To:	**Trebert-Haeberlin, Susanne STH DSC-CHSE-STH <s.trebert-haeberlin@shell.com>; Cagen, Stuart Z SCC-CF-SS <stuart.cagen@shell.com>; Teague-Lixey, Holly E SCC-HSE <holly.teague-lixey@shell.com>; Gingell, Ralph SCC-HSSE <ralph.gingell@shell.com>; Cubillas, Mary SCC-CHSE <mary.cubillas@shell.com>; Clegg, Patsy M SCC-CHSE-PC <patsy.clegg@shell.com>; Mora, Bebe G SCC-CHSE <bebe.mora@shell.com>; Hulse, Michael SCC-CHSEMH <michael.hulse@shell.com>; Antrican, Susan O SCC-CHSE <susan.antrican@shell.com>; Semmler, Klaus K DSC-CHSE-KS <klaus.semmler@shell.com>; Greenhough, John JA SC-OELS/0 <john.greenhough@shell.com>**
From:	**Priston, Robert A SC-CHSE-BP </O=SHELL/OU=OPC/CN=RECIPIENTS/CN=SNRPR1>**
Cc:	**Williams, Elizabeth J SCCA-HSE <elizabeth.williams@shell.com>; Snyder, Phil J SCC-HSE-OE <phil.snyder@shell.com>**
Bcc:	
Received Date:	**2005-06-13 09:16:01 GMT**
Subject:	**RE: CT Toxicology estimates 2005, 2006 & 2007**

Susanne,
Sorry, but I don't know what CT budgets cover so I cannot provide a definitive answer.

It may be that some budget needs to be in place for phys chem characterisation of our substances in preparation for REACH for, although consortia may do much of the registration, there will a need for producers to provide, what I think may be quite detailed phys chem on our chemical substances and this may have to be provided by ourselves as a producer rather under the umbrella of a consortium.

I enclose a draft technical guidance document that was discussed in CEFIC on Friday. This is prepared by a Task Force within CEFIC under contract from the EU Commission i.e. it will be influential and indicates the current thinking. The information being asked for appears extensive to me and it is apparently very similar, if not identical, to the dataset required for registering a New Chemical Subtance currently under the Dangerous Substances Directive. Do we have all of this information currently on our substances? If not is this may be something that needs to be produced by CT?

Regads,
Bob

R A J Priston

Shell Chemicals Limited
Shell Centre, London SE1 7NA, United Kingdom
Tel: +44 (0) 207 934 2796 Fax: 7155
Mobile: 07 816 013 101
Email: robert.priston@shell.com
Internet: http://www.shell.com

-----Original Message-----
From: Trebert-Haeberlin, Susanne STH DSC-CHSE-STH
Sent: 12 June 2005 18:47
To: Cagen, Stuart Z SCC-CF-SS; Teague-Lixey, Holly E SCC-HSE; Priston, Robert A SC-CHSE-BP
Subject: RE: CT Toxicology estimates 2005, 2006 & 2007

Thanks, from the European side there is no extra budget needed as this is planned into the annual fees we pay for SSC, CEFIC PO/PG and ISOPA.

Bob,

any additions from your perspective??
Susanne

Dr. Susanne Trebert Haeberlin
Global Product Steward/Toxicology Adviser
SMPO and Sadaf BU

Deutsche Shell Chemie GmbH
Rheinland Raffinerie Wesseling
Ludwigshafener Straße 1
D-50389 Wesseling - Germany

Tel. +49 6073 73 11 76
Fax. +49 6073 73 11 77
Mobile +49 172 672 1403

-----Original Message-----
From: Cagen, Stuart Z SCC-CF-SS
Sent: Freitag, 10. Juni 2005 22:38
To: Teague-Lixey, Holly E SCC-HSE
Cc: Trebert-Haeberlin, Susanne STH DSC-CHSE-STH
Subject: RE: CT Toxicology estimates 2005, 2006 & 2007

Thanks. I think I put down about 90,000 USD for SIRC dues

Stuart Cagen

Shell Chemical LP
One Shell Plaza, 910 Louisiana, Houston, TX 77002-4916

Tel: +1 713 241 1407 **Fax:** 3325 **Other Tel:** +1 832 646 3987
Email: stuart.cagen@shell.com
Internet: http://www.shell.com/chemicals

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-----Original Message-----
From: Teague-Lixey, Holly E SCC-HSE
Sent: Friday, June 10, 2005 2:50 PM
To: Cagen, Stuart Z SCC-CF-SS
Cc: Trebert-Haeberlin, Susanne STH DSC-CHSE-STH
Subject: RE: CT Toxicology estimates 2005, 2006 & 2007

Stuart,

My apologies for the confusion. I made the assumption Susanne was copied on this email. She usually handles budgeting since she is the Global Product Steward for SMPO. We will provide you the requested data as soon as possible.

Thanks for your patience,
Holly

-----Original Message-----
From: Cagen, Stuart Z SCC-CF-SS
Sent: Tuesday, June 07, 2005 12:10 AM
To: Gingell, Ralph SCC-HSSE; Cubillas, Mary SCC-CHSE; Clegg, Patsy M SCC-CHSE-PC; Mora, Bebe G SCC-CHSE; Teague-Lixey, Holly E SCC-HSE; Hulse, Michael SCC-CHSEMH; Antrican, Susan O SCC-CHSE; Semmler, Klaus K DSC-CHSE-KS
Cc: Williams, Elizabeth J SCCA-HSE; Snyder, Phil J SCC-HSE-OE
Subject: RE: CT Toxicology estimates 2005, 2006 & 2007

All:

I was asked to provide something this week. Note I have responded; not also the uncertainty regarding most of the values.

I am anticipating some real values from solvents and EO/EG real soon.

Patsy: you and I need to calibrate our Shanghai cost assumptions. I came up with a much higher '06 value.

Thanks << Message: RE: CT Toxicology estimates 2005, 2006 & 2007 >>

Stuart Cagen

Shell Chemical LP
One Shell Plaza, 910 Louisiana, Houston, TX 77002-4916

Tel: +1 713 241 1407 **Fax:** 3325 **Other Tel:** +1 832 646 3987
Email: stuart.cagen@shell.com
Internet: http://www.shell.com/chemicals

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-----Original Message-----
From: Cagen, Stuart Z SCC-CF-SS
Sent: Wednesday, June 01, 2005 2:27 PM
To: Gingell, Ralph SCC-HSE; Cubillas, Mary SCC-CHSE; Clegg, Patsy M SCC-CHSE-PC; Mora, Bebe G SCC-CHSE; Teague-Lixey, Holly E SCC-HSE; Hulse, Michael SCC-CHSEMH; Antrican, Susan O SCC-CHSE; Semmler, Klaus K DSC-CHSE-KS
Cc: Williams, Elizabeth J SCCA-HSE; Snyder, Phil J SCC-HSE-OE
Subject: RE: CT Toxicology estimates 2005, 2006 & 2007

I've heard from Susan. Please respond as soon as feasible.

Thanks

Stuart

Stuart Cagen

Shell Chemical LP
One Shell Plaza, 910 Louisiana, Houston, TX 77002-4916

Tel: +1 713 241 1407 **Fax:** 3325 **Other Tel:** +1 832 646 3987
Email: stuart.cagen@shell.com
Internet: http://www.shell.com/chemicals

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-----Original Message-----
From: Cagen, Stuart Z SCC-CF-SS
Sent: Tuesday, May 17, 2005 10:26 AM
To: Gingell, Ralph SCC-HSE; Cubillas, Mary SCC-CHSE; Clegg, Patsy M SCC-CHSE-PC; Mora, Bebe G SCC-CHSE; Teague-Lixey, Holly E SCC-HSE; Hulse, Michael SCC-CHSEMH; Antrican, Susan O SCC-CHSE; Semmler, Klaus K DSC-CHSE-KS
Cc: Williams, Elizabeth J SCCA-HSE; Snyder, Phil J SCC-HSE-OE
Subject: FW: CT Toxicology estimates 2005, 2006 & 2007

ALL:

This is a request for US Tox R&D:

As before, please send me expected budget values for 2005 (I suppose they mean actual), 2006 and 2007, as per the note below.

They are asking for a response by June 3. How about getting values to me by May 31st so I have some time to compile and possibly ask follow up questions. OK ?

Thanks

Stuart

Stuart Cagen

Shell Chemical LP
One Shell Plaza, 910 Louisiana, Houston, TX 77002-4916

Tel: +1 713 241 1407 **Fax:** 3325 **Other Tel:** +1 832 646 3987
Email: stuart.cagen@shell.com
Internet: http://www.shell.com/chemicals

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-----Original Message-----
From: Van den Brakel, Peter P GSSIC-GSFTP
Sent: Tuesday, May 17, 2005 3:28 AM
To: Cagen, Stuart Z SCC-CF-SS
Cc: Fleming, Gary L GSSCC-GSFTP
Subject: CT Toxicology estimates 2005, 2006 & 2007

Stuart,

The budgetprocess has started for collecting best estimates for 2005, 2006 & 2007.

Appreciate if you could fill in the YELLOW area in the attached

Excelsheet and return it to me. As reference you can find 2005 budget and previous 2006 estimate.

<< File: Budget 2006 Toxicology.xls (Compressed) >>

You would help me very much if you return this back to me **Friday 3rd June** at the latest.

Thanks in advance,

with kind regards,
peter

Attachments:

R00009 RIP 3.10 TGD text proposal chapters 2 4 and 5 IEG.doc

INSERT YOUR PICTURE(S) IN THIS CELL

Technical Guidance Document for characterisation and checking of Substance Identity

REACH Implementation Project 3.10

Joint Research Centre
Institute for Health and Consumer Protection
Toxicology and Substances Unit

26 May 2005

9P7801.01

A COMPANY OF

ROYAL HASKONING

HASKONING NEDERLAND B.V.
ENVIRONMENT

Barbarossastraat 35
P.O. Box 151
Nijmegen 6500 AD
The Netherlands
+31 (0)24 328 42 84 Telephone
+31 (0)24 322 81 70 Fax
info@nijmegen.royalhaskoning.com E-mail
www.royalhaskoning.com Internet
Arnhem 09122561 CoC

Document title	Technical Guidance Document for characterisation and checking of Substance Identity REACH Implementation Project 3.10
Document short title	TGD Substance Identity Check
Status	First draft TGD structure
Date	26 May 2005
Project name	TGD Substance Identification in REACH
Project number	9P7801.01
Client	Joint Research Centre Institute for Health and Consumer Protection Toxicology and Substances Unit
Reference	9P7801.01/R00006/SCH/Nijm

Drafted by	Anouk Schwegler	
Checked by	Han Blok	
Date/initials check	……	……
Approved by	Onno Jongerius	
Date/initials approval	……	……

ROYAL HASKONING

CONTENTS

2 DEFINITIONS AND ABBREVIATIONS

2.1 Definitions

The definitions used in this Technical Guidance Document are listed and explained in table 2.1.

Table 2.1.: Definitions

Definition	Description	Reference
Actor in the supply chain*	All manufacturers and/or importers and/or downstream users.	R01
Additive	Auxiliary agent intentionally added to enhance the stability of the substance.	New
	A constituent which has been intentionally added to stabilize the substance	new (REACH Alliance)
Agency*	A central Agency will be in charge of the day-to-day management of REACH.	R15-2
Article*	Article means an object composed of one or more substances or preparations which during production is given a specific shape, surface or design determining its end use function to a greater degree than its chemical composition does.	R01
Biocide (Biocidal product)*	Active substances and preparations containing one or more active substances, put up in the form in which they are supplied to the user, intended to destroy, deter, render harmless, prevent the action of, or otherwise exert a controlling effect on any harmful organism by chemical or biological means. [Directive 98/8/EC]	R15-2
Chemical	A synonym for substance.	R15-2
Company*	A generic term that covers manufacturer, importer or only representative. The term M/I/R is also used for the same concept.	R15-2
Competent authority*	Competent authority means the authority or authorities or bodies established by the Member States to carry out the obligations arising from the REACH Regulation.	R01
Consortium leader*	The company providing registration information on behalf of the other members of the consortium. Also called “the one manufacturer or importer” in [REACH_PR1, 10 (1)].	R15-2
Consortium*	Grouping of companies for the purposes of registration.	R15-2
Constituent	A quantity of molecules with identical structural formulas as defined by a single CAS registry number which is present in a chemical substance from its manufacturing process.	new (Cefic)
	any single species that can be characterised by its unique chemical formulae, mineralogical composition or physico-chemical properties	new (REACH Alliance)
Distributor*	Means any natural or legal person established within the Community, including a retailer, who only stores and places on the market a substance, on its own or in a preparation, for third parties;	R01

Definition	Description	Reference
Downstream user*	Any natural or legal person established within the Community, other than the manufacturer or the importer, who uses a substance, either on its own or in a preparation, in the course of his industrial or professional activities. A distributor or a consumer is not a downstream user. A re-importer exempted pursuant to Article 4(2)(c) shall be regarded as a downstream user. Formulators and industrial users of chemicals. Companies that use substance professionally or industrially (on their own, in preparations). Example: a manufacturer who mixes different chemicals to make ink, or uses the ink to print leaflets.	R01
Existing substance	An "existing" chemical substance is in the EU defined as any chemical substance listed in the **E**uropean **IN**ventory of **E**xisting **C**ommercial **S**ubstances (EINECS), an inventory containing 100,195 substances. The EINECS lists all substances which were on the EU market between 1 January 1971 and 18 September 1981. The EINECS inventory was drawn up by the European Commission to meet the requirements of Article 13 of Directive 79/831/EEC. EINECS was published in the Official Journal of the European Communities in 1990 (OJ C146A, 15 June 1990, page 1-1802).	new
Import*	Means the physical introduction into the customs territory of the Community;	R01
Importer*	Any natural or legal person established within the Community who is responsible for import (The physical introduction into the customs territory of the Community).	R01
Impurity	Substance that may have been present in the starting materials or is the result of secondary or incomplete reactions. While it is present in the final product it was not intentionally added, nor does it enhance the commercial value of that substance.	new
Information requirement*	Annexes IV to IX specify the information requirements, the information that shall be submitted for registration and evaluation purposes according to Articles 9, 11 and 12, 39, 40 and 44. For the lowest tonnage level, the standard requirements are in Annex V, and every time a new tonnage level is reached, the requirements of the corresponding Annex have to be added to the dossier and the updated dossier resubmitted. For each registration the precise information requirements will differ, according to tonnage, use and exposure.	R15-2
Intermediate	Intermediate means a substance that is solely manufactured for and consumed in or used for chemical processing in order to be transformed into another substance. One distinguishes between: • Non-isolated intermediate • . On site isolated intermediate • . Transported isolated intermediate	R01

Definition	Description	Reference
Inventory*	Examples of inventories are: • ELINCS (European List of Notified Chemical Substances); • EINECS (European Inventory of Existing Commercial Chemical Substances); • TSCA inventory in the USA (Toxic Substance Control Act); • Domestic Substances List Canada (DSL) ; • Australian Inventory of Chemical Substances (AICS); • Inventory of Existing and New Chemical Substances in Japan (ENCS); • Philippines Inventory of Chemicals and Chemical Substances (PICCS).	R15-2
IUCLID	IUCLID is a database and management system for the administration of data on chemical substances. This system was initially developed to fulfil European requirements for the evaluation and control of the risks of existing chemical substances. IUCLID has been designed for entering and storing in a relational database the information on the properties of substances in an agreed upon format for use in regulatory submissions. IUCLID can generate reports from information entered into the data base in formats suitable to meet the reporting requirements of the US EPA HPV Chemical Challenge program, the EU Existing Chemicals program, the EU Biocides program and the OECD SIDS program.	R15-2
M/I/R*	M/I/R is a shortcut term to designate manufacturer, importer or only representative. The term company is also used with the same meaning.	R15-2
M/I/R/DU*	M/I/R/DU is a shortcut term to designate a M/I/R or a downstream user.	R15-2
Main constituent	The constituent in a real substance that makes (as a general rule) >80% (w/w) of the composition of that substance.	new
Major constituent	The constituent in a real substance that makes (as a general rule) between 10 and 80% (w/w) of the composition of that substance.	New
Manufacturer*	Any natural or legal person established within the Community manufacturing (producing and extracting substances in the natural state) a substance within the Community.	R01
Manufacturing*	Means production and extraction of substances in the natural state.	R01
Mono-constituent substance	A real substance in which one type of molecule is present for at least 80% (w/w).	new
New substance	A synonym for notified substance.	new
Non-isolated intermediate	Means an intermediate that during synthesis is not intentionally removed (except for sampling) from the equipment in which the synthesis takes place. Such equipment includes the reaction vessel, its ancillary equipment, and any equipment through which the substance(s) pass(es) during a continuous flow or batch process as well as the pipe work for transfer from one vessel to another for the purpose of the next reaction step, but it excludes tanks or other vessels in which the substance(s) are stored after the manufacture.	R01

Definition	Description	Reference
Notified substance	Notified substance means a substance for which a notification has been submitted and which could be placed on the market in accordance with Directive 67/548/EEC. A harmonised EU notification scheme for new chemical substances, manufactured or imported within EU industries, was introduced for new substances as part of the 6th Amendment to Directive 67/548/EEC, concerned with the classification, packaging, and labelling of dangerous substances. The 6th Amendment (Directive 79/831/EEC) was adopted in September 1979 and came into force in all Member States on 18th September 1981. New substances, introduced to the EU market subsequently, form a cumulative index, the **E**uropean **LI**st of **N**otified **C**hemical **S**ubstances (ELINCS), which is periodically updated.	R01
Only representative*	A natural or legal person established outside the Community who manufactures a substance imported into the Community on its own, in preparations or in articles may by mutual agreement appoint a natural or legal person established in the Community to fulfil, as his only representative, the obligations on importers regarding the registration of substances. The representative shall also comply with all other obligations of importers under the Regulation. The non-Community exporter shall inform the importer(s) within the same supply chain of the appointment. These importers shall be regarded as downstream users for the purposes of the Regulation.	R15-2
On-site isolated intermediate	Means an intermediate not meeting the criteria of a non-isolated intermediate and where the manufacture of the intermediate and the synthesis of (an)other substance(s) from that intermediate take place on the same site, operated by one more legal entities.	R01
Pesticide*	Pesticides, also know as “plant protection products”, are active substances and preparations containing one or more active substances, put up in the form in which they are supplied to the user, intended to: 1) protect plants or plant products against all harmful organisms or prevent the action of such organisms, in so far as such substances or preparations are not otherwise defined below; 2) influence the life processes of plants, other than as a nutrient, (e.g. growth regulators); 3) preserve plant products, in so far as such substances or products are not subject to special Council of Commission provisions on preservatives; 4) destroy undesired plants; or 5) destroy parts of plants, check or prevent undesired growth of plants. [Council Directive 91/414/EEC, 2 (1)]	R15-2

Definition	Description	Reference
Phase-in substance	A substance which over the 15 years preceding the entry into force of this Regulation meets at least one of the following criteria: it was manufactured in or imported into the Community, or the countries acceding to the European Union on 1 May 2004, by a manufacturer or importer and is listed in the European Inventory of Existing Commercial Chemical Substances (EINECS); it was manufactured in the Community, or in the countries acceding to the European Union on 1 May 2004, but not placed on the market by the manufacturer or importer; it was placed on the market in the Community, or in the countries acceding to the European Union on 1 May 2004, and between 18 September 1981 and 31 October 1993 inclusive it was also placed on the market by the manufacturer or importer and was considered as having been notified in accordance with the first indent of Article 8 (1) of Directive 67/548/EEC, as amended by Directive 79/831/EEC, but does not meet the definition of a polymer set out in Directive 67/548/EEC, as amended by Directive 92/32/EEC.	R01
Placing on the market*	Supplying or making available, whether in return for payment or free of charge, to a third party. Import into the customs territory of the Community shall be deemed to be placing on the market;	R01
Poly-constituent substance	A substances with a defined composition in which more than one constituent is present in a concentration ≥ 10% (w/w).	New
Polymer	A substance consisting of molecules characterised by the sequence of one or more types of monomer units. Such molecules must be distributed over a range of molecular weights wherein differences in the molecular weight are primarily attributable to differences in the number of monomer units. A polymer comprises the following: a simple weight majority of molecules containing at least three monomer units which are covalently bound to at least one other monomer unit or other reactant; less than a simple weight majority of molecules of the same molecular weight. In the context of this definition a 'monomer unit' means the reacted form of a monomer substance in a polymer;	R01
Potential registrant*	A manufacturer or importer desiring to register his substance and who is looking for already available data before submitting a registration.	R15-2
Preparation	Mixture or solution composed of two or more substances. A preparation is a deliberate physical mixture of more than one substance with the absent of chemical reaction(s) after mixing.	R01
Product and process orientated research and development*	Means any scientific development related to product development, the further development of a substance in the course of which pilot plant or production trials are used to develop the production process and/or to test the fields of application of the substance;	R01
Real substance	The 'real substance' can be defined as those substances that: - Fall under the legal definition of a substance in REACH; - Are produced in or imported into the Community; - Have to be identified sufficiently and uniquely as part of the registration process in REACH.	new
Registrant*	The manufacturer or the importer submitting a registration.	R01

Definition	Description	Reference
Registration dossier*	Information to provide in the context of a registration defined in Article 9 or 15-16. It consists of a technical dossier and, when required, a Chemical Safety Report. Annexes IV to IX set out the requirements for generating information on the substance to be registered.	R15-2
Registration*	The manufacturers and importers submit information in a standardised format, to demonstrate that they are managing their chemicals safely.	R15-2
Restriction*	Restriction means any condition for or prohibition of the manufacture, use or placing on the market.	R01
Site*	Means a single location, in which, if there is more than one manufacturer of (a) substance(s), certain infrastructure and facilities are shared;	R01
Submission	A submission is a general term that encompasses any communication of information by the industry to the Agency. The registration of a substance is an example of submission.	R15-2
Substance	A chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition.	R01
Technical dossier*	Part of a registration dossier containing information on the substance and information on risk management measures. It does not include the chemical safety report that documents the choice of these measures. The precise content of the technical dossier is defined in as well as in the Annexes IV to IX.	R15-2
Tonnage threshold*	Volume based criteria for different requirements under REACH, formulated as “X tonnes/year per manufacturer/importer”. The tonnage threshold will affect registration deadlines.	R15-2
Transported isolated intermediate	Means an intermediate not meeting the criteria of a non-isolated intermediate and transported between or supplied to other sites;	R01

2.2 Abbreviations

The abbreviations used in this Technical Guidance Document are listed and explained in table 2.2.

Table 2.2: Abbreviations

Abbreviation	Meaning	Reference
AIS		
CAS	Chemical Abstracts Service See www.cas.org	R15-2
CEFIC	Conseil Européen de l'Industrie Chimique / European Chemical Industry Council See www.cefic.be and www.cefic.org	R15-2
C&L	Classification & Labelling	R15-2
CMR	Carcinogenic, Mutagenic of toxic to Reproduction	R15-2
CA	Competent Authority	R15-2
CSA	Chemical Safety Assessment	R15-2
CSR	Chemical Safety Report	R15-2
EC	European Commission	R15-2
ECA	European Chemicals Agency	R15-2
ECB	European Chemicals Bureau	R15-2
EINECS	European Inventory of Existing Commercial Chemical Substances	R15-2
ELINCS	European List of Notified Chemical Substances	R15-2
ESIS	European Substances Information System	R15-2
GHS	Globally Harmonised System for classification and labelling of chemicals	R15-2
HPV	High Production Volume	R15-2
INCI	International Nomenclature of Cosmetic Ingredients	
ISO	International Organization for Standardisation.	
IUCLID	International Uniform Chemical Information Database	R15-2
IUPAC	International Union of Pure and Applied Chemistry See www.iupac.org/dhtml_home.html	R15-2
JRC	Joint Research Centre	R15-2
MS	Member State	R15-2
NCD	New Chemicals Database	R15-2
OECD	Organisation for Economic Cooperation and Development	R15-2
PBT	Persistent, Bio-accumulative and Toxic	R15-2
PPORD	Product and Process Orientated Research and Development	R15-2
PPP	Plant Protection Product	R15-2
QSAR	Quantitative Structure Activity Relationship	R15-2
REACH	Registration, Evaluation and Authorisation of CHemicals	R15-2
RIP	REACH Implementation Project	R15-2
SDS	Safety Data Sheet	R15-2
TSCA	Toxic Substance Control Act (USA)	R15-2
UNEP	United Nations Environment Programme See www.unep.org	R15-2
US-EPA	United States Environment Protection Agency See www.epa.gov	R15-2

Abbreviation	Meaning	Reference
VPVB	Very Persistent Very Bio-accumulative substance	R15-2

3 FRAMEWORK FOR SUBSTANCE IDENTIFICATION IN REACH

3.1 Introduction

3.2 Substance definition

3.3 Framework for substance identification in REACH

3.4 Framework for substance identification in IUCLID 5

4 PRACTICAL GUIDANCE FOR SUBSTANCE IDENTIFICATION IN REACH

4.1 Introduction

This section provides guidance for the actual substance identification process by explaining how to record and check the identity of substances during (pre-) registration within REACH.

This practical guidance is meant for all substances. However, different categories are recognised, for which the rules and criteria for the substance identification parameters are known to be different. Therefore, the user is guided firstly via a decision tree (as shown in 4.2) to the appropriate identification process for the category of substance.

The appropriate substance identification processes as identified in the decision tree will be worked out in detail in the subsequent paragraphs. So section 4.3.1 provides guidance on the actual substance identification for a mono-constituent substance and section 4.3.2 for substances with more than one constituent. Section 4.4 and the following paragraphs give specific guidance for categories within UVCB substances known to have an identical substance identification process.

Finally in section 4.5 the workflow for checking the substance identity (to recognise if your substance is the same as an already registered substance) is worked out.

4.2 Real substances, constituents and categories

A "*real" substance* is a substance that is produced in or imported into the Communities and that requires a registration. A "real" substance can be a substance containing only one main constituent or can be a (defined or undefined) mixture of several constituents.

Each "real" substance should be described uniquely according to the different constituent compositions, keeping in mind the following:

- A *main constituent* makes (as a general rule) at least 80% of the composition of a real substance;
- A *major constituent* makes (as a general rule) between 10 and 80% of the composition of a real substance;
- *Additives* are intentionally added for reasons of stability or conservation.
- *Impurities* are constituents that have been in or used as starting materials or derived (unintentionally) by the reaction process. As a rule impurities present >=1% have to be identified and quantified, or at any lower concentration in case relevant for the classification or hazard profile;

The identification process of a real substance must be done based on the substance identification parameters of REACH Annex IV.

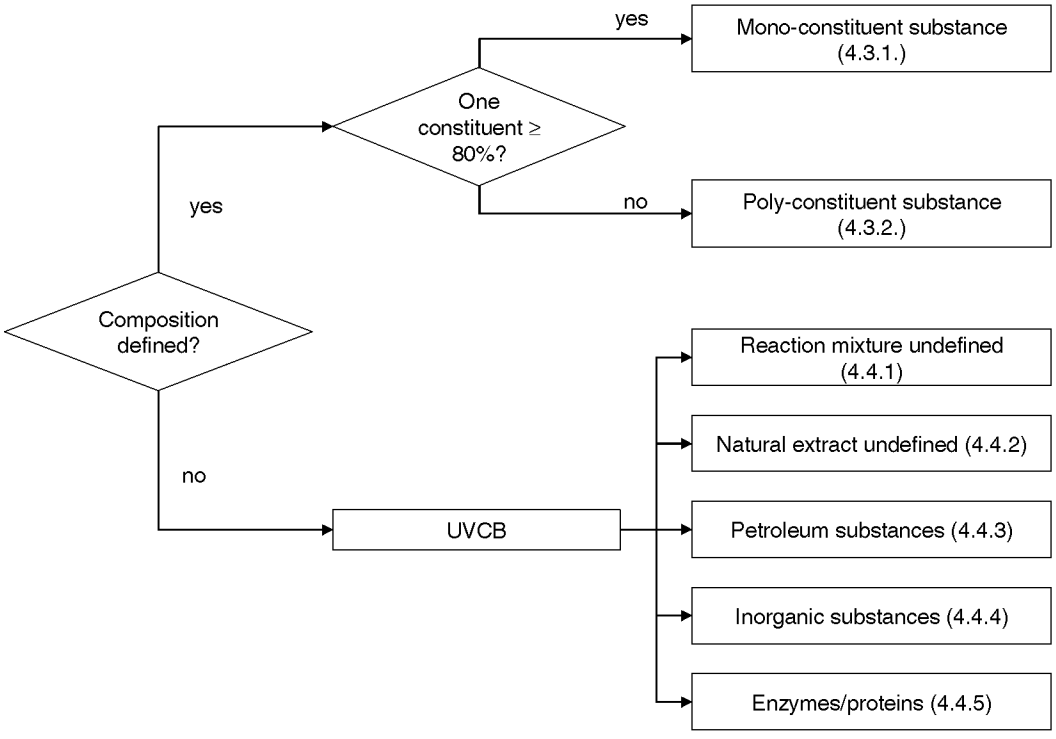
There are typically two kinds of substances:
- Substances with a known composition (mono-constituent substances, poly-constituent substances).
- UVCB substances (Substances of Unknown or Variable composition, Complex reaction products or Biological materials). These substances include e.g. reaction mixtures with an unknown or only partly known composition, extracts from organisms of natural origin etc.

The identification process has to be differentiated for substances with a defined composition and for substances with an undefined or variable composition:
- Real substances with a defined composition are uniquely identified by the one main constituent (mono-constituent substance) or by the major constituents (poly-constituent substance).
- For UVCB substances in general no precise composition is known. In case composition is partly known, these are to be identified based on those known constituents. In addition all other available information which identifies the substance should be given. In case of reaction mixtures these may be characterised by starting materials, reaction type and physical and analytical properties as boiling point range, molecular weight fraction, analytical finger prints and/or other parameters which identify the substance. In case of natural extracts, petroleum substances etc. the characterisation may be based on the original natural material, the type of extraction and other purification or reaction steps and other parameters. In all cases identification can be given in descriptions, the main type of molecules with a range for homologues.

Because the substance identification process may differ significantly between substances with a defined and an undefined composition, a categorisation is used in this TGD, as shown in figure 4.1. This categorisation is a tool to assist the user with the recording of the substance identity.

Per category the registrant is guided through the rules & criteria to record a real substance of that category uniquely. It is the registrant's responsibility to select the most appropriate category and to record the substance identity in line with the rules and criteria for that category. If the registrant has good reasons to deviate from the substance identification rules and criteria of the TGD, the reasons for deviation must be justified.

Figure 4.1: Decision tree for determining the appropriate substance identification process



Substance of defined composition

Substances with a defined composition can be categorised as *mono-constituent substances* or *poly-constituent substances.*

Mono-constituent substances are typically defined by one main constituent present at 80% (w/w) or more, and containing up to 20% (w/w) impurities and/or additives.

				Examples (MS04)
Main constituent	**Content**	**Impurity**	**Content (%)**	**Registered substance**
m-xylene	91%	o-xylene	5	m-xylene
o-xylene	87%	m-xylene	10	o-xylene

Poly-constituent substances are typically defined by more than 1 major constituent, each present at ≥10% (w/w) and <80% (w/w).

				Example (MS04)
Major constituents	**Content**	**Impurity**	**Content (%)**	**Registered substance**
m-xylene	50	p-xylene	5	Mixture of m-xylene and o-xylene
o-xylene	45			

Main and major constituents should be defined on a molecular basis with molecular weight, molecular formula and structural formula. The IUPAC name, the CAS and EC name and number (if available) should be given.

For impurities and additives the IUPAC-name, CAS-number, EC-number and molecular formula for those present at >1% should be specified. Impurities and additives present in a lower concentration range should be specified if relevant for the hazard profile of the substance.

Spectral data and chromatographic characterisation have to be given for the real substance. Spectral data and chromatographic characterisations can be given for the main and major constituents separately.

UVCB Substances

UVCB substances are Substances of Unknown or Variable composition, Complex reaction products or Biological materials.

These are substances that cannot be defined in general terms of chemical identity of the constituents (e.g. not possible to determine the precise structure, molecular formula or molecular weight), but which can be considered as meeting the criteria for true chemical substances. In order to be able to identify UVCB substances, an alternative set of rules and criteria are set.

- Rea*ction mixtures of undefined composition*, that can be characterised by starting materials and process type in addition with other characterisation of the reaction mixture;

		Examples
EINECS number	**EINECS Name**	**CAS-number**
284-268-6	Hexanedioic acid, reaction products with diethylenetriamine, epichlorhydrin-quaternized	84836-82-8
282-615-6	Benzaldehyde, reaction products with N,N-diethylbenzenamine and N,N-dimethylbenzenamine, oxidized	84281-72-1

- *Substances of natural origin of undefined composition* are typically characterised by the species of plants or micro-organism or animal that is the source in addition with other characterisation of the molecules. For instance they can be characterised by the type of extraction and further isolation processes, e.g. the solvent used, distillation, purification, fermentation steps etc.

		Examples
EINECS number	**EINECS Name**	**CAS-number**
307-876-6	Lavender, Lavandula officinalis, ext., sulfurized, silver salts	97766-16-0
273-578-7	Meet extracts, beef	68990-09-0

- *Petroleum substances* [to be described]

		Examples
EINECS number	**EINECS Name**	**CAS-number**
265-101-6	Residual oils (petroleum), solvent refined	64742-01-4
265-129-9	Gas oils (petroleum), chemically neutralized	64742-29-6

- *Inorganic substances* [to be described]

		Examples
EINECS number	**EINECS Name**	**CAS-number**
231-545-4	Silicon dioxide	7631-86-9
283-938-5	Bentonite, ferrian	84776-13-6

- *Enzymes and proteins* [to be described]

		Examples
EINECS number	**EINECS Name**	**CAS-number**
259-747-8	Coenzyme A, sodium salt	55672-92-9

In many cases of UVCB substances additional tools for characterisation must be used to identify the substance, e.g. boiling point range or sector specific definitions like colour and odour indexes etc.

How to use the decision tree to record the substance identity for registration

The first step a registrant needs to do is to determine by the decision tree and descriptions in this paragraph what category for substance identification is applicable and most appropriate to identify the substance uniquely. It is the responsibility of the registrant to select the most appropriate category for his real substance.

It must be stressed that for example the existence of a subcategory 'inorganic substances' under UVCB's does not mean that all inorganic substances must fall under that subcategory. An inorganic substance can also be identified as a mono-constituent substance or poly-constituent substance if the composition is defined.

The second step is to collect the relevant substance identification information and prepare the registration dossier in line with the rules and criteria for that specific category in the TGD. For each category a specific overview has been described of the substance identification parameters to be used and the rules & criteria to record the substance identity in a separate paragraph:

- For the substance identification process of mono-constituent substances go to paragraph 4.3.1;
- For poly-constituent substances go to paragraph 4.3.2;
- For the identification of substances within one of the UVCB categories go to the corresponding paragraph in section 4.4.

The final step is to record the substance identity in IUCLID 5 for the actual registration process in line with the instructions of the IUCLID 5 manual and other relevant TGD's if applicable. This step is outside the scope of this TGD.

4.3 Guidance on the identification of substances of defined composition

4.3.1 Mono-constituent substances

A *mono-constituent substance* is defined as a real substance in which one type of molecule is present for at least 80% (w/w). All substances with one molecule present at more than 80% (w/w) can be considered as a mono-constituent substance. That means that e.g. reaction mixtures and natural substances can also fall within the definition of mono-constituent substance if the composition is known.

Example: Cellulose pulp is a natural substance which is per definition composed of cellulose and impurities. In EINECS different grades of cellulose (> 80%) are listed as mono-constituent substance: Cellulose, EINECS number 232-674-9

This '80%-rule' is also applied for the registration of new substances for ELINCS. Deviation from that rule is possible, but only with a justification.

This paragraph describes the rules and criteria that should be used to record the identity of the mono-constituent substance uniquely.

In case the registrant has good reasons to deviate from the 80% rule, this has to be done with a justification.

Justification for deviation: …… …… ……
Possible examples for a justified deviation are: - *If the single constituent is <80% but the real substance can be shown to have similar physical and biological properties leading to the same classification requirements as other mono-constituent substances with the same identity that fulfil the 80% rule.* - *If the composition information contains more constituents (or at a different percentage) relevant for the proper classification & labelling this should be justified.* - *Etcetera*
ISSUE I-10: Issue of how to deal with working with rules for justification. What is the level of guidance to be included in the TGD. CEFIC will prepare a text proposal.

Name and other identifiers

IUPAC name or other international chemical name [Main constituent]

As a general rule a mono-constituent substance is named after its main constituent (the constituent available ≥80%). Therefore, the English IUPAC name of the main constituent must be given. In case a IUPAC name cannot be derived, other international chemical names can be given instead, if a correct reference can be given of the internationally accepted nomenclature, like the ISO name.

For technical guidance see: section 5.1 *For practical guidance see: section 6*

Other names ……

All other names can be given, including other chemical names, trade names or abbreviations. Other names may also include internal company names or names from sector specific inventories, like colour index names, INCI names, etc.
For technical guidance see: section 5.2 *For practical guidance see: section 6*

EC number ……
EC name ……

The EC number and EC name of the main constituent shall be given, where applicable. The EC-number is the official EU registration number for the substance and together with the EC name listed in the EINECS, ELINCS or NLP Inventory. Check the applicability of the EC-number with the registered substance.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

CAS number ……
CAS name ……
Other CAS numbers ……

The CAS-number and the CAS-name of the main constituent must be given, in case available. *In case more than one CAS number exists for the substance, give also the other CAS-numbers. As a general rule, the CAS-number related to the EC-number must be given as the main CAS-number.* *Forms for application for CAS-numbers are included in the Annex to this TGD.*	
Example:	**Lavandin grosso:** CAS USA 8022-15-9 CAS EINECS: 91722-69-9
ISSUE I-1 for double CAS-numbers for one substance need to be checked	
For technical guidance see: section 5.4 *For practical guidance see: section 6*	

Other identity code ……

In case other identity codes are available for the real substance, those can be given. In case a standard is available for the real substance, like an ISO standard, the reference to that standard should be given here. Other identity codes can include Colour Index Numbers, AIS numbers, other sector related numbers and internal company codes.
For technical guidance see: section 5.5 *For practical guidance see: section 6*

Molecular and structural formula

Molecular formula (Hill Method) ……
Molecular formula (CAS Method) ……
Structural formula ……
SMILES code ……

The molecular formula of the main constituent must be given in line with the Hill method. In case available the molecular formula should also be given according to the CAS method. The structural formula should also be given for the main constituent. The SMILES notation of the main constituent needs to be given if applicable.
For technical guidance see: section 5.6 *For practical guidance see: section 6.2*

Information on optical activity ……

The information of the optical activity of the main constituent must be given if applicable and appropriate.
For technical guidance see: section 5.7 *For practical guidance see: -*

Molecular weight ……
Molecular weight range ……

The molecular weight of the main constituent should be given. A molecular weight range will only be applicable in specific cases, for example for a group of homologues or a mixture of oligomers.
For technical guidance see: section 5.8 *For practical guidance see: -*

Composition information

Degree of purity of the substance:
Typical concentration of the main constituent ……w/w%
Lower limit ……w/w%
Upper limit ……w/w%

For a mono-constituent substance the concentration of the main constituent should be given as the degree of purity of the real substance. The concentration should be provided as a typical concentration and as a concentration range. In case of a variable concentration, choose a range relevant for the substance.
For technical guidance see: section 5 *For practical guidance see: -*

Nature and order of magnitude of impurities:

	IUPAC name	CAS number	EC number	Mol. formula	w/w% or ppm
A					
B					

Impurities present in a concentration >1% (or above any lower concentration limit, if relevant for the

classification) should be specified. For those impurities at least one of the following identifiers should be given: - *the IUPAC name or if not to be derived another international accepted chemical name;* - *CAS-number;* - *EC number;* - *Molecular or structural formula.* *For each impurity, the concentration (range) should be given (as w/w% or ppm).* *As a genral rule, the total concentration of impurities is <20%.*
For technical guidance see: section 5 *For practical guidance see: -*

Total concentration of non-specified impurities: ……w/w%

Nature and order of magnitude of any additives:

	IUPAC name	CAS number	EC number	Mol. formula	w/w% or ppm
A					
B					

Additives present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For additives at least one of the following identifiers should be given: - *the IUPAC name or if not to be derived another international accepted chemical name;* - *CAS-number;* - *EC number;* - *Molecular or structural formula.* *For each additive, the concentration (range) should be given (as w/w% or ppm).*
For technical guidance see: section 5 *For practical guidance see: -*

Analytical information

Spectral data — Refer to relevant annex to the registration

Spectral data are needed to confirm the structure assigned to the mono-constituent substance. Several spectroscopic methods are used for spectra (ultra –violet, infra-red, nuclear magnetic resonance or mass spectrum). Not all methods are suitable for all classes of compounds. Methods and insights how to use the methods is subject of continuous changes.
ISSUE I-13: Some analytical methods cannot be used in special cases (e.g. UV for certain structures)
For technical guidance see: section 5.10 *For practical guidance see: section 6.2*

High-pressure liquid chromatogram, gas chromatogram — Refer to relevant annex to the registration

A chromatogram must be given to confirm the composition of the real substance, if possible.
For technical guidance see: section 5.11 *For practical guidance see: section 6.2*

Description of analytical methods or bibliographical references	Refer to relevant annex to the registration

An overview of the analytical methods or the appropriate bibliographic references for the identification of the substance and where appropriate for the identification of the impurities and additives needs to be given. This information should be sufficient to allow methods to be reproduced.
ISSUE I-14: Concern of industry is that the analytical information (REACH Annex IV, 2.3.7) need to be entered twice (for substance identification and as part of the registration dossier). Question whether it is an endpoint or a substance identifier
For technical guidance see: - *For practical guidance see: -*

4.3.2 Poly-constituent substances

Poly-constituent substances are substances with a defined composition in which more than one major constituent is present in a concentration ≥ 10% (w/w) and < 80% (w/w). As a result, more than one constituent is relevant for the identity of the real substance.

All substances, also natural substances and reaction mixtures can be poly-constituent substances as long as the composition is defined.

The identification of a poly-constituent substance is a combination of the identifiers of the real substance as such (CAS-number, EC-number, name etc of the substance as such), the composition information and the identifiers of the major constituents (names, CAS-numbers, EC-numbers, etc) of that real substance.

For impurities and additives the IUPAC-name, CAS-number, EC-number and molecular formula for those present >1% should be specified. Impurities and additives present in a lower concentration range should be specified if relevant for the hazard profile of the substance.

This paragraph describes the rules and criteria that should be used to record the identity of the poly-constituent substance.

Name and other identifiers

IUPAC name or other international chemical name	Mixture of [major constituents]

As a general rule, the name of a poly-constituent substance is based on names of the major constituents (constituents present ≥10% and < 80%). The generic format for the name for of this category is 'Mixture of [names of the major constituents]'. The names of the major constituents are the English IUPAC names. In case a IUPAC name cannot be derived, other international chemical names can be given as well, if a correct

reference is given of the internationally accepted nomenclature like ISO names.
For technical guidance see: section 5.1 *For practical guidance see: section 6*

Other names ……

All other names can be given, including other chemical names, trade names or abbreviations under which the real substance will be marketed in the Community etc. Other names may also include internal company names or names from sector specific inventories, like colour index names, INCI names, etc.
For technical guidance see: section 5.2 *For practical guidance see: section 6*

EC number ……
EC name ……

The EC number and EC name of the real substance must be given, in case available. The EC-number is the official EU registration number for the substance and together with the EC name listed in the EINECS, ELINCS or NLP Inventory. Check the applicability of the EC-number with the registered substance.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

CAS number ……
CAS name ……
Other CAS numbers ……

The CAS-number and the CAS-name of the real substance must be given, in case available. *In case more than one CAS number exists for the substance, give also the other CAS-numbers. As a general rule, the CAS-number related to the EC-number must be given as the main CAS-number.* *Forms for application for CAS-numbers are included in the Annex to this TGD.*
For technical guidance see: section 5.4 *For practical guidance see: section 6*

Other identity code ……

In case other identity codes are available for the real substance, those can be given. In case a standard is available for the real substance, like an ISO standard, the reference to that standard should be given here. Other identity codes can include Colour Index Numbers, AIS numbers, other sector related numbers and internal company codes.
For technical guidance see: section 5.5 *For practical guidance see: section 6*

Name and other identifiers of the major constituents

The names and other identifiers of the major constituents need to be identified for all major constituents present in the real substance.

	IUPAC names or other international chemical names:
A	
B	

The English IUPAC names of the major constituents must be given. As a result of the general rules for naming poly-constituent substances, these names are the names included in the name of the real substance. In case IUPAC names cannot be derived, other international chemical names can be given instead, if a correct reference can be given of the internationally accepted nomenclature, like the ISO name.
For technical guidance see: section 5.1 *For practical guidance see: section 6*

	Other names:
A	
B	

For all major components, other names can be given, including other chemical names, colour index names, trade names or abbreviations. Other names may also include internal company names. This might also

include the IUPAC names in all languages available.
For technical guidance see: section 5.2 *For practical guidance see: section 6*

	EC number	EC name
A		
B		

The EC-number and EC name of the major constituents must be given, in case available. The EC-number is the official EU registration number for the substance and together with the EC name listed in the EINECS, ELINCS or NLP Inventory. Check the applicability of the EC-number with the registered substance.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

	CAS number	CAS name
A		
B		

The CAS-number and the CAS-name must be given for the major constituents, in case available. As the CAS-number is one of the most important identifiers of substances in industry, it is very important to know the CAS-number. Forms for application for CAS-numbers are included in the Annex to this TGD.
For technical guidance see: section 5.4 *For practical guidance see: section 6*

	Other identity code - type	Code
A		
B		

In case other identity codes are available for the major constituents, those can be given. These can include Colour Index Numbers, AIS numbers, and other sector related numbers. Other identity codes can also include internal company codes.
For technical guidance see: section 5.5 *For practical guidance see: section 6*

Molecular and structural formula

	Molecular Formula		Structural formula	SMILES code
	Hill method	CAS method		
A				
B				

The molecular formula of the major constituents should be given according to the Hill methodology. In case available the molecular formula should also be given according to the CAS method. The structural formula of the major constituents should also be given. The SMILES notations of the major constituents need to be given if applicable.
For technical guidance see: section 5.6 *For practical guidance see: -*

	Information on optical activity
A	
B	

Optical activity should be given for either the real substance or for all major constituents.
For technical guidance see: section 5.7 *For practical guidance see: -*

	Molecular weight or molecular weight range
A	
B	

For a poly-constituent substance the molecular weights of the major constituents should be given. Molecular weight ranges will only be applicable in specific cases, for example for a group of homologues or a mixture of oligomers.
For technical guidance see: section 5.8 *For practical guidance see: -*

Composition information

	Typical concentration (w/w%)	Lower limit (w/w%)	Upper limit (w/w%)
A			
B			

For a poly-constituent substance the concentration of the major constituents should be given as the degree of purity of the real substance. The concentrations should be provided as a typical concentration and as a concentration range. In case of a variable concentration, choose a range relevant for the constituent.
For technical guidance see: section 5 *For practical guidance see: -*

Nature and order of magnitude of impurities:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
a					
b					

Impurities present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For those impurities at least one of the following identifiers should be given: - *the IUPAC name or if not to be derived another international accepted chemical name;* - *CAS-number;* - *EC number;* - *Molecular or structural formula.* *For each impurity, the concentration (range) should be given (as w/w% or ppm).* *As a rule, the total concentration of impurities is <20%.*
For technical guidance see: section 5 *For practical guidance see: -*

Total concentration of non-specified impurities: ……w/w%

Nature and order of magnitude of any additives:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Additives present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For additives at least one of the following identifiers should be given: - *the IUPAC name or if not to be derived another international accepted chemical name;* - *CAS-number;* - *EC number;* - *Molecular or structural formula.* *For each additive, the concentration (range) should be given (as w/w% or ppm).*
For technical guidance see: section 5 *For practical guidance see: -*

Analytical information

Spectral data Refer to relevant annex to the registration

In most cases spectral data are not useful for poly-constituent substances. In those cases where spectral data provides information on the composition of the poly-constituent substance, this information should be given. Several spectroscopic methods are used for spectra (ultra –violet, infra-red, nuclear magnetic resonance or mass spectrum). Not all methods are suitable for all classes of compounds. Methods and insights how to use the methods is subject of continuous changes.
For technical guidance see: section 5.10 *For practical guidance see: -*

High-pressure liquid chromatogram, gas chromatogram	Refer to relevant annex to the registration

A chromatogram must be given to confirm the composition of the real substance, if possible.
For technical guidance see: section 5.11 *For practical guidance see: section 6.2*

Description of analytical methods or bibliographical references	Refer to relevant annex to the registration

An overview of the analytical methods or the appropriate bibliographic references for the identification of the substance and where appropriate for the identification of the impurities and additives needs to be given. This information should be sufficient to allow methods to be reproduced.

4.4 Guidance on the identification of UVCB's

UVCB substances are substances of Unknown or Variable composition, Complex reaction products or Biological materials. UVCB substances are not-well-defined substances such as reaction products, plant products, post-reacted naturally occurring substances or naturally occurring substances. UVCB's may not have a precise chemical name and they usually do not have a complete chemical structure diagram associated nor a specific molecular formula.

UVCB-substances cover different categories of substances, requiring different rules and criteria for the identification. In this section the following sub categories of UVCB's are included:

- reaction mixtures of undefined composition (see 4.4.1);
- natural extracts of undefined composition (see 4.4.2);
- petroleum substances (see 4.4.3);
- inorganic substances (see 4.4.4);
- enzymes & proteins (see 4.4.5);

4.4.1 Reaction mixtures of undefined composition

A reaction mixture is considered as a real substance. A reaction mixture can fall under the category of well defined composition (see 4.3) but when the composition is not well-known it will fall under the UVCB sub category 'reaction mixtures of undefined composition'. Some examples of typical entries of reaction mixtures of undefined composition (MS04):

Nonanedioic acid, reaction products with 2-amino-2-methyl-1-propanol
Formaldehyde, reaction products with diethylene glycol and phenol
1,4-Benzenediol, reaction products with aniline, branched octyl styryl derivs.
Linseed oil, reaction products with high-temp. coal tar pitch, sulfurized

Identification of these reaction mixtures cannot be based on the composition of the substance. Other identifiers are necessary to uniquely identify the real substance. These are the starting materials of the reaction mixture, process descriptions, physical-chemical properties. It is important to be aware that the chosen identifiers determine the bandwidth of the registered substance and therefore the range of substances considered the same as the registered substance.

Name and other identifiers

IUPAC name or other international chemical name	Reaction product of [starting materials]

As a general rule reaction mixtures of undefined composition are named after the starting materials of the reaction. The generic format for the name for of this category is 'Reaction product of [names of the starting materials]'. The names of the starting materials are the English IUPAC names. In case a IUPAC name cannot be derived, other international chemical names can be given as well, if a correct reference is given of the internationally accepted nomenclature, like the ISO name.

In case the names of starting materials cannot be given, the name of the real substance can also be based on an indication of the reaction process.
Example: | *Slags, copper refining (L08)*
ISSUE I-15: The suggested naming conventions at SEG01 and IEG01 for reaction mixtures of undefined composition is what to do if the same substance is prepared with some (slightly) different starting materials
For technical guidance see: section 5.1 *For practical guidance see: section 6*

Other names ……

All other names can be given for the reaction mixture, including trade names or abbreviations under which the real substance will be marketed in the Community etc. Other names may also include internal company names or names from sector specific inventories, colour index names, INCI names, etc.
For technical guidance see: - *For practical guidance see: -*

EC number ……
EC name ……

The EC number and EC name of the real substance must be given, in case available. The EC-number is the official EU registration number for the substance and together with the EC name listed in the EINECS, ELINCS or NLP Inventory. Check the applicability of the EC-number with the registered substance.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

CAS number ……
CAS name ……
Other CAS numbers ……

The CAS-number and the CAS-name of the real substance must be given, in case available. *In case more than one CAS number exists for the substance, give also the other CAS-numbers. As a general rule, the CAS-number related to the EC-number must be given as the main CAS-number.* *Forms for application for CAS-numbers are included in the Annex to this TGD.*
For technical guidance see: section 5.4 *For practical guidance see: section 6*

Other identity code ……

In case other identity codes are available for the real substance, those can be given. In case a standard is available for the real substance, like an ISO standard, the reference to that standard should be given here. Other identity codes can include sector related numbers and internal company codes.
For technical guidance see: - *For practical guidance see: -*

Name and other identifiers of the major constituents

In the case of reaction mixtures of undefined composition it is possible that one or more constituents are known to be present in the reaction mixtures. In case such constituents are present at concentrations > 10%, these should be registered as major constituents of the real substance.

	IUPAC names or other international chemical names:
A	
B	

The English IUPAC names of the known major constituents must be given. In case IUPAC names cannot be derived, other international chemical names can be given instead, if a correct reference can be given of the internationally accepted nomenclature, like the ISO name.

For technical guidance see: section 5.1
For practical guidance see: section 6

	Other names:
A	
B	

For all known major components, other names can be given, including other chemical names, colour index names, trade names or abbreviations. Other names may also include internal company names. This might also include the IUPAC names in all languages available.

	EC number	EC name
A		
B		

The EC-number and EC name of the known major constituents must be given, in case available.

For technical guidance see: section 5.3
For practical guidance see: section 6

	CAS number	CAS name
A		
B		

The CAS-number and the CAS-name must be given for the known major constituents, in case available.

For technical guidance see: section 5.4
For practical guidance see: section 6

	Other identity code - type	Code
A		
B		

In case other identity codes are available for the major constituents, those can be given. These can include Colour Index Numbers, AIS numbers, and other sector related numbers. Other identity codes can also include internal company codes.
For technical guidance see: section 5.5 *For practical guidance see: section 6*

Molecular and structural formula

	Molecular Formula		Structural formula	SMILES code
	Hill method	CAS method		
A				
B				

The molecular formulas of the known major constituents should be given according to the Hill methodology. In case available the molecular formulas should also be given according to the CAS method. The structural formulas should also be given for the major constituents. The SMILES notations of the major constituents need to be given if applicable.

For technical guidance see: section 5.6
For practical guidance see: -

Information on optical activity ……

Optical activity should be given for either the real substance or for all major constituents if applicable and appropriate.

For technical guidance see: section 5.7
For practical guidance see: -

	Molecular weight or molecular weight range
A	
B	

For known major constituents in a reaction mixture of undefined composition the molecular weights should be given. Molecular weight ranges will only be applicable in specific cases, for example for a group of homologues or a mixture of oligomers.

For technical guidance see: section 5.8
For practical guidance see: -

Composition information for the real substance

	Typical concentration (w/w%)	Lower limit (w/w%)	Upper limit (w/w%)
A			
B			

The concentrations of the known major constituents should be given. The concentrations can be provided as a typical concentration or as a concentration range. In case of a variable concentration, choose a range relevant for the constituent.

For technical guidance see: section 5
For practical guidance see: -

Nature and order of magnitude of impurities:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Impurities known to be present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For those impurities at least one of the following identifiers should be given:

- *the IUPAC name or if not to be derived another international accepted chemical name;*
- *CAS-number;*
- *EC number;*
- *Molecular or structural formula.*

For each impurity, the concentration (range) should be given (as w/w% or ppm).

For technical guidance see: section 5
For practical guidance see: -

Total concentration of non-specified impurities: ……w/w%

Nature and order of magnitude of any additives:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Additives known to be present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For additives at least one of the following identifiers should be given:

- *the IUPAC name or if not to be derived another international accepted chemical name;*
- *CAS-number;*
- *EC number;*
- *Molecular or structural formula.*

For each additive, the concentration (range) should be given (as w/w% or ppm).

For technical guidance see: section 5
For practical guidance see: -

Analytical information

Spectral data	Not applicable
High-pressure liquid chromatogram, gas chromatogram	Not applicable

Description of analytical methods or bibliographical references	Not applicable

For reaction mixtures of undefined composition spectral data and chromatograms will not give relevant information on the identity of the real substance.

Process descriptions

Especially in case when little or nothing is known about the composition of the reaction mixture, other identifiers must be given in order to identify the substance. One important option is information about the manufacturing process in which the substance is derived.

Description of processes used in the manufacture of the real substance: …… ……
An identification parameter for reaction mixtures of undefined composition is a process description. It is up to the registrant to decide the level of information provided.

Other identification parameters

Besides composition information and information on the process other characteristics of the substance can be given. As many characteristics must be given in order to identify the substance as clear as possible.

Starting products of the reaction product:

	IUPAC name	CAS number	EC number	Mol. formula	Ratio (%)
A					
B					

In case starting materials were identified in the registration of the real substance, additional information should be given on these starting materials. This information includes IUPAC name, CAS-number and EC-number, molecular formula and ratio in the reaction process.

Generic description of type of molecules (e.g. esters) ……

Range of homologues ……

Boiling point range or cut off ……°C

Finger print techniques ……

Technical specification ……

Particle size distribution or cut off ……

Sieve fraction ……

4.4.2 Natural extracts of undefined composition

		Examples (L08)
EINECS nr	**EINECS name**	**Additional description in EINECS**
289-609-2	Beet, Beta vulgaris repacea, ext.	Extractives and their physically modified derivatives such as tinctures, concretes, absolutes, essential oils, oleoresins, terpenes, terpene-free fractions, distillates, residues, etc., obtained from Beta vulgaris rapacea, Chemopodiaceae.
305-979-0	Oils, animal, sulfonated, sodium salts	

This paragraph only includes guidance for natural extracts of undefined composition. Natural extracts of defined composition can be considered as mono- or poly-constituent substances (see 4.3).

The main rule for natural extracts is to name them after the genus and species of the organism where the substance originates from. Besides that, other identifiers should be given for the purpose of identification. The identifiers chosen and ranges given determine the bandwidth of the substance and therewith the range of other substances to be included under that same registration. This is illustrated by an example from the previous system (L08):

EINECS nr	**EINECS name**	**Additional description in EINECS**
232-282-8	Coconut oil	Extractives and their physically modified derivatives. It consists primarily of the glycerides of the fatty acids capric, lauric, myristic, oleic and palmitic. (Cocus nucifera, Palmae).

Covers the coconut oils within the following ranges:

Length of carbon chain and degree of unsaturation	**Name of fatty acid**	**Range of content (%)**
C8:0	Caprylic acid	7.8 – 9.5
C10:0	Capric acid	4.5 – 9.7
C12:0	Lauric acid	44 – 51
C14:0	Myristic acid	13 – 18.5
C16:0	Palmitic acid	7.5 – 10.5
C18:0	Stearic acid	1 – 3
C18:1	Oleic acid	5 – 8.2
C18:2	Linoleic acid	1.0 – 2.6

Name and other identifiers

IUPAC Name or other international	

Chemical Name	……
Extracts of biological origin are to be named after the genus and species of the originating plant or non-mammal. For mammals the name can be given based on the organ of origin. Other identifiers as extraction method or process temperature can be included in the name as well.	
For technical guidance see: - *For practical guidance see: -*	

Other names ……

All other names can be given for the substance, including trade names or abbreviations under which the real substance will be marketed in the Community etc. Other names may also include internal company names and sector-related names.
For technical guidance see: - *For practical guidance see: -*

EC number ……
EC name ……

The EC number and EC name of the real substance must be given, in case available. The EC-number is the official EU registration number for the substance and together with the EC name listed in the EINECS, ELINCS or NLP Inventory. Check the applicability of the EC-number with the registered substance.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

CAS number ……
CAS name ……
Other CAS numbers ……

The CAS-number and the CAS-name of the real substance must be given, in case available. *In case more than one CAS number exists for the substance, give also the other CAS-numbers. As a general rule, the CAS-number related to the EC-number must be given as the main CAS-number.* *Forms for application for CAS-numbers are included in the Annex to this TGD.*
For technical guidance see: section 5.4 *For practical guidance see: section 6*

Other identity code ……

In case other identity codes are available for the real substance, those can be given. In case a standard is available for the real substance, like an ISO standard, the reference to that standard should be given here. Other identity codes can include sector related numbers and internal company codes.
For technical guidance see: - *For practical guidance see: -*

Name and other identifiers of the major constituents

In the case of natural extracts of undefined composition it is possible that one or more constituents are known to be present in the real substance. In case such constituents are present at concentrations > 10%, these should be registered as major constituents of the real substance.

	IUPAC names or other international chemical names:
A	
B	

The English IUPAC names of the known major constituents must be given. In case IUPAC names cannot be derived, other international chemical names can be given instead, if a correct reference can be given of the internationally accepted nomenclature, like the ISO name.
For technical guidance see: section 5.1 *For practical guidance see: section 6*

	Other names:
A	
B	

For all known major components, other names can be given, including other chemical names, colour index names, trade names or abbreviations. Other names may also include internal company names. This might also include the IUPAC names in all languages available.

	EC number	EC name
A		
B		

The EC-number and EC name of the known major constituents must be given, in case available.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

	CAS number	CAS name
A		
B		

The CAS-number and the CAS-name must be given for the known major constituents, in case available.
For technical guidance see: section 5.4 *For practical guidance see: section 6*

	Other identity code - type	Code
A		
B		

In case other identity codes are available for the major constituents, those can be given. These can include Colour Index Numbers, AIS numbers, and other sector related numbers. Other identity codes can also include internal company codes.		
For technical guidance see: section 5.5 *For practical guidance see: section 6*		

Molecular and structural formula

	Molecular formula	Structural formula	SMILES code
A			
B			

The molecular formulas of the known major constituents should be given according to the Hill methodology. In case available the molecular formula should also be given according to the CAS method. Structural formulas should also be given for the known major constituents. The SMILES notations of the major constituents need to be given if applicable.
For technical guidance see: section 5.6 *For practical guidance see: -*

Information on optical activity ……

Optical activity should be given for all major constituents if applicable and appropriate.
For technical guidance see: section 5.7 *For practical guidance see: -*

	Molecular weight or molecular weight range
A	
B	

For known major constituents in a natural extract of undefined composition the molecular weights should be given. Molecular weight ranges will only be applicable in specific cases, for example for a group of homologues or a mixture of oligomers.
For technical guidance see: section 5.8 *For practical guidance see: -*

Composition information

	Typical concentration (w/w%)	Lower limit (w/w%)	Upper limit (w/w%)
A			
B			

The concentrations of the known major constituents should be given. The concentrations can be provided as

a typical concentration or as a concentration range. In case of a variable concentration, choose a range relevant for the constituent.
For technical guidance see: section 5 *For practical guidance see: -*

Nature and order of magnitude of impurities:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Impurities known to be present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For those impurities at least one of the following identifiers should be given:

- *the IUPAC name or if not to be derived another international accepted chemical name;*
- *CAS-number;*
- *EC number;*
- *Molecular or structural formula.*

For each impurity, the concentration (range) should be given (as w/w% or ppm).

For technical guidance see: section 5
For practical guidance see: -

Total concentration of non-specified impurities: ……w/w%

Nature and order of magnitude of any additives:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Additives known to be present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For additives at least one of the following identifiers should be given:

- *the IUPAC name or if not to be derived another international accepted chemical name;*
- *CAS-number;*
- *EC number;*
- *Molecular or structural formula.*

For each additive, the concentration (range) should be given (as w/w% or ppm).

For technical guidance see: section 5
For practical guidance see: -

Analytical information for the real substance

Spectral data	Not applicable
High-pressure liquid chromatogram, gas chromatogram	Not applicable
Description of analytical methods or bibliographical references	Not applicable

For natural extracts of undefined composition spectral data and chromatograms will not give relevant information on the identity of the real substance.

Process descriptions

Especially in the case when little or nothing is known about the composition of the natural extract, other identifiers must be given in order to identify the substance. One important option is information about the manufacturing process in which the real substance is derived.

The level of information determines the bandwidth of registration and therefore, determines which substances can be considered as the same substance and which cannot.

Description of processes used in the manufacture of the real substance: …… …… …… ……
An important identification parameter for natural extracts is the extract process description. It is up to the registrant to decide the level of information provided.
For technical guidance see: *For practical guidance see:*

Other identification parameters

Generic description of type of molecules (e.g. esters)	……
Range of homologues	……
Boiling point range or cut off	……°C

4.4.3 Petroleum substances

Petroleum substances are substances of very complex and variable composition. The starting materials used in the petroleum refining industry may be crude oil or any specific refinery stream obtained by one or more processes. The composition of the final products depends on the crude oil used for the manufacture as the composition of the crude oil varies depending on the place of origin. Therefore, there is a natural, process independent variation in composition of petroleum products. (L08)

For the naming of petroleum substances terms and definitions were laid down for the purpose of TSCA compilation (I13). And in the process of compiling EINECS the same identification rules were used. For the purpose of substance identification in REACH these terms and definitions are continued specifically for petroleum substances.

The terms and definitions for identification of petroleum substances include the stream's source, general composition, carbon number, boiling range or other appropriate physical characteristics, and predominant hydrocarbon type. In specific instances the definitions state that the stream contains benzene or 4- or 6-membered condensed ring aromatic hydrocarbons at certain concentrations.

From the process of identification of petroleum substances in the past, a list of CAS-numbers was compiled of petroleum substances in EINECS. That list of CAS-numbers is included in Annex x to this TGD. A substance included in that list is considered to be in the category of petroleum substances for the purpose of identification.

Name and other identifiers

IUPAC name or other international chemical name	……
For the identification of petroleum substances It is highly recommended to give the name according to the worldwide nomenclature and used within the European Union. Based on the CAS-number of the substance that name can be obtained from the EINECS inventory	
For technical guidance see: - *For practical guidance see:*	
Other names	……
Other names for the substance can be included. These include names under which the substance is put on the market within the European Union. These can also include internal company names.	
For technical guidance see: *For practical guidance see:*	
EC number EC name	…… ……
The EC number and EC name of the petroleum substance shall be given, where applicable. The EC-number	

is the official EU registration number for the substance and together with the EC name listed in the EINECS, ELINCS or NLP Inventory. (see Annex-x)	
For technical guidance see: *For practical guidance see:*	
CAS number CAS name	…… ……
The CAS-number and the CAS-name of the petroleum substance must be given. As a general rule the CAS-number of the petroleum substance is the starting point for the definition and identification of the substance.	
For technical guidance see: section 5.4 *For practical guidance see: section 6*	
Other identity code	……
Other identity codes for the substance can be given. These include numbers under which the substance is put on the market within the European Union. These can also include internal company numbers.	
For technical guidance see: section 5.5 *For practical guidance see: section 6*	

Name and other identifiers of the major constituents

In case constituents are known to be present at concentrations >10%, those major constituents should be identified.

	IUPAC names or other international chemical names:
A	
B	

The English IUPAC names of the known major constituents must be given. In case IUPAC names cannot be derived, other international chemical names can be given instead, if a correct reference can be given of the internationally accepted nomenclature, like the ISO name.
For technical guidance see: section 5.1 *For practical guidance see: section 6*

	Other names:
A	
B	

For all known major components, other names can be given, including other chemical names, trade names or abbreviations. Other names may also include internal company names. This might also include the IUPAC names in all languages available.
For technical guidance see: section 5.2 *For practical guidance see: section 6*

	EC number	EC name
A		
B		

The EC-number and EC name of the known major constituents must be given, in case available.
For technical guidance see: section 5.3 *For practical guidance see: section 6*

	CAS number	CAS name
A		
B		

The CAS-number and the CAS-name must be given for the known major constituents, in case available.
For technical guidance see: section 5.4 *For practical guidance see: section 6*

	Other identity code - type	Code
A		
B		

In case other identity codes are available for the major constituents, those can be given. Other identity codes can include internal company codes.
For technical guidance see: section 5.5 *For practical guidance see: section 6*

Molecular and structural formula

	Molecular formula	Structural formula	SMILES code
A			
B			

The molecular formula of the known major constituents should be given according to the Hill methodology. In case available the molecular formula should also be given according to the CAS method. Structural formulas should also be given for the known major constituents. The SMILES notations of the major constituents need to be given if applicable.
For technical guidance see: section 5.6 *For practical guidance see: -*

Information on optical activity ……

Optical activity should be given for all known major constituents if applicable and appropriate.
For technical guidance see: section 5.7

For practical guidance see: -

	Molecular weight or molecular weight range
A	
B	

For a petroleum substance the molecular weights of the known major constituents should be given. Molecular weight ranges will only be applicable in specific cases, for example for a group of homologues or a mixture of oligomers.

For technical guidance see: section 5.8
For practical guidance see: -

Composition information

	Typical concentration (w/w%)	Lower limit (w/w%)	Upper limit (w/w%)
A			
B			

For a petroleum substance the concentration of the known major constituents, if appropriate, should be given. The concentrations can be provided as a typical concentration and as a concentration range. In case of a variable concentration, choose a range relevant for the constituent. Be aware that the given concentration range is important identifier in the process of checking if it is the same substance.

For technical guidance see: section 5
For practical guidance see: -

Nature and order of magnitude of impurities:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Impurities present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For those impurities at least one of the following identifiers should be given:

- *the IUPAC name or if not to be derived another international accepted chemical name;*
- *CAS-number;*
- *EC number;*
- *Molecular or structural formula.*

For each impurity, the concentration (range) should be given (as w/w% or ppm).

For technical guidance see: section 5
For practical guidance see: -

Total concentration of non-specified impurities: ……w/w%

Nature and order of magnitude of any additives:

	IUPAC name	CAS number	EC number	Mol. formula	% or ppm
A					
B					

Additives present in a concentration >1% (or above any lower concentration limit, if relevant for the classification) should be specified. For additives at least one of the following identifiers should be given:

- *the IUPAC name or if not to be derived another international accepted chemical name;*
- *CAS-number;*
- *EC number;*
- *Molecular or structural formula.*

For each additive, the concentration (range) should be given (as w/w% or ppm).

For technical guidance see: section 5
For practical guidance see: -

Analytical information for the real substance

Spectral data	Not relevant
High-pressure liquid chromatogram, gas chromatogram	Not relevant
Description of analytical methods or bibliographical references	Not relevant

As petroleum substances are mixtures of undefined or variable composition, spectral data and chromatogram results give no information relevant for the identification.

4.4.4 Inorganic substances

- Aluminate (Al6O114-), barium strontium (4:1:7)
- Ferrate (Fe12O192-), strontium (1:1)
- Bismuth, compd. with europium (1:1)
- Europium selenide (EuSe)
- Copper, compd. with zinc (1:1)

4.4.5 Enzymes & proteins

Enzymes were principally reportable for EINECS. Consequently, about 400 enzymes are listed in EINECS.
Different ways to describe these enzymes have been used for the report:

Common functional description without further specification

EINECS-No	CAS-No	Enzyme
2329074	9035-82-9	Dehydrogenase
2326686	9003-99-0	Peroxidase
2327449	9013-05-2	Phosphatase
2326560	9002-13-5	Urease

Organism where the enzyme is isolated from

EINECS-No	CAS-No	Enzyme
2325609	9000-85-5	Amylase, bacterial
2327428	9013-01-8	Amylase, fungal
2326267	9001-72-3	Proteinase, pancreatic
2575208	51931-23-8	Proteinase, Bacillus subtilis

Substrate specificity

EINECS-No	CAS-No	Enzyme
2559165	42616-25-1	Lyase, methionine
2325860	9001-16-5	Oxidase, cytochrome
2327496	9013-66-5	Peroxidase, glutathione

Problematic entries: enzymes which are described by a generic entry and by specific characteristic properties like substrate specificity or source organism

EINECS-No	CAS-No	Enzyme
2329074	9035-82-9	Dehydrogenase
2328479	9029-06-5	Dehydrogenase, alanine
2328704	9031-72-5	Dehydrogenase, alcohol
2328290	9028-36-8	Dehydrogenase, D-lactate
2328442	9028-85-7	Dehydrogenase, formate
2328374	9028-54-0	Dehydrogenase, galactose
2328369	9028-53-9	Dehydrogenase, glucose

2326707	9004-06-2	Elastase
2544536	39445-21-1	Elastase (pig pancreas)

The question is under the present legislation and will be under REACH: Is an enzyme covered by an EINECS entry or not? Furthermore, it is not clear if an enzyme with a specific functionality which is isolated from a genetically modified organism (GMO) is legally identical to an (wild type) enzyme with the same activity but which is isolated from a "natural" source as listed in EINECS.

If only a generic entry of an enzyme exists (e.g. only the function of the enzyme without the source organism) then only this function is possibly relevant for the decision whether the enzyme is a phase-in-substance or not.

Is there a possibility to differentiate e.g. between an enzyme which is isolated from a natural source without using biotechnological methods or an enzyme which is produced and isolated from a GMO?

If a generic entry exists a natural (not modified) or artificial (modified) enzyme which fulfils the enzymatic function of this class may not be notified because the generic entry covers all subclasses. "Modified" means here, compared to the naturally occurring enzyme (MS04).

4.5 Workflow for checking substance identity

Text proposal not yet prepared

5 TECHNICAL GUIDANCE PER SUBSTANCE IDENTIFICATION PARAMETER

5.1 Name(s) in the IUPAC- or other International nomenclature

For registration the English IUPAC name or another well defined internationally accepted name of the substance needs to be given.

A IUPAC name is based on the international standard chemical nomenclature set by the international organisation IUPAC, the International Union of Pure and Applied Chemistry. The IUPAC nomenclature is a systematic way of naming chemical compounds, organic and inorganic. In IUPAC nomenclature, prefixes, suffixes and infixes are used to describe the type and position of functional groups in the compound.

penta-1,3-dien-1-ol, in this example the prefix is 1,3-pent-, the infix is -die- and the suffix is –ol; -en- is the basis of the name, the root name.

The set of rules were developed over the years and are continuously changing to deal with new components of molecular diversity and possible conflicts or confusions that have been identified. The rules set by IUPAC can be only used for well defined substances.

Below some general guidance on the structure of an IUPAC name is listed. For detailed support please use the guidance listed in 5.2.

Organic substance

1. Identify the number of C-atoms in the longest continuous chain of carbon atoms; This number of C-atoms determines the prefix, the first part, of the root name:

Number of carbon atoms	Root
1	meth-
2	eth-
3	prop-
4	but-
5	pent-
6	hex-
7	hept-
8	oct-
N	….

2. Determine the saturation of the chain; the saturation of the chain determines the suffix, the second part, of the root name:

Saturation	Bonds	Suffix
Unsaturated	Double	-ene
	Triple	-yn
Saturated	-	-ane

In case of multiple double or triple bonds the number of bonds is indicated with ‘mono’, ‘di’, ‘tri’ etc before the suffix.

Pentene with 2 double bonds: pentadiene

3. Combine prefix, suffix and additions to the root name;

   NB: For the root name IUPAC approved trivial and semi-systematic names may be used as well.

Benzene, toluene, etc.

4. Identify substituents and/or functional groups: carbon or non-carbon groups attached to the chain of carbon atoms identified under 1;

5. Determine the order of precedence of the substituents and/or functional groups;

6. Add the suffix for the first substituent/functional group in order of precedence;

7. Add the prefix for the other substituents and functional groups in alphabetical order.

Precedence	Group	Formula	Suffix	Prefix
1	Carboxylic acid	R-COOH	-oic acid	Carboxy
2	Ester	R-CO-O-R	-oate	*None*
3	Amide	R-$CONH_2$	-amide	Carbamoyl
4	Cyanide	R-CN	-nitrile	Cyano
5	Aldehyde	R-CHO	-al	Oxo
6	Ketone	R-CO-R	-one	Oxo
7	Alcohol	R-OH	-ol	Hydroxyl
8	Thiol	R-SH	-thiol	Mercapto
9	Amine	R-NH_2	-amine	Amino

Inorganic substance
Naming of inorganic substances is based on a set of rules, of which the most basic rules are presented below:

1 Single atom anions are named with an -ide suffix

O^{2-} is oxide

2 Simple ionic compounds are names with the cation followed by the anion; For cations taking on multiple charges, the charge is written using Roman numerals in parentheses immediately following the element name);

Cu^{2+} is copper(II)

3 Hydrates are named as the ionic compound followed by a numerical prefix and -hydrate. The numerical prefixes are mono-, di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, deca-.

$CuSO_4 \cdot 5H_2O$ is "copper(II) sulphate pentahydrate"

4 Inorganic molecular compounds are named with a prefix (see hydrates) before each element. The more electronegative element is written last and with an -ide suffix.

CO_2 is carbon dioxide, and CCl_4 is carbon tetrachloride.

5 Acids are named by the anion formed when dissolved in water.
a If an acid forms an anion named -ide, it is named hydro-ic acid.

hydrochloric acid forms a chloride anion.

b If an acid forms an anion named –ate, the acid is named with an -ic suffix.

chloric acid dissociates to chlorate anions in water.

c If an acid forms an anion names –ite, the acid is named with an -ous suffix.

chlorous acid disassociates into chlorite anions.

3. Natural products and related components

For natural products IUPAC has developed several rules for systematic naming. In short it means that for substances extracted from a natural source the name is based, whenever possible, on the family, genus or species name of the biological material from which the substance has been extracted.

For a hypothecial protein, *Hypothecalia Examplare* the names are based on hypothecalia and/or examplare, for example Horse Examplare

If possible, the name should reflect the known or likely distribution of the natural product. If appropriate, the class or order might also be used as the basis for the name of a substance that occurs in a number of related families. The name of natural products of unknown structure should not contain any prefixes, suffixes and/or infixes used in organic nomenclature.

Condensation product of Horse examplare, Valarine added to the N-terminus Examplare-Val

Many natural occurring substances belong to well-defined structural classes, each of which can be characterised by a set of parent structures that are closely related, that is, each can be derived from a fundamental structure. The systematic name for those naturally occurring substances and their derivates can be based on the name of an appropriate fundamental parent structure.

Well known parent structures are alkaloids, steroids, terpenoids, vitamins

A fundamental parent structure should reflect the basic skeleton that is common to most substances in that class. Natural occurring substances or derivates are named after the parent structure, adding prefixes, suffixes or infixes denoting:

- modifications to the skeletal structure
- replacement of skeletal atoms
- changes in the state of hydrogenation implied by the name of the parent structure
- atoms or groups substituting hydrogen atoms of the parent structure
- configurations not already implied by the name of the parent structure, or changed from that implied

Thiamin chloride is also known as vitamin B_1

For more detailed information on systematic naming of natural products and related substances, the IUPAC should be contacted (see 6.2).

4. IUPAC name not possible to derive
If it is not possible to derive an IUPAC name for substances, other international recognised nomenclature, specific for those substances, can be used like:

- Minerals; mineralogical names
- Petroleum substances
- Colour Index Generic Names[1]
- Oil additives
- INCI (International Nomenclature Cosmetic Ingredients)[2]
- SDA names for surfactants

5.2 Other names

All relevant names and/or public identifiers in all languages under which the substance is or will be marketed in the EU are useful to be included for registration under the REACH framework. This includes trade names, synonyms, abbreviations etc. in the local market languages.

5.3 EC-number from the EINECS, ELINCS or NLP (EC Inventory)

The EC-number, i.e. the EINECS, ELINCS or NLP number, is the official number of the substance within the European Union. The EC-number can be obtained from the official publications of EINECS, ELINCS and NLP and of the European Chemicals Agency.

The EC-number consists of 7 digits of the type $x_1x_2x_3$-$x_4x_5x_6$-x_7. The first digit is dependant of the list:

List	First digit of EC-number
EINECS	2 or 3
ELINCS	4

[1] http://www.colour-index.org/, Colour Index International, Fourth Edition Online
[2] http://dg3.eudra.org/F3/inci/index.htm, Official INCI website

NLP	5

For the EC-number, a checksum is available:

$$\frac{x_1 + 2x_2 + 3x_3 + 4x_4 + 5x_5 + 6x_6}{11} = \frac{\sum ix_i}{11} = Q + \frac{x_7}{11}$$

The EC-number must be correct according to the checksum.

5.4 CAS name and CAS number

The Chemical Abstracts Service (CAS), a division of the American Chemical Society (ACS), assigns these identifiers to every chemical which enters the CAS registry database. They are assigned in sequential order to unique, new substances identified by CAS scientists. Every compound registered at the Chemical Abstracts Service has a name according to the CAS-nomenclature, which the ACS adopts after recommendations of the ACS committee on nomenclature.

CAS name

The CAS name is the name given by the Chemical Abstract Service and is different than the IUPAC name. The CAS nomenclature is based on a limited set of criteria that are not always sufficient for deriving the name for a substance. Therefore, in general it is recommended to contact Chemical Abstract Service for obtaining the correct CAS name.

In short, the basic nomenclature rules are:
- A 'main' part of the substance is selected to act as header parent.
- Substituents are listed after the header parent, which is referred to as inverted order
- When more substituents are available they are listed in alphabetical order, including the prefixes

o-Xylen-3-ol is Benzene, 1,2-dimethyl, 3-hydroxy,

CAS number

The CAS-number of a substance is the non-legislative registration number. CAS-numbers can be obtained from the Chemical Abstract Service.

The CAS-number consists of a minimum of 5 digits, split up in three parts, separated by hyphens. The second part always consists of 2 digits, the third part of 1 digit,

N_i .....N_4 N_3 – N_2 N_1 - R

For the CAS-number, a checksum is available:

$$\frac{iN_i + ...4N_4 + 3N_3 + 2N_2 + 1N_1}{10} = \frac{\sum iN_i}{10} = Q + \frac{R}{10}$$

The CAS-number must be correct according to the checksum.

Registration of a substance to CAS

The CAS registry service assigns CAS numbers to the following chemical compounds:

- Mono-constituent substances, represented by:
  - Completely defined molecular structures (i.e., all atoms and the chemical bonds joining them are known). Different positional isomers, stereo chemical isomers, and salt forms are also taken into consideration.
  - Names which clearly imply the chemical composition of the substances
- Specific ratios for salts or condensation products
- Naturally occurring minerals
- Specific alloys, ions, isotopes and elementary particles
- Complex substances, such as:
  - Chemically modified biological materials
  - Complex reaction products
  - Industrial process streams

For CAS registration the form must be used as included in 6.2 to this TGD. As stated in that form the following information is needed in general order of preference:

- Well Defined Chemical Compounds:
  - Chemical structure diagram
  - Systematic chemical name
  - Common names
  - Molecular formula
- Complex Reaction Products
  - List of reactants and nature of the reaction
  - Reaction scheme
  - Typical composition of the product
- Plant and Animal Products
  - Genus Species as well as other unambiguous common names of the source
  - Method of extraction
  - Description of further chemical processing
- Products from Industrial Processes
  - Precursors and method of preparation
  - Schematic diagram depicting the industrial process and the point where the substance is isolated
  - Process description

    Catalytic cracking, dewaxed
  - Carbon (alkyl) range

    C4 through C12
  - Physical properties

    Boiling range, viscosity, solid, slag
  - Principal chemical composition
  - Source

    petroleum, coal

- Biotechnological Products
  - Sequence data
  - Biological source information, including Genus/Species
  - Enzyme activity

For more information on, application for and finding CAS numbers and CAS nomenclature, see 5.2.

5.5 Other identity codes

Other internationally recognised identity codes can be given as well, like:
- UN number
- Colour Index Number
- Dye number
- etc.

5.6 Molecular formula, structural formula and SMILES

Molecular formula
A molecular formula identifies each type of element by its chemical symbol and identifies the number of atoms of such element to be found in each discrete molecule of the substance. Molecular formulae can be arranged according to different systems. Both the SNIF guidance (L12) and the Chemical Abstract Service acknowledge the Hill order as the only system to be used while arranging molecular formulae.

The recommended method for the identification of substances, for the purpose of REACH, is therefore also the Hill Method. For applying the Hill method the following steps can be followed:

1 Identify the elements and list the chemical symbols;
2 Arrange the elements in the correct order:
   a. Carbon containing substances:
      Each element is mentioned by its chemical symbol, in the following sequence:
      (1) Carbon;
      (2) Hydrogen;
      (3) Other element symbols in alphabetical order;

Pentane: C_5H_{12} Pentene: C_5H_{10} Pentanol: $C_5H_{12}O$

   b. Non carbon containing substances:
      Each element is mentioned in alphabetical order;

Hydrochloric acid: ClH

3 For each element, add the number of atoms, in case > 1, as subscript to the chemical symbols;

4 Add information, not related to the main structure, at the end of the molecular formula, separated by a dot or comma.

Sodium benzoate is $C_7H_6O_2$, sodium salt Copper sulphate dihydrate is $CuO_4S.2H_2O$

In case the Hill method is not possible for a specific substance, the molecular formula should be given in a different way, for example as an empirical formula, a simple description of the atoms and the ratio of the atoms available, or the formula given by the Chemical Abstract Service (see 5.2).

Structural formula
A structural formula is needed for the visualisation of the chemical structure of the molecules within the substance. The structural formula should indicate the location of the atoms, ions or groups and the nature of bonds joining them. This includes also isomerism, i.e. cis/trans, chirality, enantiomers etc.

The structure formula can be given in different formats: in the form of a molecular formula and the in form of a structural diagram.

- *Structural formula in the form of a molecular formula*

1. Write down all elements group wise and in order of appearance;

n-pentane: CH3CH2CH2CH2CH3

2. Each substituent is written down between brackets, directly after the atom to which it is connected;

2-methylbutane: CH3CH(CH2)CH2CH3

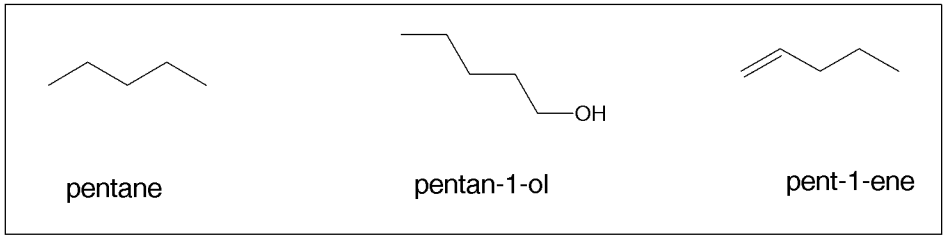
3. In case of double or triple bonds, show between the groups of elements of concern.

pent-1-ene: CH2=CHCH2CH2CH3

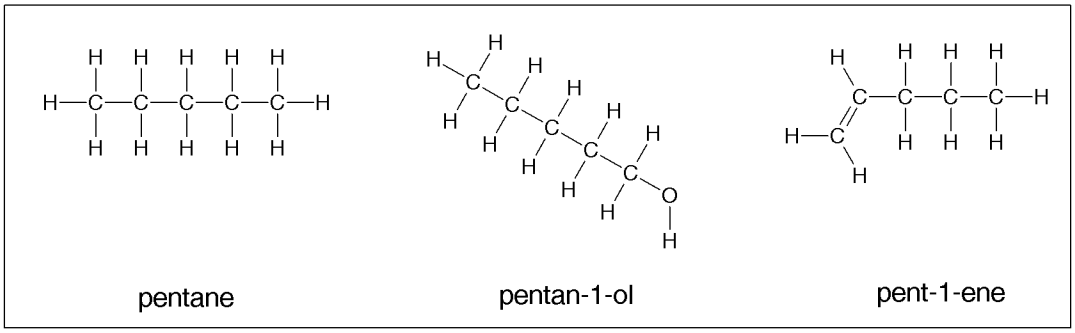
- *Structural formula in the form of a structural diagram*

For a structural diagram the elements and the bonds between the elements are visualised in a 2D or 3D picture. Several methods exist:

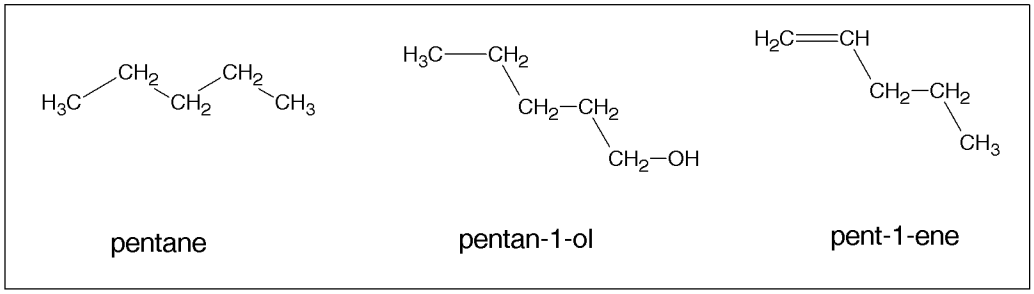
1. Showing all non-carbon elements and hydrogen attached to non-carbon elements.



2. Showing all elements by name



3. Showing carbon and hydrogen as groups (e.g. CH3), all non-carbon elements and all hydrogens not bonding to carbon.



SMILES notation

SMILES is an acronym for Simplified Molecular Input Line Entry Specification. It is a chemical notation system used to represent a molecular structure by a linear string of symbols. With standard SMILES, the name of a molecule is synonymous with its structure, it shows indirectly a two dimensional picture of the molecular structure. Since a two dimensional chemical structure can be drawn in various ways, there are several correct SMILES notations for one molecule. The basis of SMILES is the representation of a valence model of a molecule; therefore, it is not suitable to describe molecules which cannot be represented by a valence model.

SMILES notations are comprised of atoms, designated by elemental symbols, bonds, parentheses, used to show branching, and numbers, used for cyclic structures. A SMILES notation denotes a molecular structure as a graph with optional chiral indications. SMILES notations describing only the structure in terms of bonds and atoms is called a generic SMILES, a SMILES notation written with isotopic and chiral specifications is known as an isomeric SMILES.

In short the SMILES notation is based on several basic rules:

1 Atoms are represented by their atomic symbols;

2 Each atom, except for hydrogen, is specified independently;
   a. Elements in the "organic subset" B, C, N, O, P, S, F, Cl, Br and I are written without brackets and without attached H, as long as the number of H conforms to the lowest normal valence consistent with explicit bonds:

Element in "organic subset"	**"Lowest normal valence"**
B	3
C	4
N	3 and 5
O	2
P	3 and 5
S	2, 4 and 6
F	1
Cl	1
Br	1
I	1

   b. Elements in the "organic subset" are written with brackets as soon as the number of H does not conform to the lowest normal valence;

Ammonium cation is NH4+

   c. Elements other than those in the "organic subset" are written between brackets with any attached hydrogen shown

3 Aliphatic atoms are entered in upper case; aromatic atoms are entered in lower case;

benzene is c1ccccc2 and cyclohexane is C1CCCC2

4 Hydrogen is only included in case of the following situations:
   a. charged hydrogen, i.e. a proton, [H+]
   b. hydrogens connected to other hydrogens, i.e. molecular hydrogen, [H][H]
   c. hydrogens connected to other than one other atom, e.g. bridging hydrogens
   d. isotopic hydrogen specifications, e.g. deuterium ([2H])
   e. if the hydrogen is connected to a chiral atom

5 The four basic bonds are shown as follows:

Type of bond	**SMILES notation**
Single	- (not needed to show)
Double	=
Triple	#
Aromatic	Lower case letters

6 Substituents are shown by enclosure in parentheses, and immediately after the atom to which it is connected;

2-methylbutane is CC(C)CC

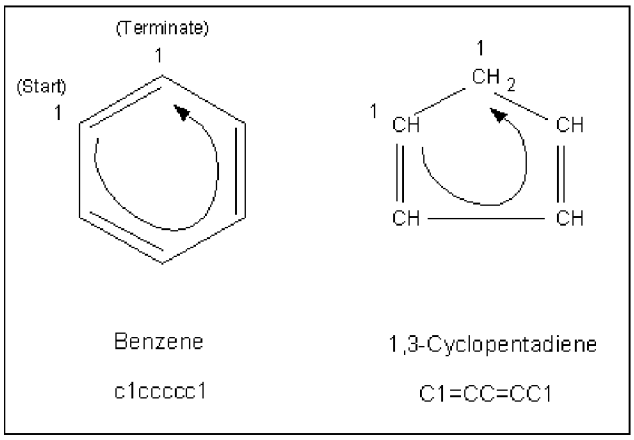
   a. Substituents are always mentioned directly after the relevant atom; it cannot follow a double or triple bond symbol;

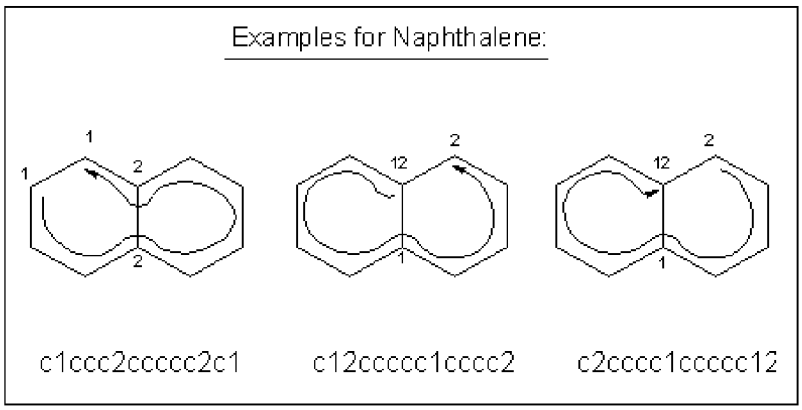
Pentanoic acid is CCCCC(=O)O

   b. Substituents within substituents are allowed;

2-(1-methylethyl)butane is CC(C(C)C)CC

7 For cyclic structures the numbers 1 through 9 are used to indicate the starting and terminating atom of the cycle.
   a. The same number is used to indicate the starting and terminating atom for each ring. The starting and terminating atom must be connected to each other.
   b. Numbers are entered immediately following the atoms used to indicate the starting and terminating positions.
   c. A starting or terminating atom can be associated with two consecutive numbers.





8 Disconnected compounds are designated as individual structures or ions separated by a dot (".").Adjacent atoms separated by dot (.) are not directly bonded to each other, e.g. Van der Waals bonding;

Aminopropene hydrochloride is C=CC(N).HCl

9 Isomeric configuration is specified by the "slash" characters "\" and "/". These symbols indicate the relative direction between two isomeric bonds. (cis ='/ \', trans = '/ /'). SMILES uses local chirality, which means that the chirality must be completely specified.

cis-1,2-dibromoethene is Br/C=C\Br trans-1,2-dibromoethene is Br/C=C/Br

10 Enantiomers or chirality are specified by the '@' symbol. The symbol '@' indicates that following neighbours of the chiral atom are listed anticlockwise. If the symbol '@@' is used, the atoms are listed clockwise. The chiral atom is noted between brackets.

2-chloro-2-hydroxypropanoic acid with specified chirality is C[C@](Cl)(O)C(=O)(O)

11 Isotopic specifications are indicated by preceding the atomic symbol with a number equal to the desired integral atomic mass. An atomic mass can only be specified inside brackets;

Carbon-13 is [13C] and Oxygen-18 is [18O]

For the determination of the SMILES notation several tools (SMILES generators) are available (see 6.2)

5.7 Information on optical activity

Optical activity is the ability of asymmetric compounds to rotate the orientation of planar polarized light. Such compounds and their mirror images are known as enantiomers and have one or more chiral centres. Although differing in geometric arrangement, enantiomers possess identical chemical and physical properties. Since each type of enantiomer affects polarized light differently, optical activity can be used to identify which enantiomer is present in a sample and therefore, also the purity of the substance. The magnitude of the rotation is an intrinsic property of the molecule.

Enantiomers always have opposite rotations; they polarize to the same extent, but in the opposite direction. The optical activity of an enantiomers mixture is therefore an indication of the ratio between the two enantiomers. A 50-50 mixture of enantiomers has an optical activity of 0.

The observed rotation depends on the concentration, the length of the sample tube, the temperature and the wave length of the light source.

In conclusion, optical activity is the parameter to define the identity of an asymmetric compound and is the only parameter to distinguish the compound from its mirror image. Therefore, if applicable and if appropriate the optical activity of the substance should be given.

The standard for optical activity is called the specific rotation. The specific rotation is defined as the observed rotation of light at 5896 angstrom, with a path length of 1 dm and in a sample concentration of 1 g/ml. The specific rotation is the observed rotation divided by the path length (dm) times the concentration (g/ml).

Optical activity can be measured with different methods. The most common are:
- Optical rotation, which observes a sample's effect on the velocities of right and left circularly polarised light beams;
- Circular dichroism, which observes a sample's absorption of right and left polarised light.

If the substance rotates the light to the right (clockwise) it is called dextrorotatory and is designated with a + sign. If it rotates light to the left (counter clockwise) it is called levorotatory and it is designated -.

5.8 Molecular weight or molecular weight range

The molecular weight is the weight of a molecule of a substance expressed in atomic mass units (amu) or in molar masses (g/mole). The molecular weight may be calculated from the molecular formula of the substance: it is the sum of the atomic weights of the atoms making up the molecule. For molecules, like proteins, undefined reaction mixtures, where one molecular weight cannot be determined, a molecular weight range can be given.

Several methods can be used to determine the molecular weight of substances:

- For determining the molecular weights of gaseous substances, Avogadro's law can be used, which states that under given conditions of temperature and pressure a given volume of any gas contains a specific number of molecules of the gas

$$PV = nRT = NkT$$

n = number of moles
R = universal gas constant = 8.3145 J/mol K
N = number of molecules
k = Boltzmann constant = 1.38066 x 10-23 J/K = 8.617385 x 10-5 eV/K
k = R/NA
NA = Avogadro's number = 6.0221 x 1023 /mol

- For liquids and solid substances the molecular weight can be determined by determination of their effects on the melting point, boiling point, vapour pressure, or osmotic pressure of some solvent.
- Mass spectrometry, a highly accurate measure method
- For molecules with high molecular weights, like proteins and viruses. The molecular weights may be determined by measurement of for example sedimentation rate in an ultracentrifuge or by light-scattering photometry etc.

5.9 Substance composition

For each substance the substance composition as combination of the relevant main constituents, additives and impurities need to be registered in line with the rules and criteria described in section 5.

Each constituent, additive or impurity needs to be properly identified by:

- Name (IUPAC name or other internationally accepted name, see 4.3.1);
- CAS number (if available, see 4.3.4);
- EC number (if available, see 4.3.3).

For each constituent, additive or impurity the appropriate concentration or concentration range needs to be identified.

5.10 Spectral data

Spectral data are needed to confirm the structure given of a mono-constituent substance or to confirm that a reaction mixture is not a preparation. Several methods can be used for spectra (ultra-violet, infra-red, nuclear magnetic resonance or mass spectrum). Not all methods are suitable for all classes of compounds. Where possible, the TGD will give guidance for the appropriate spectra to include.

For several well-used methods the following information should be indicated on the spectrum itself or in annexes:

UltraViolet-Visible (UV-VIS) spectrum
- the identity of the product
- solvent and concentration
- range
- position (and epsilon value) of main peaks
- effect of acid
- effect of alkali

Infrared Spectroscopy (IR) spectrum
- the identity of the product
- medium
- range
- results (indicate the main peaks important for the identification, e.g. interpretation of the fingerprint area)

Nuclear Magnetic Resonance Spectroscopy (NMR) spectrum
- the identity of the product
- nucleus and frequency
- solvent
- if appropriate internal or external reference
- Results (indicate the signals important for identification and the signals corresponding to the solvent and the impurities).
- for 1H NMR spectra the integration curve should be provided
- the intensity of weak NMR peaks should be increased vertically and complex patterns expanded

Mass Spectroscopy (MS) Spectrum
- the identity of the product
- accelerating voltage
- method of loading (direct insertion via GC, etc)
- Ionisation mode (Electron Impact, Chemical Ionisation, Field Desorption, etc)
- the molecular ion (M)
- significant fragments for the identification of the product
- m/z values or assignments of the peaks important for the identification of the structure
- complex patterns should be expanded

Other international recognised methods can be used as well if the spectral data will confirm the identification of the product, e.g. the structure.

The following general requirements are needed for a clear understanding and/or interpretation of the spectra:
- Note significant wavelengths or other data as appropriate;

- Provide extra information, e.g. spectra of starting materials;
- Give solvent used and/or other essential details as indicated below for some methods;
- Provide clear copies (rather than originals) with scales properly marked;
- Provide information on the concentrations used;
- Ensure the most intense substance-related peaks approach the full-scale mark.

5.11 High-pressure liquid chromatogram, gas chromatogram

A chromatogram needs to be provided to confirm the composition of the product. In others words, a chromatogram will confirm the existence of impurities, additives and the constituents of a reaction mixture. The two best known methods for separation and identification of mixtures are gas chromatography (GC) and high pressure liquid chromatography (HPLC). The two methods are based on the interaction of a mobile phase with a stationary phase, leading to a separation of the constituents of a mixture.

For GC/HPLC chromatograms the following information should be indicated on the chromatogram itself or in several annexes:

- *HPLC:*
  - The identity of the product
  - Column properties, like diameter, packing, length
  - Temperature, also if range is used
  - Composition mobile phase also range if used
  - Concentration range
  - Visualisation method, e.g. UV-VIS
  - Results (indicate the main peaks important for the identification)
- *GC:*
  - The identity of the product
  - Column properties, like diameter, packing, length
  - Temperature, also if range is used
  - Injection temperature
  - Carrier gas and pressure of carrier gas
  - Concentration range
  - Visualisation method, e.g. MS
  - Peak identification
  - Results (indicate the main peaks important for the identification)

ISSUE: HPLC is that a High-pressure liquid chromatogram or a High-performance liquid chromatogram

5.12 Description of the analytical methods

Annex IV requires describing the analytical methods or the appropriate bibliographical references for the identification of the substance and, where appropriating, for the identification of impurities and additives. This information shall be sufficient to allow the methods to be reproduced.

ISSUE I-14: Concern of industry is that the analytical information (REACH Annex IV, 2.3.7) need to be entered twice (for substance identification and as part of the registration dossier). Question whether it is an endpoint or a substance identifier

6 GUIDANCE INSTRUMENTS

6.1 Introduction

6.2 Sources of information for substance identification parameters

General

SI parameter	Source	Source description
General	http://www.sis.nlm.nih.gov/Chem/ChemMain.html	A family of databases and tools to help users search for chemical information
	http://chemfinder.cambridgesoft.com/	A free database that provides chemical structures, physical properties, and hyperlinks to more relevant information
	http://www.accelrys.com/accord/productlisting.html	Chemical software; Accord Alphabetical Product Listing
	http://www.syrres.com/esc/free_demos.htm	free online searches of the following databases: Environmental fate database KOW (online Log P) PHYSPROP (Physical properties)

Name and other identifiers

IUPAC name	http://www.iupac.org	official website IUPAC
	http://www.chem.qmul.ac.uk/iupac	IUPAC chemical nomenclature and recommendations (under authority of IUPAC)
	Nomenclature of Organic Chemistry (Blue Book) Pergamon, 1979 [ISBN 0-08022-3699]	principal IUPAC nomenclature publications, up-date expected 2006.
	A Guide to IUPAC Nomenclature of Organic Compounds (recommendations 1993) (supplementary Blue Book) Blackwell Science, 1993 [ISBN 0-63203-4882]	principal IUPAC nomenclature publications, up-date expected 2006.
	Nomenclature of Inorganic Chemistry (recommendations 1990) (Red Book) Blackwell Science, 1990 [ISBN 0-63202-4941]	principal IUPAC nomenclature publications, up-date expected July 2005.
	Biochemical Nomenclature and Related Documents (White Book) Portland Press, 1992 [ISBN 1-85578-005-4]	principal IUPAC nomenclature publications
	Principles of Chemical Nomenclature: a Guide to IUPAC Recommendations Blackwell Science, 1998 [ISBN 0-86542-6856]	introductory volume covering all types of compound
	http://www.chem.qmul.ac.uk/iumbd	IUBMB biochemical nomenclature database (under authority of IUBMB)

	http://www.acdlabs.com/products/name_lab/	commercial computerised naming program that can be very helpful in naming structures of moderate complexity , also freeware available for small molecules (IUPAC recommended)
	http://www.acdlabs.com/iupac/nomenclature	IUPAC nomenclature of organic chemistry (IUPAC recommenced)
	http://www.acdlabs.com/iupac/nomenclature, appendix R9.1	complete list of approved trivial and semi systematic root names
	http://www.chemexper.com/misc/iupac/index.html	ChemExper IUPAC site
Other names	http://www.colour-index.org	Colour Index Generic Names, Colour Index International, Fourth Edition Online
	http://dg3.eudra.org/F3/inci/index.htm	INCI (International Nomenclature Cosmetic Ingredients), Official INCI website
Other identifiers	http://www.cenorm.be	CE norms, official European CE-site
EC-number	http://ecb.jrc.it/	Official ECB site, search on EINECS, ELINCS, NLP and Annex I of 67/548/EEC
CAS number	http://www.cas.org	official website CAS registry service
	http://www.chemistry.org	official website American Chemical Society

Molecular and structural formula

SMILES	http://www2.ccc.uni-erlangen.de/services/gifcreator/	Free SMILES generator
	http://cactus.nci.nih.gov/services/translate/	Free SMILES generator
	http://www.acdlabs.com	ACDChemsketch, freeware with SMILES generator (also commercially available)

Analytical information

General	Quality control for spectral data and methods of analysis	

6.3 Specific IT Tools for substance identification

6.4 Additional guidance needs to be developed

7 REFERENCES & RELEVANT LITERATURE

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