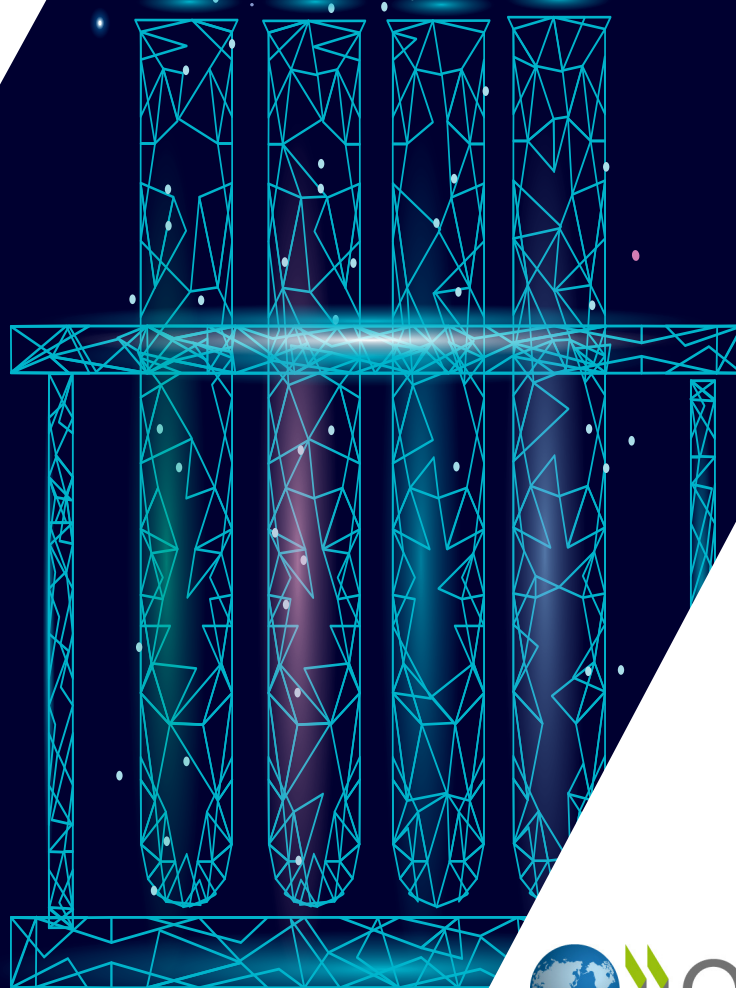




eChemPortal

eChemPortal Guidance for New Participants



 **OECD**
BETTER POLICIES FOR BETTER LIVES

 **ECHA**
EUROPEAN CHEMICALS AGENCY

eChemPortal Guidance for New Participants

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About the OECD

The Organisation for Economic Co-operation and Development (OECD) is an intergovernmental organisation in which representatives of 38 industrialised countries in North and South America, Europe and the Asia and Pacific region, as well as the European Commission, meet to co-ordinate and harmonise policies, discuss issues of mutual concern, and work together to respond to international problems. Most of the OECD's work is carried out by more than 200 specialised committees and working groups composed of member country delegates. Observers from several countries with special status at the OECD, and from interested international organisations, attend many of the OECD's workshops and other meetings. Committees and working groups are served by the OECD Secretariat, located in Paris, France, which is organised into directorates and divisions.

The Environment, Health and Safety Division publishes free-of-charge documents in twelve different series: **Testing and Assessment; Good Laboratory Practice and Compliance Monitoring; Pesticides; Biocides; Risk Management; Harmonisation of Regulatory Oversight in Biotechnology; Safety of Novel Foods and Feeds; Chemical Accidents; Pollutant Release and Transfer Registers; Emission Scenario Documents; Safety of Manufactured Nanomaterials;** and **Adverse Outcome Pathways**. More information about the Environment, Health and Safety Programme and EHS publications is available on the OECD's World Wide Web site (www.oecd.org/chemicalsafety/).

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Chapter 1. Introduction

The eChemPortal, the Global Portal to Information on Chemical Substances, is an effort of the Organisation for Economic Co-operation and Development (OECD) with contribution from governments and other stakeholders and is developed in collaboration with the European Chemicals Agency.

This guide is addressed to potential or new eChemPortal data source participants willing to know:

- Whether a data source is within the scope of the eChemPortal and how to request participation.
- How a data source can technically submit data.

Its main aim is to provide concise and practical information to help candidate participants identify the type of chemicals information shared on the eChemPortal and to define the best participation strategy for their data source.

The OECD is grateful to the members of the OECD Steering Group for the Development of the Global Portal to Information on Chemical Substances (eChemPortal) who participated in the development of this guidance and particularly the member from the EC Joint Research Centre which lead this activity.

eChemPortal new participant checklist

- [Understanding the eChemPortal purpose](#)
- [Identification of eChemPortal participation objectives](#)
- [Verification of eligibility](#)
- [Data Source definition](#)
- [Identification of contributing data type](#)
- [Requesting participation](#)
- [Identification of the technical solution](#)
- [Data mapping completion](#)
- [Adoption of a submission process](#)
- [Maintenance of Data \(submission process implementation\)](#)

Plan ahead

Although this might not be a common situation for readers of this guide, planning the contribution to the eChemPortal from the beginning of a new data dissemination programme or application is probably the most cost-effective way to participate.

By taking into consideration the content of this guide at the beginning, a data mapping and notification strategy can be taken into consideration from the start to understand efforts and gain efficiencies.

1.1. What is the eChemPortal?

The eChemPortal provides free public access to information on chemical properties and direct links to collections of information prepared for government chemical programmes at national, regional, and international levels. Access to information on existing chemicals, new industrial chemicals, pesticides and biocides is provided.

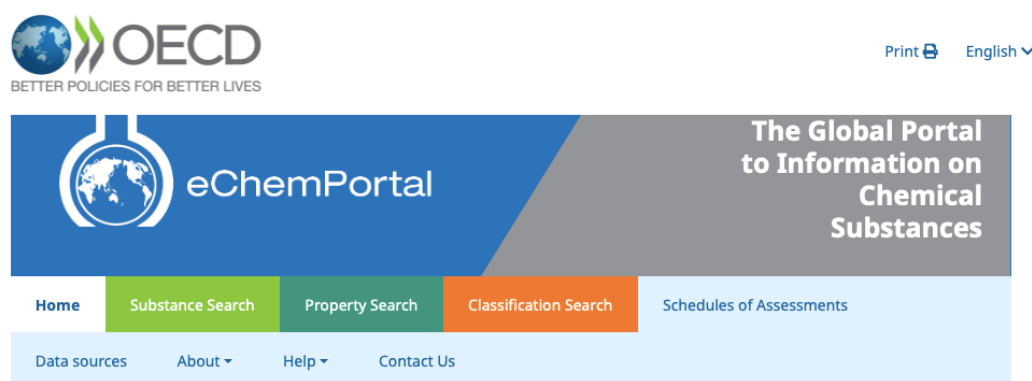
The eChemPortal also makes available chemical classification results according to national / regional hazard classification schemes or according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS).

In addition, the eChemPortal provides exposure and use information on chemicals.

The eChemPortal aims at being the preferred worldwide source of information about chemicals from authorities and international organisations.

The eChemPortal

The eChemPortal is freely accessible by the public at <https://www.echemportal.org>



Please search for information on substances and have a look at existing participating sources to familiarise yourself with the eChemPortal.

1.1.1. Roles

The Organisation for Economic Co-operation and Development (OECD) (www.oecd.org/) is responsible for the maintenance and development of the eChemPortal in collaboration with the European Chemicals Agency (ECHA) (<https://echa.europa.eu/>). It is hosted by the ECHA.

The data sources accessed through the eChemPortal are maintained by and remain the responsibility of the organisations that create them. The data and information stored in each data source are the responsibility of the data owner.

Participating data sources are responsible for ensuring links from the eChemPortal to their local data sources are updated by sending updated data to the eChemPortal administrator or the eChemPortal system.

1.1.2. Extending the eChemPortal

Holders of Internet-accessible databases or report collections prepared for government and international organisation chemical programmes on physical-chemical properties, environmental fate and pathways, ecotoxicity or toxicity of chemicals, as well as their use and exposure, are invited to participate in the eChemPortal.

1.1.3. Functionalities

The eChemPortal allows users to:

- Search data from multiple data sources simultaneously.
- Search by chemical name, chemical identifier, chemical property or effect, or classification.
- Retrieve direct links to reports and datasets and to property data in the participating data sources.
- Obtain information on classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS), when available.

1.1.4. Data format

The eChemPortal uses elements of the OECD Harmonised Templates for Reporting Chemical Test Summaries (OHTs) (www.oecd.org/ehs/templates) for data formatting in its data catalogue and search screens.

The Templates ensure consistent reporting of test study report results in summary format across regulatory programs. Corresponding XML schema enable electronic exchange between IT systems. The templates can be used to report summary test results for any type of chemical (e.g., pesticides, biocides, industrial chemicals). By using these templates, governments and industry are easily able to electronically exchange test study summary information.

The eChemPortal data notification XML format is different from but compatible with the Templates' XML format in order to be fit for the purposes of the eChemPortal.

1.2. Why provide information to the eChemPortal?

The OECD and its members countries are dedicated to protecting human health and the environment by promoting chemical safety worldwide. The eChemPortal is a key tool supporting this work. For all stakeholders, including in developing economies, the eChemPortal is a tool for finding information to support health and environment decisions concerning chemicals.

Better chemicals management is one of the objectives pursued by many countries and that is part of many international world programmes. UNEP 2006 Strategic Approach to International Chemicals management aims at for example:

*"To ensure, for all stakeholders: That information on chemicals throughout their life cycle, including, where appropriate, chemicals in products, is available, accessible, user friendly, adequate and appropriate to the needs of all stakeholders."*¹

¹ UNEP, 2006, Strategic Approach to International Chemicals Management – SAICM texts and resolutions of the International Conference on Chemicals Management, paragraph 15.b.i.

To this end, the eChemPortal provides worldwide visibility to chemical programs implemented around the globe.

The eChemPortal maximizes access to information on chemicals for all stakeholders for whom such information is critical, regulators and industry, and benefits academics, international organisations and the general public - regardless of geography or purpose. It is a significant step towards achieving long-standing international commitments to identify and make information on chemical properties publicly available.

It aims to be the global Internet portal that provides free easy access to all existing information of regulatory relevance on chemicals by linking directly to collections of information prepared for government and international organisation chemical programmes.

The eChemPortal expands the ability of governments to efficiently access information in order to share the burden of work, ensure resource efficiencies, and avoid duplication of work on assessment and, subsequently, reduce animal testing. It can help transform data into knowledge by encouraging users to build knowledge sharing communities. Such principles are those carried by open data approaches promoted by many governments.

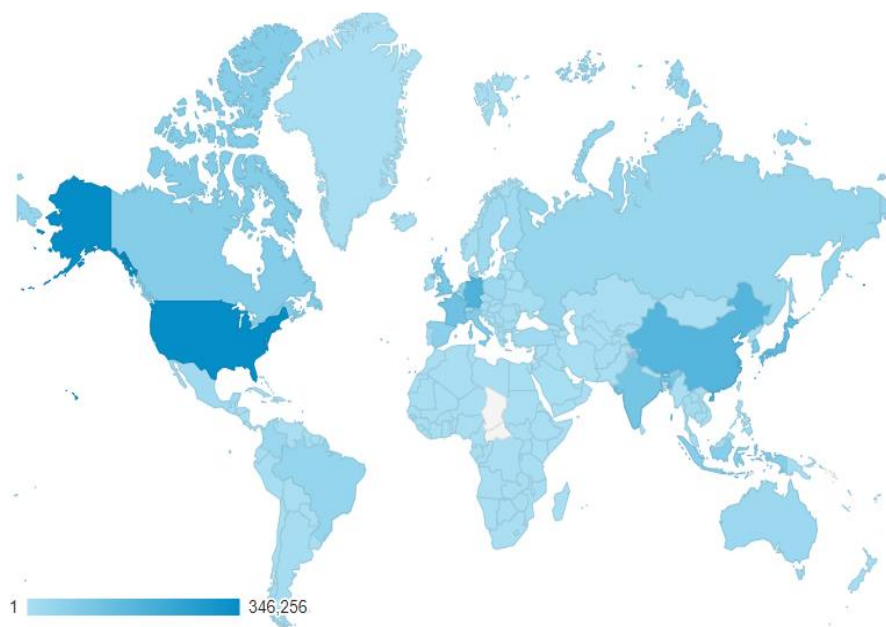
eChemPortal participation objectives

Participating in the eChemPortal offers benefits for the data provider:

- Recognition as an actor in the work to meet international Chemicals management aims.
- Visibility to the data provider's chemical programme, including in the number and geographical spread of visitors to the chemical programme's website.
- Facilitation of searches on national, regional, or international programme data without necessarily investing in a specific tool, particularly if submitting property and effects data to the eChemPortal.

The average monthly number of visits to the eChemPortal in 2022 was approximately 26,500.

Figure 1.1. Number of users who initiated at least one session during the year (Jan. 2022 - Dec. 2022)



Source: Google Analytics for Session greater than 15 seconds accessed in January 2023.

1.3. Who can contribute?

In general, the eChemPortal focuses on information submitted to government chemical or international organisation programmes at national, regional, and international levels. Stakeholders represented at the OECD Chemicals and Biotechnology Committee (CBC) are eligible to propose contributions to the eChemPortal or extension of the scope of the kind of information contained in the eChemPortal. Information on the OECD, Environment, Health and Safety Programme overseen by the OECD CBC is available here: <https://www.oecd.org/chemicalsafety/organisationoftheenvironmenthealthandsafetyprogramme.htm>.

Data sources should have a public interface presenting information on chemicals of relevance for this programme:

- chemical properties (for example found in hazard & risk assessments or test data),
- exposure and use information, and
- National classification results according to national / regional hazard classification schemes or the Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

focused on

- existing industrial chemicals
- new industrial chemicals
- pesticides
- biocides.

Data submitted to the eChemPortal ideally should be in English. However, data sources with information in a language other than English may participate with, if possible, chemical names in English for display in the search results and a remark indicating the language of the data source. Chemical names in languages other than English can be submitted as synonyms.

Chemicals repositories or inventories are not in scope of the eChemPortal as they do not provide specific information on chemicals outside of grouping or identification of substances; information on regulatory measures on chemicals is also not in the scope of the eChemPortal.

Nevertheless, and in case of doubts, the OECD welcomes all type of proposals (see 3.3 Submitting your data) and encourages potential candidates to contact the OECD at an early stage in order to check the relevance of the data source.

Eligibility criteria

- Represented at the OECD Chemicals and Biotechnology Committee (CBC)
- Data come from a government chemical programme and can be shared (if needed, including a disclaimer)
- Data are hosted on a publicly accessible website
- Data contain information on chemical substances:
 - Property information (e.g. hazard & risk assessments, test data)
 - Exposure and use information
 - National classification results, and in particular according to the GHS
 - Existing industrial chemicals
 - and/or New industrial chemicals
 - and/or Pesticides
 - and/or Biocides
- Chemical names can be submitted in English (ideally)

In case of doubt or question, please contact the OECD Secretariat: echemportal@oecd.org.

Chapter 2. Is your data suitable for the eChemPortal?

Before applying to become an eChemPortal participating data source, you should check that your data are fit for purpose and meet the eChemPortal objectives and content.

As its name indicates, the eChemPortal is an on-line global Internet portal - a collection of homogenous query table data submitted by heterogeneous third party data sources. Only enough data are collected to allow queries.

All data sources are found via the eChemPortal Substance Search by submitting the minimum data to the eChemPortal.

The eChemPortal search results link directly to information of regulatory relevance on chemicals freely available on the data source website. See section 1.3 Who can contribute? for the chemical information relevant for the eChemPortal.

Data sources with structured chemical property and effects data should consider submitting the appropriate structured data to the eChemPortal to be found also via the eChemPortal Property Search.

Data sources containing GHS chemical classifications and labelling information which has undergone a review by a regulatory body or similar international organisation should consider submitting data in a structured format to be found also via the eChemPortal Classification Search.

See section 2.2 Assessing your data for more information on the minimum data required for each search.

The eChemPortal can link to information available in different formats, for example HTML in free text or a structured online database, reports in different file formats, in different database file formats (e.g. Microsoft Excel™), as long as the information is freely available on the data source website.

Responsibilities

The data in the eChemPortal do not undergo any evaluation by the OECD. The OECD accepts no responsibility or liability whatsoever with regard to the material on the web site.

The use of the information from source databases can be subject to specific disclaimers if needed. Reproduction or further distribution of the information available via the eChemPortal is subject to copyright laws and might require the permission of the owner of that information.

For information, the "Data sources" page of the eChemPortal web site contains information on the currently participating data sources.

2.1. Understanding the eChemPortal principles

The main principle of the eChemPortal is to reference chemicals of interest prepared for governmental programmes. To this extent, the eChemPortal does not store the specific information coming from the programme.

Instead, it focuses on collecting generic “metadata” allowing the identification of the chemicals covered by the data source. “Metadata” of all participating data sources can be queried by external users. Based on the query parameters, the eChemPortal identifies data sources matching the request and provides external links to the original source web sites.

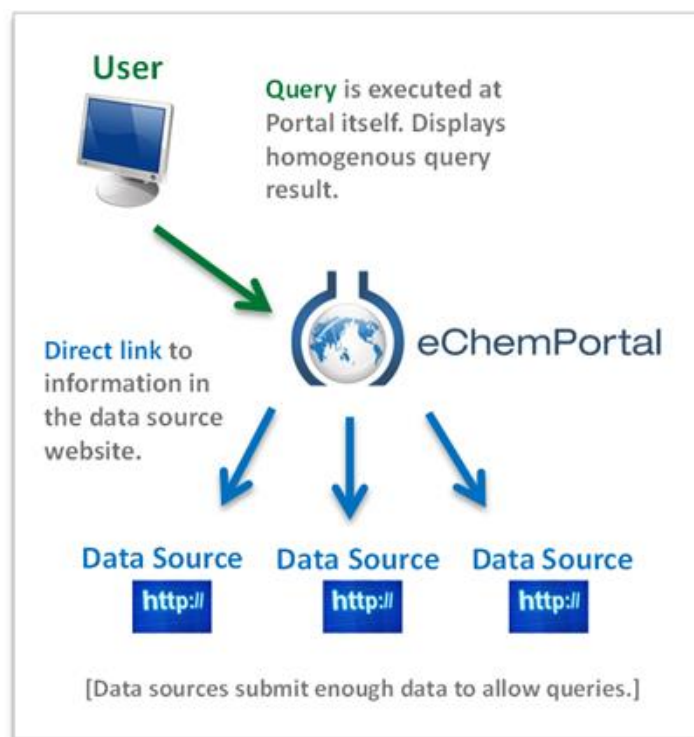
The eChemPortal does not aggregate substance records submitted by data sources under one substance identity, as it has no quality controlled chemical substance identifier index. Substance identity information is stored and displayed in the eChemPortal as it has been submitted per substance record by data sources.

Therefore, search results in the eChemPortal may display multiple records with the same substance identity from different data sources. As well, for example, search results in the eChemPortal may display multiple records with the same substance identity from the same data source, if that data source submitted a new substance record for each data set of the same substance in its local database; however, it is better if a data source submits one record per substance, for example, with a link to a substance profile page.

The eChemPortal stores and displays the so-called “original value”, i.e. the substance property and effects information seen by end users on the data source web site, as well as structured information which correspond to the search fields to allow searches to be found in the eChemPortal. Searches address the distinct database fields which correspond to the search fields. If data are retrieved, they are not displayed as such in the search results. Instead, the “original value” is displayed for each item.

The following diagram describes this process.

Figure 2.1. eChemPortal processes



The query parameters in the eChemPortal are:

- Selecting sources
- Searching for substances by:
 - Substance
 - Classification
 - Property.

The following section describes in detail the content of these parameters and what type of information is appropriate for the eChemPortal.

Current participating data sources

There are thirty-five* participating data sources from Australia, Canada, Finland, France, Germany, Japan, New Zealand, the United Kingdom, the United States, the European Union, and International Organisations.

- 31 contain information on chemical substance properties and effects.
- 11 data sources contain information on chemical classifications.
- 16 contain exposure and use information.

Types of information that can be found in participating databases reflect those information types that can be found across the entire database, not necessarily in every record found via the eChemPortal.

Some participants provide information on substance identification only and web links to information/documents on their local systems. Other participants also provide property and effects data or chemical classification and labelling data because they have the capacity to provide searchable data. (For example, their information exists in a database format and not just in a PDF document.)

The number of data sources participating in the eChemPortal is increasing continuously. The current list of data sources can be found on the eChemPortal here:

<https://www.echemportal.org/echemportal/content/participants>.

* March 2023

2.2. Assessing your data

The eChemPortal hosts two types of information on data sources:

1. The source description presenting the type of information provided by the participant programme.
2. The metadata used to search for information on chemicals.

2.2.1. Source description

The source description refers to the information contained in the eChemPortal “participating data sources”. It gives an overview of the data coming from the chemical programme to users in order to let them decide whether they would like to include a specific data source for their query.

Source description preparation

In order to assess if the data source of the participant is relevant for the eChemPortal participation and to identify what type of information could be shared, the preparation of the data source description in the eChemPortal format is valuable.

This allows participants to better understand the relevance of their data to the eChemPortal while starting the participation request, as this information is always requested.

A source description template is available for data sources upon request from the OECD Secretariat: *eChemPortal Database or Report Collection Information Description Template*.

Examples of source descriptions can be found on the eChemPortal: <https://www.echemportal.org/echemportal/content/participants>.

Example of a data source description:

Participating Data sources > CCR

Canadian Categorization Results

Type of information that can be found via eChemPortal:

Property data sets and industrial chemicals.

General information

The Canadian Environmental Protection Act, 1999 (CEPA 1999) is one of the primary tools used to prevent and reduce threats posed to Canadians and the Canadian environment by substances used or released in Canada. More than 23,000 chemical substances were in use in Canada between January 1, 1984 and December 31, 1986, when the original CEPA was being created. The law calls these "existing substances," and they are registered on the Domestic Substances List (DSL).

Under CEPA the Government of Canada was required to sort through or "categorize" all of these 23,000 existing chemical substances by 2006. Using information from Canadian industry, academic research and other countries, Government of Canada scientists worked with partners in applying a set of rigorous tools to the 23,000 chemical substances on the DSL. They were categorized to identify those that were:

- **inherently toxic** to humans or to the environment and that might be:
 - **persistent** (take a very long time to break down), and/or
 - **bioaccumulative** (collect in living organisms and end up in the food chain)
- substances to which people might have **greatest potential for exposure**.
- Additionally, substances considered a priority for assessment based on other health concerns were considered as part of this prioritization exercise.

This database contains the categorization results for substances on the Canadian Domestic substance list. Please note that information contained in this database was last updated in 2006 and some data may no longer be valid. Categorization is a first step to finding out which of these chemical substances require further attention in the form of assessment, research and/or measures to control their use or release.

For more information please see: <https://www.canada.ca/en/health-canada/services/chemical-substances.html> .

Hazard information

This Database contains the categorization results for substances on the Canadian Domestic substance list and the supporting data on:

- Inherent toxicity
- Persistency
- Bioaccumulation

Search capabilities

This Database offers a search by Chemical identification:

- CAS Number
- Chemical Name
- Type of substance

and filters by specific criteria categorization criteria:

- Meets Government of Canada Categorization Criteria?
- Meets Human Health Categorization Criteria?
- Meets Environmental Criteria for Categorization?
- Persistent (P)?
- Bioaccumulative (B)?
- Inherently Toxic to Aquatic Organisms (IT)?
- Basis for Environment Categorization (PIT, BIT, PBIT) if categorized? Results from the searches lead to specific chemical profile pages.
- Human Health - Potential for Exposure
- Human Health - Previous Assessments
- Human Health - Simple Hazard Assessment
- Human Health - Complex Hazard Assessment

Maintenance

The Government of Canada is responsible for the content of this Database containing Categorization Results from the Canadian Domestic Substance List. Categorization was completed in 2006 and the data is not planned to be updated. The database is hosted by the Organisation for Economic Cooperation and Development (OECD).

Peer review

Using information from Canadian industry, academic research and other countries, Government of Canada scientists worked with partners in applying a set of rigorous tools to the 23,000 chemical substances on the DSL.

2.2.2. Type of information for source selection in the search

Searches in the eChemPortal can be narrowed to specific sources. Groups of specific sources can be selected according to the “type” of information that the source contains. **Each data source is related to one or more of these types of information**, as defined in the source description.

Currently the types are: *Property information; Exposure and use information; GHS classifications.*

2.2.3. Search criteria

Once the data source is described and identified as relevant for participation to the eChemPortal, new participants should identify search criteria in their possession that could be used by the eChemPortal users.

Three kinds of search criteria can be sent to the eChemPortal (non-exclusive):

- Substance identifiers
- GHS classifications
- Substance properties.

Substances search

The first set of search criteria concerns substance identifiers. They provide a way for the user to look for a known substance based on existing identifiers used in various chemical inventories.

The key criteria that can be provided in order to allow the substance search are the following:

- **CAS Registry Number** (optional)
- **Other reference number or alternate CAS Registry Numbers** (optional). Supported reference numbers are:
 - CAS Registry Numbers: Unique numerical identifier assigned by the Chemical Abstracts Service (CAS).
 - EC Numbers: Unique identifier assigned to substances for regulatory purposes within the European Union by the European Commission.
 - IUBMB: International Union of Biochemistry and Molecular Biology.
 - MITI: Japanese Existing and New Chemical Substances Inventory (ENCS).
 - UN number: UN Recommendations on the Transport of Dangerous Goods.
 - NA Number: assigned by the United States Department of Transportation.
- **Chemical Name**: the main chemical name displayed in the local data source.
- **Synonym, Trade name, name in other language** (optional).
- **URL**: The URL leads directly to the full information in the local website.

Classifications search

The eChemPortal allows searches based on substance classifications according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) of the United Nations. The GHS provides an internationally harmonised approach to classification and labelling. The GHS classifies chemicals by types of hazard and proposes harmonised hazard communication elements in order to

enhance the protection of human health and the environment during the handling, transport and use of chemicals. The system is revised every two years.²

The GHS hazards are grouped into three hazard classes: Health Hazards (e.g. irritation to skin), Physical Hazards (e.g. flammability), and Environmental Hazards (e.g. hazardous to the aquatic environment). Each hazard is divided according to different severity levels: Hazard Categories (categories) (e.g. Sensitization, skin 1).

The criteria for the Classification Search in the eChemPortal are the **GHS Hazard Categories**.

Additional information may be provided to the user in the search result list:

- **Registry number (and type):** Registry number (e.g. Harmonised Classification and Labelling index number (Annex VI of CPL Regulation ((EC) No 1272/2008).
- **Substance form:** form of the substance (gaseous, liquid, nanomaterial, powder, solid, other).
- **Labelling pictogram:** The GHS includes Hazard pictograms.
- **Labelling signal word:** Danger or warning.

Properties search

The eChemPortal allows searches for information on substance property and effects. The search forms are based on the OECD Harmonised Templates (OHTs) format.

The Templates are standard data formats for reporting information on chemical properties or their effects on human health and the environment, and to describe their use and related exposure to workers, consumers and the environment. They are usually designed to report test summaries related to a particular endpoint (e.g. chemical properties such as boiling point or water solubility, environmental characteristics such as biodegradation in soil or toxicity to fish, health features such as skin irritation or genetic toxicity), for studies conducted according to OECD Test Guidelines and other national and international methods.

Data sources submit a sub-set of the endpoint property elements described in the Templates to allow the queries in the eChemPortal. The eChemPortal stores endpoint property data in the Template format. An Excel file listing all the indexed fields, is available on request from the OECD Secretariat.

Each endpoint search screen contains a number of parameters that can be defined by the user in order to perform complex queries. Cross combining substance properties searches across several endpoints ("Query blocks") is also possible.

The endpoints covered by the eChemPortal substance Property Search fall under the following information:

- Physical and chemical properties (19 OHT), e.g. Vapour pressure.
- Environmental fate and pathways (13 OHT), e.g. Phototransformation in air.
- Ecotoxicological information (15 OHT), e.g. Short-term toxicity to fish.
- Toxicological information (22 OHT), e.g. Acute toxicity: oral.

² United Nations (2019), *Globally Harmonized System of Classification and Labelling of Chemical (GHS), Eighth revised edition*, New York and Geneva, eISBN 978-92-1-004083-9

2.2.4. Links from search results

As the eChemPortal is a platform sharing key information on substance, it directs the users back to the origin of the data for complete information. The data should be therefore publicly accessible and published on the internet so that it can be referenced inside the eChemPortal.

In the eChemPortal search results, three types of links are provided which reference the Homepage of the participating database and the information related to a substance, and, for data sources participating in the search by property or classification functionality, reference the website containing the endpoint study record or the classification information, respectively.

Data sources should try to submit one URL to a chemical profile page in the substance search rather than many, if possible. The URL for the chemical profile page can be identical to the link for the endpoint study records or the classification information, depending on the content and structure of the data source website.

Identification of contributing data types

- Participants should identify the data coming from their source system that they are willing to share with the eChemPortal on (read carefully the previous section):
 - Substance identity
 - Classification
 - Properties (according to OECD Harmonised Templates indexed fields)
- Participants should check the eChemPortal requirements in order to identify to which extent their data are similar.
 - It can be identical, in which case the data are excellent candidates.
 - It can be similar but requiring some transformation or re-mapping of the data, in which case the data need to be reviewed and the transformation effort carefully estimated.
 - It can be different and incompatible (e.g. using a national classification or a non-OHT substance property); in which case the data cannot be submitted.
- Lastly, for each of the three types of information above, the participant should identify if a URL can be provided which will lead eChemPortal users to the relevant section of the data source system. For example,
 - search results on substance identity information should contain a link leading to the substance page description in the source system.
 - classification search results should lead to the classification of the substance,
 - and ideally, property search results should lead directly to the page in the source system containing the relevant endpoint study record information.

If the source system does not have a mechanism allowing the provision of specific URLs which lead the end user to a specific part of its data, a solution should be planned, if possible. It will reduce the impact of the participant contribution if end users see in the eChemPortal search results that the data source contains relevant information, but have difficulty retrieving it.

Chapter 3. Planning your participation

Taking into consideration the eligibility of data source to contribute to the eChemPortal and the type of information that can be provided, new participants can contact the OECD Secretariat to request participation and should establish a strategy in order to extract and format the information related to their data source.

These aspects are covered in this section, focusing particularly on:

- Requesting participation.
- Mapping the data from the source system to the eChemPortal format (business perspective).
- Converting the data from the source system to the eChemPortal format (technical perspective).
- Submitting the data (initial submission and update).

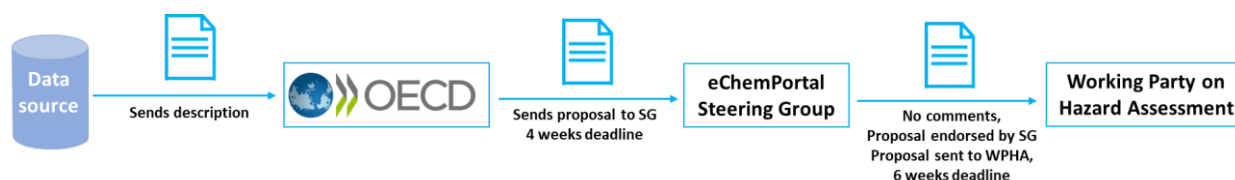
3.1. How to Request participation?

Proposals for linking new sources of data to the eChemPortal can be made by any stakeholder represented at the OECD Chemicals and Biotechnology Committee (CBC).

The decision to accept a proposal is taken by the OECD Working Party on Hazard Assessment (WPHA). OECD actively encourages additional participation; please contact the OECD Secretariat if you have any questions on how to make a proposal.

Once the description of the data source is received, the OECD Secretariat sends a proposal including the description to the eChemPortal Steering Group for a four week commenting period. If no comments are received, the proposal is considered endorsed by the Steering Group and the Secretariat sends it to the OECD Working Party on Hazard Assessment for six weeks. As soon as it is endorsed, the data source can be added. Data sources should plan in advance but should wait for endorsement before expending resources for the preparation of data.

Figure 3.1. Workflow of the endorsement process



eChemPortal new participant checklist

- Check list to request participation.
- Verify that you can contribute to the eChemPortal.
- Verify that your data are suitable for the eChemPortal.
- Contact OECD Secretariat (echemportal@oecd.org) with questions on participation and/or to request the Source description template.
- Send a completed data source definition to the secretariat, formally requesting participation.
- Wait for confirmation by the OECD Secretariat that the proposed participation has been endorsed by the OECD eChemPortal Steering Group (four weeks) and the OECD Working Party on Hazard Assessment (six weeks).

3.2. How to prepare your data?

In order to submit chemical data coming from a given programme on chemicals to the eChemPortal, the data need to be converted from the source system structure to the eChemPortal data format.

For this purpose, the data need to undergo a transformation that will map the information from the source structure to the eChemPortal format from both a content and a technical point of view.

The eChemPortal accepts XML files as input submitted in the form of notification tickets. These notification tickets can be uploaded manually or submitted automatically by a web service.

The importance of Substance identity

It is important to manage the substance identity in the source system. Indeed, users of the eChemPortal will use chemical identifiers, mainly chemical names, and chemical reference numbers.

The eChemPortal does not aggregate the submitted substance information under one substance identity, but simply stores the information provided by the submitter.

This has two main consequences:

- The more identifiers available for a chemical, the easier the substance will be retrieved in the eChemPortal.
- It is important to identify a unique name (the Chemical Name) and to report all other names as synonyms as well as all existing numerical identifiers. Therefore, it is important to manage substance identity consistently in the source system.

The CAS Registry Number is the main numerical identifier in the eChemPortal. If more than one CAS is available for a given substance, a main CAS should be identified, and the others provided as other CAS numbers.

There are three formats in which information may be submitted to the eChemPortal.

- XML files: the eChemPortal format that allow direct submission. This method requires IT skills but is easier if IT scripts can be created.
- Excel files: an intermediate format that allow conversion to XML format. This method is manageable with non-IT skills but is more difficult to handle if the list of substances in the source system is large. Text files also may be submitted for substance information.
- IUCLID files: using the IUCLID provider agent to convert IUCLID files into the eChemPortal format automatically.

3.2.1. XML based approach

The eChemPortal format for submitting notifications is XML. XML files are structured documents that implement strictly defined standards. XML documents are easy to produce for persons having prior experience.

Data are submitted in the form of “Tickets” that are XML files design to initialise, insert, update or delete substances information provided by the participants.

Complying directly with the eChemPortal requirements for the XML based approach

Documents are available upon request from the OECD Secretariat on how to comply with the eChemPortal requirements.

- **Excel of the eChemPortal catalogue:** An Excel file provides a full list of the property and classification parameters that may be submitted by data sources.
- **Guidance for Data Sources on Populating eChemPortal with Relevant Data:** provides information on how to generate XML files in the format that is required by the eChemPortal, covering substance, GHS and property information, as well as data mapping considerations.
- **XML schema:** describes technically how the XML files should comply with the eChemPortal data structure. The eChemPortal XML schema was first published in 2015 and is updated as necessary, approximately once every one or two years, in order to align with updates to the OECD Harmonised Templates (OHTs) format and the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). Currently, all previous versions of the XML ticket notifications can be submitted to the eChemPortal.

Most likely, an IT provider or department should be involved for this approach which is more technically demanding.

XML tickets have the following structure:

- Administrative data:
 - Ticket information (Ticket ID, timestamp, etc.)
 - Participant ID (Name of the participant data source in the eChemPortal)
 - Message number (if the submission is split in several files)
- Submission data
 - Type of submission (insert, delete, update, etc.)
 - Substance (link to source system, comments, etc.)

- Identification (Chemical name, CAS number, etc.)
- Classification and Labelling information (GHS based structure)
- Property information (OECD Harmonised Templates based structure).

Understanding the detailed structure of the substance properties document may represent a significant effort, especially if a mapping exercise is needed to transfer data from the source system format to the eChemPortal XML ticket notifications.

Issues to be considered for the transformation of source data

Data source managers should consider the following items when mapping data source data to the eChemPortal XML ticket notifications:

- URLs to the relevant data in the data source
- The “original value” principle of the eChemPortal
- Free text related to list fields
- Numeric ranges and numeric qualifiers
- Units of measurement
- Repeatable fields
- Source fields grouped to (repeatable) block of fields
- Mapping non-grouped source fields to grouped target fields

The *Guidance for Data Sources on Populating eChemPortal with Relevant Data* contains explanations of mapping considerations.

Examples of approaches taken to map definitions and build a software tool to generate eChemPortal XML ticket notifications

For one data source, a complete set of source data was available as MS Access and Excel tables. To map definitions and build a software tool to generate eChemPortal XML ticket notifications, the following approach was used.

- Developed a Mapping specifications document which identified which and how the source data were to be rendered in the eChemPortal format.
- Developed an input table as Excel table containing all relevant input source data, except the default values, and all specific field and phrase mapping definitions. Reference to the XML template was made through the target field codes that were used in the XML template as placeholders for the values captured from this input table.
- Developed an XML template which contained default elements and placeholders for items that needed to be extracted from the input table. The template contained the exact structure for all relevant XML elements, as prescribed by the relevant eChemPortal documentation (i.e. XML schema definitions). It reflected an Insert notification ticket.
- Developed a transformation tool as a VBA macro which extracted the relevant input data from the input table, inserted them in the XML template and generated the notification tickets as final output.

For another data source, an MS Access DB file where all the eChemPortal target fields, the relevant fields of the source database and transformation rules were included in separate tables. The outcome served as a basis for IT developers to develop an appropriate transformation tool.

3.2.2. Excel based approach

As the XML format can be quite difficult to handle by non-IT skilled users, substance and GHS classification information may be submitted in Excel format (substance information may also be submitted in *.txt format). Information on substance properties cannot be submitted in an Excel format. Substance information may be added or deleted but not updated using the Excel format.

Although more convenient for visualising the data, the Excel format is error prone as it requires a significant number of manual interventions. Building the Excel requires a grouping exercise and a clear respect of the rules as the file is parsed by a computer. This is recommended mainly for datasets with a manageable number of substance entries.

Complying directly with eChemPortal requirements for the Excel based approach

The following document is available upon request from the OECD Secretariat.

- **eChemPortal Data Template for EXCEL TXT:** Guidelines on how to prepare the Excel table (or *.txt file) for submission of substance or substance and classification and labelling to the eChemPortal are available in the document.

Example of a substance submission with the Excel based approach

The Excel based approach is often used by data sources submitting substance identity information only or both substance identity and classification and labelling information with a minimum of technical effort.

	A	B	C	D	E	F	G	H	I	J	K	L
	DATABASE	CAS_NO	OTHER_N	INO_TYPE	CHEMICAL_NAME	NAME_TYPE	SYNONYMS	SYNONYM_NAME_TYPE	SMILES	DOC_TITLE	URL	OPERATION
1	IPCHEM	26244-33-7			(2,3-dihydro-3,3-dimethyl-2-oxo-benzofuran-5-yl methane)		2-keto-ethofumesate					https://ip ADD
2	IPCHEM	338-45-4			(z)-mevinphos							https://ip ADD
3	IPCHEM	3567-62-2			1-(3,4-dichlorophenyl)-3-methyl-uree							https://ip ADD
4	IPCHEM	2327-02-8			1-(3,4-dichlorophenyl)-urea		3,4-dichlorophenyluree					https://ip ADD
5	IPCHEM	56046-17-4			1-(4-isopropylphenyl) urea		didemethylisoproturon					https://ip ADD
6	IPCHEM	34123-57-4			1-(4-isopropylphenyl)-3-methylurea		desméthylisoproturon					https://ip ADD
7	IPCHEM	34123-57-4			1-(4-isopropylphenyl)-3-methylurea		desméthylisoproturon					https://ip ADD
8	IPCHEM	1300-21-6			1-2 dichloroethane							https://ip ADD
9	IPCHEM	107-04-0			1-bromo-2-chloroéthane							https://ip ADD
10	IPCHEM	71-36-3			1-butanol							https://ip ADD
11	IPCHEM	5131-66-8			1-butoxy-2-propanol							https://ip ADD
12	IPCHEM	106-89-8			1-chloro-2,3-epoxy-propane		epichlorohydrine					https://ip ADD
13	IPCHEM	106-89-8			1-chloro-2,3-epoxy-propane		epichlorhydrin					https://ip ADD
14	IPCHEM	97-00-7			1-chloro-2,4-dinitrobenzene		1-chlor-2,4-dinitrobenzol					https://ip ADD
15	IPCHEM	97-00-7			1-chloro-2,4-dinitrobenzene		chloro-1 dinitrobenzène-2,4					https://ip ADD
16	IPCHEM	97-00-7			1-chloro-2,4-dinitrobenzene		2,4-dinitrochlorobenzene					https://ip ADD
17	IPCHEM	121-73-3			1-chloro-3-nitrobenzene		3-nitrochlorobenzene					https://ip ADD
18	IPCHEM	121-73-3			1-chloro-3-nitrobenzene		chloronitrobenzène-1,3					https://ip ADD
19	IPCHEM	121-73-3			1-chloro-3-nitrobenzene		1-chlor-3-nitrobenzol					https://ip ADD
20	IPCHEM	100-00-5			1-chloro-4-nitro-benzene		1-chlor-4-nitrobenzol					https://ip ADD
21	IPCHEM	100-00-5			1-chloro-4-nitro-benzene		chloronitrobenzène-1,4					https://ip ADD
22	IPCHEM	100-00-5			1-chloro-4-nitro-benzene							https://ip ADD

Areas that need attention when preparing data in the Excel format

As mentioned above, the Excel format is error prone. The following areas need special attention to avoid common errors:

- File format requirements, e.g. UTF-8 encoding, no hidden special characters, a heading line, only one data sheet, pre-defined formats and values for specific data elements
- CAS number fields should be formatted as “text” fields so as not to be interpreted as “date” fields.
- Lines with multiple synonyms or numbers need to be placed directly below the master row.
- The maximum size for submission of an Excel file is 50 MB. If a file is too large and has to be split into more than one file, multiple lines forming a record for a substance should be contained in the same file.

3.2.3. Using IUCLID 6

The IUCLID (International Uniform Chemical Information Database) can submit data on chemical properties and effects from IUCLID Dossiers to the eChemPortal through an IUCLID Provider Agent.

IUCLID (International Uniform Chemical Information Database) is a software application designed to record, store, maintain and exchange data on the intrinsic and hazard properties of chemical substances or mixtures, as well as the uses of these substances and the associated exposure levels. The IUCLID 6 (latest version) software (containing no data) can be freely downloaded from the web site of the European Chemicals Agency (ECHA) and installed on a desktop for use by one specific user and on a server or

Cloud to be used in a multi-user environment. For information on the availability of the IUCLID Provider Agent, contact ECHA.

Users willing to choose this approach would need nevertheless to convert the data from their source system to the IUCLID application. Such an approach would require less technical skills but could be demanding in terms of entering the data. An IUCLID Data Uploader application meant to make this import easier is available.

For systems storing natively on the IUCLID format, using the IUCLID Provider Agent is most likely the best approach and should be considered for new source systems to be build.

As well, the IUCLID server version can be opened to the public as a read-only interface, allowing not only submission of stored data to the eChemPortal, but also use of IUCLID as a platform from which information can be made available and to which the eChemPortal can link.

For more information, see <https://iuclid6.echa.europa.eu/>.

Adoption of a submission strategy

- Based on the three options described above,
 - the XML based approach
 - the Excel based approach
 - using IUCLID 6,the participant needs to choose the most appropriate option.
- Depending on the scope of the data submitted (both in volume and in type of data), the participant data source needs to choose one option, taking into account that generating the notification format can take time and resources. The technical generation usually does not require an important effort for an IT provider, but it needs to be planned sufficiently in advance in most governmental organisations.
- The submission should also not be considered as a one-off task. Indeed, the update of data to the eChemPortal is essential to meet successfully the goals of the Portal and is the responsibility of the participant.

Example of the International Chemical Safety Cards

The International Chemical Safety Cards (ICSC) provide safety and health information on 1,700 chemicals in a concise format and in multiple languages, aimed principally at use in workplaces. The ICSCs are a joint activity of two International Organisations – the World Health Organization and the International Labour Organization. The ICSCs are freely accessible via the internet and the underlying content is stored in a structured database – two features which make the ICSCs suitable to participate in the Substance Search of the eChemPortal. For International Organizations, the objective of information products such as the ICSCs is to disseminate information on hazardous chemicals as widely as possible to assist users to manage chemicals safely.

Participating in the eChemPortal would increase the visibility of the ICSCs and increase the number of global visitors accessing the ICSCs. This was a clear benefit, in line with the objectives of the participating organizations. However, in order to participate in the eChemPortal a one-time investment of funds was required to commission the programming of an “export function” (a utility within the ICSC database) to generate a spreadsheet with the required substance identity information in the template required for upload to the eChemPortal, and hence to be included in the Substance Search. Since this bespoke utility became operational, the ICSC Secretariat has been able to upload ICSC data to the eChemPortal on demand, according to a schedule dictated by how often the underlying data in the ICSCs have been updated (at least annually).

This proportionate, one-off investment of resources by management has achieved the objective of participating in the Substance Search without requiring to make changes to the structure or content of the underlying database.

3.3. Submitting your data

Submitting the data depends on the way the notification tickets were prepared (in Excel or XML files).

For both approaches, it is very important for the submitter to keep track of all past submissions and to define a process for maintaining in synchronisation the source data with the eChemPortal notifications. The use of a versioning system is recommended for this purpose.

As teams evolve over time, it is also very important to keep information about the decision process and the choices that were taken during the preparation of the submitted data.

3.3.1. Excel based approach

For the Excel based notifications, the Excel file should be sent to the eChemPortal administrator. The Excel files are converted by the administrator and uploaded to the web site.

Figure 3.2. Data flow from the Excel file to the eChemPortal



The database owner sends an index in an Excel file according to the established template. The OECD Secretariat performs some data quality checks in order to avoid common errors. This Excel file is fed in the eChemPortal back-office that will generate the XML tickets. At this stage, errors that may occur are data quality errors. Once the XML tickets are generated, they are uploaded in the eChemPortal back-office and the tickets are inserted one by one in order. If an error occurs, the ticket is blocked and, once the error is corrected, the whole process has to be started again.

3.3.2. XML based approach

When a new participant is added to the eChemPortal, the eChemPortal assigns a UUID (Universally Unique Identifier) to the participant, which is guaranteed to be unique across all data providers of the system. The participant uses this UUID in the XML ticket notifications that are communicated to the eChemPortal.

Additionally, the participant receives a URL to be used for sending the payload to the eChemPortal. The eChemPortal Participant can then send payloads (notification tickets) to the eChemPortal by performing a HTTPS POST to the URL provided.

The XML tickets can contain data for either one substance or data for multiple substances. However, in the case of tickets carrying property data, it is recommended to use only one substance in a ticket; otherwise, it is difficult to trace the substances and provide help on validation errors.

Single notification tickets can be uploaded using an eChemPortal feeding URL.

The eChemPortal Participant starts the indexing process by sending an Init notification ticket, which are followed by Insert ticket(s) and as appropriate, by Add / Update / Delete ticket(s). The Update ticket updates previously submitted substance information, property endpoints, or classification and labelling information. The Delete ticket deletes the whole substance dataset.

If the upload of any notification ticket fails, the access to the eChemPortal URL is blocked. The eChemPortal informs the data source administrator.

Even though the XML tickets have been validated and no upload failures have occurred, it is recommended to verify that the transferred source data are shown correctly in eChemPortal searches. To this end a number of test searches should be done. If unwanted search results are observed, the mapping definitions should be optimised as appropriate.

For the testing exercises, the OECD should be requested to grant access to a test version of the eChemPortal to avoid interfering with the live version.

3.3.3. Using the provider agent

IUCLID stores data in both (editable) raw data in Substance datasets and in "Dossiers", write-protected snapshots of (selected) raw data. The IUCLID Provider Agent only transfers data from Dossiers to the eChemPortal and does not transfer structured GHS information.

The IUCLID Provider Agent provides a user-interface to manage and check the notification process, loads dossier information from IUCLID, transforms the IUCLID format data to the eChemPortal XML format and submits the XML ticket notifications to the eChemPortal.

More information on the IUCLID Provider Agent is available from the European Chemicals Agency.

3.4. Maintaining and updating your data

Regular updates are requested from participants. It is important to plan.

Updates can occur for different reasons:

- Major update of the source system from a content point of view
- Provision of additional information
- On regular basis (e.g. yearly) if the source system is continuously fed with new data.

It is useful to keep key records and document the submission process to facilitate repeating the process when an update of data needs to be sent to the eChemPortal.

Considering progressive submission

Sharing information with the eChemPortal can be achieved progressively, playing on different parameters such as:

- Number of substances
- Type of information notified to the eChemPortal (in order):
 - Substances
 - Classifications
 - Properties
- Notification approach
 - Manual
 - Automated

For example, a participant can start by submitting substance identity information and then at a later stage information on substance properties.

Chapter 4. Modification history

Version	Date	Modification
1	March 2023	First version of this document.

The eChemPortal, the Global Portal to Information on Chemical Substances, is an effort of the Organisation for Economic Co-operation and Development (OECD) with contribution from governments and other stakeholders and is developed in collaboration with the European Chemicals Agency.

This guide is addressed to potential or new eChemPortal data source participants willing to know:

- Whether a data source is within the scope of the eChemPortal and how to request participation.
- How a data source can technically submit data.

Its main aim is to provide concise and practical information to help candidate participants identify the type of chemicals information shared on the eChemPortal and to define the best participation strategy for their data source.

oe.cd/echempportal

