

# Substance identity - screening of the registration dossiers

Issue type 2, 6, and 7

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# Substance identity IT screening campaign

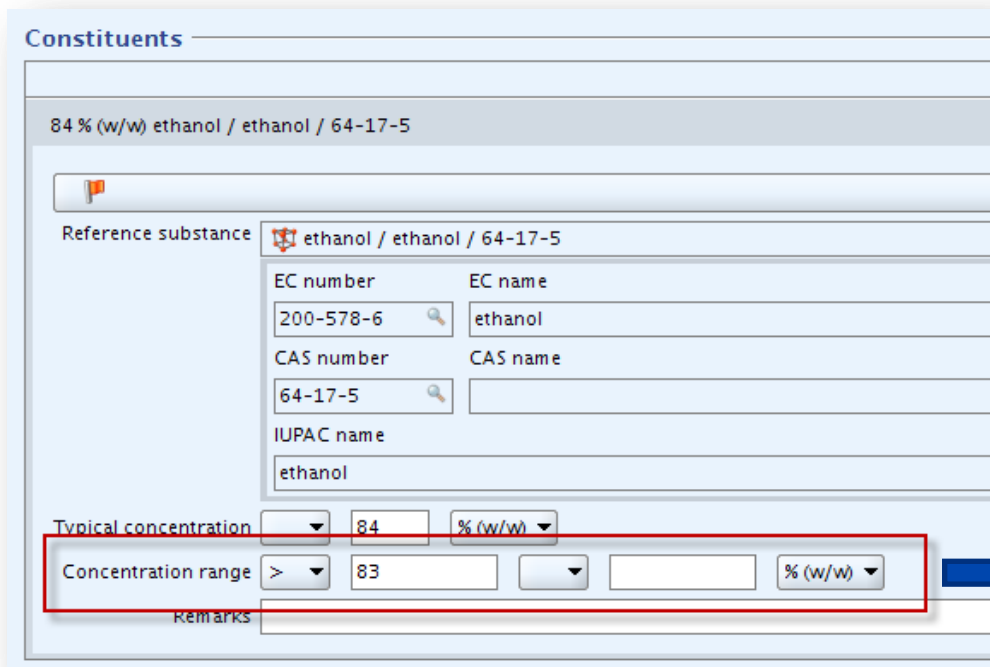
Scope defined by 10 Issue types:

1. Missing concentration ranges
2. Typical concentration outside of concentration range
3. Composition reported with no constituents
4. Low or ambiguous degree of purity for well-defined substances
5. Unidentified constituent or impurity present at significant concentration
6. Well-defined substance with inconsistency between degree of purity and constituent concentrations
7. Well-defined substance with inconsistency between degree of purity and impurity concentrations
8. No spectral and analytical information provided
9. Additives without stabilising function
10. Inconsistent identifiers of constituents, impurities and additives

## **Please take into consideration the following preliminary remarks:**

- In IUCLID section 1.2 (Substance composition), the degree of purity and the concentration (for constituents, impurities, and additives) are expected to be reported as ranges, i.e. indicating the lower and upper limits.
- These values should be based on analytical data, and should be representative of the substance as manufactured/imported. Regulatory values (e.g. 80-100%) should not be used (unless they are representative of analytical data).

- For the IT-tool screening, some assumptions were made in the case of missing values to make a specific interpretation of the ranges according to the values provided in the dossier. Therefore, in some cases, the issue may be solved by simply filling in the missing values.



The screenshot shows the 'Constituents' section of an IT-tool interface. At the top, it displays '84 % (w/w) ethanol / ethanol / 64-17-5'. Below this, there is a 'Reference substance' section with a search icon and the text 'ethanol / ethanol / 64-17-5'. This section contains several input fields: 'EC number' (200-578-6), 'EC name' (ethanol), 'CAS number' (64-17-5), 'CAS name' (empty), and 'IUPAC name' (ethanol). At the bottom of the form, there are three rows of input fields: 'Typical concentration' (84 % (w/w)), 'Concentration range' (> 83 % (w/w)), and 'Remarks' (empty). A red box highlights the 'Concentration range' field, and a blue arrow points from this box to the explanatory text on the right.

The concentration range is assumed to be >83 and <100 % (w/w)

*Please note that, in general, the examples in this presentation are invented to illustrate and explain the different issue types better. Please note that these examples are only for illustration of these issue types and without any practical or scientific considerations.*



# **Issue type 2: Typical concentration outside of concentration range**

**➔ (IUCLID section 1.2)**



## Issue type 2: Typical concentration outside of concentration range

### Example

#### Excerpt from the information letter:

***"Typical concentration outside of concentration range.***

*The typical concentration of the constituent with reference substance name "xxxx" and IUPAC name "xxxx" in the composition with name "xxxx" and local UUID "xxxxxxxxxxxxxxxxxxxxxxxxxxxx" is outside the concentration range."*

Constituents

0.8 % (w/w) methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate / methyl octadeca-9,12,15-tri...

EU: REACH

Reference substance: methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate / methyl octadeca-9,12,15-tri...


EC number	206-102-3	EC name	methyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate
CAS number	301-00-8	CAS name	
IUPAC name	methyl octadeca-9,12,15-trienoate		

Typical concentration: 0.8 % (w/w)

Concentration range: >= 1 % (w/w) to <= 20 % (w/w)

Remarks:

This example is relative to constituents, but the shortcomings apply to impurities and additives as well





**Issue type 6:  
Well-defined substance  
with inconsistency  
between degree of purity  
and constituent  
concentrations**

**→ (IUCLID section 1.2)**



## **Issue type 6: Well-defined substance with inconsistency between degree of purity and constituent concentrations.**

### **Example 1: mono-constituent substance**

#### **Excerpt from the information letter:**

***“Well-defined substance with inconsistency between degree of purity and constituent concentrations.*”**

*The composition with name “xxxx” and local UUID “xxxxxxxxxxxxxxxx” contains the constituent with reference substance name “xxxx” and IUPAC name “xxxx” for which the reported typical concentration and/or concentration range suggest that it can be present at a higher concentration than the maximum degree of purity.”*

**Substance composition**

Ethanol for webinar

Name: Ethanol for webinar

Brief description:

Composition ID: L-0ed32ceb-8b9e-4dcf-9eb2-af6acc1c80b1

**Degree of purity**

> 80 < 90 % (w/w)

**Constituents**

95 % (w/w) ethanol / ethanol / 64-17-5

Reference substance: ethanol / ethanol / 64-17-5

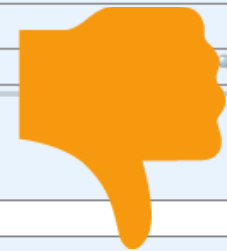
EC number	200-578-6	EC name	ethanol
CAS number	64-17-5	CAS name	
IUPAC name	ethanol		

Typical concentration: 95 % (w/w)

Concentration range: > 80 < 100 % (w/w)

Remarks:

The maximum degree of purity (90 %) is not consistent with the typical concentration (95 %) and the upper limit of the concentration range (100 %)



## Substance composition

Ethanol for webinar

Name

Brief description

Composition ID

**Degree of purity**

% (w/w)

**Constituents**

90 % (w/w) ethanol / ethanol / 64-17-5

Reference substance

EC number	EC name
<input type="text" value="200-578-6"/>	<input type="text" value="ethanol"/>
CAS number	CAS name
<input type="text" value="64-17-5"/>	<input type="text"/>
IUPAC name	
<input type="text" value="ethanol"/>	

Typical concentration  % (w/w)

**Concentration range**   % (w/w)

Remarks

For **mono-constituent** substances, the degree of purity must correspond to the concentration range of the constituent.



## Issue type 6: Well-defined substance with inconsistency between degree of purity and constituent concentrations

### Example 2: multi-constituent substance

Excerpt from the information letter:

***"Well-defined substance with inconsistency between degree of purity and constituent concentrations.***

*The composition with name "xxxx" and local UUID "xxxxxxxxxxxxxxxxxxxx" contains an inconsistency between the degree of purity and the concentration ranges of the constituents. The maximum concentration of the constituent with reference substance name "xxxx" and IUPAC name "xxxx" is 70 % (w/w) and when added to the minimum concentrations of the remaining constituents (30 % (w/w)) is higher than the maximum degree of purity (90 % (w/w))."*

**Substance composition**

Ethanol for webinar

Name: Ethanol for webinar

Brief description:

Composition ID: L-71d7017a-75e1-4df4-8c48-e38b0c137680

**Degree of purity**

> 71 < 90 % (w/w)

**Constituents**

60 ethanol / ethanol / 64-17-5

Reference substance: ethanol / ethanol / 64-17-5

Typical concentration: 60 % (w/w)

Concentration range: > 40 < 70 % (w/w)

Remarks:

40 % (w/w) methanol / methanol / 67-56-1

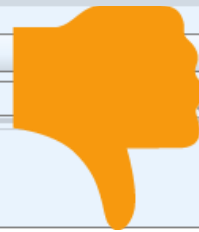
Reference substance: methanol / methanol / 67-56-1

Typical concentration: 40 % (w/w)

Concentration range: > 30 < 50 % (w/w)

Remarks:

The maximum degree of purity (90 %) is not consistent with the sum of the maximum concentration of one constituent and the minimum concentration of the other(s) (70+30 %)



## Substance composition


Ethanol for webinar

Name: Ethanol for webinar

Brief description:

Composition ID: L-71d7017a-75e1-4df4-8c48-e38b0c137680


**Degree of purity**



> 78 < 96 % (w/w)

**Constituents**

58 % (w/w) ethanol / ethanol / 64-17-5




Reference substance: ethanol / ethanol / 64-17-5

Typical concentration: 58 % (w/w)

Concentration range: > 52 < 62 % (w/w)

30 % (w/w) methanol / methanol / 67-56-1



Reference substance: methanol / methanol / 67-56-1

Typical concentration: 30 % (w/w)

Concentration range: > 25 < 40 % (w/w)

Remarks:

For **multi-constituent** substances, the degree of purity must correspond to the overall concentration range of the constituents.



**Issue type 7:  
Well-defined substance  
with inconsistency  
between degree of purity  
and impurity  
concentrations**

**→ (IUCLID section 1.2)**





## **Issue type 7: Well-defined substance with inconsistency between degree of purity and impurity concentrations.**

### **Example 1: shortcomings concerning the maximum degree of purity**

**Excerpt from the information letter:**

***"Well-defined substance with inconsistency between degree of purity and impurity concentrations***

*The composition with name "xxxx" and local UUID "xxxxxxxxxxxxxx" contains in total 2 impurities for which the sum of the minimum concentrations (12 % (w/w)) is inconsistent with the maximum degree of purity (100 % (w/w))."*

## Substance composition

Ethanol for webinar

Name: Ethanol for webinar

Brief description:

Composition ID: L-71d7017a-75e1-4df4-8c48-e38b0c137680

**Degree of purity**

> 95 < 100 % (w/w)

**Constituents**

ethanol / ethanol / 64-17-5

**Impurities**

8 % (w/w) methanol / methanol / 67-56-1

Reference substance: methanol / methanol / 67-56-1

Typical concentration: 8 % (w/w)

Concentration range: > 7 < 9 % (w/w)

Remarks:

7 % (w/w) water / water / 7732-18-5

Reference substance: water / water / 7732-18-5

Typical concentration: 7 % (w/w)

Concentration range: > 5 < 8 % (w/w)

A maximum degree of purity of 100 % cannot be reached when the impurities are present at a minimum concentration of 12 %



## **Issue type 7: Well-defined substance with inconsistency between degree of purity and impurity concentrations.**

### **Example 2: shortcomings concerning the minimum degree of purity**

#### **Excerpt from the information letter:**

#### ***"Well-defined substance with inconsistency between degree of purity and impurity concentrations***

*The composition with name "xxxx" and local UUID "xxxxxxxxxxxxxx" contains in total 2 impurities for which the sum of the maximum concentrations (8 % (w/w)) is inconsistent with the minimum degree of purity (90 % (w/w))."*

**Substance composition**

Ethanol for webinar

**Degree of purity**

> 90 < 98 % (w/w)

**Constituents**

96 % (w/w) ethanol / ethanol / 64-17-5

**Impurities**

2 % (w/w) methanol / methanol / 67-56-1

Reference substance methanol / methanol / 67-56-1

Typical concentration 2 % (w/w)

Concentration range > 1 < 5 % (w/w)

Remarks

2 % (w/w) water / water / 7732-18-5

Reference substance water / water / 7732-18-5

Typical concentration 2 % (w/w)

Concentration range > 1 < 3 % (w/w)

**Additives**

A minimum degree of purity of 90 % cannot be reached when the maximum concentration of the impurities is 8 %



**Substance composition**

Ethanol for webinar

Name: Ethanol for webinar

Brief description:

Composition ID: L-71d7017a-75e1-4df4-8c48-e38b0c137680

**Degree of purity**

> 83 < 92 % (w/w)

**Constituents**

90 % (w/w) ethanol / ethanol / 64-17-5

**Impurities**

6 % (w/w) methanol / methanol / 67-56-1

Reference substance: methanol / methanol / 67-56-1

Typical concentration: 6 % (w/w)


Concentration range: > 5 < 9 % (w/w)

4 % (w/w) water / water / 7732-18-5

Reference substance: water / water / 7732-18-5

Typical concentration: 4 % (w/w)

Concentration range: > 3 < 8 % (w/w)



Both minimum and maximum limits in the degree of purity are consistent with the concentration ranges of the impurities

## Practical hints for avoiding/correcting shortcomings

- Many of the shortcomings presented in this section are caused by missing data, and especially missing ranges.
- Therefore, always provide the degree of purity and the concentration (for constituents, impurities, and additives) as ranges, i.e. indicating the lower and upper limits.
- Report representative values for the substance as manufactured/imported, based on the analytical data.

## Practical hints for avoiding/correcting shortcomings (cont.)

- Be consistent with the units (% (w/w) and ppm recommended)
- Do not create blocks for non-existing constituents/impurities/additives (empty blocks).
- A practical guidance on how to report the substance composition in IUCLID section 1.2 can be found in the **Data Submission Manual Part 18 - How to report the substance identity in IUCLID 5 for registration under REACH**, available on the ECHA website.

# Thank you

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