Overview

- Introduction
- Required data for substance identity purposes
- Dossier preparation (introduction)
- Substance identity of
  - Mono-constituent substances
  - Multi-constituent substances
  - … with additional identifiers
- Dossier preparation (mono & multi-constituent substances)

- BREAK

- Substance identity of UVCB substances
- Dossier preparation (UVCB substances)

UVCB substance

- **U**nknown or
- **V**ariable composition
- **C**omplex reaction product or
- **B**iological origin

UVCB substance

- Composition not (completely) known

  OR

- Composition very variable

  OR

- Many constituents

→ “Reaction products of [starting material IUPAC name] and [starting material IUPAC name] and …”

UVCB substance

- Naming according to
  - Source (starting material) and
  - Production process (synthesis / refinement)
- Other identification parameters
  - Ratio of starting materials
  - Relevant process conditions (solvent, temperature…)
    → in the description

UVCB subtypes

- Biological source, refinement
- Biological source, synthesis
- Chemical or mineral source, synthesis
- Chemical or mineral source, refinement

Specific types of UVCB substances:

- Substances obtained from oil or oil like sources
- Variation in carbon chain length
- Enzymes

UVCB subtypes

- Biological source, refinement
  - Lavender, Lavandula hybrida, ext. → Lavender, Lavandula hybrida, essential oil
- Biological source, synthesis
  - Acetylation products of Lavender, Lavandula hybrida, ext.

UVCB subtypes

- Chemical or mineral source, synthesis
  - Reaction products of acetophenone and formaldehyde and cyclohexylamine and methanol and acetic acid

- Chemical or mineral source, refinement
  - Oxirane reaction products with ammonia, intermediate fraction

UVCB specific types

- Substances obtained from oil or oil like source
- Variation in carbon chain length
- Enzymes

Substances obtained from oil or oil like source

Identification by

- Starting material
- Process (list of 26 processes for EINECS)
- Boiling range (or other phys. prop.)
- Carbon range
  - carbon count refers to all carbons in a molecule
  - defined ranges for certain processes, narrower ranges are covered
- Typical composition
  - “alkane”, “hydrocarbon”, “aromatic hydrocarbon”, …

Substances obtained from oil or oil like source

- In addition to source and process
  - Generic description of composition
    - type of constituents: “hydrocarbons”
    - carbon range: C12-30
  - Boiling range (usually in description)

- → Substance identity based partially on chemical composition

UVCB specific types

- Substances obtained from oil or oil like source
- Variation in carbon chain length
- Enzymes

Variation in carbon chain length

- Formalised system of generic descriptions developed
- Based on the chemical composition of the substance
- Not applicable to well defined substances

Variation in carbon chain length

- Alkyl descriptor
  - C12-18 (even numbered, C18 unsaturated)
    → any source
  - Palm-kernel alkyl
    → only natural sources
- Functionality descriptor
  - Amine, alcohol, fatty acids
- Salt descriptor (if required)
  - Sodium, potassium, …

e.g. “C12-18 (even numbered, C18 unsaturated) alkyl sulfonate, sodium salt”

Variation in carbon chain length

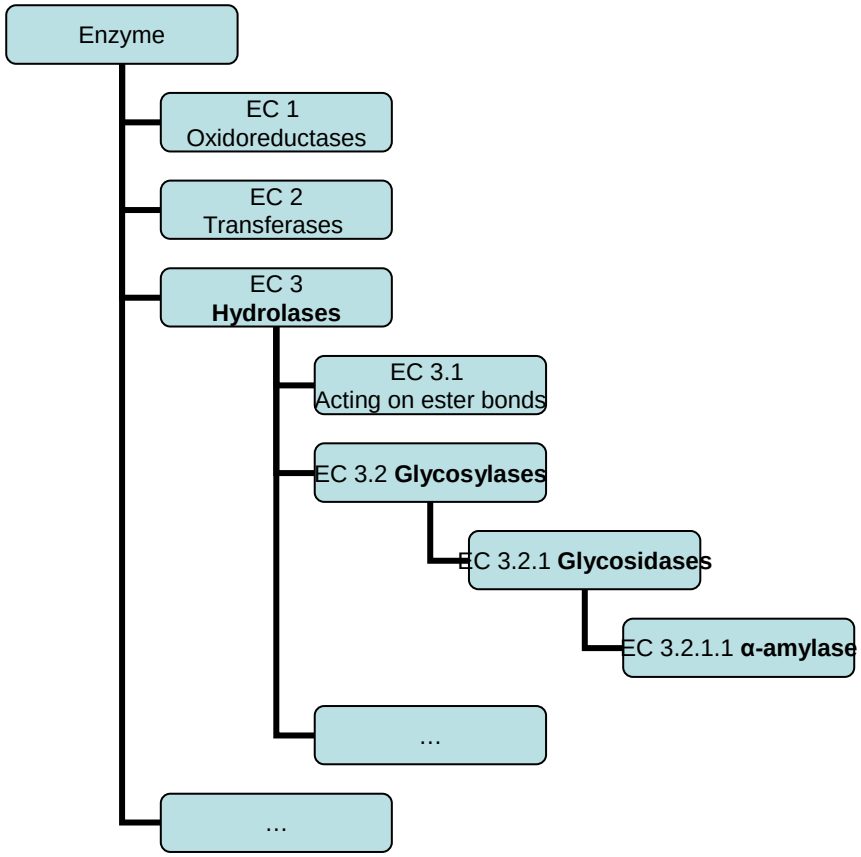
- Alkyl descriptor specification
  - If not indicated:
    linear, saturated, all chain lengths present
  - Otherwise specify:
    branched, unsaturated, C18 unsaturated, even numbered, …
- Alkyl descriptor scope
  - Chain length range ≠ natural source description
  - C12-18 ≠ C14-18 (range ≠ narrow range)

UVCB specific types

- Substances obtained from oil or oil like source
- Variation in carbon chain length
- Enzymes

Enzymes

- Main identifier is catalytic activity
- Naming according to International Union of Biochemistry and Molecular Biology (IUBMB) rules
- http://www.chem.qmul.ac.uk/iubmb/nomenclature/



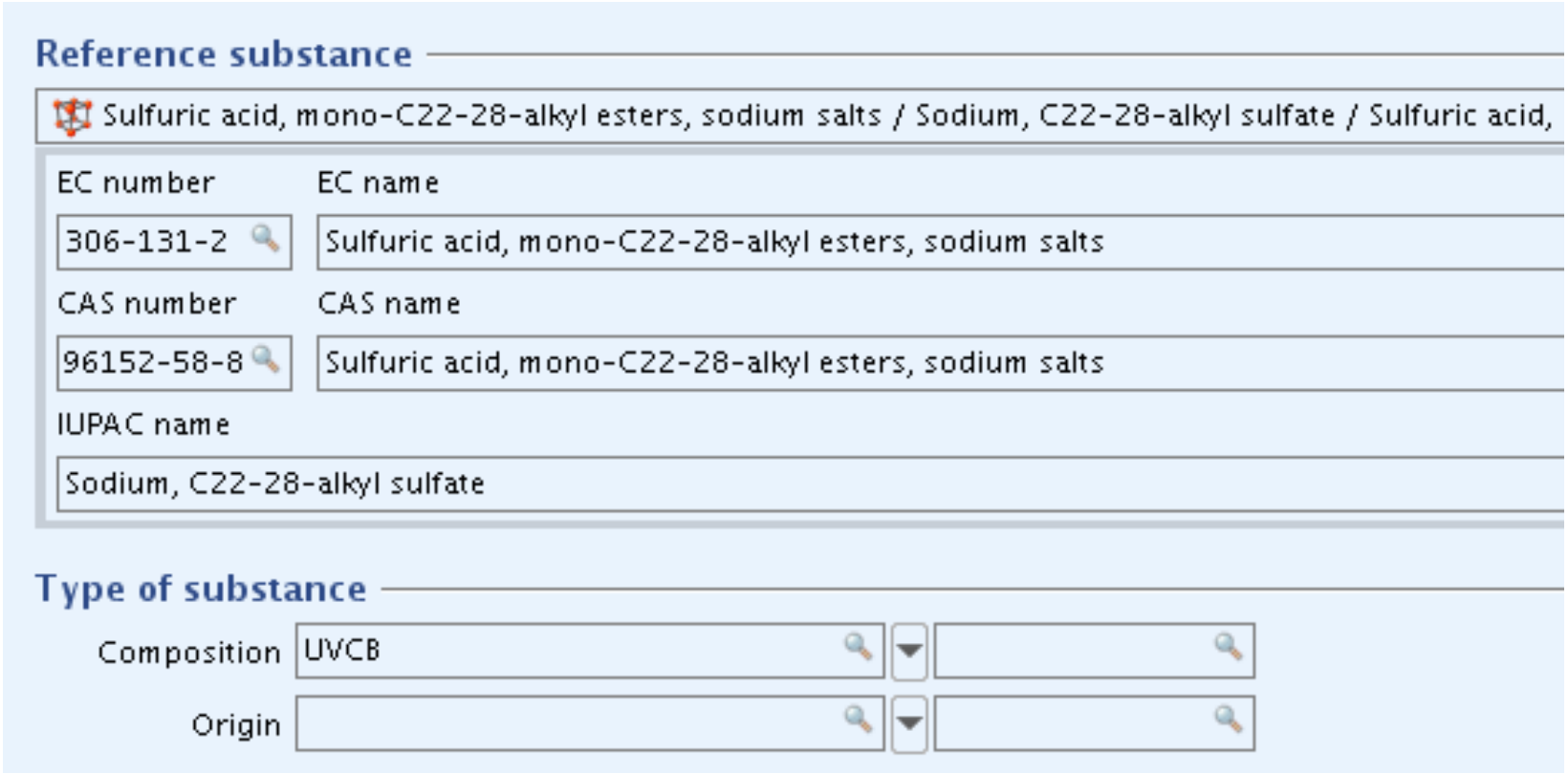
UVCB Data requirements

- Identification
  - Provide generic structure when possible (not always reasonable → not mandatory)
- Composition
  - Groups of constituents acceptable
  - Grouping consistent with analytical data

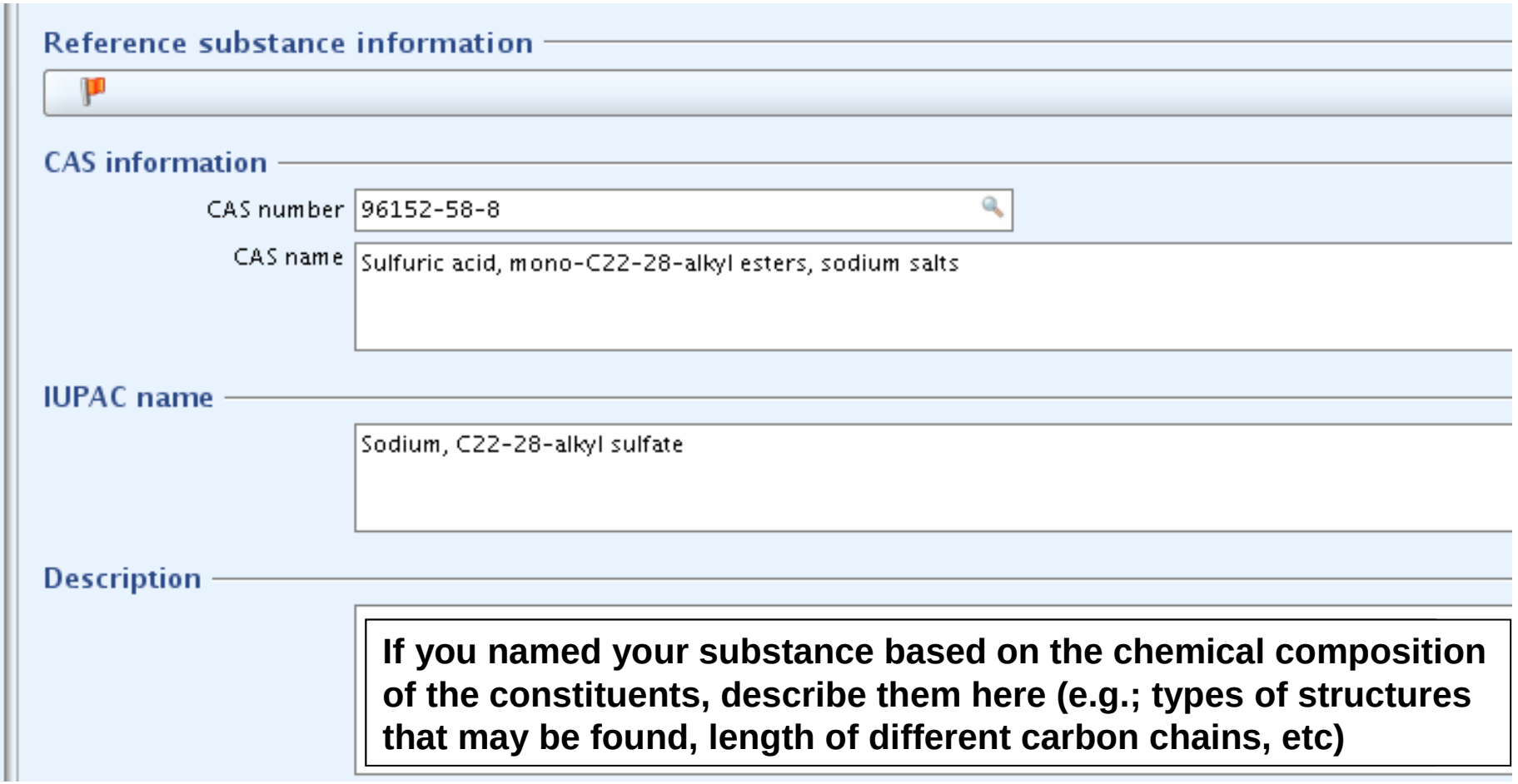
IUCLID 5 Dossiers

Dossier preparation for UVCB substances

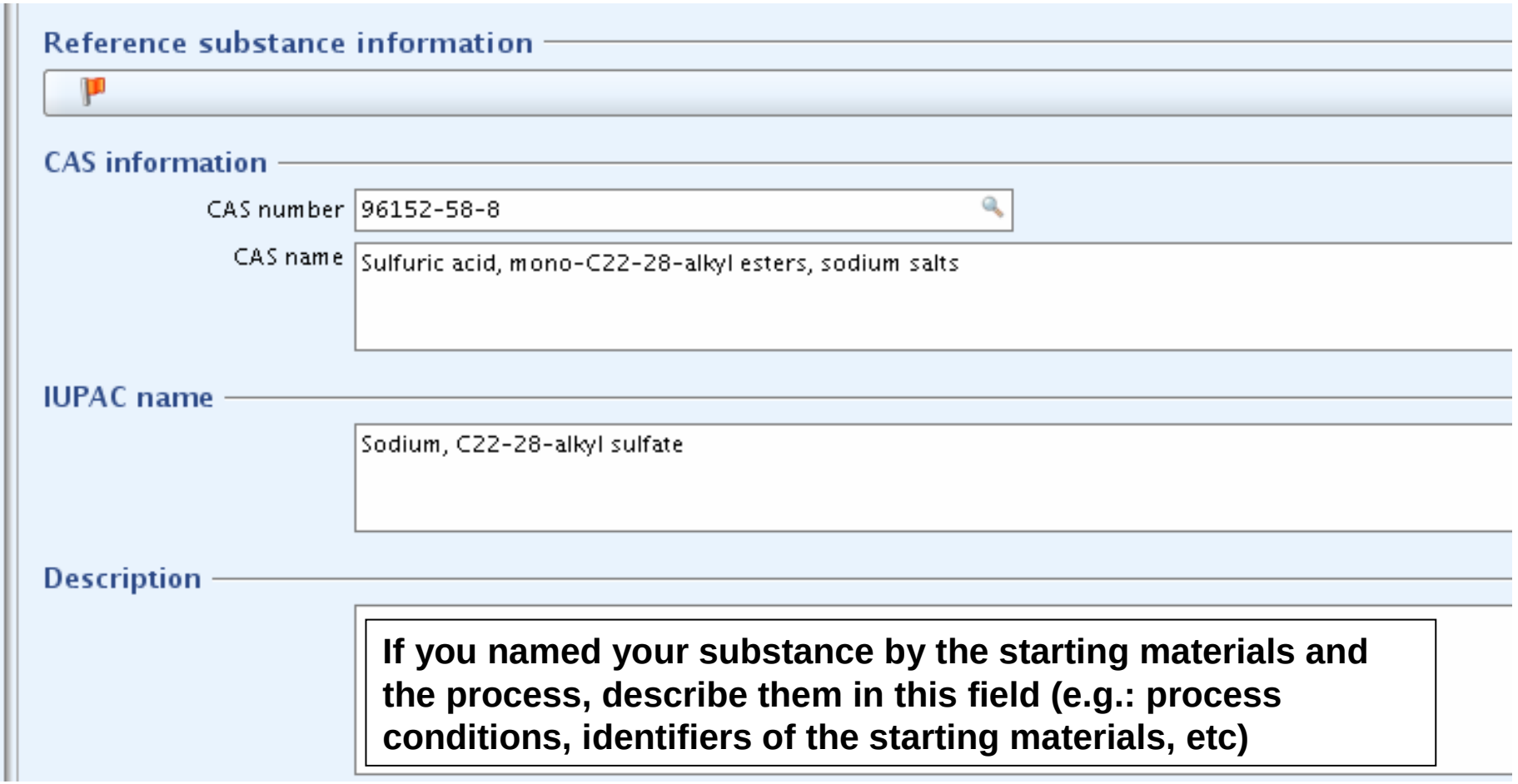
1.1 Identity


Reference substance
Sulfuric acid, mono-C22-28-alkyl esters, sodium salts / Sodium, C22-28-alkyl sulfate / Sulfuric acid,
EC number
EC name
306-131-2
Sulfuric acid, mono-C22-28-alkyl esters, sodium salts
CAS number
CAS name
96152-58-8
Sulfuric acid, mono-C22-28-alkyl esters, sodium salts
IUPAC name
Sodium, C22-28-alkyl sulfate
Type of substance
Composition
UVCB
Origin

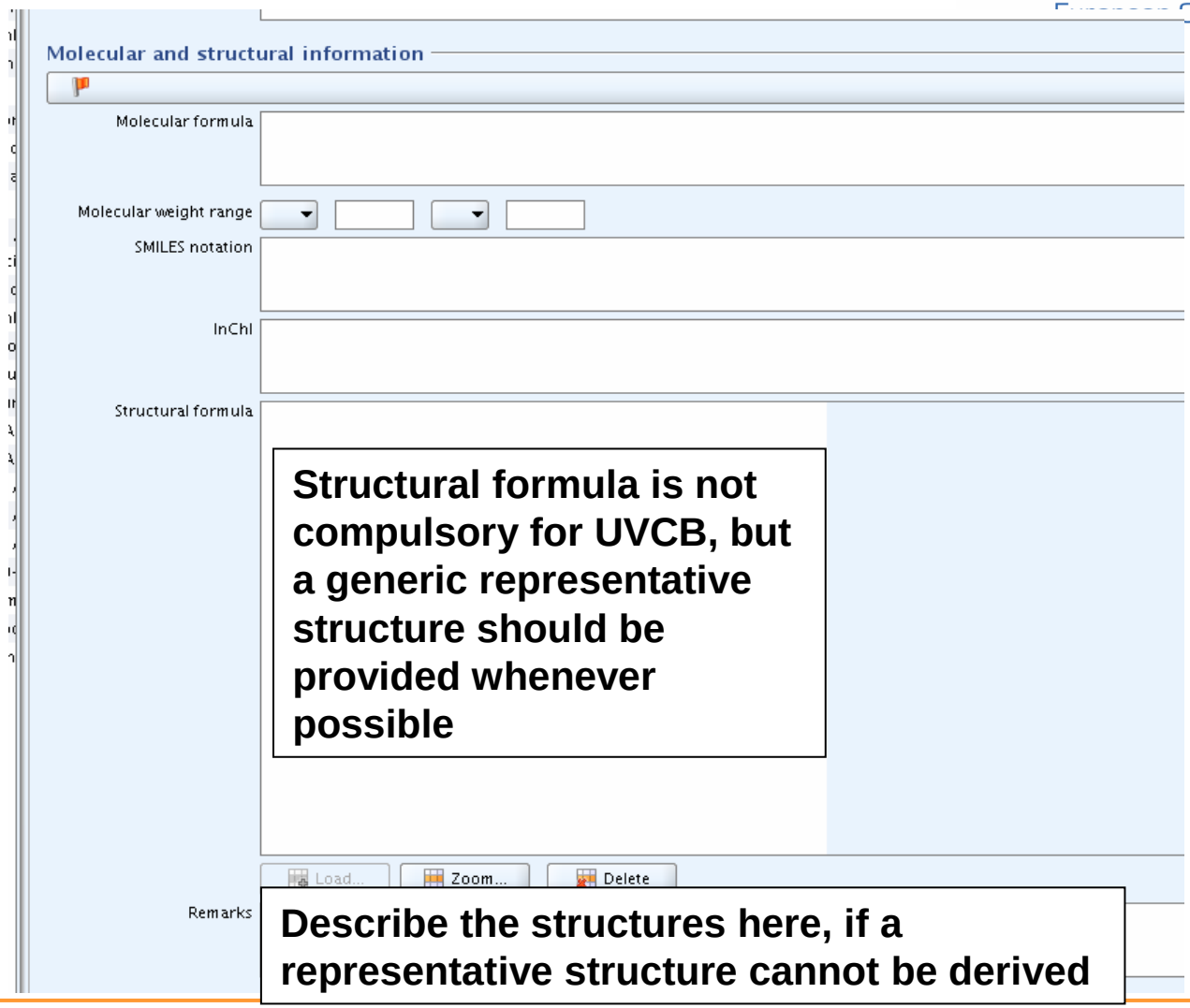
1.1 Identity (reference substance)



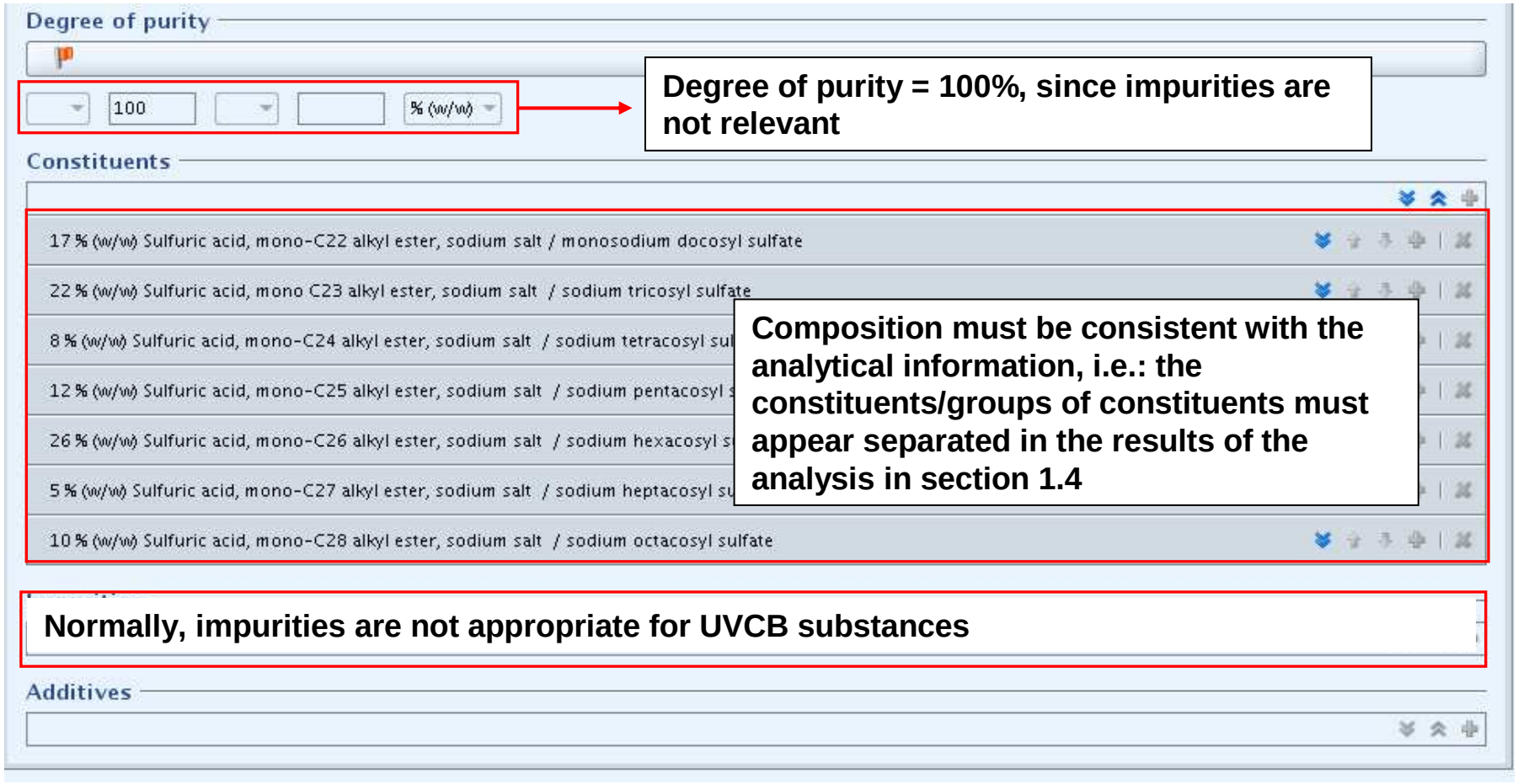
1.1 Identity (reference substance)

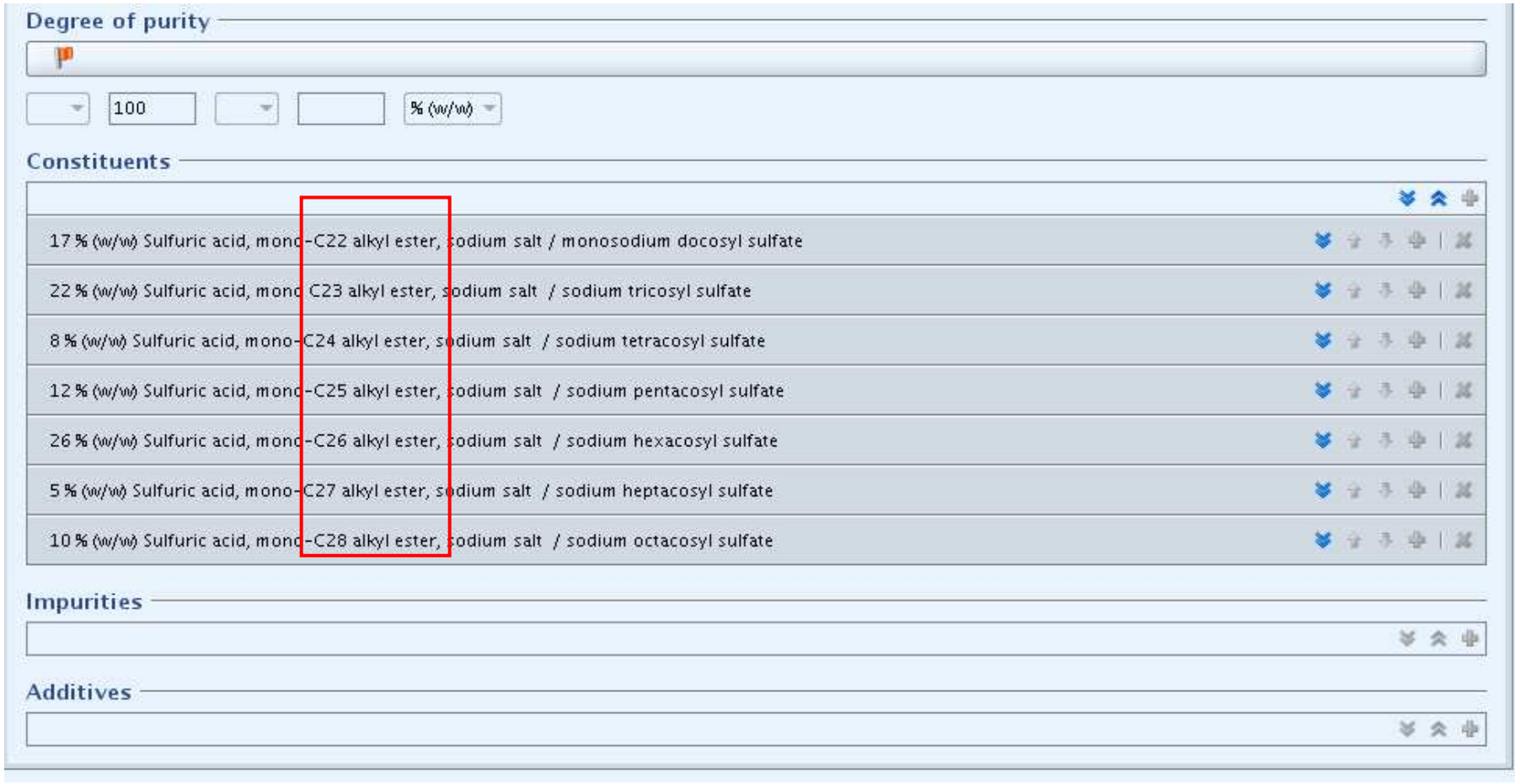


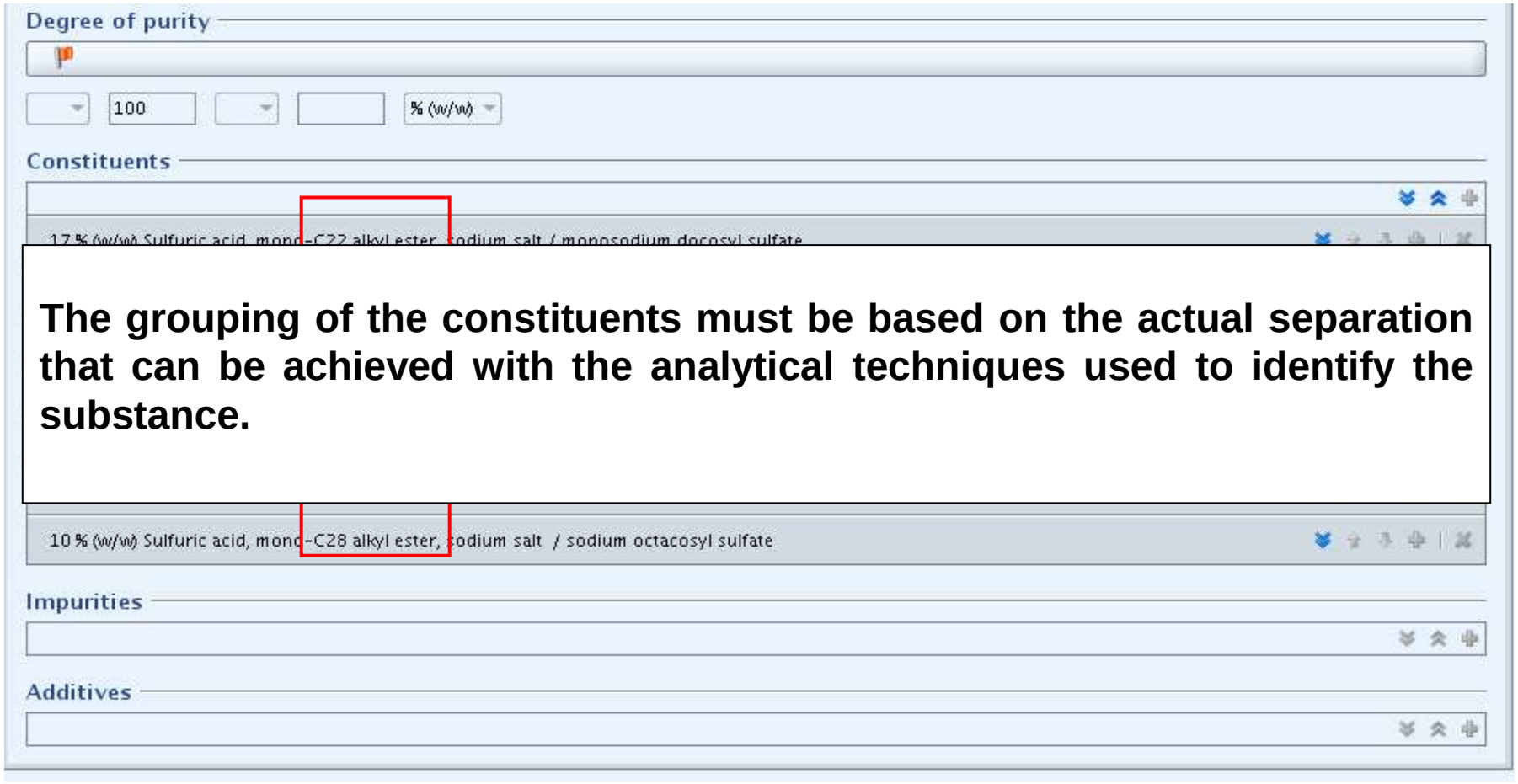
1.1 Identity (reference substance)



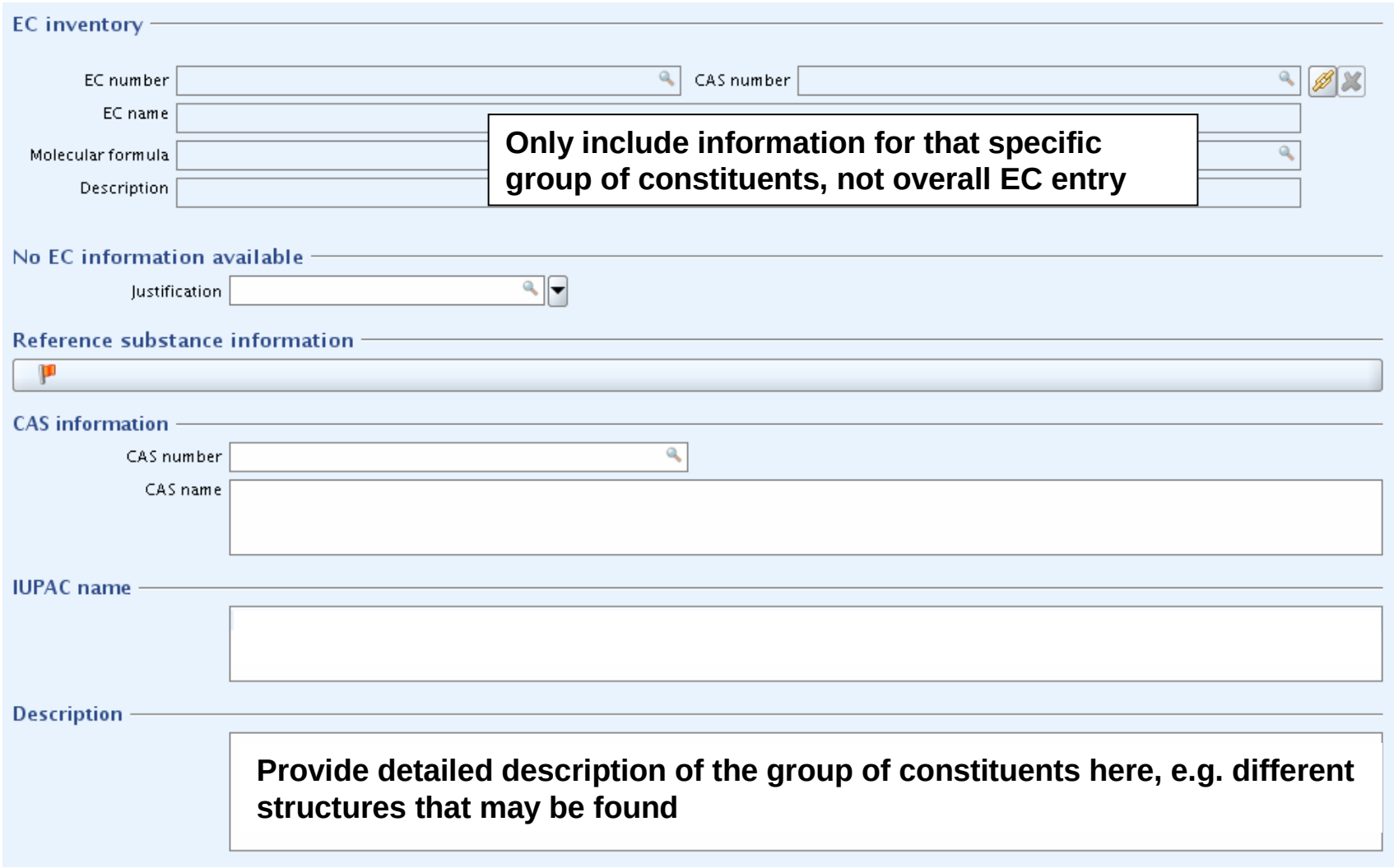
1.2 Composition



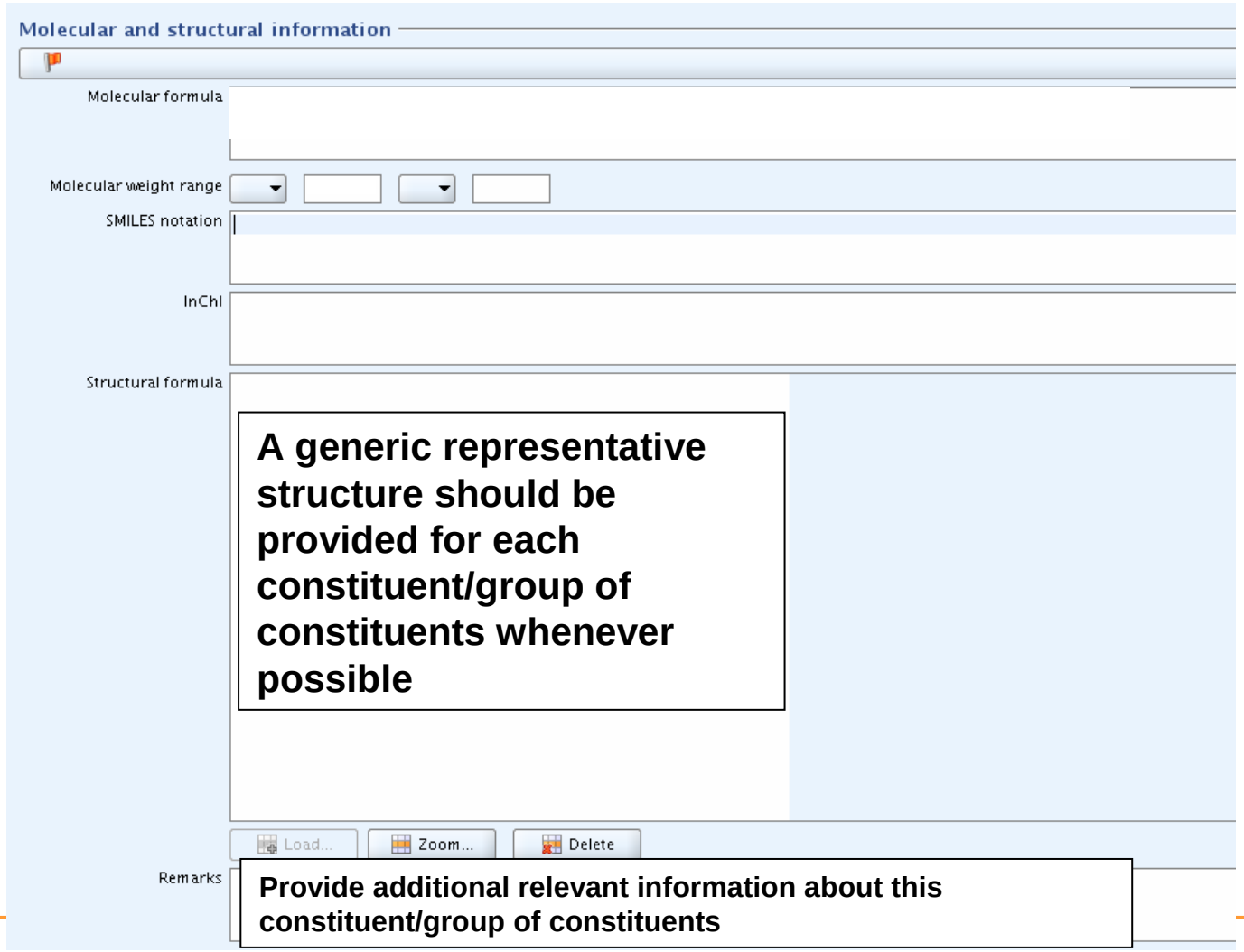

Degree of purity
100
% (w/w)
Constituents
17 % (w/w) Sulfuric acid, mono-C22 alkyl ester, sodium salt / monosodium docosyl sulfate
22 % (w/w) Sulfuric acid, mono-C23 alkyl ester, sodium salt / sodium tricosyl sulfate
8 % (w/w) Sulfuric acid, mono-C24 alkyl ester, sodium salt / sodium tetracosyl sulfate
12 % (w/w) Sulfuric acid, mono-C25 alkyl ester, sodium salt / sodium pentacosyl sulfate
26 % (w/w) Sulfuric acid, mono-C26 alkyl ester, sodium salt / sodium hexacosyl sulfate
5 % (w/w) Sulfuric acid, mono-C27 alkyl ester, sodium salt / sodium heptacosyl sulfate
10 % (w/w) Sulfuric acid, mono-C28 alkyl ester, sodium salt / sodium octacosyl sulfate
Impurities
Additives


Degree of purity
100
% (w/w)
Constituents
17 % (w/w) Sulfuric acid, mono-C22 alkyl ester, sodium salt / monosodium docosyl sulfate
The grouping of the constituents must be based on the actual separation that can be achieved with the analytical techniques used to identify the substance.
10 % (w/w) Sulfuric acid, mono-C28 alkyl ester, sodium salt / sodium octacosyl sulfate
Impurities
Additives

1.2 Composition: groups of constituents



1.2 Composition



Summary

- Required data for substance identity purposes
- Substance identity of
  - Mono-constituent substances
  - Multi-constituent substances
  - UVCB substances
- Dossier preparation for substance identity