

# 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

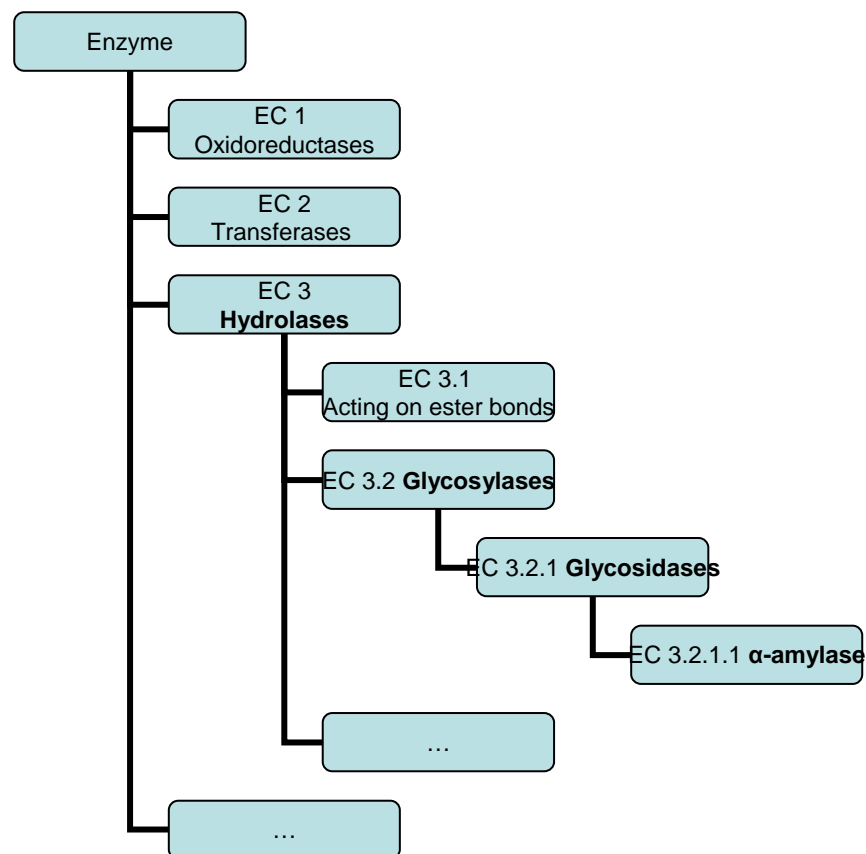
- Alkyl descriptor specification
  - If not indicated:  
linear, saturated, all chain lengths present
  - Otherwise specify:  
branched, unsaturated, C18 unsaturated, even numbered, ...
- Alkyl descriptor scope
  - Chain length range  $\neq$  natural source description
  - C12-18  $\neq$  C14-18 (range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

## Reference substance information



## CAS information

CAS number 96152-58-8

CAS name Sulfuric acid, mono-C22-28-alkyl esters, sodium salts

## IUPAC name

Sodium, C22-28-alkyl sulfate

## Description

**If you named your substance based on the chemical composition of the constituents, describe them here (e.g.; types of structures that may be found, length of different carbon chains, etc)**

# 1.1 Identity (reference substance)

## Reference substance information



## CAS information

CAS number 96152-58-8

CAS name Sulfuric acid, mono-C22-28-alkyl esters, sodium salts

## IUPAC name

Sodium, C22-28-alkyl sulfate

## Description

**If you named your substance by the starting materials and the process, describe them in this field (e.g.: process conditions, identifiers of the starting materials, etc)**

## 1.1 Identity (reference substance)

**Molecular and structural information**

Molecular formula

Molecular weight range

SMILES notation

InChI

Structural formula

**Structural formula is not compulsory for UVCB, but a generic representative structure should be provided whenever possible**

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Remarks **Describe the structures here, if a representative structure cannot be derived**

# 1.2 Composition

**Degree of purity**

100 % (w/w)

**Degree of purity = 100%, since impurities are not relevant**

**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

**Composition must be consistent with the analytical information, i.e.: the constituents/groups of constituents must appear separated in the results of the analysis in section 1.4**






















**Normally, impurities are not appropriate for UVCB substances**

**Additives**

**Degree of purity**

% (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	  
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**Impurities**

**Additives**



**Degree of purity**

% (w/w)

**Constituents**

17 % (w/w) Sulfuric acid, mono-C22 alkyl ester, sodium salt / monosodium docosyl sulfate
10 % (w/w) Sulfuric acid, mono-C28 alkyl ester, sodium salt / sodium octacosyl sulfate

**Impurities**

**Additives**

**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.**

# 1.2 Composition: groups of constituents

**EC inventory**

EC number  CAS number

EC name

Molecular formula

Description

**Only include information for that specific group of constituents, not overall EC entry**

**No EC information available**

Justification

**Reference substance information**

**CAS information**

CAS number

CAS name

**IUPAC name**

**Description**

**Provide detailed description of the group of constituents here, e.g. different structures that may be found**

# 1.2 Composition

**Molecular and structural information**

Molecular formula

Molecular weight range

SMILES notation

InChI

Structural formula

**A generic representative structure should be provided for each constituent/group of constituents whenever possible**

Load... Zoom... Delete

Remarks

**Provide additional relevant information about this constituent/group of constituents**

# Summary

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