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Pre-release

EU-SRS

Chemicals EU-SRS User Guide

Guidance on naming and building chemical records in EU-SRS

Disclaimer

This document is created as part of deliverable D2.8 EU-SRS Data Management Plan of Unicom Work Package 2: Implement IDMP – Substance Management in Europe.

This guide will be a living document, used by the Substances Validation Group (SVG) for creation and maintenance of substances in EU-SRS.

The current version is a pre-release. Your feedback, if any, is welcomed by **8 December 2022**. Comments can be sent to Steven de Wit (e-mail: s.d.wit@cbg-meb.nl).

Your feedback will be considered when preparing the official release which will be submitted as Unicom deliverable to the European Commission in January 2023.

Document control

This document is subject to a regular review by the Substance Validation Group (SVG). It is a living document, and changes will be captured in the version history section.

Document ownership

This document is owned by the SVG.

Revision history

Version	Date	Changes made	Author(s)
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List of abbreviations

Abbreviation	Complete Form
AL	Additional Listing Name
ATC	Anatomical Therapeutic Chemical Classification System
BAN	British Approved Name
CAS	Chemical Abstracts Service
CV	Controlled Vocabulary
DN	Display Name
eAF	electronic Application Form
EP	European Pharmacopoeia
EDTA	Ethylenediaminetetraacetic acid
EU	European
EMA	European Medicines Agency
EDQM	European Directorate for the Quality of Medicines and HealthCare
EU-SRS	European Substance Registration System
FDA	Food and Drug Administration
G-SRS	Global Substance Registration System
INN	International Nonproprietary Name
INNM	Modified Nonproprietary Name
ISO IDMP	International Organization for Standardization Identification of Medicinal Products
IUPAC	International Union of Pure and Applied Chemistry
JAN	Japanese Accepted Name
Ph. Eur.	European Pharmacopoeia
pINN	proposed INN
PT	Preferred Term
rINN	Recommended Non-proprietary Name
RMS	Referentials Management Services
SMILES	Simplified Molecular Input Line Entry System
SmPC	Summary of Product Characteristics
SMS	Substance Management Service
SMSID	Substance Management Service Identifier
SPOR	Substances, Products, Organisations & Referentials
SVG	Substance Validation Group
UNII	Unique Ingredient Identifier
US	United States

Abbreviation	Complete Form
USAN	United States Adopted Name
USP	United States Pharmacopeia
WHO	World Health Organization
xEVMPD	Extended EudraVigilance Medicinal Product Dictionary

1 Introduction

The EU Network is currently implementing the ISO IDMP standards in a phased programme based on the four domains of master data in pharmaceutical regulatory processes: substance, product, organisation and referential (collectively referred to as “SPOR”) master data. ISO IDMP compliant business services for the central management and supervision of data in each of the four SPOR areas will be established through an iterative and incremental delivery approach. Through the Substance Management Services (SMS) of the SPOR programme EMA will provide the EU network centralised substance data management services.

EU-SRS will become the scientifically rigorous back-end for the Substance Management Services of SPOR. EU-SRS will be accessible to the EU regulatory network, enabling the unambiguous identification of substances used in medicinal products based on their scientific properties in accordance with ISO IDMP standard 11238 and ISO IDMP technical specification standard 19844. EU-SRS allows the unique identification of substances which will support various purposes including the enhancement of traceability of pharmacovigilance, non-clinical, clinical and quality findings with a high degree of precision to substances by their scientific identity.

The Substance Validation Group is responsible for building substance records in EU-SRS. In addition, the SVG defines guidance and best practices for substances management in EU-SRS (per substance type).

1.1 Purpose

The purpose of this document is to provide practical guidance for the registration of chemical substances in EU-SRS.

1.2 Scope

Registration of human and veterinary chemical substances are in scope of this document.

This document is intended to be used together with the EU-SRS Substance Maintenance Process which describes the workflow between EMA and SVG (under development).

2 Defining a chemical substance

In order to ensure good quality chemical substances records, which is built in a well-organized, and harmonised way, rules have been established and agreed upon within the SVG together with relevant partners. References to external documentation are made where necessary. This chapter provides general guidance on how to define chemical substances.

The concepts required for the unique identification and description of substances are described in the ISO 11238 IDMP standard on substances. Guidelines for implementing ISO 11238 are provided in the technical specification ISO/TS 19844. Although ISO 11238 does not provide any guidance on substance nomenclature, it does provide a structure for the capture of names and codes that are used to refer to a substance. This section aims to provide supplementary guidance and should be read in conjunction with the standard and technical specification.

2.1 Definition

Placeholder for definition from ISO/TS 19844:2018 (approval pending).

According to ISO 11238, the following substances can be registered as Chemical:

- ▶ Stoichiometric single molecular entity
- ▶ Salts of chemically defined substances
- ▶ Solvates
- ▶ Cyclic peptides
- ▶ Peptides derived largely from non-proteinogenic amino acids
- ▶ Extensively-modified oligonucleotides
- ▶ Isotopes
- ▶ Peptides with <3 amino acids
- ▶ Proteins with <40 amino acids*

*alternative definition will be chemical to capture the molecular structure of the protein

3 Naming of a chemical substance

This chapter provides details around naming of Chemical substances in EU-SRS and SMS.

3.1 Name types

EU-SRS contains name type information. ISO 11238 list several name types. Within the EU-SRS, examples of name types are:

- ▶ **Official names:** This name type contains comprehensive information about the name. It is chosen for names that are assigned by an official organisation. According to the EU Directive, the International Nonproprietary Name (INN) and the European Pharmacopoeia must be followed in the EU.
- ▶ **Systematic names:** For chemical substances, the systematic names are formed according to the IUPAC rules. It can also be used for other systematic names (e.g. CAS name).
- ▶ **Codes:** Synonyms that represent company codes.
- ▶ **Common names:** Usage for first designation of recognised trivial names that have an additional systematic designation. An alternative for "official name".

3.2 Naming convention

Each unique substance receives an SMSID from SMS, and each SMSID has Preferred Term, which is characterised as 'Display Name' in the system. The Preferred Term is the name most accurately describing the substance at a given time and could change during the lifetime of a substance.

The Preferred Term is used in several forms visible to industry. Going forward, it is planned that these forms (such as eAF) will also display the aliases.

3.2.1 Preferred term

Every record in EU-SRS (independently of the level) has a preferred term. According to Directive 2001/83/EC the Preferred Term of a substance should be selected from the priority ranking of the following reference sources and name type:

1. European Pharmacopoeia (Ph. Eur.) (Official Name Type)

NOTE: There are cases where the Ph. Eur. name and the INN name are not aligned or where the monograph definition does not give sufficient level of depth. For these cases, a case-by-case analysis should be performed to determine which name would most accurately describe the substance and this name should be included as an alias (Table 1).

Table 1. Situation in which the Ph. Eur. Name is included as PT and INN is included as an alias, in which the INN describes the substance more accurately.

Ph. Eur. Title (included as PT)	INN (included as Alias)
Fosfomycin calcium	Fosfomycine calcium monohydrate
Chloroquine sulfate	Chloroquine sulfate monohydrate

2. Recommended International Non-Proprietary Name (rINN) (Official Name Type)

NOTE 1: An INN for a new chemical entity does not routinely specify the stereoisomeric state of the molecule in the non-proprietary name. If stereochemistry has been determined, then this information is presented in the chemical name(s) to identify the substance. An INN can, therefore, represent the racemic mixture (e.g. ibuprofen), the levo-isomer (e.g. amifostine), or the dextro-isomer (e.g. butopamine).

NOTE 2: Modified INN will be generated according to the WHO publications "International Nonproprietary Names Modified" and "Names for radicals, groups & others Comprehensive list".

3. Other official name type with EU jurisdiction (INCI, BAN, etc.) (Official Name Type)
4. Verified common name (Common Name Type)

NOTE: This refers to the names that are commonly used but are not assigned by official organization.

5. International Union of Pure and Applied Chemistry (IUPAC) name (Systematic Name Type)

NOTE: Different formats are accepted for systematic names. If the format used is correct according to any of these acceptable formats, the systematic name is to be kept and no other formats need to be added.

6. Other systematic name (Systematic Name Type)
7. Company code (Code Type)

NOTE: A company code can be temporarily used as a Preferred Term only if no other name is available in the public domain, e.g. for substances under development. Once another name becomes available, the company code should be changed into an alias and another term should become the Preferred Term.

3.2.2 Aliases

Aliases are valid alternative names for a Preferred Term, according to valid reference sources. SMS provides aliases when available. In addition to the sources/name types used for preferred terms, the following sources can also be used for aliases:

- ▶ Proposed INN (pINN) (Official Name Type)
- ▶ United States Approved Name (USAN) (Official Name Type)
- ▶ United States Pharmacopoeia (USP) (Official Name Type)
- ▶ Japanese Approved Name (JAN) (Official Name Type)
- ▶ Official name in other jurisdiction, e.g. AAN (Official Name Type)

The EU-SRS Preferred Term should be written in European English. Any US English term is however to be kept as an alias. Differences in spelling between the EU and the US are included in Table 2.

Table 2. Differences in spelling in the EU and US.

EU English	US English	Comment
-oxide	-oxyde	Use of “i” in UK, and “y” in US
-f-	-ph-	Pronounce “F” see examples below
alfa	alpha	For proteins
alpha	alpha	For chemical systematic name
aluminium	aluminum	Translation from Latin can be different
-ilate	-ylate	Examples provided in the first four entries below
besilate	besylate	
camsilate	camsylate	
mesilate	mesylate	
tosilate	tosylate	
colour	color	
sulfate*	sulfate*	
sulfuric	sulphuric	

* Note: USAN and USP use ‘Sulfate’ instead of ‘sulphate’. Additionally, ‘sulphate’ was used in British English until 2011, explaining why older records could have different spelling.

3.2.3 Invalid substance names

Not acceptable names include:

- ▶ Product names: Product names should not be inserted as substance names. This applies also in cases where in official reference sources they are reported as a synonym of the substance (e.g. Calcium gluconate 50 mg/ml).
- ▶ Pharmaceutical product characteristics as part of the substance name, e.g. 'For Injection', 'For Solution for Infusion' are acceptable in the dictionary only if these are referring in a specific Pharmacopoeia monograph and be classified as Specified Substance Group 3. Otherwise, the term is not considered to be valid.
- ▶ The expression of the strength is different from the concentration of a substance; in this case the information can be included in the name according to the definition of Specified Substance Group 1. (e.g.: Hydrochloride 1 N)
- ▶ Substance names in the form 'substance name (as solvated/salt/prodrug)' (e.g. Clopidogrel (as hydrochloride) or Abacavir (as abacavir sulfate))
- ▶ Multiple substance names or Substance Type; A substance is considered not valid when the name refers to a class of substances or when more substances are listed (e.g. separated with commas, pluses: Vitamin C, Acerola, Propolis).
- ▶ Molecular formulas used as name (e.g. HCl instead of Hydrochloride)
- ▶ Non-converted CAS name writing (e.g. 'benzamide, 4-amino-N-(((2S)-1-ethyl-2-pyrrolidiny)methyl)-5-(ethylsulfonyl)-2-methoxy-' instead of '4-amino-N-(((2S)-1-ethyl-2-pyrrolidiny)methyl)-5-(ethylsulfonyl)-2-methoxybenzamide')

Exceptions to the rules for invalid naming

- ▶ Exception to the above rules: in case an invalid name is the most known and commonly used name, but only as an alias (e.g. EDTA is accepted as an alias for Edetic acid)

3.3 Examples of correct naming

For organic substances the syntax is the following:

<Active moiety>, <(Basic or Acid)>, <Salt>, <Hydrate>

Only stoichiometric moieties are acceptable.

Examples of correct naming of Chemicals are listed in Table 3.

Table 3. Examples of correct naming of chemical substances.

Preferred Term	Comment
Halometasone monohydrate	The Preferred Term should specify hydrate with mono-, di- or x-hydrate. -di, -tri and so on describes more than one H ₂ O-molecule; -sesqui describes 1.5 H ₂ O; -hemipenta describes 2.5 H ₂ O *Only the term of 'hydrate' is allowed in case of a Non-stoichiometric substance or in case that the amount of water is variable (Substance type: Mixture). When this is the case the record should have a property 'Water content' which is defining the amount of water in the substance. -monohydrate means one H ₂ O-molecule in the crystal lattice
Emetine dihydrochloride	The Preferred Term should specify salt with mono-, di- or x- salt
perindopril tert-butylamine	The Preferred Term should specify salt with mono-, di- or x- salt
Yttrium (90y) edotreotide	Radiopharmaca
2-{4-[2-(7,8-dimethyl[1,2,4]triazolo[1,5-a]pyridin-6-yl)-3-(propan-2-yl)-1H-indol-5-yl]piperidin-1-yl}acetamide	Systematic names are accepted as an alias when following any official naming convention. However, when a systematic name is newly added as a Preferred term, it is preferred to follow IUPAC writing, as this format is often used by INN and applicants.
2-phenylphenol 3-fluorophenmetrazine	Use of 1-/2-/3- instead of <i>ortho-/meta-/para-</i> as prefix

4 Building Chemical Records

4.1 Duplicate check

The first step of any registration should be to ensure that the substance is not already available in EU-SRS, to prevent from adding a duplicate. To ensure there is no duplicates, different elements can be used for verification, such as: different names, company codes, molecular formula, structure, systematic name (or parts of systematic name in different order) and database IDs. The approach for duplicates check should be determined case-by-case. If duplicates are found, further investigation is required to determine if it's a true duplicate.

4.2 General information

Each substance is unique in EU-SRS. Select Register then Chemical from one of the various options explained in the Registration Page Navigation Options section of this document. Select "Register a chemical" from the "Register a Substance" menu. The chemical registration form will be displayed (see Figure 1Figure 1). Section cards are collapsible to ease navigation, however the elements in this form are:

- ▶ Overview
- ▶ Names
- ▶ Structure
- ▶ Codes
- ▶ Relationships
- ▶ Notes
- ▶ Properties
- ▶ References

Overview

Registering New Chemical

Definition Type *
Primary

Definition Level
Complete

☐ Deprecated

[Record Level Access](#)

Substance tags
Enter new tags (and press Enter after each entry) or select from suggested tags below

Definitional References ⁰ [Create new](#) [Definition Access](#)

Names [Add Names](#)

Structure

Codes [Add Codes](#)

Relationships [Add Relationships](#)

Notes [Add Notes](#)

Properties [Add Properties](#)

References [Add References](#)

Figure 1. A form for registering a new Chemical in EU-SRS.

According to ISO 11238, the structure of a chemical substance must be captured during registration. The molar mass, molecular formula and stereochemistry are generated from the structure. Unknown positions in the stereochemistry must be clearly identified. Ratios of proportions (for salts, hydrates) must be taken into account. Variable compositions (or composition ranges) must be included.

Mandatory fields for chemicals are:

- ▶ a substance identity/molecular structure
- ▶ at least one name
- ▶ at least one definitional reference

4.3 Overview

For the registration of a new chemical in EU-SRS, some general information needs to be entered first (see Figure 2). Additional explanation of the EU-SRS fields is included in Appendix 5.4.

Figure 2. Overview of general information to be registered.

1. Definition Type - hover over and select the down arrow to activate the Edit drop-down. There are two options:
 - a. Primary
 - b. Alternative - Chemical alternative definition of a protein, nucleic acid, polymer, ring/open sugar etc. Once Alternative is selected a Primary Substance Search field appears

Note: Type the Primary Substance name in search box and select. As you begin, typing a list containing those letters will appear. Make a selection and then select search and the Primary Substance will populate. After submission, the system generates a relationship connecting both definitions. Alternative definition registration is similar to Primary definitions, but Names and Codes are not included.

2. Definition Level – select the down arrow to activate the Edit drop-down.
 - a. Always try to enter a Complete definition
 - b. Incomplete are allowed for incompletely defined substances.
 - c. Representatives are too complex to define completely
3. Deprecated box: selecting this box means it is semi-deleted, or a candidate for deletion. There are other flags for deprecation elsewhere in EU-SRS, but that one also tells the browse/search functions not to show this record unless you specifically click the box allowing it to show.
4. Record Level Access: some substances are public in which case set the Record Level Access to Public by deselecting Protected under Record Level Access. Some substance are private in which case the option Protected should be selected. Private means not readily available in public sources, domains, website, etc. (e.g., SciFinder, PubChem).
5. Definitional Reference(s):
 - a. Select the Create new + button
 - b. The Add Reference screen appears and additional fields will be displayed

Note: Select the down arrow next to Source Type. Use the scroll on the right to navigate and select a Source Type. Source Text/Citation – identifies where the information comes from. Based on the release sensitivity: Check Public Domain if public (If public, add Tags for Public-Domain-Release). Update the Access by deselecting PROTECTED, if applicable. Select Save.

In order to make something Public it has to be made public three times:

- ▶ Undo the lock
- ▶ Select the Public Domain checkbox
- ▶ Enter the Tag as Public Domain Release

Public Domain checkbox should be added for all public references. Every public name should have at least one reference with Public Domain checkbox. Public Domain Release Tag should be used for public records and added to the record when the lock is opened.

Click on Create new + to add more references or select a previously used ref by clicking on reuse to select a previous substance reference.

4.4 Names

Currently, the following name types are to be used:

- ▶ **Official names:** This name type contains comprehensive information about the name. It is chosen for names that are assigned by an official organisation. According to the EU Directive, the International Non-proprietary Name (INN) and the European Pharmacopoeia must be followed in the EU.
- ▶ **Systematic names:** For chemical substances, the systematic names are formed according to the IUPAC rules. It can also be used for other systematic names (e.g. CAS).
- ▶ **Codes:** Synonyms that represent company codes.
- ▶ **Common names:** Usage for first designation of recognised trivial names that have an additional systematic designation. An alternative for "official name".

Names can be added with "Add Names +". Depending on the type, additional information is displayed. The language of the names is set to English by default. At the same time, the name is always present as "public".

For the correct mapping of the Preferred Term in SMS versus the Preferred Term in EU-SRS, the correct ticking of Display Name (DN) is crucial.

Option 1: SMS Preferred Term and EU-SRS Preferred Term (= Display Name) are the same

- ▶ In EU-SRS, the Preferred Term is selected as Display Name, and the Additional Listing Name is also ticked

Option 2: SMS Preferred Term and EU-SRS Preferred Term (= Display Name) are not the same

- ▶ In EU-SRS:
 - ▶ Preferred term is indicated as Display Name
 - ▶ SMS Preferred Term is indicated as Additional Listing Name
- ▶ In SMS:
 - ▶ The public term is indicated as Preferred Term
 - ▶ The EU-SRS Preferred Term is indicated as alias, with name source "Substance Validation Group"

Note that there are several reasons why in SMS the Preferred term is not the EU-SRS Preferred Term:

- ▶ The action to change the Preferred Term is postponed due to technical reasons
- ▶ The EU-SRS Preferred Term is a confidential term, and can therefore not be marked as Preferred Term; in SMS the PT is always a public term

Table 4 describes the different situations of correct mapping of the PT in SMS versus EU-SRS.

Table 4. Correct mapping of PT in SMS versus in EU-SRS.

Situation	SMS		EU-SRS	
	Name	Name Reference	Display Name (DN)	Additional Listing Name (AL)
SMS PT = EU-SRS PT	SMS PT = EU-SRS PT	-	Yes	Yes
SMS PT ≠ EU-SRS PT	Alias SMS = EU-SRS PT	Substance Validation Group	Yes	No
	SMS PT = EU-SRS Alias		No	Yes

4.4.1 Official name

The name of the substance is entered under Name, then the name type is selected under Type. Languages ("Languages": English), Jurisdiction are selected from the drop-down lists.

DN AL Name * Mevidalen resolve Type * Official Name Access

Standardized Name

Languages English Domains Jurisdiction EUROPEAN UNION

Figure 3. Registering an Official Name.

Chemical record can include more than one Official name, but just one name can be used as Display name (DN). The status of the official name is associated with the given jurisdiction. It is possible that an official name is a valid name in EU jurisdiction and other official name will be used in e.g. US jurisdiction.

For the official name, "Naming Organization" should be added (Figure 4). This is done with the "plus" sign next to "Naming Organization" when clicking on „Naming Organization“. If it is selected, the corresponding organization (BAN, EP, INCI, INN, JAN, USAN) can be selected. If more than one organization is to be registered, additional "Naming Organizations" must be added using the "plus" sign.

Naming Organizations +

Delete	Naming Organization	Deprecated
	USAN	<input type="checkbox"/> Deprecated
	INN	<input type="checkbox"/> Deprecated

Figure 4. Registering Naming Organizations.

For Official Names it is mandatory to add the Jurisdiction to the relevant Naming Organization. This always corresponds to the countries for which this designation can be used. Table 5 shows the naming organizations that can be used for official names. It also shows how to correctly include the Jurisdiction when the Official Name is included as the Display Name or as an Alias.

Table 5. Listing of naming organizations and corresponding jurisdictions.

Naming organization	Description	Jurisdiction if Official Name is included as	
		Display Name	Alias
EP	European Pharmacopeia	EU	-
INN	International Nonpriority Name	EU	EU
USAN	United States Adopted Name	US*	US
USP	United States Pharmacopeia	US*	US
BAN	British Adopted Name	EU	GB
BP	British Pharmacopeia	EU	GB
JAN	Japanese Adopted Name	JP**	JP
INCI	International Nomenclature of Cosmetic Ingredients	EU	-

*If USAN/USP is the same as INN: then substance will get two Naming Organizations:

1. INN (Jurisdiction EU)
2. USAN (Jurisdiction US)

If USAN/USP is not the same as INN, then INN will be included as DN (Jurisdiction EU), USAN/USP will be included as Alias (Jurisdiction US)

**If JAN is the same as INN: then substance will get 2 Naming Organizations:

1. INN (Jurisdiction EU)
2. JAN (Jurisdiction JP)

If JAN is not the same as INN, then INN will be included as DN (Jurisdiction EU), JAP will be included as Alias (Jurisdiction JP)

Subsequently, the references for the corresponding name must be entered (Figure 5). References can be added with "Create new +". A dialogue window opens for this purpose. Using "add reference", the information on the source type (see the list of "Source types" used at the end of the document) and the "Citation" (free text for the actual citation) can be inserted. A checkmark should be placed next to "Public Domain" for the public names.

Source Type *
INN List

Source Text/Citation *
INN proposed List 124

☐ Public Domain

URL

Source Id

Tags

Delete Upload Document

Apply to

Source Type *
INN List

Source Text/Citation *
INN recommended List 86

☒ Public Domain

URL

Source Id

Tags

Delete Upload Document

Apply to

Add reference

Figure 5. Registering references.

Further references can be entered in general, taking into account the list for "Source type" at the end of the document (see Appendix 0). Selection for the respective term takes place by "reuse".

Reuse Substance References

☒ Filter Out System / Validation references

Apply	Type	Citation	Public Domain	Access
<input type="checkbox"/>	STN (SCIFINDER)	STN	Yes	Public
<input checked="" type="checkbox"/>	SRS	FDA-SRS	Yes	Public
<input type="checkbox"/>	INN_LIST	INN CN	Yes	Public
<input type="checkbox"/>		IUPAC	Yes	Public
<input checked="" type="checkbox"/>	CAS	CAS	Yes	Public
<input checked="" type="checkbox"/>	USANCOUN	USAN	Yes	Public
<input checked="" type="checkbox"/>	INN_LIST	INN proposed List 124	Yes	Public
<input checked="" type="checkbox"/>	INN_LIST	INN recommended List 86	Yes	Public

Cancel Save

Figure 6. Reuse of substance references.

4.4.2 Systematic Name

The systematic name of the substance is entered under the tab "Name", then the name type is selected under "Type". As with the first name, the references are opened and saved in a new dialogue window ("reuse") (Figure 7).

Figure 7. Registering of systematic names using HTML codes.

The IUPAC (= INN description: systematic name in the INN list) are mapped as references. Other systematic names (e.g. CAS name) can also be entered. This is the preferred name in SciFinder. The relevant references are attached.

When entering systematic names and synonyms, care must be taken to ensure IUPAC-compliant display. The use of HTML meta-language ensures the correct use of Greek letters, Roman numerals, superscript and subscript, among others. The list of HTML codes to be used can be found in Appendix 5.1. Non-converted CAS names should not be used.

4.4.3 Alias

Under the tab "Name" the name of the substance is added, then the name type is selected under "Type". English "Languages" is set by the program. No tick must be set for Display Name „DN“ or Additional Listing Name „AL“. The company codes can be entered with different spellings, depending on the reference database used (Figure 8).

Figure 8. Registering company code with different spelling.

For the locked synonyms (protected, non-public), the access lock must be closed, and in the options under the lock symbol, a tick is set for "Protected".

4.5 Structure

A molecular structure should be included for registering a chemical. This can be done in two ways:

- ▶ By using relevant SMILES
- ▶ By drawing the molecular structure

Under the "Structure" tab, a structure must be displayed for Chemical substance (Figure 9).

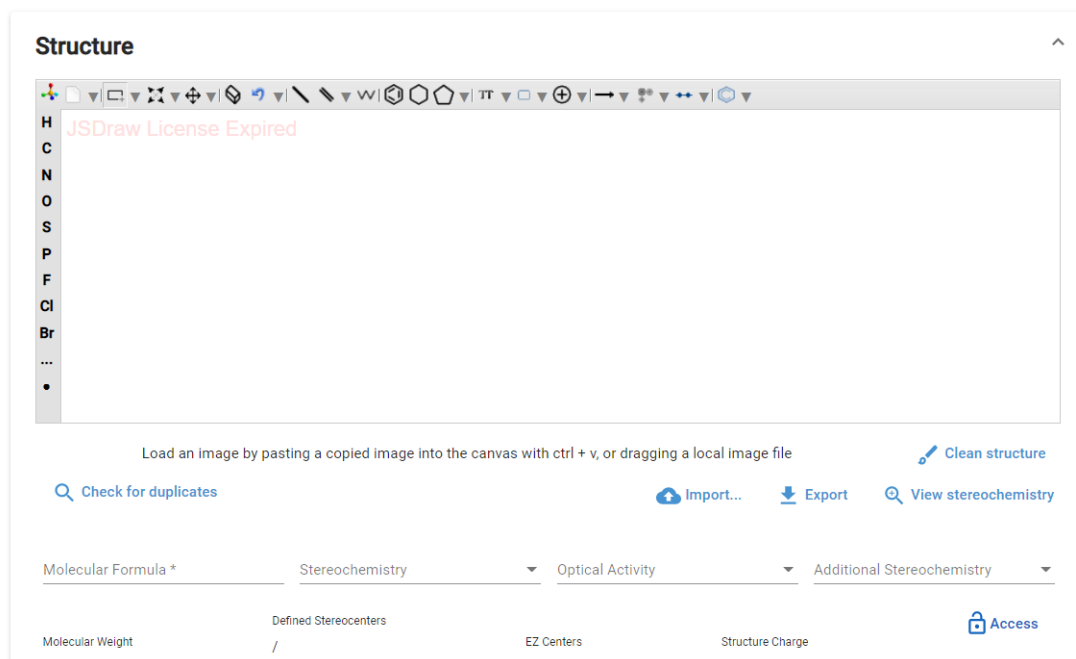
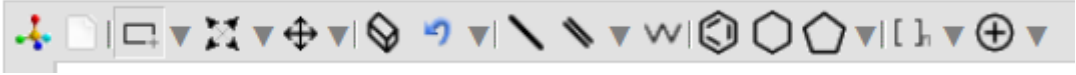










Figure 9. Drawing tool for registering a molecular structure.

4.5.1 Drawing tool for molecular structures

For chemicals, it is required to insert the molecular structure by using the drawing tool. Instructions for using the drawing tool are included below.

Table 6. Instructions for the horizontal part of the drawing tool.

	
	JSDraw V5.2.0 (java script editor for chemical structure and biologics)
	Clear all contents (new page)
	„Triangle“ for whole list of different tasks mainly for the selection of the structure
	„Triangle“ for whole list of different tasks changing the position of the structure (up to the middle), increasing, reducing, rotation
	„Triangle“ for whole list of different tasks changing the position of the structure, every direction possible
	Eraser
	„Triangle“ for whole list of different tasks back / forward arrow
	Single bond








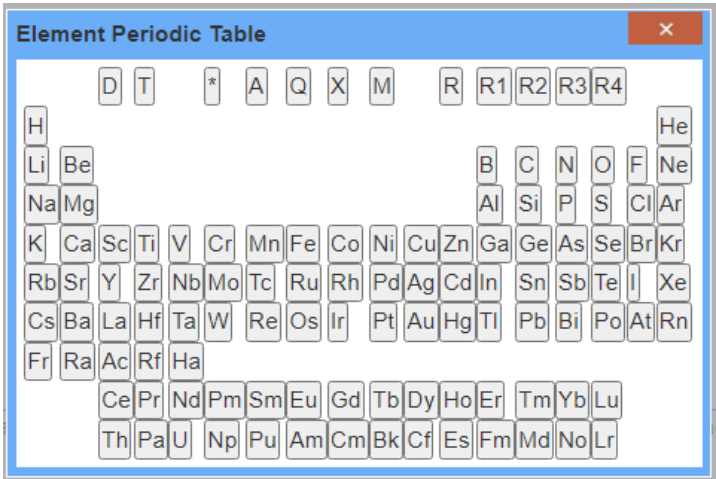
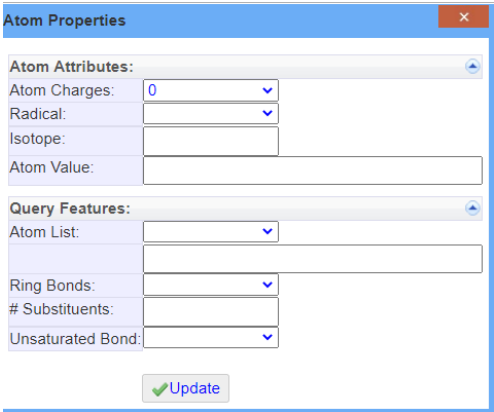
	<p>„Triangle“ for whole list of different tasks</p> <p>Other bonds</p>
	<p>Chain tool</p>
	<p>+ „Triangle“ for whole list of different tasks</p>
	
	
	<p>„Triangle“ for whole list of different tasks</p> <p>Brackets for e.g. polymers</p>
	<p>„Triangle“ for whole list of different tasks</p> <p>+ and – for ions</p>

Table 7. Instructions for the vertical part of the drawing tool.

<div style="display: flex; flex-direction: column; align-items: center;"> <div>H</div> <div>C</div> <div>N</div> <div>O</div> <div>S</div> <div>P</div> <div>F</div> <div>Cl</div> <div>Br</div> <div>...</div> <div>●</div> </div>	<div style="display: flex; align-items: center;"> <div style="width: 30px; height: 30px; background-color: #ccc; margin-right: 10px;"></div> <div> <p>Element periodic table:</p>  </div> </div>
	<div style="display: flex; align-items: center;"> <div style="width: 30px; height: 30px; background-color: #ccc; margin-right: 10px;"></div> <div> <p>Atom properties:</p>  </div> </div>

4.5.2 Entering of the Structure

The structure can be drawn using the drawing tool (Figure 9) or inserted as SMILES. For this purpose, SMILES can be copied from reference databases (e.g. SciFinder, G-SRS) (Figure 10) and then pasted in the structure area (Figure 11).

:

CAS

SciFinder[®]

Substances ▾

mevidalen

^

Other Names and Identifiers

Canonical SMILES

O=C(N1C(C=2C=CC=C(C2CC1CO)CCC(O)(C)C)CC=3C(Cl)=CC=CC3Cl

Isomeric SMILES

C(CC(C)(C)O)C1=C2C([C@H](C)N(C(C3=C(Cl)C=CC3Cl)=O)[C@@H](CO)C2)=CC=C1

Figure 10. SMILES as found in SciFinder.

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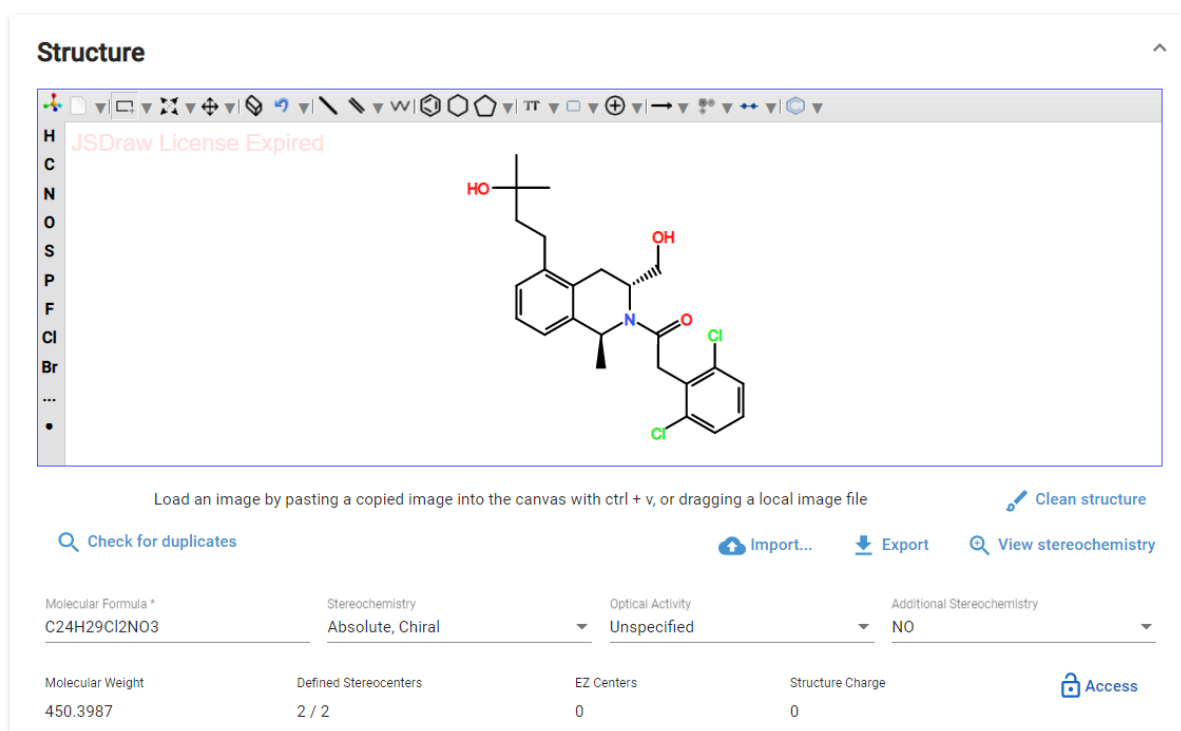



Figure 11. Molecular structure pasted in drawing tool.

Based on the displayed structure, both the molecular formula and the molecular weight are generated. The information on the stereochemistry is also obtained from the molecular structure.

The structure may be rotated by clicking on the rotate button: . An atom in the structure is marked by clicking on it. With a further click (+hold) in the image, the structure can be rotated as desired (Figure 12).

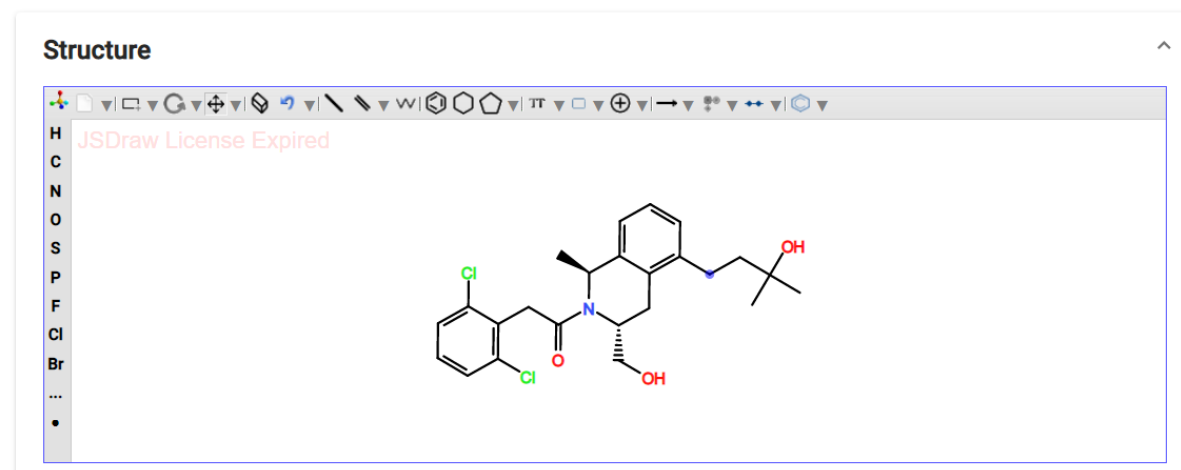


Figure 12. Rotated molecular structure.

Entering a reference is required for registering a molecular structure. However, this reference is not entered in the structure, but at the very top of the data set under "Definition Reference":

Figure 13. Registering a definitional reference.

If the structure can be released, definitional reference(s) should be inserted. Examples of possible references for the definition:

- ▶ INNs INN list reference
- ▶ Pharmacopoeia pharmacopoeia reference
- ▶ General reference confirmation of the structure (e.g. CAS, G-SRS)

If publication of the dataset is allowed, the Access lock icon should be opened. To enable the release, a tag “Public Domain Release” must be inserted at a definitional reference at this time. The release of the record should only be done finally when all information on the substance has already been entered.

4.6 Codes

The code section in edit mode includes substance identifiers from other databases, RMS category, RMS domain and ATC code. In browse mode all those codes will be displayed in two different sections. Substance identifiers from other databases will be displayed as identifier. RMS category, RMS domain and ATC code will be shown as classifications.

4.6.1 Substance identifiers from other databases

The codes of the substance can be selected from the code system drop down list. Type of the code is also defined by the drop-down list. There are several types that can be selected from the list:

- ▶ Primary: to be used if the code uniquely describes the structure
- ▶ Generic (family): is selected if the code is not precisely specified and can be assigned to several substances, whole family
- ▶ Superseded: is set if the code number is already deprecated
- ▶ Alternative: is used when there are two codes that correctly describe the same structure. It is often found on SciFinder for recently recorded substance.

To enter the CAS No., CAS is selected from the “Code System” drop-down list (Figure 14). The type is set as described above. Cas No. is then inserted under Code.

The screenshot shows the 'Registration of CAS ID' form. At the top, there are four dropdown menus: 'Code System *' (set to CAS), 'Code System Type' (set to CHEMICAL), 'Type' (set to PRIMARY), and 'Code #' (set to 1638667-79-4). To the right of these is an 'Access' button with a lock icon. Below these are three text input fields: 'Url', 'Code text' (with placeholder 'Enter text here'), and 'Comments' (with placeholder 'Enter text here'). At the bottom left, there is a 'References' section with a count of 1. At the bottom right, there are two buttons: 'Create new' with a plus icon and 'Reuse' with a download icon, followed by a small downward arrow.

Figure 14. Registration of CAS ID.

CAS No. is a single identifier that requires a reference. Figure 15 shows how to enter a reference for CAS ID.

The screenshot shows the 'Add Reference' dialog box. It contains several input fields: 'Source Type *' (set to STN (SCIFINDER)), 'Source Text/Citation *' (set to STN), a checked 'Public Domain' checkbox, and an 'Access' button with a lock icon. Below these are three more input fields: 'URL', 'Source Id', and 'Tags'. At the bottom left, there are two links: 'Upload Document' with a cloud icon and 'Use Previous Substance Reference'. At the bottom right, there are 'Cancel' and 'Save' buttons.

Figure 15. Reference for CAS ID.

Other codes (e.g. FDA-UNII, SMSID, xEVMPD, INN, EDQM) are included in the same manner, but they do not require a reference. EU-SRS will automatically construct URLs for the following Code Systems which can be accessed in the hyperlink on the view page. An overview of code systems and associated hyperlinks is included in Table 8

Table 8. Code systems and associated hyperlinks.

Code System	Hyperlink
CAS	ChemIDplus (from 2023: CAS Common Chemistry)
FDA-UNII	G-SRS
PubChem	PubChem
INN	The School of INN
EDQM	Knowledge Database EDQM
NCI Thesaurus	NIH National cancer institute

4.6.2 RMS category and domain

The classification of the substance is entered under code section. To enter the “category” or “domain”, RMS is selected from the “Code System” drop-down list. The type is set to “Generic (family)” and the number of the category is added under “Code”.

The screenshot shows a registration form with the following fields and values:

- Code System ***: RMS (not in CV)
- Code System Type**: (empty)
- Type**: GENERIC (FAMILY)
- Code ***: 100000000012
- Access**: (lock icon) Access ^
- Url**: (empty)
- Code text**: Enter text here
- Comments**: Enter text here
- References**: 0
- Create new**: (+) ^

Figure 16. Registration of RMS domain.

Neither category nor domain need a reference. The use of the type generic is mandatory.

Some CVs have overlap with SMS and are managed in RMS. These CVs include:

- ▶ **Domain:** to indicate for which domain the substance is used for. This can be either human use or veterinary use (Table 9)
- ▶ **Category:** to indicate the substance type in EU-SRS (Table 9)

Table 9. Applicable RMS codes for Domain and Category for chemicals.

RMS Code	Domain
100000000012	Human use
100000000013	Veterinary use
RMS Code	Category
100000075670	Chemical

4.6.3 ATC code

The ATC Code level 5 of the substance is entered under code section. The “WHO-ATC” is selected from the “Code System” drop-down list. The type is set to “Generic (family)” and the number of the category is added under “Code” (Figure 17).

Code System *
WHO-ATC

Code System Type
PHARMCLASS

Type
GENERIC (FAMILY)

Code *
R02AX02

Access

Url

Code text
Enter text here

Comments
Enter text here

References 0

Create new Reuse

Figure 17. Registration of ATC Code using the example of ATC of Ibuprofen.

ATC code does not require a reference. The use of the type “Generic (family)” is mandatory. “Code system type”: “Pharmclass” is generated by the system.

NOTE: Check the information in the browse mode. If ATC code is shown there under tab Identifier, it means that this code is not yet stored. In such a case inform the key user.

In such cases it is also possible to build the hierarchy tree from the WHO-ATC hierarchy itself by adding the levels in “Code text” one after the other in the following way: “ATC| Level 1| Level 2| Level 3| Level 4| Level 5”. In this way ATC Code will also be displayed as Classification in browse mode.

4.7 Notes

Notes are generated automatically and includes system validation messages.

4.8 Properties

Additional substance details can be added to the “Properties” card (Figure 18). However, Properties are less relevant for chemicals than for other substance types. For some substances, pharmacokinetics information may already be available. The following are the most commonly measured pharmacokinetic characteristics: T_{max} , C_{max} , Volume of distribution and Dose. The “Pharmacokinetic” is selected from “Property type” drop-down list. The name of characteristic is specified under “Name”. Parameters can be added optionally. They are specified in a free text field. The low and high limits are shown under Amount.

Name *
Tmax (not in CV)

Property Type *
PHARMACOKINETIC (not in CV)

Defining
☐ Referenced Substance

Access

Parameters +

FOOD EFFECT - [1.34 to 1.96] hours (average) - ORAL DOSE

Amount

Type **	Average	Low	High	Low Limit	High Limit	Units	Non-numeric Value
		1	2			hours (not in ...)	ORAL DOSE

Access

Figure 18. Registration of pharmacokinetics using the example of Ibuprofen.

4.9 Relationships

Relationships can only be generated for existing data sets.

4.9.1 Active Moiety

If a salt is entered, the basic substance must be registered first. In the "Salt" data set, the basic substance is then inserted at this point (Figure 19). The basic substance is often the active substance of the salt and can be expressed in relation to the associated substance. If an active substance is selected at the salt level, this salt is linked in the hierarchy of the parent substance.

Example: Mevidalen hydroxybenzoate is the salt of mevidalen. In the salt dataset, Mevidalen hydroxybenzoate, active moiety (mevidalen) is inserted.

Relationships

[Add Relationships +](#)
[Collapse All](#)



Mevidalen

Related Substance

Type *
ACTIVE MOIETY

Access Mediator Substance

Qualification Interaction Type

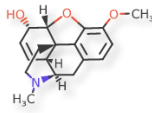
Comments
Enter text here

Figure 19. Registration of active moiety.

Under "Related Substance", a name (preferably the longest part of the name) or CAS No. can be searched for and the desired substance selected. „Active moiety" is selected as "Type" from the drop-down list. It is not necessary to enter references.

4.9.2 Impurities

Impurities are also assigned under "Relationships" (Figure 20). Only impurities of Ph. Eur. monographed substances are registered. In order to create a relationship between an impurity and the related substance, the impurity must already be registered before registering the related substance in the database. The procedure is similar for all "Relationships". In the field "Related Substance", the substance can be found and selected from the database by means of the name or the CAS No.. Under "Type", the relationship between the substance and its "Relationship" is selected. For the impurities, "Impurity -> Parent" (it means: "it is an impurity of the registered substance") must be selected.



Related Substance

Type *
IMPURITY -> PARENT

Access Mediator Substance

Qualification
Ph. Eur.

Interaction Type
CHROMATOGRAPHIC PURI...

Comments
Enter text here

Codeine

Amount

Type ** Average Low High Low Limit High Limit Units Non-numeric V... Access

0.2 %

References 1

Create new Reuse

Type	Citation	Public Domain	Access	Edit	Deselect	Tags
EP	Ph. Eur. 10.0/1244	Yes	Public			Apply to

Figure 20. Registration of Impurities.

Qualification (Ph. Eur.) and method of investigation described in the monograph are specified. Under Amount certain maximum permissible value of this impurity is included. Reference defines the source for this specification.

4.9.3 Other relevant Relationships

All relations that have an arrow in their name can be registered to both basis substance and the related record. Other record gets the reverse relations added automatically. All relevant relationships are included in Table 10.

Table 10. Listing of relevant relationships.

Relationship	Comment
Active moiety	results in generation of the hierarchy
BASIS OF STRENGTH	results in generation of the hierarchy
DEGRADENT->PARENT	
DIASTEREOISOMER->EPIMER	
ENANTIOMER->ENANTIOMER	
ENANTIOMER->RACEMATE	
EPIMER->DIASTEREOISOMER	
IMPURITY->PARENT	generates new tab (Impurities) in browse mode
INDUCER->TRANSPORTER	
INHIBITOR->TARGET	
METABOLITE ACTIVE->PARENT	

Relationship	Comment
METABOLITE->PARENT	
PARENT ORGANISM->PART/FRACTION	
PARENT->DEGRADENT	
PARENT->IMPURITY	is automatically generated at the child record under Relationships when 'impurity --> parent' is registered
PARENT->METABOLITE	
PARENT->METABOLITE ACTIVE	
PARENT->SALT/SOLVATE	can be recorded for the base substance as well as for the salt/solvate. This relation leads to a link between both data sets and allows a change from basis substance to all relevant salts.
PART/FRACTION->PARENT ORGANISM	
RACEMATE->ENANTIOMER	
SALT/SOLVATE->PARENT	can be recorded for the base substance as well as for the salt/solvate. This relation leads to a link between both data sets and allows a change from basis substance to all relevant salts.
TARGET->INHIBITOR	
TRANSPORTER->INDUCER	

4.10 References

References can be included directly during the registration of names, codes or relationships, etc. Alternatively, registration can be started by recording all references, which are then used in the course of registering further information. References can be added, updated, or removed from this card. Public Domain checkbox should be added for all public references. Every public name should have at least one reference with Public Domain checkbox. Public Domain Release Tag should be used for public records and added to the record when the lock for the full dataset is opened. This is then equivalent to the release for public of the dataset. The complete list of valid references can be found in Appendix 3.

4.11 Completion of Registration

To complete the registration of "Chemical", a "Definition Reference" must be inserted. If the record is allowed to be published, the Access lock icon should be opened.

The data set is not saved and inserted into the database until "Submit" is selected. A dialogue window appears (Figure 21). If all messages are highlighted in green, click on "Dismiss All" and then on "Submit". The data set can now be viewed with "View Substance" in the browse mode.

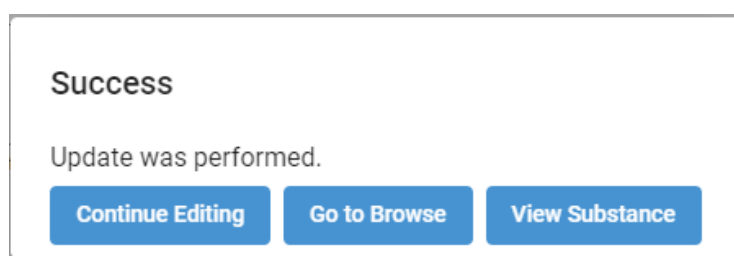


Figure 21. Notification of completed substance registration.

If messages with a yellow background appear, these details must first be checked for correctness. Registration can still take place. Messages with a red background do not allow registration. These errors must first be corrected in the data set so that registration can subsequently take place.

NOTE: Please make sure that the editing of the substance mode does not exceed 120 min. If this time is exceeded, submission is not possible.

4.12 Verification of completed record

After completion of the registration, the whole record should be verified in browse mode (Figure 22). If the record has been verified, it should be approved and pushed to the production environment.

Overview	>					
Structure	>					
Names 5	>					
Identifiers 6	>					
Notes 2	>					
Audit Info	>					
References 10	>					
Moieties 1	>					

Names					
Search					
Name	Type	Language	Details	References	
mevidalen ✓	Official Name	English	View	View	
2-(2,6-dichlorophenyl)-1-[(1 <i>S</i> ,3 <i>R</i>)-3,4-dihydro-3-(hydroxymethyl)-5-(3-hydroxy-3-methylbutyl)-1-methyl-2(1 <i>H</i>)-isoquinolinyl]ethanone	Systematic Name	English	View	View	
2-(2,6-dichlorophenyl)-1-[(1 <i>S</i> ,3 <i>R</i>)-3-(hydroxymethyl)-5-(3-hydroxy-3-methylbutyl)-1-methyl-3,4-dihydroisoquinolin-2(1 <i>H</i>)-yl]ethan-1-one	Systematic Name	English	View	View	
LY 3154207	Code	English	View	View	
LY3154207	Code	English	View	View	

Figure 22. Extract from the browse mode.

4.13 Concept upgrade

Some chemicals were registered as concepts during the data load in EU-SRS. Under Concept, chemicals can also be registered in the simplified registration procedure. These records can be found in Browse mode in this way by using of RMS Chemical Category: 10000075670. The data sets under Concept can be upgraded to correct chemical record when the complete information on the substance is available.

For the Concept upgrade to “Chemical” the following steps are necessary:

1. Go to the field “Advanced Features” in the headline.
2. Click in the scroll down menu on “Change Substance Class”.
3. Choose the applicable substance class in the field ‘New Class’.
4. Check the names under Names after which the chemical record was opened.
5. Continue with the steps described from section 4 above.

4.14 Change Reason

If a substance is updated (e.g. new name added), the reason for creating a new version must be recorded under Change reason. This tab appears only from the second version. So, it is not present at the first registration. In order to simplify the future search, a short valid reason should be given if possible. Examples of change reasons are summarized in Table 11. Selecting multiple change reasons is possible, e.g. name, codes, relationships.

Table 11. Examples of change reasons.

Change reason	Comment
Name	Name was added/removed
Codes	Code was added/removed
PT	Preferred Term was changed
Structure	Update of structure
Substance	Whole review of the record
References	References were added/removed
Relationships	Relationship was added/removed
Properties	Properties was added/removed
Modification	Modification was added/removed

5 Appendix

5.1 HTML code elements for displaying special characters

HTML Code	HTML View
₂	x ₂
²	x ²
←	←
→	→
<	<
>	>
±	±
Α	Α
α	α
Β	Β
β	β
Γ	Γ
γ	γ
Δ	Δ
δ	δ
Ε	Ε
ε	ε
Ζ	Ζ
ζ	ζ
Η	Η
η	η
Θ	Θ
θ	θ
Ι	Ι

HTML Code	HTML View
ι	Ι
Κ	Κ
κ	κ
Λ	Λ
&lambd;	λ
Μ	Μ
μ	μ
Ν	Ν
ν	ν
Ξ	Ξ
ξ	ξ
Ο	Ο
ο	ο
Π	Π
π	π
Ρ	Ρ
ρ	ρ
Σ	Σ
σ	σ
Τ	Τ
τ	τ
Υ	Υ
υ	υ
Φ	Φ
φ	φ
Χ	Χ

HTML Code	HTML View
χ	Χ
Ψ	Ψ
ψ	ψ
Ω	Ω
ω	ω
±	±
ß	ß
Ä	Ä
ä	ä
Ö	Ö
ö	ö
Ü	Ü
ü	ü
§	§
¯	-
Ⅰ	I
Ⅱ	II
Ⅲ	III
Ⅳ	IV
Ⅴ	V
Ⅵ	VI
Ⅶ	VII
Ⅷ	VIII
Ⅸ	IX
Ⅹ	X
Ⅺ	XI

HTML Code	HTML View
Ⅻ	XII
ⅩⅢ	X III
ⅩⅣ	X IV
ⅩⅤ	X V
ⅩⅥ	X VI
ⅩⅦ	X VII
ⅩⅧ	X VIII
ⅩⅨ	X IX
ⅩⅩ	X X

5.2 Valid source types and citations

Source Type	Citation	Comment
EMA LIST	SMS	Reference for SMS Names Tag: Public domain release for Public dataset
EMA LIST	SVG	Reference for Public names without valid public source Tag: Public domain release for Public dataset
CAS	CAS (SciFinder)	Reference for Names
STN (SCIFINDER)	STN	Reference for CAS ID in tab Codes
CHEMID	ChemIDplus	
CHEMSPIDER	ChemSpider	
PUBCHEM	PubChem	
FDA_SRS	FDA-GSRS	
FDA_SRS	G-SRS	
CLINICALTRIALS	AdisInsight or USNCT or ICTRP	
IUPAC	IUPAC Name	
INN List	INN description	INN chemical name, definitional name from INN list. The chemical substances are supposed to be IUPAC names.
INN List	INN recommended List No	the number of the published recommended INN list. Tag: Public domain release can be added for Public dataset. Link to pdf file of list can be also added.
INN List	INN proposed List No.	the number of the published proposed INN list. Tag: Public domain release can be added for Public dataset. Link to pdf file of list can be also added.
EUROPEAN PHARMACOPOEIA	Ph. Eur.: Issue, monograph number	e.g. Ph. Eur.: 10.0, 2118
BRITISH PHARMACOPOEIA	BP year	e.g. BP2022
USP/NF	USP issue	e.g. USP42

Source Type	Citation	Comment
MARTINDALE	Martindale year	e.g. Martindale 2022
BAN	BAN	Britisch Approved Name
JAN	JAN	Japanese Accepted Names
AAN	AAN	Australian Approved Name
USAN Coun	USAN	To be used for the USAN designation
USAN Coun	USAN description	To be used for USAN chemical names
JAN	JAN	Japanese Accepted Names
AAN	AAN	Australian Approved Name
International nomenclature of cosmetic ingredients	INCI	
NCI DRUG DICTIONARY	NCI drug dictionary	
NCI THESAURUS	NCI thesaurus	
ORPHAN DRUG	Orphan.desig:FDA Orphan.desig:EU	

5.3 List of relevant databases for substances

When additional information concerning a substance is needed, the following databases can be used as a reference:

Database	Description
INN	The INN Programme assigns International Nonproprietary Names to medicinal substances through a broad consultative process. WHO is responsible for the INNs.
European Pharmacopoeia	The purpose of the European Pharmacopoeia is to promote public health by the provision of recognised common standards for the quality of medicines and their components. As these standards ensure that medicines reaching the market are safe for use by patients, it is essential that they are appropriate. Their existence also facilitates the free movement of medicinal products in Europe and beyond.
Medicines Complete	A site which guides on to several different publications, databases containing information about medicines.
Inxight: Drugs	Site provided by NIH, National Center for Advancing Translational Sciences. Information about e.g. treatment and pharmacology.
FDA Substance Registration System	Registration system in the U.S. by FDA and the U.S. National Library of Medicine (NIH), provides UNII-codes, Unique Ingredient Identifier.
G-SRS	Database built by GiNAS, NIH. This is the basis for the EU-SRS.
United States Approved Names	This is a site for USAN, where to find the approved names, provided by American Medical Association, AMA.
Japanese Accepted Names	This is a site for JAN, where to find the approved names, as part of the Japanese Pharmacopoeia.
PubChem	Chemical information from authoritative sources provided by U.S. National Library of medicine, NIH
European Union Food Additives	This database can serve as a tool to inform about the food additives approved for use in food in the EU and their conditions of use. It is based on the Union list of food.
EU CosIng	CosIng is the European Commission database for information on cosmetic substances and ingredients.
European Chemicals Agency	ECHA is an agency of the European Union and the site provides data from registration dossiers.

Database	Description
EC Active substance database	Site from the European Commission and it provides General index of products by active substance.
Merck Index	Online version of the Merck index, regarded as the most authoritative and reliable source of information on chemicals, drugs and biologicals. Now this trusted resource is available online from the Royal Society of Chemistry.
EU Orphan Database	Site from the European Commission and it provides The Community Register of orphan medicinal products.
FDA Orphan substance database	Site from FDA and it provides The Community Register of orphan medicinal products.
Index Nominum	This is an International Database of Pharmaceutical Substances and Preparations, provided by Wissenschaftliche Verlagsgesellschaft Stuttgart
International Pharmacopoeia	International Pharmacopoeia provided by WHO.
Scifinder	Research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.
FDA Inactive Database	Site provided by FDA with a database of Inactive ingredients.

5.4 EU-SRS field guidance for registering and/or editing of a chemical

EU-SRS field name	Field details
Overview	
Preferred Term	Decide if the name complies to the PT rules listed in section 3.2.1 for registration in EU-SRS.
Definition Type	Always Primary.
Definition Level	Always Complete.
Deprecated	Relevant for a Deprecated Record.
Record Level Access	If no box is ticked the record is public. If it should be non public choose 'PROTECTED'. 'PROTECTED' means that the record cannot be exported.
Substance tags	<i>Not applicable.</i>

EU-SRS field name	Field details
Definitional References	Field linked to Reference section.
Names	
Name (Display Name/Preferred Term in EU-SRS)	<p>Each record needs a Preferred term, which is the displayed name in EU-SRS.</p> <p>Necessary details: Choose a name type, Language always 'English', tick 'DN' (= Display Name)', choose a naming organisation, check if a public reference is given. Detailed information on the single fields can be found below.</p>
Name (Additional name in EU-SRS, could be PT in SMS)	May be added, but the Display Name is sufficient. If there is a record in SMS (which is not necessarily the case), the common name used as PT in SMS should always be included as alias in the record as an Additional Listing Name ('Common Name').
Type	<p>Each name type can be chosen, as appropriate. If it is possible to choose between more than one name type, the following prioritisation should be used: Official Name, Common Name, Systematic Name, Company Code, Brand Name .</p> <p>The Official Name is any name used by an Official Naming body. An Official Naming Body is any organization allowed to Name a Substance.</p> <p>PT = appropriate name type (e.g., 'Official Name', 'Systematic Name'), Alias = PT in SMS = 'Common Name', Other Alias = 'Common Name' or other name type</p>
Access	If the information in the record is confidential, Access can be set to 'PROTECTED', but the name should have a public and a confidential reference.
DN	DN = Display Name: Tick box to indicate what name should be the Display Name in EU-SRS (= Preferred Term in EU-SRS). Mandatory for the EU-SRS-PT.
AL	<p>AL = Additional Listing Name: Field is mandatory for the SMS-PT (not to be ticked for other aliases).</p> <p>If EU-SRS-PT is the same as SMS-PT both check boxes should be used.</p>
Standardized Name	<i>Not applicable.</i>
Languages	Always English.
Domains	<i>Not applicable.</i>
Jurisdiction	<p>Field is optional when an 'Official Name' type is selected.</p> <p>Example: USAN would have Jurisdiction United States.</p>
References	At least one public reference is needed per name. References can be newly created or reused.

EU-SRS field name	Field details
Naming Organization	Field is only displayed if 'Official Name' type is chosen. If displayed it is conditional. Mandatory when the organization are INN, EP., USAN, BAN, JAN, AAN, INCI.
Structure	
Structure	Load an image by pasting a copied image into the canvas with ctrl + v, or dragging a local image file.
Molecular Formula	Filled in by the system.
Stereochemistry	Filled in by the system.
Optical Activity	Filled in by the system.
Additional Stereochemistry	Filled in by the system.
Stereo Comments	Additional field for possible comments. Free text field.
Codes	
Code system	<p>SMSID is always mandatory unless an SMSID is not available - then the SMS team will be asked for. Preferably other public sources are added when available, e.g., INN, EDQM, CAS, PubChem, Wikipedia.</p> <p>Classification: Besides the codes from the source databases used, the classification of the substance is entered under code section, which is relevant for searching. To enter the 'category' or 'domain', RMS is selected from the drop-down list.</p>
Code System Type	<i>This is a default value (automatically filled in and managed by Admin).</i>
Type	In nearly all cases default 'Primary' (code uniquely describes the substance). When the code is tied to a group/used for classification (Code system 'RMS') use 'Generic (Family)'. Superseded is set if the code is already deprecated.
Code	<p>Alpha numeric value.</p> <p>Classification: A list of all RMS categories and domains is shown in Table 9. Relevant is the code for the domain 'Human use' or 'Veterinary use' and the category 'Polymer'</p>
Access	Set to Public from the system after the import from SMS (standard = Public).
URL	Will be generated automatically
Code Text	<i>Not applicable.</i>
Comments	<i>Not applicable.</i>

EU-SRS field name	Field details
References	For CAS ID add STN reference
Relationships	
Related Substance	can be selected directly by the search from the dataset
Type (purpose hierarchy)	'Active Moiety' and 'Basis of strength' is selected if the substance is to be assigned to a higher-level data set (e.g. Ibuprofen is the active moiety of Ibuprofen sodium)
Type (purpose not hierarchy)	All relations that have an arrow in their name can be registered to both basis substance and the related record. Other record gets the reverse relations added automatically. For more information see section 4.6.3.
Access	<i>Not applicable.</i>
Mediator Substance	<i>Not applicable.</i>
Qualification	Ph. Eur.: is registered for Ph. Eur. impurities of monographed substances (for relationship: 'Impurity → Parent').
Interaction Type	investigation described in the monograph are specified (e.g. HPLC) (for relationship: 'Impurity → Parent').
Notes	
Note	Field is optional and automatically populated by the system.
References	<i>Not applicable.</i>
Access	<i>Not applicable.</i>
Properties	
Name	Density, Mol_Weight: Number Average, Mol_Weight:Weight Average, Particle size, Viscosity:Dynamic, Viscosity:Kinematic can be selected from the drop-down list.
Property Type	Chemical, Enzymatic or Physical can be selected as Property type from the drop-down list
Defining	Default is empty Tick box. The check mark can be set if the requirements are mandatory. It is also used in the family of substances that differ in their certain properties
Referenced Substance	<i>Not applicable.</i>
Parameters	<i>Not applicable/</i>
Amount	appears as a pop-up window. The type information 'mol ratio' or 'weight ratio' can be registered, as mean value (Average), or range (Low Limit and High Limit). Units can be selected, but it is not

EU-SRS field name	Field details
	mandatory. Access is set to Public from the system after the import from SMS (standard = Public).
References	<i>Not applicable.</i>
Access	<i>Not applicable.</i>
References	
Source Type	CV-List; Mandatory field; Additional value not in CV is possible as temporary value (note: be careful with adding a new value, this needs to be communicated with the technical team).
Source text/Citation	Mandatory field and should represent the related value of the type.
Public Domain	Default is Public (Tick box), but it may be set 'Non-Public' in combination with a public reference.
Access	Default is 'Public'. Confidential = tick 'PROTECTED'.
URL	This field is optional .
Source Id	<i>Not applicable.</i>
Upload a Document	This field is optional.
Tags	This field should be populated by at least one value ('Public domain release') and if applicable other values.
Change Reason	
Change Reason	Add the reason of the change of the record that led to the creation of a new version. Use short notes (if something was added, edited or removed), e.g. Name, Code, RMS, Reference, Naming Organization.