

# PlastChem Database User Guide

## (v1.1)

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**Reference to the database:** Martin Wagner, Laura Monclús, Hans Peter H. Arp, Ksenia J. Groh, Mari E. Løseth, Jane Muncke, Zhanyun Wang, Raoul Wolf, Lisa Zimmermann (2024) State of the science on plastic chemicals – PlastChem database (**version 1.1**)

**Repository of the database and updates:** <https://zenodo.org/communities/plastchem/>

**Details on the methods** used to set the database can be found in the PlastChem Report: <http://dx.doi.org/10.5281/zenodo.10701706>

## Content of the PlastChem database

The PlastChem database provides all information associated with the report. The database is organized in eleven spreadsheets within an Excel file (Table 1).

**Table 1.** Overview of the spreadsheets of the PlastChem database and their content.

| Worksheet                     | Content                                                                                                                                                                                                    |
|-------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| List of abbreviations         | Contains the description of all the abbreviations used in the PlastChem database.                                                                                                                          |
| Explanation sections database | Contains a description of all the items included in the database, including the list of sources and an explanation of the scoring system.                                                                  |
| Overview database             | Contains a short version of the PlastChem database summarizing the most essential information for a quick overview.                                                                                        |
| Full database                 | Contains the full list of chemicals in the PlastChem database and the associated information.                                                                                                              |
| MEA List                      | Contains the list of chemicals that are currently regulated under selected Multilateral Environmental Agreements (MEA), that is, the Basel, Stockholm and Minamata Conventions, and the Montreal Protocol. |
| Red List                      | Contains the list of chemicals of concern (Red List), as classified according to the PlastChem scoring system (Hazard Score of 1 or 2).                                                                    |
| Orange List                   | Contains the list of less hazardous chemicals (Orange List), as classified according to the PlastChem scoring system (Hazard Score of 0.5).                                                                |
| Watch List                    | Contains the list of chemicals for which a hazard assessment is considered or ongoing (Watch List) by the regulatory sources (Hazard Score of 0.25).                                                       |
| White List                    | Contains the list of non-hazardous chemicals (White List), as classified according to the PlastChem scoring system (Hazard Score of 0).                                                                    |
| Grey List                     | Contains the list of chemicals without hazard information (Grey List), as classified according to the PlastChem scoring system.                                                                            |
| Duplicates                    | Contains the duplicated chemicals not included in the database.                                                                                                                                            |

The full database and the following spreadsheets are organized into 10 sections, each highlighted in a different colour to enhance clarity and ease of navigation (Table 2).

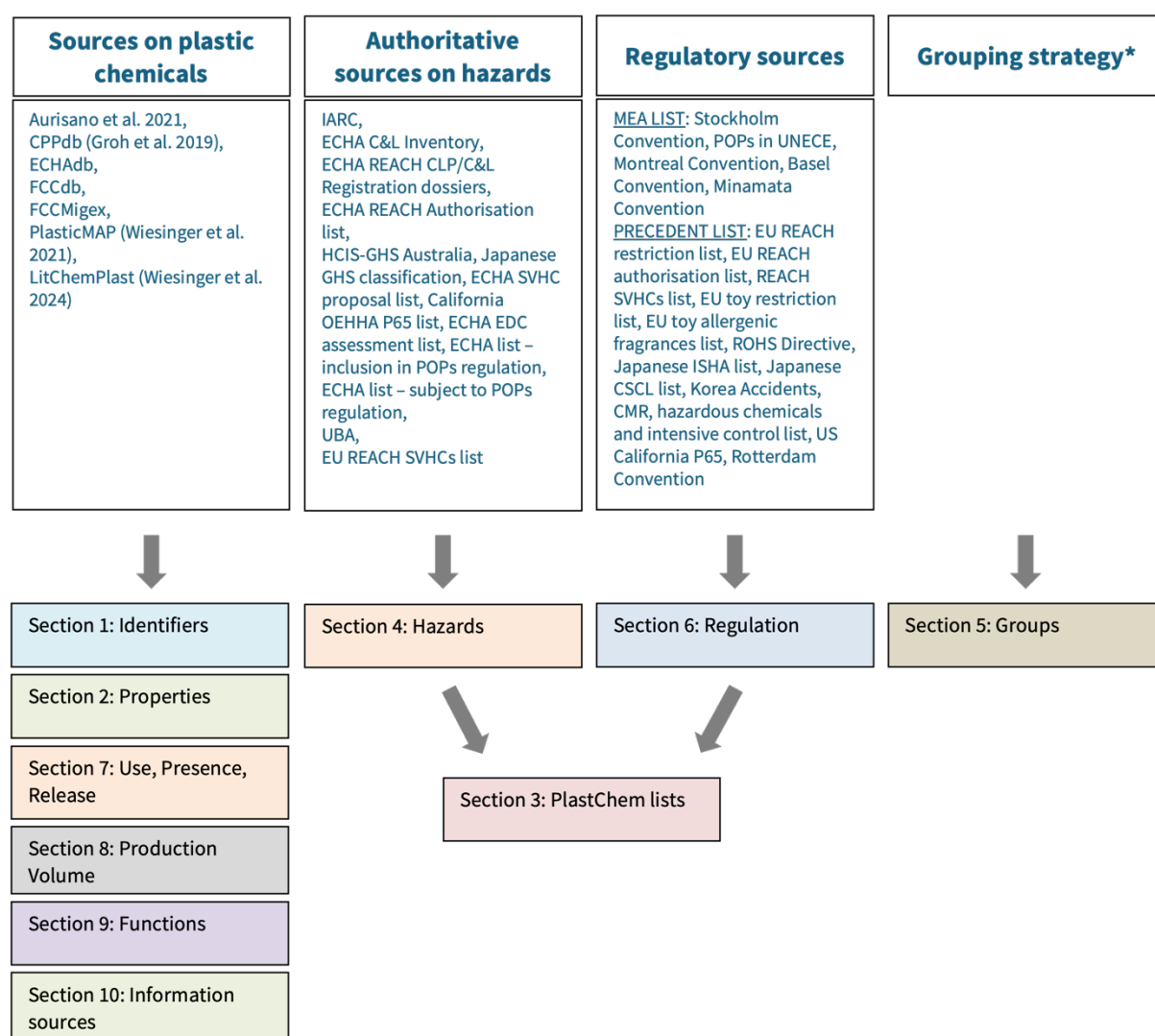
**Table 2. Overview of the sections of the PlastChem database and its content.**

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>1 – IDENTIFIERS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Unique identifiers for each chemical, including a PlastChem identification number, CAS Registry Numbers (CASRN), legacy CASRNs, the chemical's name according to <a href="#">PubChem</a> and the <a href="#">International Union of Pure and Applied Chemistry</a> (IUPAC).                                                                                                                                                                                                                                                                                                                                                                                                            |
| <b>2 – PROPERTIES</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Chemical properties, including molecular formula, molecular weight, canonical and isomeric SMILES ( <a href="#">Simplified Molecular Input Line Entry System</a> ), Inchi Key ( <a href="#">International Chemical Identifier</a> ), predicted octanol-water partition coefficient, exact mass, topological polar surface area, complexity and formal charge of a chemical.                                                                                                                                                                                                                                                                                                            |
| <b>3 – PLASTCHEM LISTS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Lists of chemicals provided in the PlastChem Report that classify chemicals based on their hazard properties and regulatory status. <ul style="list-style-type: none"> <li>• Red List: Chemicals of concern</li> <li>• Orange List: Less hazardous chemicals</li> <li>• Watch List: Chemicals that are currently under evaluation or pending classification</li> <li>• White List: Chemicals evaluated and concluded not hazardous</li> <li>• Grey List: Chemicals lacking hazard information</li> <li>• MEA List: Chemicals globally regulated under Multilateral Environmental Agreements</li> <li>• Precedent List: Chemicals regulated in specific regions or countries</li> </ul> |
| <b>4 – HAZARD INFORMATION</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| Hazard information for each chemical summarized with an overall <b>Hazard Score</b> , offering a quick and comprehensive overview of its hazard status. The score indicates whether the chemical is of concern, less concern, under evaluation, non-hazardous, or lacks hazard data. Additionally, detailed scores for hazard classes and traits are provided for deeper insight.                                                                                                                                                                                                                                                                                                      |
| <b>5 – GROUPS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Group(s) in which a chemical is classified in according to its structure. Additional information on priority groups and ECHA grouping is provided.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <b>6 – REGULATION</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Regulatory status for each chemical summarized. The <b>MEA_List</b> column outlines the chemical's regulation under existing Multilateral Environmental Agreements and the <b>Precedent_List</b> column indicates whether the chemical is regulated at a regional or national level. Additional details on specific regulations are provided.                                                                                                                                                                                                                                                                                                                                          |
| <b>7 – USE, PRESENCE, RELEASE</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Evidence of commercial use, presence, and release of a chemical from plastics is consolidated into an overall <b>UPR_Summary</b> , offering a quick overview of the available data. For more detailed insights, separate summaries are provided for each component: <b>Use</b> , <b>Presence</b> and <b>Release</b> . Additional details on the polymer type in which a chemical is used, detected to be present or to be released from are provided in the additional columns.                                                                                                                                                                                                        |
| <b>8 – PRODUCTION VOLUME</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| Production volume information for a chemical.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| <b>9 – FUNCTIONS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Harmonized function(s) of a chemical and additional information from the original sources.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| <b>10 – INFORMATION SOURCES</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| Information sources used to ensemble the PlastChem database and the original names of the chemicals as used in these sources.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

## Establishing the database

The PlastChem database was established by compiling and harmonizing information from seven previous databases, retrieving additional and updated information on the hazard classification and regulatory status, and by grouping chemicals based on their structure (Figure 1). The hazard information was compiled and harmonized from 15 authoritative sources (Section 4) and was used together with the regulatory status (Section 6) to classify the chemicals in various PlastChem Lists (Section 3).

Detailed information on the methods can be found in the PlastChem Report (<http://dx.doi.org/10.5281/zenodo.10701706>).



**Figure 1. Workflow for setting up the PlastChem database.** \*Grouping strategy is described in detail in the Annex A6 from the PlastChem report.

# PlastChem Scoring Systems

The PlastChem database incorporates three distinct scoring systems.

## 1. Binary scores in sections 2, 3, 5, 6, 9, and 10.

This system assigns a value of 1 to indicate the availability of information for a chemical in the specific column, while leaving the field blank when no information is available.

## 2. Hazard Scoring System in section 4.

This system assigns values ranging from 0 to 2 to represent the level of hazardousness:

- **0:** The chemical is considered non-hazardous.
- **0.25:** The hazardousness of the chemical is under review or evaluation.
- **0.5:** The chemical is classified less hazardous.
- **1:** The chemical is classified hazardous → chemical of concern
- **2:** The chemical is classified as very hazardous → chemical of concern
- **Blank:** No hazard information available.

Section 4 contains two additional scoring systems.

- **Hazard Score Sum** represents the sum of the four hazard criteria applied in framework, which include: Persistence\_Score, Bioaccumulation\_Score, Mobility\_score, and Toxicity\_Score. It ranges from 0 to 8.
- **Evidence Score:** It is the number of sources consulted that classify a chemical as hazardous across all the evaluated hazard traits. It ranges from 0 to 31.

## 3. Use, Presence, Release Scoring System in section 7

This system assigns values ranging from 0 to 2 to represent the level of evidence for a chemical being used or present in plastics, or being released from plastics.

- **0:** Analyzed in a scientific study and not detected in plastics.
- **0.25:** Analyzed in a scientific study with inconclusive results.
- **0.5:** Listed as commercially used in plastic.
- **1:** Analyzed and detected as present in plastics through extraction experiments.
- **2:** Analyzed and detected as being released from plastics via migration experiments.
- **Blank:** No information available.

# How to retrieve information and practical examples of how to use the database

## How to use the database

To obtain information from the database, users can start by reviewing the *Overview database*, which provides a comprehensive general overview of the available data. For more complete information, users are suggested to review the *Full Database*, where all the information from PlastChem is available. If you require specific details, you can navigate directly to relevant spreadsheets, such as the *MEA List*, *Red List*, *Orange List*, *Watch List*, *White List*, or *Grey List*.

To extract the information of interest, use the filter feature in Microsoft Excel located in the top rows of the spreadsheet. Navigate to the column that contains the information you want to filter for, click on the grey arrow  to open the filter function for that column. Check or uncheck the score you want to filter for to receive a list of chemicals with the selected score. Note that you can combine filters from multiple columns to refine your selection of chemicals. Please also note that you need to remove filters if you want to start a new query.

If you need assistance with using the filter tool, you can visit the Microsoft Support page following the link: [Filter data in a range or table - Microsoft Support](#). This method allows you to efficiently find and analyse the data you need.

## Use Case 1: How many chemicals of concern are used or detected in plastic? And how many of these are released from PE?

Step 1 – Select chemicals of concern.

- Navigate to **Section 4: Hazard Information**.
  - Uncheck “Select all” and filter for chemicals with a **Hazard Score** of 1 and 2 in column AE.
- This will provide you with the full list of chemicals of concern

Step 2 – Select the chemicals of concern known to be used or detected in plastic.

- Proceed to **Section 7: Use, Presence, Release (UPR)**.
- Filter for chemicals with a **UPR\_summary** score of 1 (column FA), which reflects the chemicals that are known to be used or have been detected in plastic.
- To determine how many of these chemicals have specific data on their use in plastics, further filter for **Use** score 1 (column FB).
- For specific data on their presence, filter for **Presence** score 1 (column FC).
- For specific data on their release, filter for **Release** score 1 (column FD).
- Note that you need to clear the filter for your previous selection if you do not want to combine filters (e.g., chemicals with use and release data).

Step 3 – Identify how many of these chemicals are released from PE.

- Remove the filters for **UPR\_summary**, **Use**, **Presence**, **Release** → this will return you to the list of all chemicals of concern
- Continue in Section 7: Use, Presence, Release (UPR) to identify how many chemicals are released specifically from PE.

- Filter for a **PE\_combined** score of 2 (release) in column FF.
- This will provide a list of chemicals of concern that have been shown to be released from PE

## Use Case 2: How many chemicals are CMRs and are regulated under MEA?

Step 1 – Select CMR chemicals.

- Navigate to **Section 4: Hazard Information**.
- Filter for chemicals with **CMR** score of 1 and 2 in column AO, which identify the chemicals that are carcinogenic, mutagenic and/or toxic for reproduction.
- To further determine how many of these chemicals have specific data on carcinogenesis, filter for **Carcinogenic** score 1 and 2 (column AL).
- For specific data on Mutagenesis, filter for **Mutagenic** score 1 and 2 (column AM).
- For specific data on Reproduction, filter for **Reproduction** score 1 and 2 (column AN).
- Note that you need to clear the filter for your previous selection if you do not want to combine filters (e.g., chemicals that are carcinogenic and reprotoxic).

Step 2 – Select the CMR chemicals that are regulated under MEAs.

- Remove all filters except the one applied to the column CRM (column AO).
- Proceed to **Section 6: Regulation**.
- Filter for chemicals with **MEA\_list** score of 1 (column V), which identify the chemicals that are regulated under an MEA.

→ This will provide a list of CMR chemicals regulated globally

## Use Case 3: How many chemicals in the Red List have information for their functions?

Step 1 – Select the chemicals listed in the Red List.

- Navigate to **Section 3: PlastChem lists**.
- Filter for **PlastChem\_lists** Red\_list in column U. An alternative approach is to use the spreadsheet “Red List” which contains the pre-filtered list of chemicals of concern.

Step 2 – Select the chemicals listed in the Red List that have information in their functions.

- Proceed to **Section 9: Functions**.
- Filter for **Functions\_information** score 1 in column HB, which reflects which chemicals have information on their functions.

→ This will provide you with a list of Red List chemicals (chemicals of concern that are not regulated globally) that have information on their functions.

Step 3 – Pinpoint specific functions.

- To further identify which function(s) the chemical performs, proceed to the following columns in the section (columns HD and following) and filter score 1 in the function of interest.

### Use Case 4: Which priority groups have more than 50% of their members classified as chemicals of concern?

Step 1 – Select the priority groups of chemicals of concern.

- Navigate to **Section 5: Groups**.
- Filter for **priority\_groups** score 1 in column AZ.

Step 2 – Pinpoint a specific priority group of concern.

- Proceed to select the priority group of concern of interest in the following columns with score of 1. For instance, filter aromatic\_amines (column BA) for score 1 to select all aromatic amines.

→ This will provide the number of chemicals in the selected priority group.

Step 3 – Identify the % of chemicals that are of concern in the selected priority group of concern.

- Proceed to **Section 4: Hazard**.
- Filter for chemicals with **Hazard\_score** of 1 and 2 in column AE.

→ This will provide the number of chemicals of concern in the selected priority group.

### Use Case 5: How many chemicals with aquatic toxicity are regulated at a regional or national level?

Step 1 – Select the chemicals that are toxic for the aquatic environment.

- Navigate to **Section 4: Hazards**.
- Filter for chemicals with **Aquatic\_toxicity** scores 1 and 2 in column AR.

Step 2 – Determine regulated chemicals.

- Proceed to **Section 6: Regulation**.
- Filter for chemicals with **Precedent\_list** score of 1 in column EC

→ This provides a list of chemicals with aquatic toxicity that are regulated regionally or nationally.

Step 3 – Pinpoint specific legislation.

- Check the **Precedent\_names** column for the relevant legislation linked to each chemical.
- Alternatively, use individual legislation-specific columns to refine your search. For instance, filter for score 1 in California\_P65 (column EJ) to identify chemicals regulated under California Proposition 65 in the US.