REACH-IT Data Submission Manual

Part 17 - How to derive a Public Name for a substance for use under the REACH Regulation

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http://echa.europa.eu/reach/helpdesk/echahelp_en.asp

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1 Introduction

A coherent system for deriving public names for substances is needed to increase the usefulness of the publication of substance-specific information by ECHA on its website, in particular in the context of:

- Publication of information from registrations according to Article 119 of the REACH Regulation[1]
- Publication of testing proposals according to Article 40(2) of the REACH Regulation

This document advises industry on how to derive a public name for a substance for which the IUPAC name[2] is claimed as confidential[3] within a registration dossier in accordance with Article 10(a)(xi) of the REACH Regulation.

This manual does not cover inorganic substances.

2 Principles and purpose of Public Names for Substances in the context of REACH

The underlying principle of a 'public name' (sometimes referred to as a 'masked name', 'generic name' or 'disguised name') is that the chemical identity of the substance is revealed to the maximum extent possible, but without disclosing trade secrets or other confidential information that would potentially harm the commercial interests of the registrant or any other party concerned. It should be noted that ECHA publishes information on substances on its website in accordance with the principles set out in Article 119. For example this includes trade names, which have not been claimed confidential.

One of the characteristics of a suitable public name is such that it should permit a scientist to gain sufficient knowledge of the chemical structure as to allow understanding of the intrinsic properties. It will often also be necessary to make professional judgements based on knowledge of similar substances having similar properties due to the same or similar chemical groups and substructures of the published substance. Hence the public name must allow interested parties to do this; otherwise a key purpose of the provisions in REACH which provide for communication of information on substances would be compromised. In the particular case of a public call for scientifically valid data on a registered substance in the context of the evaluation of a testing proposal, if the public name does not provide adequate information on the chemical structure the effectiveness of the public consultation would be compromised.

If the IUPAC name of the substance is successfully claimed as confidential it will not be made publicly available nor will the structural information for that substance. If no other non-confidential substance identifier is available (e.g. an EINECS name), a public name will be disseminated.

[1] Regulation (EC) No 1907/2006 OJ L 396, 30.12.2006, p. 1 and Corrigendum L136/3 29.5.2007, Corrigendum OJ LL141/22, 31.5.2008, p.22, Corrigendum L 143/55, 3.6.2008, p.1 and Corrigendum OJ L 36, 5.2.2009, p. 84 and Amendments

[2] The IUPAC name is the chemical name in accordance with the nomenclature of the **I**nternational **U**nion of **P**ure and **A**pplied **C**hemistry

[3] How to make a confidentiality claim for the IUPAC name in accordance with Article 119(2)(f) or (g) of the REACH Regulation is described in the REACH-IT Data Submission Manual, Part 16 – Confidentiality Claims (http://echa.europa.eu/doc/reachit/dsm_16_confidentiality_claims.pdf)

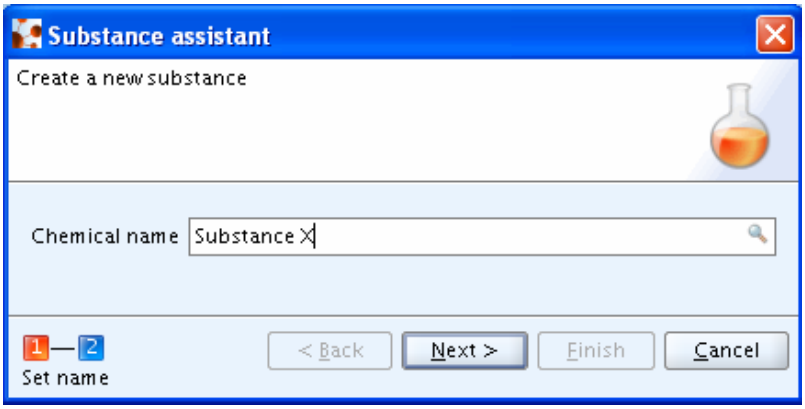
This manual provides rules for registrants on how to generate a public name for most substances. In some aspects it may not be fully comprehensive and therefore registrants and ECHA will need to use their professional judgement. The manual will be updated on the basis of experience in generating public names.

3 Where to include the public name?

If the registrant makes a confidentiality claim for the IUPAC name he is required to provide an appropriate public name (masked name) for ECHA to use for dissemination purposes. In the absence of an adequate public name, a confidentiality claim for the IUPAC name cannot be accepted by ECHA. Registrants are requested to include the public name in their registration dossier in the 'public name' field of IUCLID.

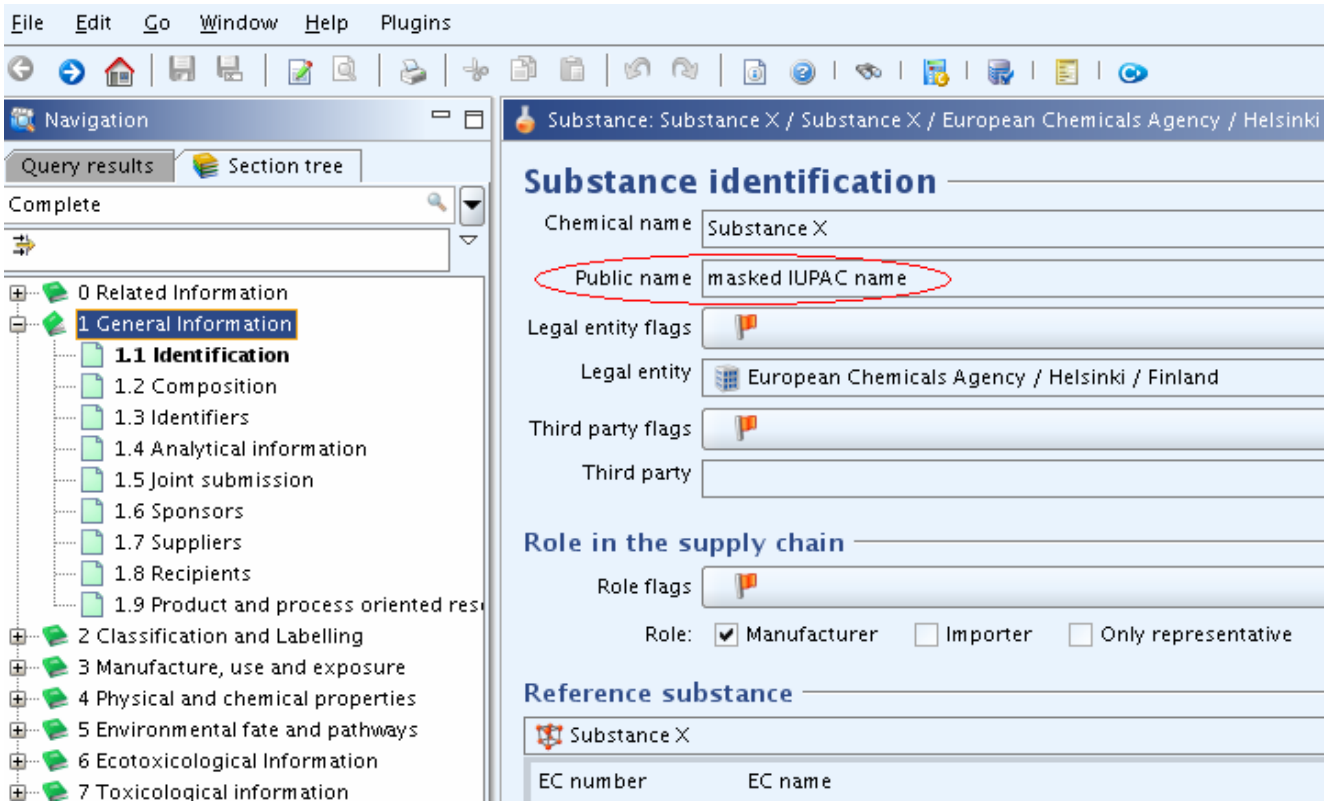
When the user creates a substance following the steps as indicated by IUCLID

Figure 1 : Creating a substance in IUCLID



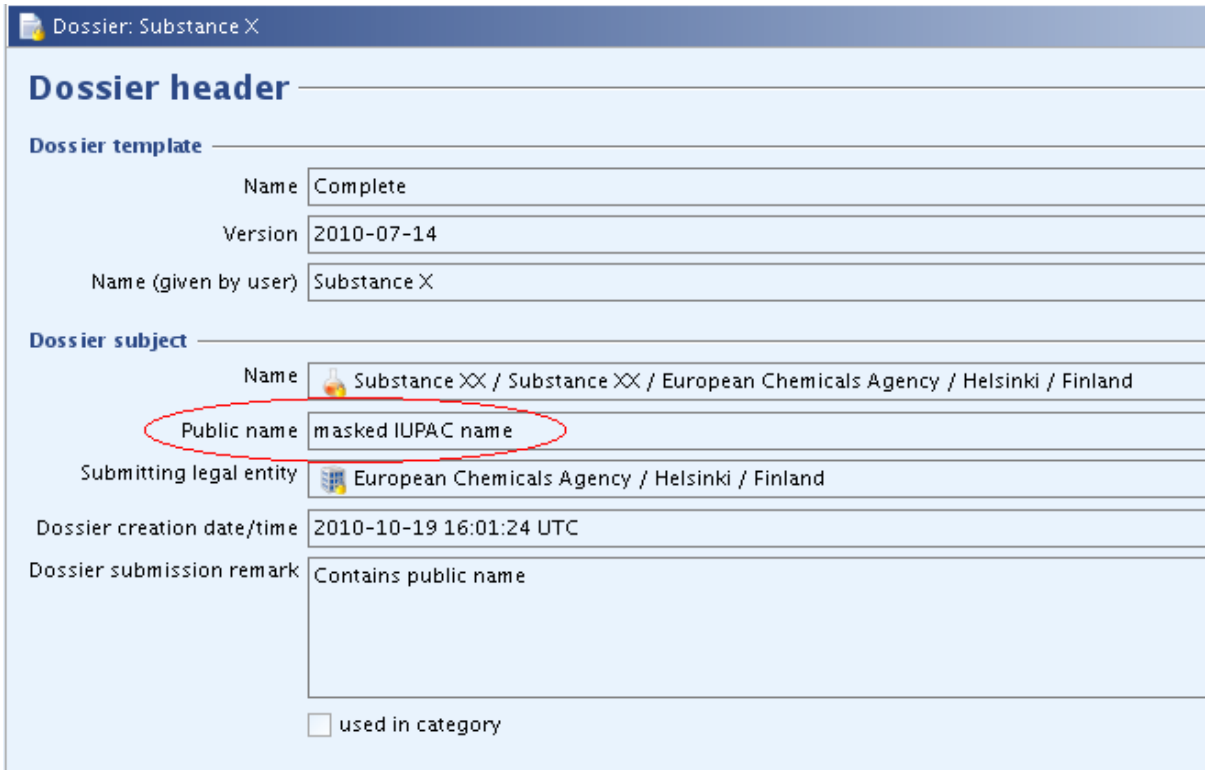
he will arrive at the substance identification screen where he can include the masked name in the public name field as indicated in the next screen shot.

Figure 2 : Location of the public name field in IUCLID



Once the dossier is created the given public name will appear in the dossier header in the public name field.

Figure 3 : Appearance of the public name in the dossier header in IUCLID



Note – If the IUPAC name is claimed confidential, the justification for the confidentiality claim will also need to include a masking justification for the public name. In case of one level masking, this will be a simple statement on what is masked in the public name. In case of two or three levels of masking also a valid well-reasoned justification of why the second/third level masking is necessary is required (see example in Annex II). Absence of any of these elements will lead to a rejection of the claim and publication of the IUPAC name.

Note – If a claim on the IUPAC name has been accepted by ECHA, no structural information is disseminated. This includes the composition of the substance, hence information on the individual constituents.

4 Advice on how to mask IUPAC names for Substances

The system to derive a public name from the IUPAC name has been developed by ECHA for use under REACH. The approach is based on the well-established concept of 'masked names' used in the Canadian version of the US EPA scheme, and we are grateful for the assistance from Environment Canada in their experience with operating a similar scheme for public names.

The system allows different elements of the chemical name to be 'masked' in order to conceal the full description of different parts of the chemical structure. The rules presented below describe how to derive a public name for dissemination by illustrating the masking of various structural elements from the IUPAC name with a single level of masking. The use of these rules in combination is considered multiple masking. Two to three levels of masking

may be permitted if the registrant provides an acceptable justification for each level of masking.

The system provides guidance to Manufacturers, Importers and Only Representatives wishing to claim the IUPAC name as confidential when submitting a registration dossier in accordance with Article 10, 17 or 18 of the REACH Regulation.

There are inherent differences between naming well-defined substances with a definite chemical structure and naming UVCB substances for which in most cases a structural diagram cannot be depicted. Each of these possibilities is addressed separately.

4.1 Well-defined substances

Substances of well defined chemical composition are named according to the main constituent(s). These are mono-constituent or multi-constituent substances. A mono-constituent substance is named by the main constituent using the IUPAC nomenclature rules[4]. A multi-constituent substance is named as a reaction mass of the main constituents of the substance with the generic format: "Reaction mass of [IUPAC name of main constituent 1 and IUPAC name of main constituent 2 and IUPAC name of main constituent 3]". It should be noted that only main constituents typically ≥10% contribute to the name. More information on the different types is given in section 4.2 of the Guidance document for identification and naming of substances under REACH.[5]

The name of well-defined substances usually discloses the following structural information:

- the identity of the parent structure (i.e. a chain of carbon atoms, a ring system, or a coordinated metal)
- the identity, number, and position of chemical group(s) that are attached to the parent structure(s) or to other chemical groups
- the identity and number of counter ions (for salts)
- the stereo-chemistry

Public names may be created for well-defined substances by masking structurally-descriptive fragments of the IUPAC name. One degree of masking can be applied without providing a justification. Multiple masking (two to three levels) may be permitted if the registrant provides an acceptable justification for each additional level of masking. The rules for the different types of masking are given below.

The IUPAC name of a well-defined substance is masked taking into account the following:

- the locant(s) that indicate(s) the position(s) of a specific chemical group
- the multiplicative prefixes that specify the number of a given chemical group (e.g. di-, tri-, and/or tetramethyl)
- the identity (but not position and number) of a given chemical group (e.g. sulfonyl)
- the identity of a given parent structure, (e.g. a chain or ring system)
- the locant(s) of substituent chemical group(s) for a given parent structure

[4] http://www.acdlabs.com/iupac/nomenclature/
[5] http://guidance.echa.europa.eu/docs/guidance_document/substance_id_en.pdf

4.1.1 Masking options

One option is to mask one parent group (or multiple occurrences of the same parent group).

An alternative option (but not in addition to the first) is to mask one other structural element. This covers masking of:

- the locant with or without multiplicative prefixes
- the identity of a chemical group
- the cation or anion
- the stereochemistry

4.1.2 Parent Masking

A parent structure that is in general a chain of carbon atoms with either single, double or triple bonds, or a ring system with one or more fused rings may be masked by using one of the following masking terms:

- alkane or alkyl (e.g. to mask octadecane or octadecanyl)
- alkene or alkenyl (e.g. to mask ethene or ethenyl)
- alkyne or alkynyl (e.g. to mask acetylene* or ethynyl, propyne or 1-propynyl / 2-propynyl)
- arene or aryl (e.g. to mask benzene, or phenyl)
- alicycle or alicyclic (e.g to mask cyclohexane or cyclohexyl, cyclohexene or cyclohexenyl)
- polycycle or polycyclic (e.g. to mask naphthalene or naphthyl, spiroundecane or spiroundecanyl)
- heteromonocycle or heteromonocyclic (e.g. to mask thiophene or thienyl, morpholine or morpholinyl)
- heteropolycycle or heteropolycyclic (e.g. to mask quinoline or quinolyl, xanthene or xanthenyl)

* It should be noted that for some substances the trivial name is preferred and retained by IUPAC.

Note - Only one such parent group or multiple occurrences of the same parent group should be masked.

Masking of (an) additional parent group(s) is considered multiple masking and needs to be justified by the registrant. ECHA may refuse to accept multiple masking if the justification cannot be considered as valid.

4.1.3 Substituent Masking

In cases where (a) functional group(s) is/are attached to the parent structure(s) or to other chemical groups, the IUPAC name may be masked by using the following masking terms:

- halo or halide (e.g. to mask fluoro, chloro, or fluoride, chloride)

- *substituted* is used for substituents where no generic name can be established e.g. amino, hydroxy, oxo
- *stereo-isomer(s) of* is used for isomers where the specific stereochemistry should not be revealed (e.g. to mask *cis*- and *trans*- or R- and S-isomer(s))

If there is more than one of the same chemical group, then the addition of the prefix 'poly' should be considered:

- polyamino (e.g. to mask diamino) or polyhydroxy (e.g to mask trihydroxy).

Note – In case of organometallic substances and organo coordinated metal complexes the organic moiety can be masked according to the rules as described in this manual. However, the metal atom should not be masked in the chemical name.

In case of organic salts, only alkali and alkaline earth metals can be masked.

- alkali metal , e.g. sodium, potassium
- earth alkali metal , e.g. calcium, magnesium

It is possible to mask the organic part of a given salt using the rules outlined in this manual.

Note - Masking of individual parts of a functional group should generally be avoided as this may result in potentially misleading name changes e.g. oxygen in a carboxyl or amide group should not be masked as this would result in renaming the groups as substituted alcohol and substituted amine respectively, which are different substances from their precursors.

Note - Only one such substituent or multiple occurrences of the same substituent should be masked.

Masking of (an) additional substituent(s) is considered multiple masking and needs to be justified by the registrant. ECHA may refuse to accept multiple masking if the justification cannot be considered as valid.

Note – This manual does not cover inorganic substances.

Multi-constituent substances can be masked by applying the rules to the name of each constituent of the substance as described in this manual, hence:

Reaction mass of [*masked* IUPAC name of main constituent 1] and [*masked* IUPAC name of main constituent 2] and [*masked* IUPAC name of main constituent 3]

A **list of examples** of masked names is given in the Annex 1. These examples are merely used for illustrative purposes and are of substances already published elsewhere. They cover a relatively broad range of both substance type and masking possibilities.

4.2 UVCB Substances

UVCB substances are substances of Unknown or Variable composition, Complex reaction products or Biological materials, which cannot be sufficiently identified by their chemical composition because:

- the number of constituents is relatively large and/or
- the composition is, to a significant part, unknown and/or
- the variability of the composition is relatively large or poorly predictable

As a consequence UVCB substances, in contrast to well-defined substances, are named by a combination of source and process.

In general, UVCB substances are named as "Reaction products of [names of the starting materials]" and these names should be given in the English language using the IUPAC nomenclature. For these cases where the UVCB name includes elements in IUPAC nomenclature, the masking rules in this manual can be applied.

4.2.1 UVCB sub-types

Among the UVCB substances there are four UVCB sub-types for which the naming convention employed is dependent upon whether the source is biological or not and whether the process is a synthesis or a refinement. Substances derived from biological sources are named according to their genus, species, family and process, whereas those derived from chemical sources are described by their starting materials and the process. For these UVCB sub-types masking of the name is not recommended as these substances are by definition not well-defined. Relevant details that may be commercially sensitive are likely to be included in the description of the process of the individual UVCB sub-type. However, it should be noted that such information is not disseminated unless already published on EINECS[6].

4.2.2 Specific types of UVCB substances

For other types of UCVB substances which have more specified variability, namely substances with variation in the carbon-chain lengths, substances from oil (petroleum) or oil like sources (e.g. coal) and enzymes, individual naming conventions are used.

More information regarding the different UVCB sub-types and specific types of UVCB substances is given in section 4.3 of the Guidance document for identification and naming of substances under REACH[7].

4.2.2.1 Substances with variation in the carbon-chain length

Substances with variation in the carbon-chain length, e.g. paraffins and olefins are substances either derived from natural fats or oils or produced synthetically. They are systematically named using alkyl, functionality and/or salt descriptor(s).

The **alkyl descriptor** C x-y describes the number of carbon atoms in the carbon-chain length(s) of the alkyl group(s), e.g. C8-12 corresponding to the carbon numbers C8, C9, C10, C11 and C12.

[6] European Inventory of Existing Chemical Substances
[7] http://guidance.echa.europa.eu/docs/guidance_document/substance_id_en.pdf

The **functionality descriptor** identifies the functional group of the substance, e.g. amine, ammonium, carboxylic acid.

The **salt descriptor**, identifies the cation / anion of any salt, e.g. sodium (Na^+), potassium (K^+) / carbonate (CO_3^{2-}), chloride (Cl^-).

Note – In general the alkyl descriptor C x-y refers to saturated, linear alkyl chains comprising all chain length from x to y. If the carbon chain is branched and/or unsaturated and/or only even numbered this needs to be indicated in the name.

More details on the naming convention can be found in section 4.3.2.1 of the Guidance document for identification and naming of substances under REACH.

4.2.2.2 Substances obtained from oil or oil like sources

Substances from oil sources (petroleum) can be obtained through various different processes, e.g. distillation, gasification, cracking, and are usually named by the stream source, the refinery process and general composition or characteristics. If the substance contains aliphatic and/or aromatic and/or cyclic hydrocarbons and has a boiling range, this information is included in the description. The same approach is applied for substances from oil like sources. As this specific type of UVCB substance is very complex, variable and of partly undefined composition, masking of the name may not be appropriate in all cases. It should be noted that information provided in the description of this specific UVCB type is not disseminated unless already published on EINECS[8].

4.2.2.3 Enzymes

Enzymes are named according to the IUBMB nomenclature conventions[9]. The IUBMB classification system provides a unique four digit number for each enzyme type and catalytic function. The name of the enzyme as well as the IUBMB number (i.e. the Enzyme Commission Number (EC number)) is used for the identification of a specific enzyme. Enzymes names are masked by disguising the fourth digit of the IUBMB number. Some examples are illustrated in Annex I.

5 Justifying the Use of Additional Masking

The rules presented in this document describe the masking of various structural elements from the IUPAC name in order to derive a public name with a single level of masking. There may be specific circumstances where additional levels of masking are justified. The examples provided in Annex I illustrate one level masking as well as some instances of two-level masking (also indicated as double masking). A maximum of three levels may be permitted; one level may be used without justification, however each subsequent level (2nd and 3rd level) has to be accompanied by a valid justification. The reasons why more than one level of masking is necessary shall be clearly stated and explained by the registrant. A template for confidentiality claim justifications is provided in section 6 of this document and in

[8] European Inventory of Existing Chemical Substances
[9] http://www.chem.qmul.ac.uk/iupac/jcbn/index.html#6

the REACH-IT Data Submission Manual, Part 16[10] on Confidentiality Claims. Its use is strongly recommended.

Note – For confidentiality claims of the IUPAC name under REACH Article 119(2)(f) or (g), in addition to a valid justification of the potential harm of disclosure to the commercial interest, a public name must be provided, otherwise the claim cannot be accepted by ECHA.

When making a confidentiality claim on the IUPAC name also details of the masking performed should be included together with justifications for two and three-level masking where relevant, as outlined in the confidentiality claims justification template (http://echa.europa.eu/doc/reachit/ECHA_confidentiality_claim_template.rtf)

Note – ECHA can only consider a confidentiality request for the IUPAC name admissible and accept the claim as valid if an adequate public name, and if applicable, a valid justification as to why two or three levels of masking are necessary, is provided.

Absence of any other mandatory elements for claiming confidentiality will also lead to a rejection of the confidentiality claim for the IUPAC name. (see Data Submission Manual 16 – Confidentiality Claims for details)

[10] How to make a confidentiality claim for the IUPAC name in accordance with Article 119(2)(f) or (g) of the REACH Regulation is described in the REACH-IT Data Submission Manual, Part 16 – Confidentiality Claims (http://echa.europa.eu/doc/reachit/dsm_16_confidentiality_claims.pdf)

6 Confidentiality Claim template

6.1 Template

--- Company Letterhead ---
(Template copied to company headed document)

Declaration:

We, [Registrants name], claim [Insert short summary of information] confidential in accordance with REACH Article 119(2)([Insert relevant sub section]).

We, [Registrants name], hereby declare that, to the best of our knowledge as of today ([Date]), and in accordance with the due measures of protection that we have implemented, a member of the public should not be able to obtain access to the information claimed confidential without our consent or that of the third party whose commercial interests are at stake, and in particular that the information is not publicly available in any of the following public databases: [Insert databases].

Demonstration of Commercial Interest:

Description of the nature of the registrant's commercial interest and demonstration that this commercial interest is worthy of protection by the non-disclosure of information. Demonstration of the specific measures the registrant has taken to keep the information claimed confidential secret to date.

Demonstration of Potential Harm:

Explanation of why release of the information claimed confidential would be likely to cause potential harm to the commercial interest and the specific nature of those harmful effects. A causal link between disclosure and such harmful effects should be clearly explained.

Limitation to Validity of Claim:

The period of time for which the claim will be valid: until a certain date, until the occurrence of a particular event (which should be clearly specified), or indefinitely.

Contact Person

Name and contact details of a designated person to deal with any queries which may arise during the assessment by ECHA of the confidentiality claim justification.

Masking Justification for Public Name: (Only required if IUPAC Name claimed confidential)

One-Level Masking

No Justification required – simply state what is masked in the IUPAC name.

Two-Level Masking

Statement of what is masked in the IUPAC Name, and a well-reasoned justification of why the second level masking is necessary.

Three-Level Masking

Statement of what is masked in the IUPAC Name, and a well-reasoned justification of why the third level masking is necessary.

6.2 Instruction on using the template

It is strongly recommended that a copy of this template is completed when claiming confidentiality of the IUPAC name under REACH Article 119(2) (f) or (g). The template structure should be copied to a company headed MS Word document, and each section should be completed with the details appropriate to the confidentiality claim made. The resulting file should be saved in pdf format and named using the following structure, to identify clearly the confidentiality claim flag and piece of information to which the justification applies:

Justification – *[IUCLID Section where confidentiality claim is located] – [Type of Confidentiality Claim]*.**pdf**

For example:

Justification 1.1 - IUPAC name – one level masking.pdf

Justification 1.1 - IUPAC name – two-level masking.pdf

Justification 1.1 - IUPAC name – three-level masking.pdf

More information on confidentiality claims can be found in REACH-IT Data Submission Manual, Part 16[11] on Confidentiality.

An example template is provided in Annex II which illustrates where and how to include the respective masking justifications for the IUPAC name in the standard confidentiality claim template.

[11] How to make a confidentiality claim for the IUPAC name in accordance with Article 119(2)(f) or (g) of the REACH Regulation is described in the REACH-IT Data Submission Manual, Part 16 – Confidentiality Claims (http://echa.europa.eu/doc/reachit/dsm_16_confidentiality_claims.pdf)

7 Further information

IUPAC Nomenclature of Organic Chemistry

http://www.chem.qmul.ac.uk/iupac/

http://www.acdlabs.com/iupac/nomenclature/

IUPAC nomenclature of Inorganic Chemistry

http://old.iupac.org/publications/books/rbook/Red_Book_2005.pdf

http://old.iupac.org/publications/books/author/connelly.html

IUBMB nomenclature conventions

http://www.chem.qmul.ac.uk/iupac/jcbn/index.html#6

Guidance document for identification and naming of substances under REACH

http://guidance.echa.europa.eu/docs/guidance_document/substance_id_en.pdf

REACH-IT Data Submission Manual, Part 15 – Dissemination: How to determine what will be published on the ECHA website from the registration dossier

http://echa.europa.eu/doc/reachit/dsm_15_dissemination_manual.pdf

REACH-IT Data Submission Manual, Part 15 – Dissemination: Technical annex for IUCLID section 1, 2, 3

http://echa.europa.eu/doc/reachit/dsm_15_dissemination_annex_1-3.pdf

REACH-IT Data Submission Manual, Part 16 - Confidentiality Claims: How to make confidentiality claims, and how to write Art 119(2) confidentiality justifications

http://www.echa.europa.eu/doc/reachit/dsm_16_confidentiality_claims.pdf

REACH-IT Data Submission Manual, Part 16 - Confidentiality template instructions

http://www.echa.europa.eu/doc/reachit/dsm_16_annex-confidentiality_template_instructions.pdf

Appendix 1 Examples of Substances

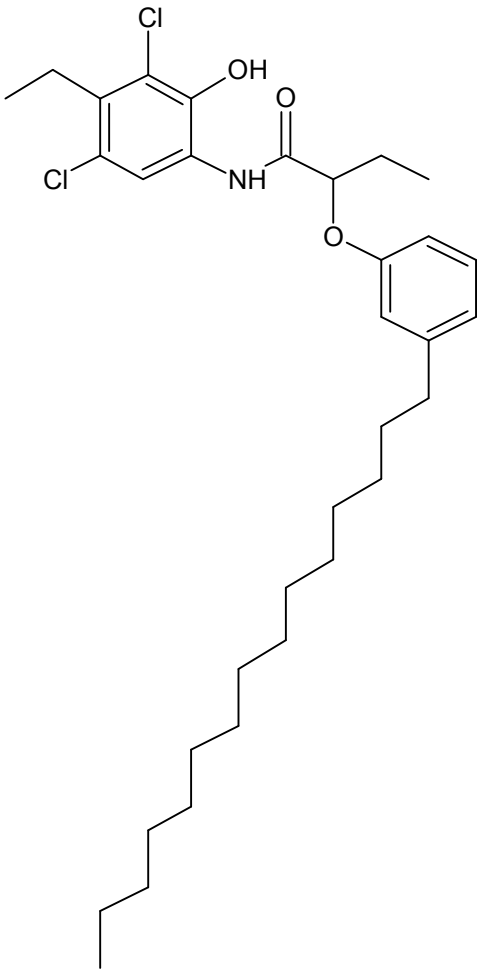
Appendix 1.1 Well-Defined Substances

Appendix 1.1.1 Mono-constituent substances

Appendix Figure 1. Example 1

Fully Defined Name

N-(3,5-dichloro-4-ethyl-2-hydroxyphenyl)-2-(3-pentadecylphenoxy)butanamide



Single Masking	Acceptable Masked Name
Number of chlorine atoms	N-(polychloro-4-ethyl-2-hydroxyphenyl)-2-(3-pentadecylphenoxy)butanamide
Chlorine atoms	N-(3,5-dihalo-4-ethyl-2-hydroxyphenyl)-2-(3-pentadecylphenoxy)butanamide
Hydroxyl group	N-(3,5-dichloro-4-ethyl-2-*substituted*phenyl)-2-(3-

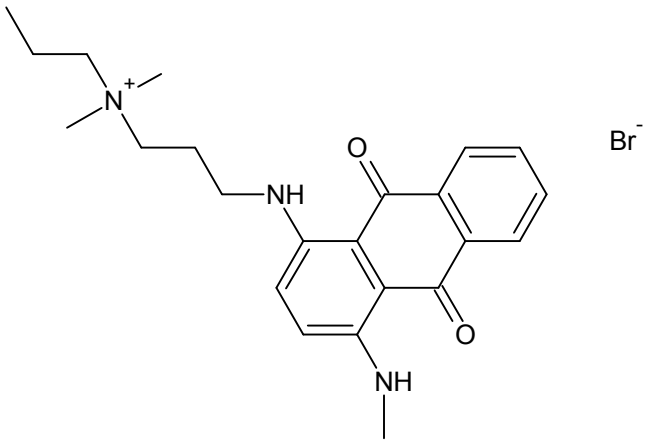
Single Masking	Acceptable Masked Name
	pentadecylphenoxy)butanamide
Ethyl group	N-(3,5-dichloro-4-alkyl-2-hydroxyphenyl)-2-(3-pentadecylphenoxy)butanamide
Pentadecyl group	N-(3,5-dichloro-4-ethyl-2-hydroxyphenyl)-2-(3-alkylphenoxy)butanamide
Butane parent	N-(3,5-dichloro-4-ethyl-2-hydroxyphenyl)-2-(3-pentadecylphenoxy)alkanamide

Double Masking	Acceptable Masked Name
Butane parent (plus parent locant)	N-(3,5-dichloro-4-ethyl-2-hydroxyphenyl)-(3-pentadecylphenoxy)alkanamide

Appendix Figure 2. Example 2

Fully Defined Name

N,N-Dimethyl-3-{[4-(methylamino)-9,10-dioxo-9,10-dihydroanthracen-1-yl]amino}-N-propylpropan-1-aminium bromide



Single Masking	Acceptable Masked Name
Bromine anion	N,N-Dimethyl-3-{[4-(methylamino)-9,10-dioxo-9,10-dihydroanthracen-1-yl]amino}-N-propylpropan-1-aminium salt
Oxo groups	N,N-Dimethyl-3-{[4-(methylamino)-9,10-di*substituted*-9,10-dihydroanthracen-1-yl]amino}-N-propylpropan-1-aminium bromide
Methyl groups	N,N-Dialkyl-3-{[4-(methylamino)-9,10-dioxo-9,10-dihydroanthracen-1-yl]amino}-N-propylpropan-1-aminium bromide
Propyl group	N,N-Dimethyl-3-{[4-(methylamino)-9,10-dioxo-9,10-dihydroanthracen-1-yl]amino}-N-alkylpropan-1-aminium bromide
Propane parent	N,N-Dimethyl-3-{[4-(methylamino)-9,10-dioxo-9,10-dihydroanthracen-1-yl]amino}-N-propylalkan-1-aminium bromide
Anthracene parent	N,N-Dimethyl-3-{[4-(methylamino)-9,10-dioxo-9,10-dihydrocarbopolycycl-1-yl]amino}-N-propylpropan-1-aminium bromide

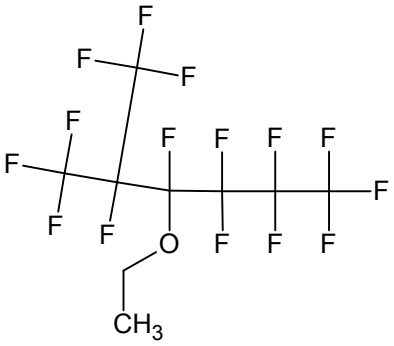
Double Masking	Acceptable Masked Name
Anthracene parent (plus parent locants)	N,N-Dimethyl-3-{[(methylamino)-dioxo-dihydro-carbopolycyclyl]amino}-N-propylpropan-1-aminium

Double Masking	Acceptable Masked Name
	bromide
Propane parent (plus parent locants)	Dimethyl{[4-(methylamino)-9,10-dioxo-9,10-dihydroanthracen-1-yl]amino}propylalkanaminium bromide

Appendix Figure 3. Example 3

Fully Defined Name

3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)hexane



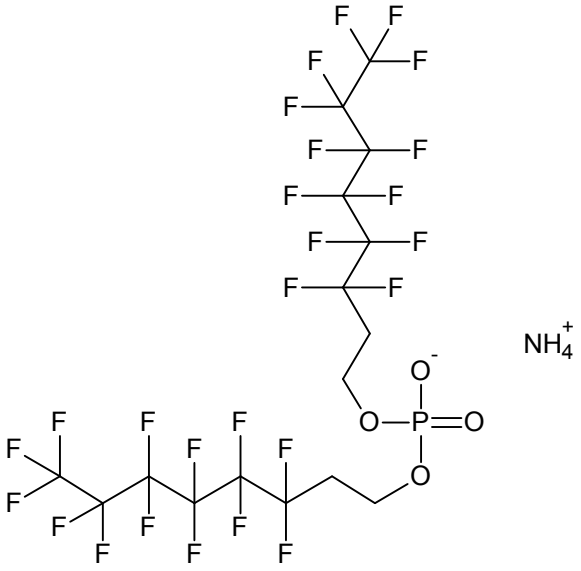
Single Masking	Acceptable Masked Name
Number of fluorine atoms	3-ethoxy-polyfluoro-2-(polyfluoromethyl)hexane
Fluorine atoms	3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecahalo-2-(trihalomethyl)hexane
Ethoxy group	3-(alkoxy)-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)hexane
Hexane parent	3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)alkane

Double Masking	Acceptable Masked Name
Hexane parent (plus parent locants)	Ethoxydodecafluoro(trifluoromethyl)alkane

Appendix Figure 4. Example 4

Fully Defined Name

Ammonium bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) phosphate



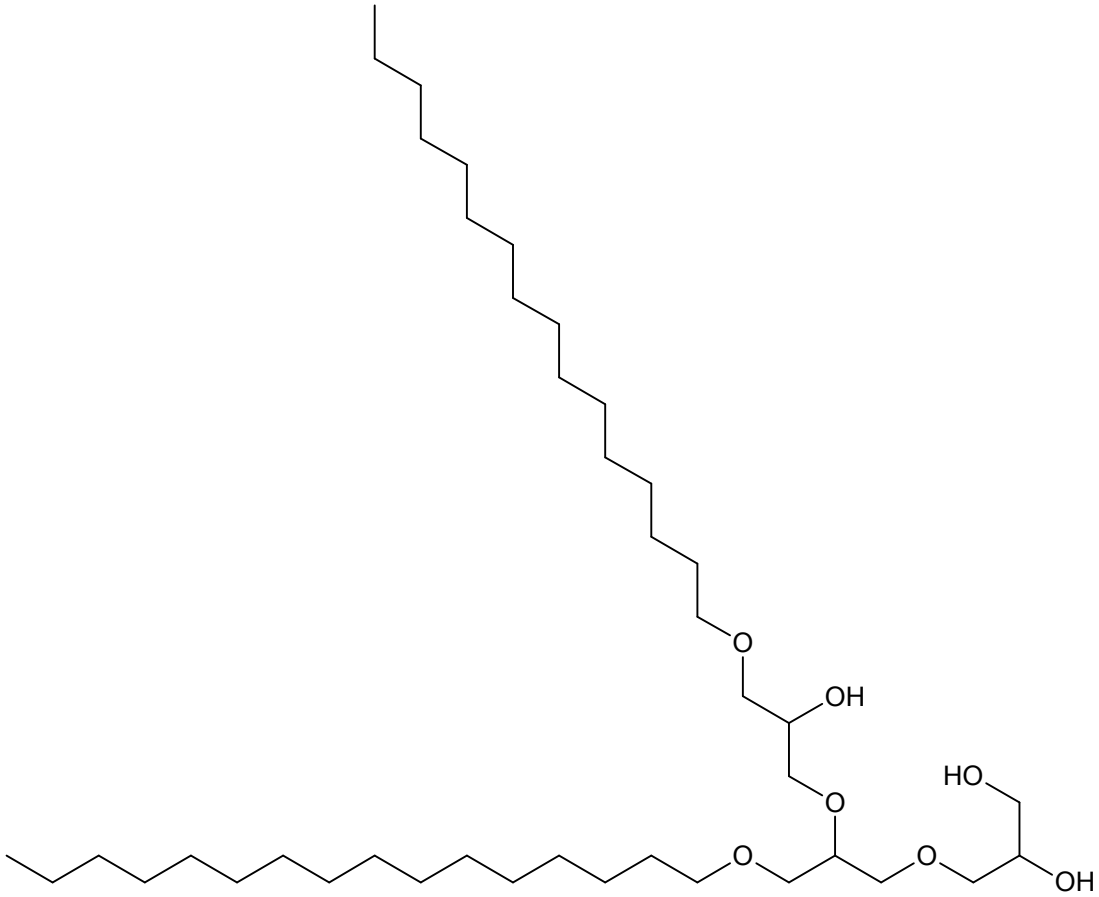
Single Masking	Acceptable Masked Name
Fluorine atoms	Ammonium bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecahalooctyl) phosphate
Number of fluorine atoms	Ammonium bis(polyfluorooctyl) phosphate
Ammonium cation	bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) phosphate salt
Octane parent	Ammonium bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoroalkyl) phosphate

Double Masking	Acceptable Masked Name
Octane parent (plus parent locants)	Ammonium bis(tridecafluoroalkyl) phosphate

Appendix Figure 5. Example 5

Fully Defined Name

6,9-bis(hexadecyloxymethyl)-4,7-dioxanonane-1,2,9-triol



Single Masking	Acceptable Masked Name
Hydroxyl group positions	6,9-bis(hexadecyloxymethyl)-4,7-dioxanonanetriol
Hydroxyl groups	6,9-bis(hexadecyloxymethyl)-4,7-dioxanonane-1,2,9-tri*substituted*
Hexadecyl groups	6,9-bis(alkoxymethyl)-4,7-dioxanonane-1,2,9-triol
Nonane parent	6,9-bis(hexadecyloxymethyl)-4,7-dioxaalkane-1,2,9-triol

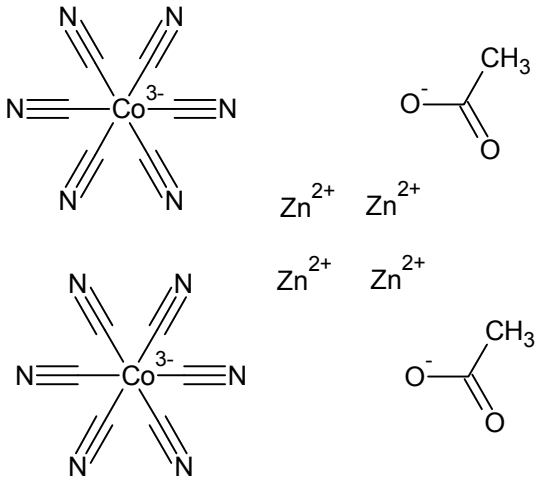
Double Masking	Acceptable Masked Name
Nonane parent (plus parent locants)	bis(hexadecyloxymethyl)dioxaalkanetriol

Appendix Figure 6. Example 6

Fully Defined Name

Tetrazinc diacetate bis-hexakis(cyano-κC)cobaltate(3-)

$Zn(II)_4([Co(III)(CN)_6]^{3-})_2(CH_3COO^-)_2$



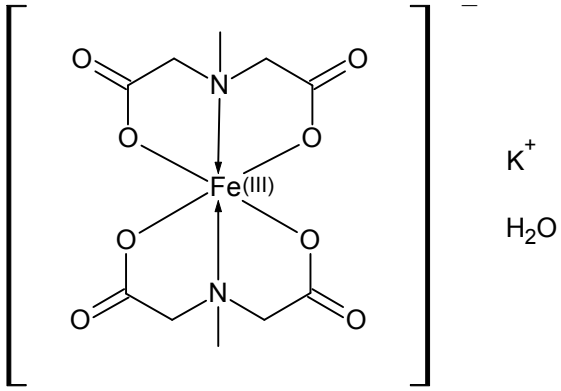
Single Masking	Acceptable Masked Name
Cyano groups	Tetrazinc diacetate bis-hexakis(*substituted*-κ)cobaltate(3-)
Acetate groups	Tetrazinc dialkanoate bis-hexakis(cyano-κC)cobaltate(3-)

Double Masking	Acceptable Masked Name
Acetate and Cyano groups	Tetrazinc dialkanoate bis-hexakis(*substituted*-κ)cobaltate(3-)

Appendix Figure 7. Example 7

Fully Defined Name

Potassium bis[2,2'-(methylimino-κN)diacetato-κO(2-)]ferrate(1-) monohydrate



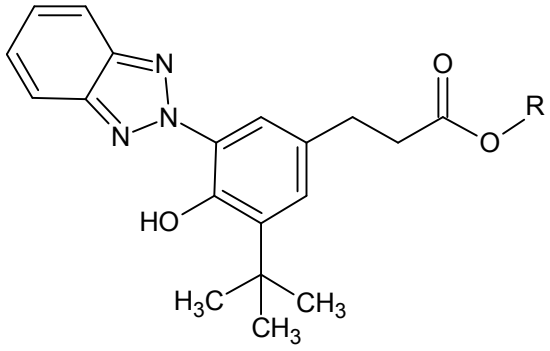
Single Masking	Acceptable Masked Name
Potassium cation	Alkali metal bis[2,2'-(methylimino-κN)diacetato-κO(2-)]ferrate(1-) monohydrate
Methyl groups	Potassium bis[2,2'-(alkylimino-κN) diacetato-κO(2-)]ferrate(1-) monohydrate
Amine groups	Potassium bis[2,2'-(methyl*substituted*-κ)diacetato-κO(2-) derivative]ferrate(1-) monohydrate

Double Masking	Acceptable Masked Name
Amine groups (plus locants)	Potassium bis[(methyl*substituted*)diacetato-κO(2-) derivative]ferrate(1-) monohydrate

Appendix Figure 8. Example 8

Fully Defined Name

C7-C9 (linear and branched) alkyl 3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]propionate



R = C_7 - C_9

Single Masking	Acceptable Masked Name
Hydroxyl group	C7-C9 (linear and branched) alkyl 3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-*substituted* phenyl]propionate
Methyl groups	C7-C9 (linear and branched alkyl 3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dialkylethyl)-4-hydroxyphenyl]propionate
C7-C9 alkyl group	(linear and branched) alkyl 3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]propionate
Benzotriazol parent	C7-C9 (linear and branched) alkyl 3-[3-(2H-heteropolycycl-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]propionate
Phenyl parent	C7-C9 (linear and branched) alkyl 3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyaryl]propionate
Propane parent	C7-C9 (linear and branched) alkyl 3-[3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]alkanoate

Double Masking	Acceptable Masked Name
Benzotriazol parent (plus parent locants)	C7-C9 (linear and branched) alkyl 3-[3-(heteropolycyclyl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]propionate

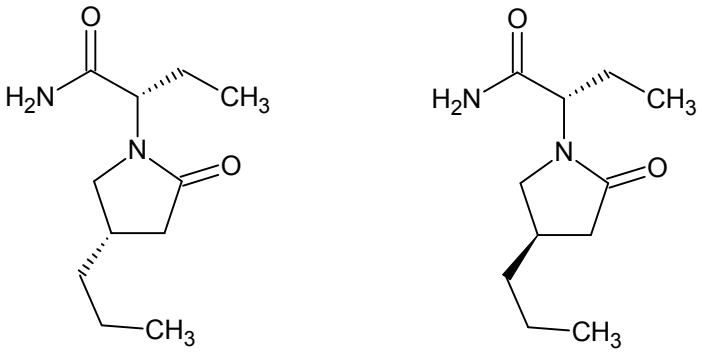
Double Masking	Acceptable Masked Name
Phenyl parent (plus parent locants)	C7-C9 (linear and branched) alkyl 3-[(2H-benzotriazol-2-yl)(1,1-dimethylethyl) hydroxyaryl]propionate
Propane parent (plus parent locants)	C7-C9 (linear and branched) alkyl [3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxyphenyl]alkanoate

Appendix 1.1.2 Multi-constituent substances

Appendix Figure 9. Example 9

Fully Defined Name

Reaction mass of (2S)-2-[(4R)-2-oxo-4-propylpyrrolidin-1-yl]butanamide and (2S)-2-[(4S)-2-oxo-4-propylpyrrolidin-1-yl]butanamide



Single Masking	Acceptable Masked Name
Stereochemistry	Stereoisomers of 2-[2-oxo-4-propylpyrrolidin-1-yl]butanamide
Oxo group	Reaction mass of (2S)-2-[(4R)-2-*substituted*-4-propylpyrrolidin-1-yl]butanamide and (2S)-2-[(4S)-2-*substituted*-4-propylpyrrolidin-1-yl]butanamide
Propyl group	Reaction mass of (2S)-2-[(4R)-2-oxo-4-alkylpyrrolidin-1-yl]butanamide and (2S)-2-[(4S)-2-oxo-4-alkylpyrrolidin-1-yl]butanamide
Butane parent	Reaction mass of (2S)-2-[(4R)-2-oxo-4-propylpyrrolidin-1-yl]alkanamide and (2S)-2-[(4S)-2-oxo-4-propylpyrrolidin-1-yl]alkanamide
Pyrrolidine parent	Reaction mass of (2S)-2-[(4R)-2-oxo-4-propylheteromonocycl-1-yl]butanamide and

Single Masking	Acceptable Masked Name
	(2S)-2-[(4S)-2-oxo-4-propylheteromonocycl-1-yl]butanamide

Double Masking	Acceptable Masked Name
Butane parent (plus parent locants)	Reaction mass of (S)-[(4R)-2-oxo-4-propylpyrrolidin-1-yl]alkanamide and (S)-[(4S)-2-oxo-4-propylpyrrolidin-1-yl]alkanamide
Pyrrolidine parent (plus parent locants)	Reaction mass of (2S)-2-[(R)-oxopropylheteromonocyclyl]butanamide and (2S)-2-[(S)-oxopropylheteromonocyclyl]butanamide

Appendix Figure 10. Example 10

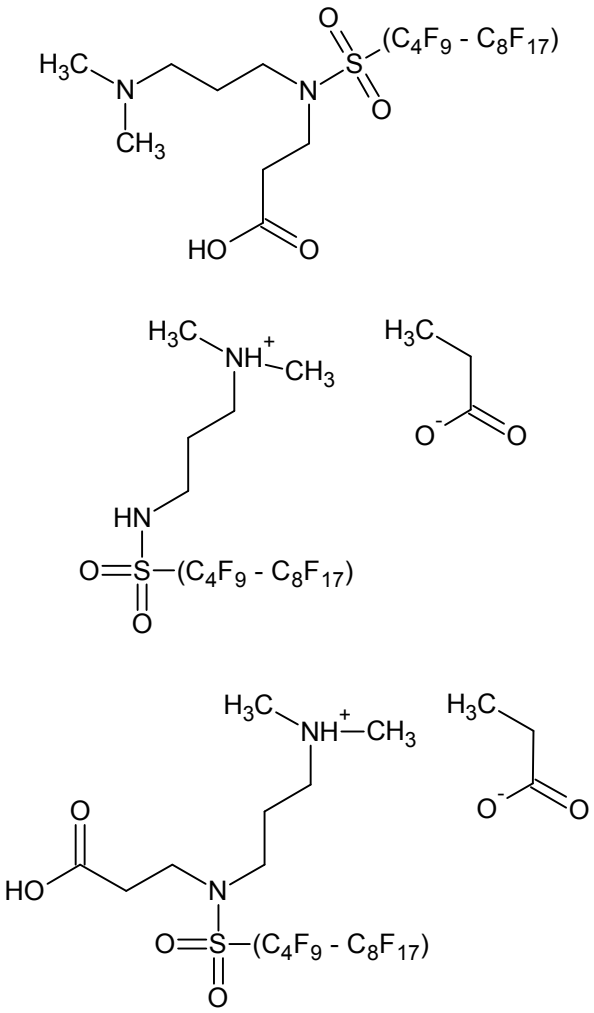
Fully Defined Name

Reaction mass of

N-[3-(dimethylamino)propyl]-N-[(perfluoro-(C4-8)-alkyl)sulfonyl]-β-alanine and

N,N-dimethyl-3-{[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}propan-1-aminium propanoate and

3-{(2-carboxyethyl)[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}-N,N-dimethylpropan-1-aminium propanoate



Single Masking	Acceptable Masked Name
Methyl groups	Reaction mass of N-[3-(dialkylamino)propyl]-N-[(perfluoro-(C4-8)-alkyl)sulfonyl]-β-alanine and

Single Masking	Acceptable Masked Name
	N,N-dialkyl-3-{[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}propan-1-aminium propanoate and 3-{(2-carboxyethyl)[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}-N,N-dialkylpropan-1-aminium propanoate
Propanoate group	Reaction mass of N-[3-(dimethylamino)propyl]-N-[(perfluoro-(C4-8)-alkyl)sulfonyl]-β-alanine and N,N-dimethyl-3-{[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}propan-1-aminium alkanoate and 3-{(2-carboxyethyl)[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}-N,N-dimethylpropan-1-aminium alkanoate
Propane parent	Reaction mass of N-[3-(dimethylamino)alkyl]-N-[(perfluoro-(C4-8)-alkyl)sulfonyl]-β-alanine and N,N-dimethyl-3-{[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}alkan-1-aminium propanoate and 3-{(2-carboxyethyl)[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}-N,N-dimethylalkan-1-aminium propanoate

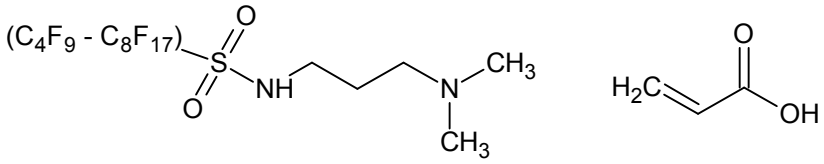
Double Masking	Acceptable Masked Name
Propane parent (plus parent locants)	Reaction mass of N-[(dimethylamino)alkyl]-N-[(perfluoro-(C4-8)-alkyl)sulfonyl]-β-alanine and N,N-dimethyl{[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}alkanaminium propanoate and {(2-carboxyethyl)[(perfluoro-(C4-8)-alkyl)sulfonyl]amino}-N,N-dimethylalkanaminium propanoate

Appendix 1.2 UVCB substances

Appendix Figure 11. Example 11

Fully Defined Name

Reaction products of N-[3-(dimethylamino)propyl]perfluoro-(C4-8)-alkylsulfonamide and acrylic acid



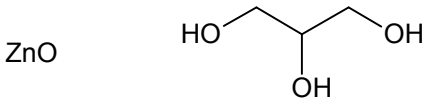
Single Masking	Acceptable Masked Name
Methyl groups	Reaction products of N-[3-(dialkylamino)propyl]perfluoro-(C4-8)-alkylsulfonamide and acrylic acid
Propyl group	Reaction products of N-[3-(dimethylamino)alkyl]perfluoro-(C4-8)-alkylsulfonamide and acrylic acid
Number of fluorine atoms	Reaction products of N-[3-(dimethylamino)propyl]polyfluoro-(C4-8)-alkylsulfonamide and acrylic acid
Fluoro groups	Reaction products of N-[3-(dimethylamino)propyl]perhalo-(C4-8)-alkylsulfonamide and acrylic acid
Propenyl group (propenoic acid/acrylic acid)	Reaction products of N-[3-(dimethylamino)propyl]perfluoro-(C4-8)-alkylsulfonamide and alkenoic acid

Double Masking	Acceptable Masked Name
Propyl group (plus locants)	Reaction products of N-[(dimethylamino)alkyl]perfluoro-(C4-8)-alkylsulfonamide and acrylic acid

Appendix Figure 12. Example 12

Fully Defined Name

Reaction products of Zinc Oxide and Glycerol



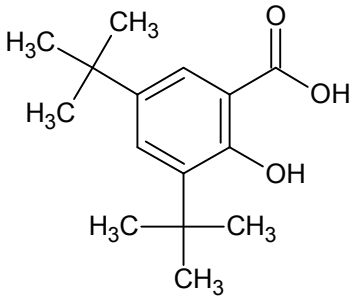
Single Masking	Acceptable Masked Name
Hydroxyl groups (glycerol)	Reaction products of Zinc Oxide and 1,2,3-tri*substituted* propane
Propyl parent (glycerol)	Reaction products of Zinc Oxide and alkane-1,2,3-triol

Double Masking	Acceptable Masked Name
Propyl parent (plus parent locants) (glycerol)	Reaction products of Zinc Oxide and alkanetriol

Appendix Figure 13. Example 13

Fully Defined Name

Reaction product of 3,5-di-tert-butylsalicylic acid and aluminium sulfate



$Al_2(SO_4)_3$

Single Masking	Acceptable Masked Name
Hydroxyl group (3,5-di-tert-butylsalicylic acid)	Reaction product of 3,5-di-tert-butyl-2-*substituted*-benzoic acid and aluminium sulfate
Tert-Butyl groups (3,5-di-tert-butylsalicylic acid)	Reaction product of 3,5-di-tert-alkyl-salicylic acid and aluminium sulfate
Benzene parent (3,5-di-tert-butylsalicylic acid)	Reaction product of 3,5-di-tert-butyl-1-carboxyl-2-hydroxy-arene and aluminium sulfate

Double Masking	Acceptable Masked Name
Benzene parent (plus locants) masked (3,5-bis-tert-butylsalicylic acid)	Reaction product of di-tert-butyl-carboxyl-hydroxy-arene and aluminium sulfate

Appendix 1.2.1 Enzymes

Example 14

Full Defined Name

(R,R)-butane-2,3-diol:NAD+ oxidoreductase, EC 1.1.1.4
Reaction: (R,R)-butane-2,3-diol + NAD+ = (R)-acetoin + NADH + H+

Public Name

Oxidoreductase with NAD+ or NADP+ as acceptor, EC 1.1.1

Example 15

Fully Defined Name

S-adenosyl-L-methionine hydrolase, EC 3.3.1.2
Reaction: S-adenosyl-L-methionine + H2O = L-homoserine + methylthioadenosine

Public Name

Thioether and trialkylsulfonium hydrolases, EC 3.3.1

Example 16

Fully Defined Name

(S)-4-hydroxymandelonitrile hydroxybenzaldehyde-lyase, EC 4.1.2.11
Reaction: (S)-4-hydroxymandelonitrile = cyanide + 4-hydroxybenzaldehyde

Public Name

EC 4.1.2 Aldehyde-Lyases, EC 4.1.2

Appendix 2 Example – Claim on IUPAC Name under Article 119(2)(f)

Example Corporation
1234 South Lime Street, London AZ5 12T, UK
Tel +44 1 123 4567 Fax +44 1 123 4568
www.examplecorporation.com

Declaration:

We, Example Corporation, claim the IUPAC Name of ExampleSubstance confidential in accordance with REACH Article 119(2)(f).

We, Example Corporation, hereby declare that, to the best of our knowledge as of today (10th July 2010), and in accordance with the due measures of protection that we have implemented, a member of the public should not be able to obtain access to the information claimed confidential without our consent or that of the third party whose commercial interests are at stake, and in particular that the information is not publicly available in any of the following public databases: eChemPortal.

Demonstration of Commercial Interest:

To produce thin film coatings Example Corporation has performed combinatorial experiments to add different organic groups a base plastic monomer, which has resulted in the discovery of the substance covered by this dossier. Such experimentation required substantial investments of time and resources to develop the particular functionalities unique to our SampleProduct range, which arise from the use of the substance covered by this dossier. These particular functionalities represent the major selling point for out SampleProduct range, and represent our major competitive advantage in the coatings market.

Demonstration of Potential Harm:

Disclosure of the IUPAC name of the substance covered by this dossier would allow our competitors to replicate directly the functionalities of our Sample Product range without the need to test a whole variety of organic groups. Disclosure would also allow our competitors to deduce certain of the alternatives explored by Example Corporation, as well as revealing the likely future direction of our product development research. Such immediate replication of the functionalities of our SampleProduct range would harm the market position of Example Corporation, and the ability to deduce the future direction of our product development would allow competitors the opportunity to develop more quickly their own competing products thereby reducing our period of maximum market share.

Limitation to Validity of Claim:

The claim for confidentiality on the IUPAC name of ExampleSubstance should remain valid for a period of six years, in accordance with REACH Article 119(2)(f).

Contact Person

Questions on this confidentiality claim should be directed to John Q. Smith, REACH Implementation Manager Example Corporation, 1234 South Lime Street, London AZ5 12T, UK
+44 1 123 4567; j.smith@examplecorporation.com

Masking Justification for Public Name - Only required if IUPAC Name claimed confidential

One Level Masking of IUPAC Name - Example 3 (see Appendix 1.1.1)

Number of fluorine atoms masked.

Two-Level Masking of IUPAC Name

Hexane parent and number of fluorine atoms masked, and a valid well-reasoned justification why the second level masking is necessary by the registrant.

Three-Level Masking of IUPAC Name

Ethoxy group, Hexane parent and number of fluorine atoms masked, and a valid well-reasoned justification why the third level masking is necessary by the registrant.

European Chemicals Agency, PO Box 400, Annankatu 18, FI-00121 Helsinki, Finland. **http://echa.europa.eu**