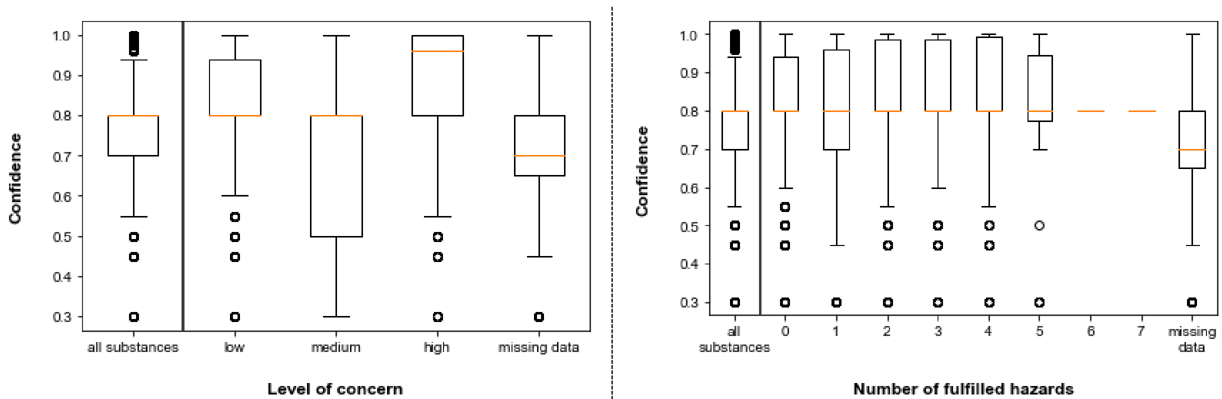

Figure S26: Confidence score comparison for the identification of plastic monomers, additives and processing depending on levels of concern (left) and numbers of hazards fulfilled (right).

S3 COMPARISON OF CHEMICAL USAGE IN OTHER MATERIALS

The potential health and environmental impacts of plastic monomers, additives and processing aids are difficult to compare to those of chemicals used in other materials, due to several factors such as unclarity in chemical demand, their hazards, releases and exposure. Similarly to plastics (i.e. more than 10000 substances may be employed; about 3% of all substances on the global market), production of other materials may also employ a large diversity of substances (paper: 17000; textiles: 3500; wood products: 1000; food additives: 3000 substances).[13–18]

Globally, production of thermoplastics requires 222 million t/yr monomers and 18 million t/yr plastic additives [plasticizers: 7.5 million t/yr, other plastic additives (excluding processing aids): 10 million t/yr], i.e. 27 % (monomers) and 2.2 % (plastic additives) of the global demand of chemicals (820 million t/yr).[19–21] Global chemicals demand for other materials may fall in similar ranges as plastic additives (paper: 51 million t/yr; textiles: 29 million t/yr, food additives: 27 million t/yr).[14–17]

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