Substance Identity in REACH

Study on Substance Identity (SID) in REACH. Analysis of SID and substance sameness of complex substances.

Final Report

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Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs
Directorate D — Consumer, Environmental and Health Technologies
Unit D1 — REACH

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EXECUTIVE SUMMARY

This study analyses approaches applied by the industry in identification of substances for registration under REACH. The study is based on a substance identity screening of 223 complex substances selected as a representative set of substances with different challenges in their identification. Based on information from registration dossiers, the study identifies key challenges in identification of complex substances in general and provides comparison of approaches taken by registrants of different groups of substances. The study does not aim at assessing compliance of registration dossiers with REACH.

The analysis begins with a mapping of all registered substances which are likely to pose objective challenges for registrants and regulators in terms of identification and assessment of substance sameness when considering joint registration submissions. Over 22 % of all substances in the ECHA database of registered substances[1] as of January 2014 represented complex substances, mostly UVCBs[2].

The screening of substance identity information from registration dossiers of the selected set of complex substances revealed common as well as sector-specific practices in identification of substances. The analysis groups together substances which are likely to share common substance identity features, taking into account specifics of each group. The study identifies individual substance identity elements used by registrants of substances with variable or unknown composition or other substances which cannot be unambiguously identified solely by specification of the composition. The study also discusses the role of these substance identity elements in relation to individual groups of substances based on the information provided by registrants in the screened dossiers.

The study also systematically assesses consistency of information provided by registrants of complex substances in dossiers. Since substance identity is typically very specific for each substance, consistency of information provided by registrants is vital for assessment of substance sameness when considering a joint registration.

Substance identity elements

Source and manufacturing process play the key role in identification of substances with unknown or variable composition. While it may not be technically possible to fully determine the composition or to avoid variability in the composition of these substances (e.g. in cases where compositional variability originates from intrinsic variability of the source, such as substances of biological origin), it is assumed that substances manufactured from the same sources and using the same manufacturing processes and technologies will have similar composition to allow joint registration. Reflecting the importance of source and manufacturing process and in accordance with the guidance for identification and naming of substances under REACH and CLP published by ECHA[3], source and manufacturing process were (together with the composition itself) the most frequently used identity elements specified by the registrants of the screened substances. The study systematically addresses for each group of substances whether a single source is always linked to specific manufacturing processes and vice versa and moreover, if different sources and different processes lead to substances registered within a single joint registration.

[1] http://echa.europa.eu/information-on-chemicals/registered-substances
[2] Substances of Unknown or Variable composition, Complex reaction products or Biological materials
[3] http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf

Different parameters (conditions) of encountered manufacturing processes typically greatly influence the composition of the resulting substance. Conditions of the manufacturing process (e.g. temperature, pressure, reaction time, catalysts, ratio of reaction agents, etc.) are therefore frequently described by registrants across all groups of substances.

Other substance identity elements are used with highly variable frequency across the studied groups of substances and are therefore more group-specific.

Grouping of substances sharing similar substance identity features

To select a representative set of substances for the substance identity screening, identified complex substances were organised into groups of substances likely to share similar substance identity features. The grouping was based solely on publically available information, mainly on the information available in the ECHA database of registered substances. The grouping system was developed solely for the purpose of the selection of the representative set of substances to capture different issues which may be specific only to a certain group of substances.

Besides aspects relating to substance identity, the developed grouping of substances takes into consideration also statistical aspects allowing comparisons between individual groups and sub-groups of substances. Some complex substances are covered by well-established long-term operating REACH registration consortia. Grouping of substances in this study takes into account grouping used by these consortia where appropriate. Despite being based solely on publically available information, the subsequent screening of information from the registration dossiers confirmed that the substances in individual groups often shared common substance identity elements and issues relating to their identification (especially in the case of substances and groups covered by operating consortia, where the observed consistency of used substance identity elements is generally higher).

Identified complex substances were organised into the following 13 groups of substances, further broken down into 56 sub-groups.

1. Inorganic substances
   1.1. Substances originating from combustion processes
   1.2. Substances originating from metallurgical processes
   1.3. Substances originating from calcination and smelting processes
   1.4. Other inorganic substances
2. Organic substances
   2.1. Substances with variability in alkyl chain length
   2.2. Petroleum-derived substances
   2.3. Coal-derived substances
   2.4. Other organic substances
3. Substances of biological origin
   3.1. Substances originating from fermentation process
   3.2. Substances originating from plants and animals
4. Other substances
   4.1. Chemicals with organic and inorganic part
   4.2. Organic-inorganic salts
   4.3. Others

Results

The executive summary lacks a summary of the main results.

Similarities and differences in identification of substances in individual groups were observed in various areas, including the role of source and manufacturing process, specification of additional substance identity elements as well as use of different analytical methods for the determination of composition.

Information exchange with stakeholders

Workshop on substance identity and questionnaires circulated within the study to industry associations and REACH consortia confirmed that identification of complex substances remains challenging. The stakeholders stressed out the importance of further work to define substance-specific or sector-specific criteria for assessing substance sameness. The stakeholders also appreciated the concept of substance identity profiles introduced earlier by The European Chemical Industry Council (CEFIC)[4], which proves very useful in harmonising the information exchanged by co-registrants of a substance to allow comparison of substance identity information and assessment of substance sameness. However, it was noted that the substance identity profile template, developed for well-defined substances, needs to be modified to work efficiently also for UVCBs.

Conclusions and Recommendations

The screening of the 2202 registration dossiers[5] of 223 complex substances together with the organised workshop and questionnaires distributed to industry associations and REACH consortia confirmed that substance identification and especially determination of substance sameness remain some of the most challenging aspects of the REACH Regulation.

The study revealed that substance identity information provided in the registration dossiers is typically more consistent and harmonised in cases where substance identity is systematically addressed by operating industry associations and REACH consortia. Harmonised reporting of substance identity information greatly facilitates subsequent assessment of substance sameness. The conclusions of the study therefore support activities of various sectoral organisations to harmonise the approaches in identification and determination of sameness of certain specific groups of complex substances. Furthermore, recent activities of industry associations and REACH consortia in collaboration with ECHA and other international bodies should bring further clarity regarding criteria of eligibility for joint registration (substance sameness criteria) in selected sectors.

Determining substance sameness was found to be especially challenging as substance identity is very sector-specific or even substance-specific and no widely applicable sameness assessment criteria can be developed. Developing substance-specific sameness assessment criteria proved to be an efficient way of addressing challenges in determination of sameness of substances when considering a joint registration. Substance identity profiles (SIPs) proved to be efficient instruments for harmonisation of substance identity information specified by potential co-registrants. However, developed originally for well-defined substances, modification of the model SIP is necessary for UVCBs and other complex substances.

[4] http://www.cefic.org/
[5] A maximum of 20 registration dossiers were analysed per substance

Based on the conclusions and observations made within the study, the following recommendations are proposed:

- It is highly recommended to carry on with initiated collaborative activities of ECHA, industry associations and other international bodies to develop sector-specific guidances for identification of individual groups of substances and especially for assessment of substance sameness.

- To facilitate exchange of information between potential SIEF members in assessment of substance sameness, further development of substance identity profiles (SIPs) should be considered to address specifics in identification of UVCBs.

- Annex VI of REACH, sections 2.3.5 and 2.3.6 list analytical data which shall be sufficient to enable each substance to be identified. As confirmed by the results of this study, these data are appropriate and sufficient usually only for identification of some groups of substances, especially organics. For other groups of substances, other analytical data are more appropriate for identification (e.g. data from X-ray diffraction, X-ray fluorescence or Inductively coupled plasma optical emission spectroscopy for various inorganic substances). It is therefore recommended to consider updating Annex VI, section 2.3 of REACH or to compile a compendium of analytical methods appropriate for identification of different groups of substances.

- It is recommended to support exchange of information and experience on identification of substances between registrants via workshops, both general and sector-specific, organised by stakeholders from industry as well as authorities, especially before the upcoming registration deadline in 2018.

GLOSSARY OF TERMS, ACRONYMS AND ABBREVIATIONS

AAS	Atomic Absorption Spectrometry
ACPA	Activated Carbon Producers Association
APAG	European Oleochemicals and Allied Products Group
ATC	Additive Technical Committee
BTEX	benzene, toluene, ethyl benzene and xylene
CAS RN	Chemical Abstracts Service Registry Number
Colour Index (C.I.)	Identifier for colorants, simplified commonly used term referring to Colour Index Constitution Number maintained by the Society of Dyers and Colourists and the American Association of Textile Chemists and Colorists
CONCAWE	Division of the European Petroleum Refiners Association carrying out research on environmental issues relevant to the oil industry
CTO	Crude Tall Oil
DIN	German Institute for Standardization (Deutsches Institut für Normung)
DMSO	Dimethyl sulfoxide
DSC	Differential Scanning Calorimetry
EC / List number.	The European Community number used within the European Community system for coding of chemicals
ECHA	European Chemicals Agency
ECOBA	European Coal Combustion Products Association
EFEO	European Federation of Essential oils
ESI-MS	Electrospray Ionisation Mass Spectrometry
EURASYP	European Association for Speciality Yeast Products
FAAS	Flame Atomic Absorption Spectroscopy
FAME analysis	Fatty Acid Methyl Esters analysis
FATAC	Fatty Acids Consortium
FTIR	Fourier Transform Infrared Spectroscopy
GC	Gas chromatography
GC-MS	Gas Chromatography–Mass Spectrometry
GFAAS	Graphite Furnace Atomic Absorption Spectrometry
GLC	Gas Liquid Chromatography
GPC	Gel Permeation Chromatography
GPC/SEC	Gel Permeation Chromatography/Size Exclusion Chromatography
Group / Sub-group of substances	Complex substances identified within this study were organised into 13 groups of substances, further broken down into 56 sub-groups.
H4R	Hydrocarbon Resins & Rosin Resins
HCB	Hexachlorobenzene
HOPA	Higher Olefins and Poly Alpha Olefins
HOPA	Higher Olefins and Poly Alpha Olefins
HPLC	High Performance Liquid Chromatography

HPSEG	High Performance Size Exclusion Chromatography
HSPA	Hydrocarbon Solvents Producers Association
IC	Ion Chromatography
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectroscopy
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
ICP-OES	Inductively Coupled Plasma Optical Emission Spectrometry
IFRA	International Fragrance Association
IR	Infrared Spectroscopy
KF titration	Karl Fischer titration
LAB	Linear Alkyl Benzene
LC-MS	Liquid Chromatography–Mass Spectrometry
LOA	Lower Olefins and Aromatics
MALDI-TOF	Matrix-Assisted Laser Desorption/Ionization-Time of Flight
MCCP	Medium-Chain Chlorinated Paraffin
MDI/MDA	Methylenediphenyl Diisocyanates/ Methylenediphenyl Diamine
MS	Mass Spectrometry
NLP	No-Longer Polymers
NMR	Nuclear Magnetic Resonance
NONS	Substances that have been notified under Directive 67/548/EEC
OECD	Organisation for Economic Co-operation and Development
PBDDs	Polybrominated Dibenzo-p-Dioxins
PBDFs	Polybrominated Dibenzofurans
PCB	Polychlorinated Biphenyls
PCCDs	Polychlorinated Dibenzodioxins
PCDFs	Polychlorinated Dibenzofurans
PEG	Polyethylene glycol
PSD	Particle Size Distribution
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC
Sample Set	Set of substances selected for further substance identity information assessment (screening)
SDA Number	Soaps & Detergent Association Reporting Number
SEM-EDS&WDS	Scanning Electron Microscopy- Energy Dispersive Spectroscopy & Wavelength Dispersive Spectroscopy
SID	Substance Identity
SIEF	Substance Information Exchange Forum

SIP	Substance Identity Profile
Substance	Substance as defined in Article 3 of REACH
TMP	Trimethoprim
TOC	Total Organic Carbon
TOPP	Turpentine Oil From Pulping Processes
TOS	Crude Tall Oil Soap
UVCB	Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials
UV-VIS	Ultra Violet-Visible Spectroscopy
VDLUFA	Association of German Agricultural Analytic and Research Institutes (Verband Deutscher Landwirtschaftlicher Untersuchungs- und Forschungsanstalten)
WGS&CSL	Wheat Glucose Syrups and Corn Steep Liquor
XANES	X-ray absorption near edge structure
XRD	X-ray diffraction
XRF	X-ray fluorescence

1. INTRODUCTION

1.1. Background

Substance identity (SID) is corner-stone of REACH and it is the basis for one of the key processes in REACH – registration of substances. Identification of substances defines what registrants have considered as one substance and the basis on which they have compiled a technical dossier for registration.

Since REACH was adopted in 2006, it was evident that REACH registrants would need more information on SID issues. This was the reason why ECHA developed a "guidance for identification and naming of substances under REACH"[6]. Since then, this guidance constitutes the main reference for discussions that occur in the SID area. This SID guidance document identifies four main types of substances according to their complexity (namely mono-constituent, multi-constituent, well-defined substances identified by their composition and other main identifiers and UVCB[7] substances). In addition, some industry organisations have developed "sectoral" guidance documents that may also address some SID issues. Activities of industry are supported by ECHA and other international bodies (e.g. OECD) participating on the development of these sectoral substance identification guidances (or initiating it).

It is exclusive responsibility of the registrant to identify his substance(s) as he is in the best position to know what he is manufacturing and/or importing. Article 11 of REACH requires registrants of the same substance to share toxicological and ecotoxicological information (specified by provisions of Article 10 and Annexes VII – XI of REACH) within a joint registration for that substance. Proper identification of the substance in accordance with Annex VI of REACH provides basis for considerations regarding joint submission. The substance sameness criteria applied by registrants in a joint submission will determine the identity of the substance they jointly register. The guidance lists elements on which registrants should base the sameness criteria. However, the guidance is not exhaustive and registrants may face challenges not foreseen in the guidance document, especially when it comes to determination of sameness of substances with variable or unknown composition or other complex substances.

The REACH review published on 5 February 2013[8] highlighted, among other things:

The processes so far have shown also that the definition of substance identity and the determination of sameness of substances are some of the most challenging aspects of REACH. The Commission services will keep working on improved practical implementation to further enhance the identification of substances and the efficiency of data sharing.

1.2. Objectives of the study

The study aimed at performing analysis of approaches taken by registrants within the first two REACH registration deadlines in identification of complex substances, i.e. substances posing challenges in their identification.

The objective of the study was to identify, for selected complex chemical substances, the difficulties faced by registrants to comply with the SID requirements under REACH and how they have handled these difficulties in the registration process using different elements to identify these substances.

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[6] https://echa.europa.eu/documents/10162/13643/substance_id_en.pdf

[7] Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials

[8] http://ec.europa.eu/enterprise/sectors/chemicals/documents/reach/review2012/index_en.htm

2. METHODOLOGY

The following sections summarise the tasks that were performed and the methodology that was followed in the study.

It shall be noted that the findings presented in this report are based on the information from registration dossiers reported in the ECHA database of registered substances as of August 2014. The report therefore represents what registrants considered appropriate to report in registration dossiers, the study does not in any way address compliance of the studied information with REACH (assessed by ECHA in compliance checks).

2.1. Selection of a representative set of substances for SID analysis

(a) Screening for complex substances

The representative set of substances for analysis (screening) of substance identity was selected from all substances registered or regarded as being registered under REACH as of 13 January 2014. The list of all substances registered or regarded as being registered included 13 703 entries (11 766 entries of registered substances and 1 937 substances regarded as being registered according to Article 15 of REACH – e.g. active substances used in plant protection products and biocidal products). The list includes duplicate entries in terms of substance identifiers (substance name, EC Number, CAS Registry Number (RN)). These entries originate from the database of registered substances available at the ECHA dissemination web page[9]. Although some entries had the same substance name they carry different information, for example full registration, registration as intermediate or NONS[10]), submission type (individual or joint), or composition (mono-constituent or multi-constituent or UVCB), which are taken into account as one of the criteria in selecting the Sample Set. It was therefore decided to leave these entries as extracted from the database of registered substances. Some of the duplicate entries of substances that were both registered and regarded as being registered were also not removed.

From the list of all substances that were registered or regarded as being registered, pre-selection of potential complex substances was made, using the following methodology:

1. Substances without a CAS Registry Number were selected
2. Substances with names containing a keyword indicating a complex substance were selected

[9] http://echa.europa.eu/en/information-on-chemicals/registered-substances
[10] Substances that have been notified under Directive 67/548/EEC.

Table 1 List of keywords indicating a complex substance searched for in the list of registered substances and substances regarded as being registered

Keyword				
UVCB	Product	mass	salt	name not available
Hydrocarbon	Oil	resin	rosin	Wax
Fatty	Petrol	gas	Ext	mix
Distil	condens	residu	heavy	light
Slag	Matte	dust	liquor	raffin
Fuel	Diesel	crack	coal	stabil
Derive	compd	compound	pyrolys	refin
Slime	catal	ase	satur	crude
React	between	waste	sludge	alloy
Ash	Fract	complex	tar	

Note: All keywords listed in the table were expanded with the asterisk (*) wildcard on both sides of the keyword.

3. UVCB and multi-constituent substances were selected
4. The list of the substances that were not pre-selected to the list of potential complex substances was screened and all substances with names indicating a complex substance were selected

The preliminary list of potential complex substances included 7 328 entries, including a great number of false positives as expected due to the design of the methodology. False positive entries have been removed within subsequent steps.

All entries in the list of potential complex substances, one by one, were assessed for complexity by a team of experts and the following substances were removed from the list (i.e. not regarded as complex in the sense of this study):

- Mono-constituent substances where the basic identifiers (i.e. CAS RN, EC Number and name of the substance) were considered as sufficient for clear identification of the substance
- Mono-constituent NONS where the basic identifiers (i.e. CAS RN, EC Number and name of the substance) were considered as sufficient for clear identification of the substance
- Polymer NONS
- Nanomaterials
- Selected multi-constituent substances (where the individual constituents are well-defined with given concentration ranges)

Mixtures of non-complex chemicals were regarded as non-complex (including mixtures of non-complex isomers).

As a rule of thumb, seemingly non-complex substances registered as UVCBs were regarded as being complex, assuming that the registrants have a reasoning for registering them as UVCBs.

Some substances had an "x" symbol in their molecular formula specified in the registration dossier, indicating that a substance might have variable stoichiometry and is therefore potentially complex. For these substances, it was decided that if a corresponding reference substance is defined by an exact structural formula or a single value of molecular weight is provided, the substance was regarded as being non-complex.

In assessing complexity, the team members used primarily publicly available information from REACH registration dossiers, however, other information sources were also used, including:

- ECHA website[11]
- ESIS[12]
- PubChem[13]
- Chemical Abstracts Service REGISTRY[14]
- Thomson Reuters Web of Science[15]
- General search engines, in particular Google[16]

The complete list of substances which were considered complex in the sense of this study includes 2 816 entries and is attached to this report as Annex 1.

(b) Organising the complex substances

To allow selection of a stratified representative sample set of complex substances for further SID information assessment (selecting the Sample Set), complex substances were organised (grouped) by groups and sub-groups, expecting that different SID issues might be associated with specific groups of substances. The first set of 2816 substances included 15 groups and 81 sub-groups of substances in which the complex substances were organised. Once all identified complex substances were organised by groups and sub-groups, the set of groups and sub-groups was consolidated once again, i.e. sub-groups of similar substances that are likely to share common SID issues have been merged, also taking into account number of substances in each category (there were sub-groups including only a few or even no substances, e.g. polytypes or wood-pyrolysis products). As a result, the complex substances were finally organised in the following 13 groups and 56 sub-groups:

1. Inorganic substances
   - 1.1. Substances originating from combustion processes
     - 1.1.1. Combustion process products
   - 1.2. Substances originating from metallurgical processes
     - 1.2.1. Dusts
     - 1.2.2. Leaches, sludges and residues
     - 1.2.3. Slags
     - 1.2.4. Others
   - 1.3. Substances originating from calcination and smelting processes
     - 1.3.1. Inorganic Pigments
     - 1.3.2. Mixed Metal Oxide
     - 1.3.3. Silicates
   - 1.4. Other inorganic substances
     - 1.4.1. Inorganic salts
     - 1.4.2. Zeolites
     - 1.4.3. Others

[11] http://echa.europa.eu/
[12] The ESIS database maintained formerly by the Joint Research Centre of the European Commission is no longer in operation
[13] https://pubchem.ncbi.nlm.nih.gov
[14] http://www.cas.org/products/scifinder
[15] http://www.webofscience.com
[16] http://www.google.com

2. Organic substances
    2.1. Substances with variability in alkyl chain length
        2.1.1. Acid Alkyl Derivates
        2.1.2. Acids and Salts
        2.1.3. Alcohols and Chlorides
        2.1.4. Alkyl Derivates
        2.1.5. Esters
        2.1.6. Nitrogen Derivates
        2.1.7. Others
    2.2. Petroleum-derived substances
        2.2.1. Alkyl aryl sulphonic acids, sulphonates
        2.2.2. Bitumen, modified asphalt
        2.2.3. Butylene oligomers
        2.2.4. Distillate and residual aromatic extracts (untreated/treated)
        2.2.5. Gas oils and distillate fuels
        2.2.6. Fuel oils and heavy residues
        2.2.7. Kerosines
        2.2.8. Low boiling point naphthas (gasolines)
        2.2.9. Lubricating oils, greases, base oils, petrolatums
        2.2.10. Olefins
        2.2.11. Other hydrocarbons (aliphatics, cyclic, aromatics)
        2.2.12. Paraffin and hydrocarbon waxes, slack waxes
        2.2.13. Petroleum gases
        2.2.14. Resin Oils & alkenes
        2.2.15. Foot oils
        2.2.16. Others
    2.3. Coal-derived substances
        2.3.1. Anthracene Oils
        2.3.2. Tar acids
        2.3.3. Coal Tar, Coal Tar Bases, Pitches
        2.3.4. Light Oils and naphthas
        2.3.5. Naphthalene Oils, Wash Oils
        2.3.6. Others
    2.4. Other organic substances
        2.4.1. Oligomers
        2.4.2. Pigments/Dyes
        2.4.3. Residues
        2.4.4. Resins (synthetic) and polymers
        2.4.5. Rosin Resin Derivates
        2.4.6. Others
3. Substances of biological origin
    3.1. Substances originating from fermentation process
        3.1.1. Enzymes
        3.1.2. Others
    3.2. Substances originating from plants and animals
        3.2.1. Derivates
        3.2.2. Extracts
        3.2.3. Vegetable oils
        3.2.4. Wood-derived substances
        3.2.5. Others
4. Other substances
    4.1. Substances with organic and inorganic part
    4.2. Organic-inorganic salts
    4.3. Others

The grouping scheme includes groups and sub-groups based on the nature of a substance (e.g. oleochemicals, zeolites, silicates, etc.) as well as groups and sub-groups based on the process or source of origin (e.g. petroleum-derived substances). The system of groups and sub-groups is therefore non-exclusive, i.e. a single substance can fall into several categories (typically substances with variability in alkyl chain length can often fall also into other, more specific sub-groups). In these cases, the substances were included in the category which is the most specific (e.g. the substance "Paraffin waxes and Hydrocarbon waxes C14-17, chloro, sulfochlorinated, low sulphonated, saponified" was included in the sub-group „2.2 petroleum-derived substances" > „2.2.12 paraffin and hydrocarbon waxes, slack waxes" rather than into „2.1. substances with variability in alkyl chain length" > „2.1.4 alkyl derivates").

Furthermore, some of the substances can be regarded either biological origin or organic, e.g. oleochemicals, petroleum products. With respect to the objective of the study, it was agreed that it is appropriate to group these substances within a single group or sub-group and assess the aspect of source and origin on SID rather than to separate these substances and break them into two different categories. It was therefore considered in which of these two categories to include them. Some of these substances extracted directly from biological sources are exempted from the obligation of registration under REACH and products derived from these substances are usually regarded as of chemical origin. Furthermore, the registrants themselves usually regard these substances as organic. The sub-groups "Alkyl derivates", "Oleochemicals", "Pigments and Dyes (excluding inorganic pigments) and all sub-groups of petroleum derived substances have been regarded as organic rather than as of biological origin.

The list of complex substances organised by groups and sub-groups is attached to this report as Annex 1, including 2 618 entries. 10 % are for inorganic substances, 76 % for organic substances, 11.5 % for substances of biological origin and 2.5 % do not fall into any of these major categories.

(c) Selection of a sample set

With the complex substances organised by groups and sub-groups, a representative set of substances (Sample Set) for further SID information assessment (screening) was selected, based on the following information:

- Composition
  - Mono-constituent / Multi-constituent / UVCB / UVCB 1[17] / UVCB 2[18] / UVCB 3[19] / UVCB 4[20]
- Registration type
  - Full / Intermediate
- Submission type
  - Individual / Joint
- Number of registrants
- Has a Final Decision or a Board of Appeals Decision been issued?
- Has a Compliance Check been performed by ECHA?
- Categorization (3-level)
  - Inorganic / Organic / Biological origin / By-product or recovered
    - Group
      - Sub-group
- Feedback from registrants in a call for data (see section 3.6.2 for further details)

[17] UVCB sub-type 1, where the source is biological and the process is a synthesis
[18] UVCB sub-type 2, where the source is chemical or mineral and the process is a synthesis
[19] UVCB sub-type 3, where the source is biological and the process is refinement
[20] UVCB sub-type 4, where the source is chemical or mineral and the process is a refinement

The selection of the substances for SID information assessment (screening) takes into account also the 4 UVCB sub-types (UVCB 1 / UVCB 2 / UVCB 3 / UVCB 4 are present in the list of complex substances in the ratio 121 : 1394 : 46 : 397, while being included in the representative set of substances selected for SID information assessment in the ratio 15 : 130 : 17 : 36).

The list of substances selected for substance identity assessment (screening) includes 223 substances and is attached to this report as Annex 2. Statistics regarding the number of complex substances identified within the study, number of complex substances selected for screening and number of screened dossiers is presented in the following Table 2.

Table 2 Statistics of complex substances identified within the study, substances selected for screening and number of screened.

Substance group	Number of		
	complex substances	selected substances	dossiers screened
1. Inorganic	**238**	**43**	**1338**
1.1 Substances originating from combustion processes	9	4	66
1.2 Substances originating from metallurgical processes	86	17	217
1.3 Substances originating from calcination and smelting processes	90	12	102
1.4 Other inorganic substances	53	10	106
2. Organic	**1853**	**136**	**302**
2.1 Substances with variability in alkyl chain length	741	26	228
2.2 Petroleum-derived substances	517	59	732
2.3 Coal-derived substances	47	8	96
2.4 Other organic substances	548	43	282
3. Biological origin	**264**	**31**	**82**
3.1 Substances originating from fermentation process	25	8	54
3.2 Substances originating from plants and animals	239	23	248
4. Others	**59**	**13**	**82**
4.1 Chemicals with organic and inorganic part	16	5	46
4.2 Organic-inorganic salts	30	5	31
4.3 Others	13	3	5
Sum	2414	223	2213

2.2. Substance identity information analysis and assessment

With the finalised list of substances selected for substance identity assessment (screening), the European Commission provided the project team with the substance identity data from registration dossiers of the selected substances. To allow achievement of the objectives of the study, data from the following IUCLID sections provided by registrants in accordance with Annex VI of REACH were screened:

IUCLID Section	Description of provided data	Annex VI reference
1.1. Identification	**Reference Substance Information** • EC inventory information as published in the official Journal – EC number – CAS number – EC name – Molecular formula – Description • CAS information – CAS number – CAS name • IUPAC name • Synonyms • Description • Related CAS information • Molecular and structural information – Molecular formula – Molecular weight – SMILES notation – InChI formula Structural formula	2.1.-2.2. (except 2.2.2.)
1.2. Composition	• Name of composition • Brief description of composition • Information for each constituent, impurity and additive – Reference Substance Information (see above) – Typical concentration – Concentration range – Remarks	2.3.1.-2.3.4.
1.4 Analytical information	• Information to confirm the structure and composition of the substance – Analytical protocol(s) – Description of method(s) used – Information on optical activity	2.2.2. and 2.3.5.-2.3.7.
3.1 Technological process	• Brief description of the technological process used for the manufacture of the substance	3.2.

To allow comparison of substance identity information on the level of individual substances, but across individual registration dossiers, the information from the dossiers was extracted into a standardised spreadsheet protocols. The template of the spreadsheet protocol with explanatory descriptions of individual fields is attached to this report as Annex 3.

The substance identity screening was based on 20 randomly selected registration dossiers for each of the substances (always including the dossier of the lead registrant). In cases where less than 20 registration dossiers were submitted, the screening included all submitted dossiers.

The objectives of the screening included analysis of consistency of substance identity information reported across individual dossiers, substances and substance groups, analysis of the factors determining the consistency of information provided by registrants and identification of substance identity elements provided by registrants of individual groups of substances. The aim of the screening was not to substitute in any way compliance checks performed by ECHA.

Further details on the methodology on the extraction and assessment of information in the registration dossiers are provided in the attached spreadsheet protocol template in Annex 3.

For comparison of substance identity elements used by registrants of the screened substances across individual groups and sub-groups of substances, another spreadsheet protocol referred to as the "substance group evaluation protocol" was developed. The protocol synthesises information on the substance identity elements used by registrants for substances grouped by individual groups and sub-groups, statistics of the use of individual substance identity elements and additional related information, e.g. whether the substances are covered by an operating REACH consortium or industry association or if a substance identity profile has been developed for the substances. The substance group evaluation protocol template with explanatory descriptions of individual fields is attached to this report as Annex 4.

The two attached protocol templates (substance identity information protocol – Annex 3 and substance group evaluation protocol – Annex 4) provide all relevant information on the methodology applied in substance identity information analysis and assessment.

3. RESULTS AND OBSERVATIONS

This section summarises results and observations made within the study. General results and observations are followed by results and observations specific for each of the studied groups of substances.

General observations

The following Table 3 provides statistical data regarding number of complex substances registered without CAS and EC numbers, the basic identifiers of well-defined substances.

Table 3 Statistics of complex substances registered without CAS RN and EC.

SID issue/question	Information	Number (percentage)
How many complex substances were registered without a numerical identifier (EC or CAS)?	**Registered complex substances:** **Registered without CAS RN** (1): **Registered without EC number or List number** (2)**:** **Registered without CAS RN and without EC number or List number:**	**2171** 609 (28 %) 48 (2.2 %) 47 (2.2 %)
Are the substances identified as UVCBs EINECS-listed substances?	**Total number of complex substances identified as UVCB by registrants:** **EINECS-listed complex UVCB substances:**	1 921 (3) 1 089 (57 %)
Notes: (1) For further information on substances registered without CAS RN, see Table 3a. (2) Substances registered without EC number or List number include mostly pigments and dyes and synthetic resins, as well as some hydrocarbons with variability in alkyl chain length and substances registered under their trade name. (3) For further breakdown of complex UVCB substances, see Table 3b.		

Table 3a Breakdown of substances registered without CAS RN.

		Number	%
Registered with EC 2xx-xxx-x	(EINECS List - European INventory of Existing Commercial chemical Substances)	8	(1.3 %)
Registered with EC 3xx-xxx-x	(EINECS List - European INventory of Existing Commercial chemical Substance)	1	(0.2 %)
Registered with EC 4xx-xxx-x	(ELINCS List - European LIst of Notified Chemical Substances)	97	(15.9 %)
Registered with EC 5xx-xxx-x	(No-Longer Polymers)	3	(0.5 %)
Registered with List Number 6xx-xxx-x	(Automatically assigned by ECHA to substances identified only with a CAS No.)	3	(0.5 %)
Registered with List Number 7xx-xxx-x	(Assigned manually by ECHA to validated substances from inquiries by ECHA)	66	(10.8 %)
Registered with List Number 8xx-xxx-x	(Automatically assigned by ECHA to substances identified only with a CAS No. (continuation of the 6xx-xxx-x series)	0	(0 %)
Registered with List Number 9xx-xxx-x	(Automatically assigned by ECHA to substances without a CAS No. or other numerical identifier)	384	(63.1 %)
Registered without EC number or List number		47	(7.7 %)
Total number of substances registered without CAS RN		**609**	

Table 3b Breakdown of complex UVCB substances.

		Number	%
Registered with EC 2xx-xxx-x	(EINECS List - European INventory of Existing Commercial chemical Substances)	970	(50.5 %)
Registered with EC 3xx-xxx-x	(EINECS List - European INventory of Existing Commercial chemical Substance)	119	(6.2 %)
Registered with EC 4xx-xxx-x	(ELINCS List - European LIst of Notified Chemical Substances)	76	(3.9 %)
Registered with EC 5xx-xxx-x	(No-Longer Polymers)	102	(5.3 %)
Registered with List Number 6xx-xxx-x	(Automatically assigned by ECHA to substances identified only with a CAS No.)	155	(8.1 %)
Registered with List Number 7xx-xxx-x	(Assigned manually by ECHA to validated substances from inquiries by ECHA)	85	(4.4 %)
Registered with List Number 8xx-xxx-x	(Automatically assigned by ECHA to substances identified only with a CAS No. (continuation of the 6xx-xxx-x series)	17	(0.9 %)
Registered with List Number 9xx-xxx-x	(Automatically assigned by ECHA to substances without a CAS No. or other numerical identifier)	359	(18.7 %)
Registered without EC/List number		38	(2.0 %)
Total number of complex UVCB substances		**1921**	

In addition to the data presented in the preceding tables, the following observations were made regarding the UVCB status of the registered complex substances:

- Most (80 %) complex substances as perceived in this project (substances for which the application of the substance identification provisions of REACH and the rules and conventions of the SID guidance pose objective challenges) are registered as UVCB substances.
- In some cases, substances were registered as UVCB substances, but based on the available information, registration as well-defined substances might be more appropriate.

There are some cases, where a single substance was registered as UVCB by some registrants and as well-defined by others (e.g. butane, homopolymer) or sometimes a substance was registered as UVCB (e.g. Silicic acid, calcium salt), while a very similar substance was registered as mono-constituent (e.g. Silicic acid, titanium salt).

Group-specific observations

Following sections present results and observations related to individual groups of substances. Each section, describing observations regarding a single group of substances, is organised in the same way and contains the following topics:

a) List of screened substances, including statistics of registration dossiers submitted to ECHA (number of individual submissions and joint submissions).

b) Substance identity elements – summary of SID elements used by registrants for identification of the substances within the group.

c) Composition – this section describes aggregated compositional information provided by registrants of the substances in each group. Composition is the fundamental substance identity element, providing information on identification and concentration of the (main) constituents/impurities/additives. Each registrant may decide to specify several compositions in his technical dossier. Multiple compositions are often specified by registrants of complex substances

including a high proportion of UVCBs, which are by definition often variable in their composition. Reasons for specifying multiple compositions in a single registration dossier include: one composition as agreed by the co-registrants within a SIEF and another describing registrant-specific data, another typical reason for providing multiple compositions is use of different analytical methods (e.g. elemental analysis and mineralogical analysis). Information on composition of substances in each group presented in the following sections include statistics of number of compositions specified in registration dossiers, number of constituents identified in each composition, typical constituents specified by registrants and evaluation of compositional data consistency among registration dossiers for each substance. Compositional data consistency was evaluated using the following 6-level scoring scale developed for the purposes of this study:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

d) Source – source is a mandatory substance identity element for UVCBs, which can typically not be sufficiently identified by their chemical composition. Information regarding the source as provided by the registrants in IUCLID section 3.1 were retrieved from all screened dossiers (including the dossier of the lead registrant) and are presented in aggregated manner for each substance.

e) Manufacturing process and its parameters (conditions) – manufacturing process is also a mandatory substance identity element for UVCBs. Information regarding the manufacturing process as provided by the registrants in IUCLID section 3.1 were retrieved from all screened dossiers (including the dossier of the lead registrant) and are presented in aggregated manner for each substance – each section includes a table where different manufacturing processes reported by registrants in dossiers are listed, capturing also situations where different registrants of a single substance reported different manufacturing processes.

f) Additional substance identity elements – SID elements used by registrants in addition to composition, source and manufacturing process are described and their role in identification of individual groups of substances is discussed. Additional substance identity elements used by registrants include mainly physicochemical properties, e.g. density, boiling point, flash point, pH, molecular formula descriptors such as alkyl chain length or carbon number range, description of the form of the substance including its state (e.g. solid, liquid), crystalline structure in the case of solids, form (e.g. paste, gel) as well as other group-specific substance identity elements (e.g. colour index number, Enzyme Commission number).

g) Analytical methods used – for each group of substances, the report systematically presents analytical methods used by the registrants of the screened dossiers. Presented information focuses also on the relation between the analytical methods used by the registrants and methods listed in Annex VI of REACH.

h) Consortia and industry associations – each section includes links to identified REACH consortia and industry associations which address identity of some of the substances in corresponding groups.

i) Substance identity profiles – each section includes links to identified publically available substance identity profiles regarding substances in corresponding groups.

3.1. Substance identity of complex inorganic substances

3.1.1. Substances originating from combustion processes

Substances originating from combustion processes are complex inorganic substances, typically residues or by-products. High variability in their chemical compositions is mainly determined by the source, origin, nature of the combusted materials (coal, biomass, waste, etc.) and by combustion technology and conditions of combustion. Besides ashes, this group includes also products from flue gas desulphurisation processes. This is a relatively small group containing only 9 substances.

a) Substances screened in this group

Four substances from this group were screened.

Table 4 Substances originating from combustion processes – substances selected for substance identity screening.

ID	Name (as registered)	No. of dossiers			% dossiers analysed*
		Joint	Indiv.	Total	
950	Ashes (residues), cenospheres	17	0	17	100
681	Ashes (residues), rice husk	15	0	15	100
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)	14	0	14	100
4990	The product from the burning of a combination of carbonaceous materials.	64	0	64	31

* 20 dossiers per substance were analysed as a maximum.

b) Substance identity elements

As presented in Table 5, 10 SID elements were used in studied registration dossiers for this subgroup of substances. Together with the group of 'other substances', substances originating from combustion processes is a subgroup where a low number of SID elements is typically used by registrants to characterise substances (average: 6 ± 2.2).

Table 5 Substance identity elements used by registrants in identification of substances originating from combustion processes.

Substance	950	681	4944	4990	% availability
Source	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	100
Parameters of process	✓	✓	✓		75
Composition	✓	✓	✓	✓	100
Particle size distribution	✓				25
Form of the substance	✓			✓	50
*Group-specific element**	✓			✓	50
*Common characteriser***	✓	✓			50
*Other characteriser****	✓	✓			50
No. of SID elements identified per substance	9	6	4	5	Avg. = 67
Average no. of SID elements. per group	6 ± 2.2				

* SID element specific to a certain group/sub-group of substances, in particular: specification of the gases contained within the sphere for cenospheres (950); specification of ashes – fly/bottom (4990).

** Common group-specific jargon, in particular: "ash" (950, 681).

*** Residue (950, 681).

10 SID elements were identified in this group of substances. 3 SID elements (Source, Process and Composition) were used by registrants for all substances in this group. For most substances, parameters (conditions) of the manufacturing process were also provided by the registrants. Among other SID elements used by the registrants, particle size distribution, form of the substance, crystalline structure (phase), group-specific elements (e.g. "contain carbon dioxide and nitrogen within the sphere", "fly/bottom ash"), common characterisers (e.g. "Ash") and other characterisers (e.g. "Residue") were encountered.

It can be observed that for identification of the substance 950, the number of SID elements used was significantly higher than average. The need for additional SID elements is likely linked to the nature of the substance (Ashes (residues), cenospheres) with a specific form (cenospheres), formed under certain conditions.

Composition

The registrants of the substances subject to the screening most frequently specified composition of the substances providing concentration ranges of individual constituents, together with their typical concentrations. In cases where only one of these two values was provided, concentration ranges were predominant over typical concentrations.

Some registration dossiers include several compositions, due to the following factors:

a) as a result of use of different analytical methods providing either elemental composition (expressed as elements/oxides) information or chemical speciation/mineralogy information

b) describing different samples, typically a registrant-specific sample vs. typical consortium/SIEF/SIP-defined values

Table 6 Number of compositional data specified in registration dossiers by registrants of substances originating from combustion processes.

ID	Name (as registered)	% of No. of compositions			
		1	2	3	4
950	Ashes (residues), cenospheres[1]	94	6		
681	Ashes (residues), rice husk[2]	100			
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)[3]	92			8
4990	The product from the burning of a combination of carbonaceous materials.[4]	5	75	15	5

Note: Void cells mean zero.

* Figures within the table refer to the percentage of screened registration dossiers which contain a certain number of compositions

One substance contains only 1 composition, one substance contains 2 compositions and two substances contain 4 compositions. The description of the compositions is provided in the following comments.

[1] - Composition no. 1 based on Substance Identification Profile (SIP) or on typical values.
- Composition no. 2 based on mineralogical analysis.

[2] - Single composition - 1 constituent (registered substance) and impurities (concentration range of 0-2%).

[3] - Composition no. 1 based on Substance Identification Profile (SIP) or on typical values.
- Composition no. 2 based on recalculation from silicate analysis for mixture of ash and SDA product. This composition corresponds to the substance used as the test material in the registration.
- Composition no. 3 based on results of silicate analysis for mixture of ash and SDA product.
- Composition no. 4 based on results of XRD analysis for mixture of ash and SDA product.

[4] - Composition no. 1 based on Substance Identification Profile (SIP) or on typical values.
- Composition no. 2 composition based on registrant-specific values.
- Composition no. 3 based on registrant-specific values and reflecting specifics of the product (bottom ash / fly ash).
- Composition no. 4 based on registrant-specific values reflecting different manufacturing sites.

Table 7 Number of constituents specified in registration dossiers by registrants of substances originating from combustion processes.

ID	Name (as registered)	Compositon & No. of constituents	
950	Ashes (residues), cenospheres	#1	15
		#2	15
681	Ashes (residues), rice husk		12[a]
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)	#1	9
		#2	6
		#3	13
		#4	11
4990	The product from the burning of a combination of carbonaceous materials.	#1	8
		#2	5
		#3	8
		#4	8
		#5	8
	Average number of constituents:		**10 ± 3**

[a] 11 constituents were specified as impurities

Three of the screened substances contain more than one composition, the average number of constituents specified in the screened registration dossiers is 10 ± 3.

Substance 950 - the higher number of constituents in both compositions is given by large variability of components provided by registrants based on registrant-specific values.

Substance 9044 - the high number of constituents is provided by the lead registrant based on Silicate analysis and recalculation.

Table 8 Consistency of compositional data provided in the registration dossiers for substances originating from combustion processes.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
950	Ashes (residues), cenospheres				100	6[a]	
681	Ashes (residues), rice husk						100
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)			85	15	8	
4990	The product from the burning of a combination of carbonaceous materials.	90		75	15		

Note: void cells mean zero.

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: Numbers in the cells of the table are percentages of dossiers sharing the same composition consistency score. The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

[a] Information on mineralogy and elemental composition provided

Table 9 Typical constituents specified in registration dossiers by registrants of substances originating from combustion processes.

ID	Name (as registered)	Typical constituent	
		Name	Concentration [%]
950	Ashes (residues), cenospheres	Amorphous (glassy) alumosilicate/silica	50 – 95
		Diiron trioxide	0 – 8
		Titanium oxide	0 – 2
		Naturally occurring substances	0 – 9
		Quartz	0 – 6
		Mullite	0 – 50
681	Ashes (residues), rice husk	Ashes (residues), rice husk	80 – 100
		Silicon dioxide	80 – 100
		Carbon	0 – 12
		Aluminium oxide	0 – 2
		Calcium oxide	0 – 2.5
		Magnesium oxide	0 – 2
		Dipotassium oxide	0 – 4
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)	Calcium chloride dehydrate	0 – 50
		Calcium dihydroxide	0 – 50
		Calcium sulfate dihydrate	0 – 79
		Calcium carbonate	0 – 35
		Calcium Sulphite Hemihydrate / Sulfurous acid, calcium salt, hydrate (2:2:1)	0 – 70
		Calcium fluoride	0 – 5
4990	The product from the burning of a combination of carbonaceous materials.	Silicon	3 – 45
		Calcium	2 – 42
		Aluminium	0.386 – 10
		Iron	0.25 – 18
		Magnesium	0.3 – 15
		Phosphorus	0.04 – 3
		Potassium	0.05 – 10
		Sodium	0.05 – 2.5

Screened compositional data usually include 1-2 major constituents and several other constituents. The constituents are expressed either in the form of minerals (oxides, carbonates, chlorides, sulfates, fluorides), or the composition is based on elemental analysis.

Source

Source is one of the key elements determining the chemical composition of substances originating from combustion processes, a typical group of substances where different sources clearly lead to different substances.

Table 10 Sources of substances originating from combustion processes as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
950	Ashes (residues), cenospheres	Coal
681	Ashes (residues), rice husk	Rice husk
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)	Various fuels used in the power industry
4990	The product from the burning of a combination of carbonaceous materials.	Combustible organic materials, e.g. biomass, biofuels, peat and sludge with coal, bark, sawdust, woodchips, solid recovered fuel (SRF) and supplementary fuels, etc.

Manufacturing process and its parameters (conditions)

Combustion is the central manufacturing process step for this group of substances. Besides direct combustion products, this group of substances includes also a product from the flue gas desulphurisation, where the manufacturing process includes absorption and precipitation.

The level of detail of the manufacturing process description is highly variable – in some cases it is only stated that the substance is a product of combustion, in other cases a detailed description of the manufacturing process is provided, including chemical reactions.

Together with source, parameters (conditions) of the manufacturing process are the key elements determining the chemical compositions of substances originating from combustion processes.

The only substance subject to screening without information on the parameters of the manufacturing process in any of the screened dossiers (20 out of 64) was "The product from the burning of a combination of carbonaceous materials." The other screened direct combustion process product, i.e. "Ashes (residues), rice husk" included information on the combustion temperature in some of the dossiers. Heating temperature during processing, pressure and content of moisture was specified in one of the dossiers for "Ashes (residues), cenospheres". Flue gas desulphurisation temperature and humidity have been specified in most dossiers for "Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)".

Besides the heating temperature, registrants often described the technology itself (reactor type, separation steps, etc.).

Additional substance identity elements

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Table 11 Additional substance identity elements specified by registrants of substances originating from combustion processes.

Substance identity element	Value	Substance identified with the SID element
Form of the substance	Cenospheres	Ashes (residues), cenospheres (950)
	Powder	The product from the burning of a combination of carbonaceous materials (4990)
Particle size distribution	Included in analytical methods	Ashes (residues), cenospheres (950)

c) Analytical methods

The following Table 12 and Table 13 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 12 REACH Annex VI analytical methods used by registrants of substances originating from combustion processes.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
950	Ashes (residues), cenospheres		Y				
681	Ashes (residues), rice husk				Y		
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)		Y				
4990	The product from the burning of a combination of carbonaceous materials.						Y

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 13 Additional analytical methods used by registrants of substances originating from combustion processes in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements		
		XRD	XRF	Other
950	Ashes (residues), cenospheres	Y	Y	Particle size distribution, loss on drying, loss on calcination
681	Ashes (residues), rice husk	Y	Y	FAAS, GFAAS, ICP-MS, Scanning Electron Microscopy
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)	Y	-	ICP-OES, loss on ignition, IC, total organic carbon, titration of free calcium, dissolved organic carbon, polycyclic aromatic hydrocarbons, phenol index, polychlorinated biphenyls, acid neutralisation capacity
4990	The product from the burning of a combination of carbonaceous materials.	Y	-	Scanning Electron Microscopy, chemical composition analysis, determination of trace elements

It can be observed that analytical methods explicitly mentioned in Annex VI of REACH are of limited relevance for this group of substances with predominantly inorganic constituents. In accordance with common analytical practices, X-ray diffraction has been used to provide information on chemical composition of all screened substances, supported with X-ray fluorescence in the case of "Ashes (residues), cenospheres" and "Ashes (residues), rice husk".

The set of analytical methods and techniques used for determination of chemical composition of individual substances subject to the screening reflects the inorganic nature of the substances.

d) Consortia/associations

Some of the substances screened within this group are covered by operating consortia united under the European Coal Combustion Products Association e.V. (http://www.ecoba.com/reach_ccps.html).

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 14 for direct links (where available).

Table 14 Publicly available substance identity profiles of substances originating from combustion processes.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
950	Ashes (residues), cenospheres	https://www.vgb.org/vgbmultimedia/Fachgremien/Umweltschutz/Cenospheres+ID+card+r01.pdf	Typical composition, Description of the source, process, analytical methods
4944	Product of Semi-Dry Absorption method of Flue Gas Desulphurization (SDA Product)	https://www.vgb.org/vgbmultimedia/SIP_SDA_10_2010-p-4352.pdf	RfS, Typical composition, Description of the source, process and its conditions
4990	The product from the burning of a combination of carbonaceous materials	http://www.cinerit.at/uploads/cinerit/Downloads/REACH_Registration_and_Utilization_of_Ash.pdf http://www.varmeforsk.se/files/program/askor/2_puunta_.pdf	Description and idtentification of the substance, typical composition description of the manufacturing process

3.1.2. Substances originating from metallurgical processes

Substances originating from metallurgical processes registered in accordance with REACH are complex inorganic substances, often residues or by-products. Substances in this group include dusts from metal refining, leaches, slimes, sludges and residues from various metallurgical processes as well as slags and dross metals. Chemical composition of these substances is typically variable as well as unknown to the full extent, mainly determined by the source and origin of raw materials.

a) Substances screened in this group

17 substances were selected in this group and are presented in Table 15

Table 15 Substances originating from metallurgical processes – substances selected for substance identity analysis

ID	EC / List No.	Name (as registered)	No. of dossiers			% Dossiers analysed
			Joint	Indiv.	Total	
658	273-760-6	Flue dust, zinc-refining	26	0	26	100
856	293-314-4	Leach residues, zinc ore, lead-contg.	12	0	12	100
1047	310-050-8	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.	3	0	3	100
663	273-824-3	Residues, zinc smelting	17	0	17	100
656	273-742-8	Slimes and Sludges, zinc sulfate electrolytic	7	0	7	100
648	273-723-4	Wastewater, zinc sulfate electrolytic, acid	6	0	6	100
646	273-701-4	Lead alloy, base, Pb,Sn, dross	9	0	9	100
9768	273-791-5	Lead, dross, antimony-rich	11	0	11	100
10048	266-007-8	Mill scale (ferrous metal)	71	0	71	28
327	266-002-0	Slags, ferrous metal, blast furnace	45	0	45	44
5031	932-275-6	Slags, steelmaking, elec. furnace (carbon steel production)	71	0	71	28
4769	918-168-7	Anode, copper	22	0	22	91
9644	265-997-9	Iron sinter	29	0	29	69
360	266-967-8	Matte, copper	8	0	8	100
706	282-356-9	Matte, lead	15	0	15	100
5016	932-075-9	Se-Te-Concentrate	2	0	2	100
1011	308-526-5	Waste solids, precious metal refining	7	0	7	100

* 20 dossiers per substance were analysed as a maximum.

All screened substances contain only dossiers submitted in joint submissions. One of the screened substances was registered by 71 registrants, another substance by 45 registrants followed by 3 substances with 20 – 30 registrants, 4 substances with 10 – 20 registrants and the remaining 7 substances with 2 – 10 registrants.

For the purposes of this project, substances originating from metallurgical processes have been further divided into the following sub-groups:

1. Dusts
2. Leaches, sludges and residues
3. Slags
4. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 16 Substance identity elements used by registrants in identification of substances originating from metallurgical processes.

	Dusts	Leaches, sludges and residues					Slags					Others						
	658	856	1047	663	656	648	646	9768	10048	327	5031	4769	9644	360	706	5016	1011	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process	✓			✓			✓			✓	✓		✓	✓				41
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
State		✓					✓		✓		✓				✓		✓	35
Density							✓											6
Solubility		✓	✓		✓													18
Particle size distribution													✓				✓	12
Form of the substance				✓		✓	✓	✓	✓	✓	✓							41
Crystalline structure (phase)							✓	✓			✓							18
Colour							✓			✓	✓							18
*Group-specific element**							✓		✓									12
*Common characteriser***	✓		✓		✓		✓	✓	✓	✓	✓	✓	✓	✓	✓			71
*Other characteriser****	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓					71
No. of SID elements identified per substance	6	6	6	6	6	5	12	7	8	8	10	4	7	5	5	3	5	Avg. = 46
Average no. of applied SID elmts. per sub-group	6	5.8 ± 0.4					9 ± 2					4.8 ± 1.3						
Average no. of applied SID elmts. per group		6.4 ± 2.2																

* SID element specific to a certain group/sub-group of substances, in particular: substance consisting of variable amounts of metals in either alloy form or as compounds such as oxides and silicates (646), corrosion product (10048).

** Common group-specific jargon, in particular: Dust (658), Matte (706, 1047, 360), Dross (646, 9768), Slimes and sludges (656), Ferrous slag (327, 5031), Anode (4769), Iron sinter (9644).

*** Residue (856, 1047, 663), By-product (658, 656), Secondary by-product (10048), Non-intentional by-product (327, 5031), Concentrate (9644), Wastewater, spent electrolyte, electrolytic solution (648)

Comments to Table 16:

- 14 SID elements were used by registrants of the screened substances for identification of substances in this group;

- 13 out of the 17 substances in this group were identified with 5 – 8 SID elements, 1 substance with 12 SID elements, 1 substance with 10 SID elements, 1 substance with 4 SID elements and 1 substance with 3 SID elements. The average number of SID elements used by registrants in this group is 6.4±2.2. The sub-group of Slags has the average number of SID elements used per substance significantly higher (9±2), while the average for the sub-group of Others is 4.8 ±1.3 SID elements per substance. SID elements increasing the number of used SID elements in the case of Slags are state (solid), form of the substance (e.g. particulates, solid dross, granulated), crystalline structure (e.g. spinel, larnite and several others) or its absence (amorphous) and colour (grey or grey to brown).

- Besides composition, source and manufacturing process, the most frequently used SID elements are "common characteriser" (Common group-specific jargon, e.g. matte for the sub-group "Leaches, sludges and residues" or dross or ferrous slag for the sub-group "Slags") and "other characteriser" (e.g. residue, by-product, secondary by-product, non-intentional by-product, electrolyte, and several others) used for identification of over 70 % of substances in this group, followed by parameters (conditions) of the manufacturing process (41 %), form of the substance (41 %) and state (35 %). Other SID elements were used for characterisation of less than 20 % of substances in this group.

Composition

The registrants of the substances subject to the screening most frequently specified composition of the substances providing conc**entration ranges of individual constituents together with their typical co**ncentrations in a vast majority of cases. In cases where only one of these two values was provided, frequency of use of concentration ranges and of typical concentrations was similar.

The data from the screened registration dossiers document the following specifics of substances originating from metallurgical processes:

- elemental composition is usually known and presenting very high variability in concentrations – chemical elements reported in dossiers in concentration ranges spanning over 50 % are no exceptions as presented in Table 20, due to the fact that information from elemental analysis aggregates concentrations of different compounds of individual elements (aggregating concentrations of the element no matter if the element is bound in the form of an oxide, sulphide, carbonate, etc.). Combined with the complexity and variability of sources of these substances which include various metallic residues and by-products from numerous metallurgical streams, concentration ranges of determined metals are very wide (spanning often more than 50 %).
- chemical speciation is often not determined by registrants, but it is generally much less variable thanks to sequential refinement processes where every output is the input for another process

The screening of the registration dossiers confirmed that elemental composition is provided by registrants in vast majority of cases, whereas information on chemical speciation is rarely included. According to the methodology for identification of inorganic UVCB substances (being further developed based on feedback from ECHA) developed by the European Association of Metals (Eurometaux), the elemental composition is considered as the primary key for defining composition because 1) elemental analysis is more available (widespread and samples in time) compared to speciation analysis, 2) elemental analysis is more accurate (from analytical perspective) and 3) elemental analysis allows to detect minor elements (not detectable in speciation analysis).

Some registration dossiers include several compositions, due to the following factors:

a) describing different samples (compositional data representing substances from different sources and processes/process streams)

b) composition with particular focus on constituents relevant for classification and labelling is often provided in addition to the primary (SIEF-defined) composition

These observations on composition apply to all sub-groups of substances originating from metallurgical processes.

Table 17 Number of compositions specified in registration dossiers by registrants of substances originating from metallurgical processes.

ID	Name (as registered)	% of No. of compositions				
		1	2	3	4	5
658	Flue dust, zinc-refining	15	85			
856	Leach residues, zinc ore, lead-contg.	25	58		17	
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.		33			67
663	Residues, zinc smelting	14	79		7	
656	Slimes and Sludges, zinc sulfate electrolytic	100				
648	Wastewater, zinc sulfate electrolytic, acid		83	17		
646	Lead alloy, base, Pb,Sn, dross	60	40			
9768	Lead, dross, antimony-rich	50	25	25		
10048	Mill scale (ferrous metal)	100				
327	Slags, ferrous metal, blast furnace	100				
5031	Slags, steelmaking, elec. furnace (carbon steel production)	100				
4769	Anode, copper	6		63	31	
9644	Iron sinter	100				
360	Matte, copper		13	63	13	13
706	Matte, lead	60	13	7	20	
5016	Se-Te-Concentrate	100				
1011	Waste solids, precious metal refining					100

Note: Figures within the table refer to the percentage of registration dossiers analysed that contain a certain number of compositions in each registration dossier (without referring to consistency and overlap between reported compositions).

6 out of the 17 screened substances included dossiers where all registrants reported only a single composition of their substance. In comparison with other groups of substances, this is a very low ratio, reflecting high compositional variability and variability of sources of substances in this group, complexity of their manufacturing processes as well as documenting different approaches applied by the registrants in identification of these substances as further discussed in this section. Some of the screened registration dossiers reported as much as 5 different compositions.

Table 18 Number of constituents specified in registration dossiers by registrants of substances originating from metallurgical processes.

ID	Name (as registered)	Compositon & No. of constituents	
658	Flue dust, zinc-refining	#1	19
		#2	20
856	Leach residues, zinc ore, lead-contg.	#1	17
		#2	18
		#3	21
		#4	20
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.	#1	33
		#2	34
		#3	6
		#4	6
		#5	6
663	Residues, zinc smelting	#1	11
		#2	12
		#3	5
		#4	5
656	Slimes and Sludges, zinc sulfate electrolytic		12
648	Wastewater, zinc sulfate electrolytic, acid	#1	6
		#2	8
		#3	6
646	Lead alloy, base, Pb,Sn, dross	#1	16
		#2	16
9768	Lead, dross, antimony-rich	#1	19
		#2	19
		#3	19
10048	Mill scale (ferrous metal)		6
327	Slags, ferrous metal, blast furnace		6
5031	Slags, steelmaking, elec. furnace (carbon steel production)		1
4769	Anode, copper	#1	7
		#2	7
		#3	19
		#4	13
9644	Iron sinter		1
360	Matte, copper	#1	11
		#2	11
		#3	11
		#4	11
		#5	7
706	Matte, lead	#1	26
		#2	25
		#3	24
		#4	25
5016	Se-Te-Concentrate		9
1011	Waste solids, precious metal refining	#1	44
		#2	30
		#3	8
		#4	10
		#5	8
	Average number of constituents:		**14 ± 9**

As already discussed above, some of the screened substances included dossiers reporting multiple compositions (as much as 5 different compositions in a single dossier). Among these, there were cases where the number of constituents reported for each composition varied greatly (e.g. substance "Waste solids, precious metal refining" with the lowest number of 8 constituents in one of the compositions and 44 constituents in another), as well as cases where most compositions reported the same number of constituents (e.g. substance "Matte, lead" with 4 out of 5 compositions specifying 11 constituents). Most frequently, the number of constituents reported in the registration dossiers was between 10 and 20 (applies to 20 of 47 compositions).

Table 19 Consistency of compositional data provided in the registration dossiers for substances originating from metallurgical processes.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
658	Flue dust, zinc-refining			100	85		
856	Leach residues, zinc ore, lead-contg.	83					100
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.	100			67		
663	Residues, zinc smelting	53			40		
656	Slimes and Sludges, zinc sulfate electrolytic	71			29		
648	Wastewater, zinc sulfate electrolytic, acid	83			17		
646	Lead alloy, base, Pb,Sn, dross	14	43		43		
9768	Lead, dross, antimony-rich	38	22		40		
10048	Mill scale (ferrous metal)					5	95
327	Slags, ferrous metal, blast furnace			10			90
5031	Slags, steelmaking, elec. furnace (carbon steel production)						100
4769	Anode, copper				100		
9644	Iron sinter						100
360	Matte, copper				60	40	
706	Matte, lead				100		
5016	Se-Te-Concentrate	100					
1011	Waste solids, precious metal refining	80			20		

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

Table 20 Typical constituents specified in registration dossiers by registrants of substances originating from metallurgical processes.

ID	Name (as registered)	Typical constituents		
		Name	EC/List No.	Concentration [%]
658	Flue dust, zinc-refining	Zinc	231-175-3	20 – 75
		Iron	231-096-4	0 – 22
		Lead	231-100-4	0.2 – 23
		Titanium	231-142-3	0 – 15
		Chlorine	231-959-5	0 – 10
856	Leach residues, zinc ore, lead-contg.	Zinc	231-175-3	1 – 55
		Iron	231-096-4	0 – 40
		Lead	231-100-4	0 – 94
		Sulfur	231-722-6	0 – 75
		Tin	231-141-8	0 – 35
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.	Silver	231-131-3	0 – 20
		Platinum (2+)	231-116-1	0 – 40
		Palladium (2+)	231-115-6	0.02 – 20
		Iron	231-096-4	0 – 22
		Copper	231-159-6	0 – 55
		Lead	231-100-4	0 – 10
		Nickel	231-111-4	0 – 20
663	Residues, zinc smelting	Zinc	231-175-3	40 – 89
		Aluminium	231-072-3	0 – 20
		Iron	231-096-4	0 – 10
		Lead	231-100-4	0 – 12
		Copper	231-159-6	0 – 12
656	Slimes and Sludges, zinc sulfate electrolytic	Manganese	233-828-8	25 – 60
		Lead	231-100-4	0.1 – 20
		Zinc	231-175-3	0.1 – 1
648	Wastewater, zinc sulfate electrolytic, acid	Zinc	231-175-3	1.4 – 55.2
		Sulfur	231-722-6	5.5 – 36.8
		Sulfuric acid	231-639-5	5 – 15
		Oxygen	231-956-9	40 – 50
646	Lead alloy, base, Pb,Sn, dross	Lead	231-100-4	0.5 – 90
		Copper	231-159-6	0 – 62
		Sulfur	231-722-6	0 – 20
		Zinc	231-175-3	0 – 10
		Tin	231-141-8	3 – 95
		Iron	231-096-4	0 – 10
		Antimony	231-146-5	0 – 30
9768	Lead, dross, antimony-rich	Lead	231-100-4	10 – 92
		Antimony	231-146-5	0 – 50
		Silver	231-131-3	0 – 20
		Tin	231-141-8	0 – 20
10048	Mill scale (ferrous metal)	Mill scale (ferrous metal)	266-007-8	40 – 100
327	Slags, ferrous metal, blast furnace	Slags, ferrous metal, blast furnace	266-002-0	100
5031	Slags, steelmaking, elec. furnace (carbon steel production)	Slags, steelmaking, elec. furnace (carbon steel production)	932-275-6	100

ID	Name (as registered)	Typical constituents		
		Name	EC/List No.	Concentration [%]
4769	Anode, copper	Copper	231-159-6	80 – 99.9
		Lead	231-100-4	0.001 – 5
		Nickel	231-111-4	0 – 10
		Arsenic	231-148-6	0 – 5
9644	Iron sinter	Iron sinter	265-997-9	100
360	Matte, copper	Copper	231-159-6	45 – 80
		Lead	231-100-4	0.01 – 7.5
		Arsenic	231-148-6	0.01– 1.8
		Iron	231-096-4	0 – 21.2
		Sulfur	231-722-6	1 – 30
		Zinc	231-175-3	0 – 5
706	Matte, lead	Lead	231-100-4	0 – 82
		Copper	231-159-6	0 – 62
		Sulfur	231-722-6	0 – 30
		Iron	231-096-4	0 – 80
		Nickel	231-111-4	0 – 14
5016	Se-Te-Concentrate	Dicopper telluride	Not available	0.3 – 63
		Dicopper selenide	Not available	0.3 – 70
		Copper	231-159-6	0 – 40
		Copper dihydroxide	243-815-9	0 – 47
		Copper oxide	Not available	0 – 38
1011	Waste solids, precious metal refining	Silver	231-131-3	0 – 70
		Aluminum	231-072-3	0 – 41
		Gold(1+)	231-165-9	0 – 50
		Carbon	231-153-3	0 – 50
		Iridium(3+)	231-095-9	0 – 45
		Platinum(2+)	231-116-1	0 – 50
		Palladium(2+)	231-115-6	0 – 50

Note: Concentration ranges presented in the table are derived from the screened registration dossiers, where the lowest reported concentration and the highest reported concentration was extracted to the table. It shall be noted that the constituents presented in the table are those most frequently reported by the registrants of the screened substances, the list of constituents reported by the registrants is not exhaustive.

As already discussed in previous sections, the registrants typically report compositional data as a result of elemental analysis, with some of them providing also information on chemical speciation reflecting particular chemical compounds (e.g. in the case of the substance "Se-Te-Concentrate" included in the table above, there were numerous similar cases observed within the screening of dossiers).

For various reasons discussed above as well as further below, reported concentration ranges of individual constituents are often very wide. In the previous table, there are 28 % of substances where the reported concentration ranges span over an interval of 50 % or more, 20 % of substances reported in concentration ranges spanning 30 – 50 %, 35 % of substances in concentration ranges spanning 10 – 30 % and only the remaining 17 % of substances have the reported concentration range narrower than 10 %.

Source

Similarly to substances originating from combustion processes, source is one of the key elements determining the chemical composition of substances originating from metallurgical processes.

Registered complex substances originating from metallurgical processes are often residues or by-products of numerous streams in a sequential processing of metal-containing (metal-rich) sources, where outputs from a certain process are inputs for another process. Composition of these complex substances is variable thanks to the intrinsic variability of primary (e.g. ores, ore concentrates) and subsequently also secondary sources (outputs of individual processing streams, recovered materials).

Although different sources predominantly resulted in different registrations in most cases, it has also been observed in this group of substances that even substances originating from different sources (both primary and secondary) have been registered within a single joint submission – see the substance no. 4769 (Anode, copper) in the following Table 21. Furthermore, substances originating from secondary sources (e.g. from individual processing streams) have also been typically registered jointly together with substances originating from primary sources – see e.g. the substances no. 1047 (Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.), 646 (Lead alloy, base, Pb,Sn, dross), 360 (Matte, copper) or 706 (Matte, lead) in the following Table 21.

Table 21 Sources of substances originating from metallurgical processes as reported by registrants in registration dossiers.

ID	Name (as registered)	Source(s)
658	Flue dust, zinc-refining	• Zinc-bearing materials and • Reducing agents
856	Leach residues, zinc ore, lead-contg.	• Solutions from leaching tanks or • Gas-cleaning washing towers
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.	• Primary and secondary streams resulting from the refining of copper, nickel and other base metals-containing ores and concentrates.

663	Residues, zinc smelting	• Zinc metal-bearing materials, e.g.
		  ○ Zinc/zinc oxide-rich
		  ○ Zinc or zinc alloys

656	Slimes and Sludges, zinc sulfate electrolytic	• Zinc electrolysis
648	Wastewater, zinc sulfate electrolytic, acid	• Zinc sulfate solution from electrolysis
646	Lead alloy, base, Pb,Sn, dross	• Either primary (smelting/refining of lead containing ore concentrates) or • secondary production of lead alloys (recycled lead containing materials)
9768	Lead, dross, antimony-rich	• Both primary and secondary lead bullion during the refining of crude metal
10048	Mill scale (ferrous metal)	• Steel surface during hot processing of steel products in presence of oxygen containing gases (corrosion product - ferrous oxide layer) • Scale rise like secondary product during hot processing on the surface material.
327	Slags, ferrous metal, blast furnace	• Iron bearing materials (e.g. iron ore, iron sinter), fusion with limestone (and/or dolomite) and other fluxes.
5031	Slags, steelmaking, elec. furnace (carbon steel production)	• Steel scrap with fluxes
4769	Anode, copper	• Blister and copper scrap • Copper matte or Black cooper • Raw copper from the converter furnace • Raw copper from the converter furnace - copper scraps like sheets, pipes, wire as well as certain amounts of blister copper and anode scrap
9644	Iron sinter	• Variable mixture of finely divided coke, iron ore, blast furnace dust, steelmaking dust, mill scale, other miscellaneous iron-bearing materials, limestone, and dolomite • Burnt lime and coke
360	Matte, copper	• Primary material mix (copper ore concentrates, fluxes, internal recycles of slags, flue dusts) or • secondary copper material • Briquettes, coke, converter slag and recycling materials
706	Matte, lead	• Primary and secondary lead containing materials high in sulphur • Wastes resulting from the refining of lead
5016	Se-Te-Concentrate	• Tellurium containing materials (from precious metals refining or leaching of anode slimes)
1011	Waste solids, precious metal refining	• Waste solids, precious metal refining • Materials for reclaim, precious metals with or without supports (metallic, oxide, chloride and other forms in varying concentrations)

The table summarising sources of substances originating from metallurgical processes as reported in registration dossiers documents discussed diversity and complexity of sources of substances registered in this group. Sources reported in the screened registration dossiers include primary sources (e.g. metals-containing ores and concentrates), as well as secondary sources recovered from various streams for further processing (e.g. solutions from electrolysis, solutions from leaching tanks, raw materials from converter furnaces, etc.). Sources reported by registrants in dossiers indicate that many sources of substances in this group are closely linked to manufacturing processes, as documented by several cases where the registrants reported the manufacturing process together with the source (e.g. the substance "Wastewater, zinc sulfate electrolytic, acid" with the source "Zinc sulfate solution from electrolysis").

Manufacturing process and its parameters (conditions)

There is a wide variety of manufacturing processes specified by registrants of substances originating from metallurgical processes. The combination of processing steps together with a high number of input and output streams in the metals industry creates considerable variability, as documented in the following table. A specific of this group of substances is that the processes are often iterative.

Table 22 Manufacturing processes of substances originating from metallurgical processes as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
658	Flue dust, zinc-refining	• Heating
856	Leach residues, zinc ore, lead-contg.	• Dissolution of zinc ores or concentrate in sulfuric acid and • physical separation (flotation and filtration)
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.	• Sulfuric acid-based leaching and/or • pyro-metallurgical processes
663	Residues, zinc smelting	• Melting, alloying, cleaning • Zinc melting • Refining, smelting, and alloying, and mechanical (physical) treatment of zinc-bearing materials
656	Slimes and Sludges, zinc sulfate electrolytic	• Electrolysis, anode clining
648	Wastewater, zinc sulfate electrolytic, acid	• Leaching, Refining, Electrolysis
646	Lead alloy, base, Pb,Sn, dross	• Pyrometallurgical operations: heating process (metal smelting) - treatment with chemical agents - collection of drosses
9768	Lead, dross, antimony-rich	• The oxidation process with air and/or oxygen during the pyrometallurgical refining of both primary and secondary lead bullion. The oxidation process is used to remove antimony, and possibly tin and arsenic.
10048	Mill scale (ferrous metal)	• Process steps where hot metal surfaces are growing scales: ○ Steelmaking: continuous casting, flame scarfing, ○ Hot rolling: reheating furnaces, rolling mill ○ Hot press & hot forming (minor processes for very large products)."
327	Slags, ferrous metal, blast furnace	• The manufacture of iron by thermochemical reduction of iron oxides in a blast furnace. Continuous process by the fusion of limestone (and/or dolomite) and other fluxes with the residues from the carbon source and the non-metallic components of the iron bearing materials (e.g. iron ore, iron sinter).
5031	Slags, steelmaking, elec. furnace (carbon steel production)	• Melting steel scrap in an electric arc furnace
4769	Anode, copper	• Continuous melting and refining • Converting process • Refining • Roasting
9644	Iron sinter	• Heating - thermal agglomeration
360	Matte, copper	• Roasting and smelting • Smelting • Pyrometallurgical copper production

ID	Name (as registered)	Manufacturing process
706	Matte, lead	• Smelting • Processing of wastes
5016	Se-Te-Concentrate	• Hydrometallurgical operations (e.g. leaching, precipitation) • Leaching with sodium hydroxide or water • Precipitation/ cementation from remaining solution
1011	Waste solids, precious metal refining	• Refining- not specified

It was not observed in the screened registration dossiers that different manufacturing processes applied to a single source would lead to a single substance, most likely due to the large number of combinations of manufacturing processes and processed sources (materials).

Based on information extracted from REACH registration dossiers, Description of the manufacturing process and of the combination of used processing steps therefore played the key role in identification of substances of metallurgical origin (together with source).

Registrants of the substances screened within the study also often reported parameters (conditions) of the manufacturing process (most frequently temperature) and in some cases also describe the used technology (e.g. blast furnace, electric arc furnace, hot rolling mill). However, in reporting the parameters (conditions) of the manufacturing process, the registrants often report parameters referring to the process of manufacture of the target chemical or product. Therefore, these parameters do not necessarily relate directly to the conditions of manufacture of the registered substance which may be extracted at a different stage of the manufacturing process. This applies especially to by-products and residues.

Additional substance identity elements

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Substance identity element	Value	Substance(s) identified with the SID element
State	Solid	• Leach residues, zinc ore, lead-contg. (856) • Lead alloy, base, Pb,Sn, dross (646) • Mill scale (ferrous metal) (10048) • Slags, steelmaking, elec. furnace (carbon steel production) (5031) • Matte, lead (706) • Waste solids, precious metal refining (1011)
Density	2.08 g/cm3	• Lead alloy, base, Pb,Sn, dross (646)
Solubility	Insoluble	• Leach residues, zinc ore, lead-contg. (856), Slimes and Sludges, zinc sulfate electrolytic (656)
	Dry or wet insoluble	• Residues, copper-iron-lead-nickel matte, sulfuric acid-insol. (1047)
Particle size distribution	Provided in analytical protocols in dossiers	• Iron sinter (9644), Waste solids, precious metal refining (1011)
Form of the substance	Zinc ashes and drosses	• Residues, zinc smelting (663)
	Solution	• Wastewater, zinc sulfate electrolytic, acid (648)
	Solid in a compact form or in the form of particulates.	• Lead alloy, base, Pb,Sn, dross (646)
	liquid (slag) or a solid dross	• Lead, dross, antimony-rich (9768)
	solid substance in granular shape	• Mill scale (ferrous metal) (10048)
	"Granulated (GBS) - solid of a grain size - vitreous, homogeneous structure; Air cooled (ABS) - solid of a grain size, may form blocks - crystalline structure"	• Slags, ferrous metal, blast furnace (327)
	solid of a grain size, may form blocks	• Slags, steelmaking, elec. furnace (carbon steel production) (5031)
Crystalline structure	Amorphous	• Lead alloy, base, Pb,Sn, dross (646), Lead, dross, antimony-rich (9768)
	Most frequently found mineral components are larnite, srebrodolskite, hatrurite, spinel, wuestite, free lime - calcium oxide	• Slags, steelmaking, elec. furnace (carbon steel production) (5031)
Colour	grey to brown	• Lead alloy, base, Pb,Sn, dross (646)
	Grey	• Slags, ferrous metal, blast furnace (327), Slags, steelmaking, elec. furnace (carbon steel production) (5031)

Especially conditions of the manufacturing process (typically temperature), state and form of the substance were often provided by the registrants of the screened substances.

The sub-group of slags shows the highest average number of used substance identity elements (10 ± 2), with crystalline structure (or information about absence of a crystalline structure in the case of amorphous solids) being sometimes provided in addition to the aforementioned substance identity elements.

c) Analytical methods

The following Table 23 and Table 24 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 23 REACH Annex VI analytical methods used by registrants of substances originating from metallurgical processes.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
658	Flue dust, zinc-refining						
856	Leach residues, zinc ore, lead-contg.						
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.						
663	Residues, zinc smelting						
656	Slimes and Sludges, zinc sulfate electrolytic						
648	Wastewater, zinc sulfate electrolytic, acid						
646	Lead alloy, base, Pb,Sn, dross		Y				
9768	Lead, dross, antimony-rich						
10048	Mill scale (ferrous metal)		Y				Y
327	Slags, ferrous metal, blast furnace						
5031	Slags, steelmaking, elec. furnace (carbon steel production)						
4769	Anode, copper						
9644	Iron sinter		Y				
360	Matte, copper						
706	Matte, lead	Y					
5016	Se-Te-Concentrate						
1011	Waste solids, precious metal refining						
Percentage of use of analytical methods (%)		6	18	0	0	0	6

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 24 Other analytical methods used by registrants of substances originating from metallurgical processes in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements				
		XRD	XRF	ICP-OES	AAS	Other
658	Flue dust, zinc-refining	Y		Y	Y	Electron probe micro-analysis
856	Leach residues, zinc ore, lead-contg.	Y	Y	Y	Y	
1047	Residues, copper-iron-lead-nickel matte, sulfuric acid-insol.		Y	Y		Fire Assay, Drying to constant weight, Combustion infrared detection analysis
663	Residues, zinc smelting	Y	Y	Y	Y	Wet technique (titration), Ion chromatography, Wet chemical-precipitation method
656	Slimes and Sludges, zinc sulfate electrolytic	Y	Y	Y		
648	Wastewater, zinc sulfate electrolytic, acid			Y		
646	Lead alloy, base, Pb,Sn, dross	Y	Y	Y		Scanning electron microscopy, Energy dispersive spectroscopy, Wavelength dispersive spectroscopy, HSC-Geo mass balance calculations, spark OES, Iodometric titration
9768	Lead, dross, antimony-rich	Y	Y	Y	Y	Scanning electron microscopy, Energy dispersive spectroscopy, Wavelength dispersive spectroscopy, Granulometry
10048	Mill scale (ferrous metal)	Y	Y	Y	Y	ICP-MS, ICP-AES, Energy dispersive spectroscopy, Gravimetry, LECO Combustion analysis
327	Slags, ferrous metal, blast furnace	Y	Y	Y		LECO Combustion analysis
5031	Slags, steelmaking, elec. furnace (carbon steel production)	Y	Y	Y		LECO Combustion analysis
4769	Anode, copper	Y	Y	Y	Y	Electrogravimetry, Chemical assays (ICP-OES, sequential dissolution, S & C analysis, Satmangan), Mineralogical quantification (XRD, optical micro, SEM -EDS & WDS, mineral quantification HSC-Geo mass-balance)
9644	Iron sinter	Y	Y	Y	Y	Titration, Particle size distribution (sieve test), Gravimetry, Determination of moisture, Photometry
360	Matte, copper	Y		Y	Y	Granulometry
706	Matte, lead		Y	Y	Y	Titration, Electrogravimetry, Gravimetry, Spectrophotometry
5016	Se-Te-Concentrate		Y			
1011	Waste solids, precious metal refining	Y	Y	Y		Loss on drying to constant weight, Particle Size Distribution (PSD), Specific Surface Area (N-BET)

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

It can be observed that analytical methods explicitly mentioned in Annex VI of REACH are of limited relevance for this group of substances with predominantly inorganic constituents. In accordance with common analytical practices, X-ray diffraction and X-ray fluorescence together with inductively coupled plasma optical emission spectrometry and often also atomic absorption spectrometry are the main analytical methods used by registrants for determination of chemical composition of substances of metallurgical origin.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressed by the following operating consortia and associations:

- Eurometaux – European Association of Metals - http://www.eurometaux.org/
- Zinc REACH Consortium – http://www.reach-zinc.eu/
- Lead REACH Consortium - http://www.reach-lead.eu/
- EUROSLAG - http://www.euroslag.com/
- The Iron Platform - http://www.iron-consortium.org/
- REACH Copper Consortium - http://copperalliance.eu/industry/regulatory-framework/reach
- REACH Sellenium & Tellurium Consortium - http://www.se-te-consortium.com/

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 25 for direct links (where available).

Table 25 Publicly available substance identity profiles of substances originating from metallurgical processes.

ID	Name (as registered)	Link to SIP(s)
658	Flue dust, zinc-refining	http://www.reach-zinc.eu/doc/menu_163/UP_2013-01-11_07-27-29_flue_dust_zinc_refining.pdf
856	Leach residues, zinc ore, lead-contg.	http://www.reach-zinc.eu/doc/menu_165/UP_2010-10-05_08-09-39_COMP_Leach_res_Zn_ore_Pb_cont.pdf
663	Residues, zinc smelting	http://www.reach-zinc.eu/doc/menu_173/UP_2013-03-06_06-04-53_Residues_zinc_smelting.pdf
656	Slimes and Sludges, zinc sulfate electrolytic	http://www.reach-zinc.eu/doc/menu_171/UP_2013-04-25_11-09-24_Slimes__sludges.pdf
648	Wastewater, zinc sulfate electrolytic, acid	http://www.reach-zinc.eu/doc/menu_169/UP_2013-01-11_08-21-54_Wastewater_Zn_sulphate.pdf
646	Lead alloy, base, Pb,Sn, dross	http://www.reach-lead.eu/substanceinfo/batch/Lead%20alloy%20base%20Sn%20Pb%20dross.zip
9768	Lead, dross, antimony-rich	http://www.reach-lead.eu/substanceinfo/batch/Lead%20dross%20antimony%20rich.zip
10048	Mill scale (ferrous metal)	http://www.iron-consortium.org/assets/files/TWG/Analysis-MillScale-V2_100717.pdf
327	Slags, ferrous metal, blast furnace	http://www.alfaacciai.it/wp-content/uploads/2011/03/CSR-ferrous-slags-all-new-14-11-13-Version-4-13-estratto-pag4-7.pdf
5031	Slags, steelmaking, elec. furnace (carbon steel production)	http://www.alfaacciai.it/wp-content/uploads/2011/03/CSR-ferrous-slags-all-new-14-11-13-Version-4-13-estratto-pag4-7.pdf
9644	Iron sinter	http://www.iron-consortium.org/assets/files/Guidance/Analysis-SinterV4_100910.pdf
706	Matte, lead	http://www.reach-lead.eu/substanceinfo/batch/Matte%20lead.zip

Substance Identity Profiles for substances in this group usually define concentration ranges of individual constituents, most frequently in the form of elemental composition, but in some cases the SIPs provide information also on the chemical speciation of certain constituents, some of the encountered SIPs also present suitable techniques for analyses of the substances. Sameness criteria based on other additional elements (e.g. grain size distribution) were also encountered in some SIPs.

3.1.3. Substances originating from calcination and smelting processes

Complex inorganic substances originating from calcination and smelting processes registered in accordance with REACH include mixed metal oxides (often used as inorganic pigments) and a large group of silicates. Despite chemical composition of these substances being known in most cases, it is typically variable. Substances in this group include mainly solids with properties determined to a great extent by their crystalline structure.

a) Substances screened in this group

Table 26 lists the 12 substances originating from calcination and smelting processes selected for substance identity screening.

Table 26 Substances originating from calcination and smelting processes – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed*
		Joint	Indiv.	Total	
9439	Hematite, chromium green black	11	0	11	100
9636	iron cobalt chromite black spinel	13	0	13	100
10344	nickel iron chromite black spinel	12	0	12	100
11694	zinc iron chromite brown spinel	15	0	15	100
9617	Ilmenite (FeTiO3), conc.	3	0	3	100
10056	Molybdenum sulfide (MoS2), roasted	29	0	29	69
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel	4	0	4	100
457	Flue dust, portland cement	78	0	78	26
9390-1	glass, oxide, chemicals	2	1	3	100
41	Silicic acid, aluminum sodium salt	11	0	11	100
45-47	Silicic acid, calcium salt	7	2	9	100
175	Silicic acid, titanium salt	1	0	1	100

* 20 dossiers per substance were analysed as a maximum.

Comments to Table 26:

2 of the screened substances contain besides dossiers from joint submissions also individual submission dossier(s). One of the screened substances was registered by 78 registrants, another by more than 20 registrants and the rest by up to 15 registrants.

For the purposes of this project, substances originating from metallurgical processes have been further divided into the following sub-groups:

1. Inorganic pigments
2. Mixed metal oxides (other than inorganic pigments)
3. Silicates

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 27 Substance identity elements used by registrants in identification of substances originating from calcination and smelting processes.

	Inorganic Pigments					Mixed Metal Oxides		Silicates					
	5078	9439	9636	10344	11694	9617	10056	41	45-7	175	457	9390-1	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	92
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	92
Parameters of process	✓	✓	✓	✓	✓		✓	✓	✓		✓	✓	83
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
State		✓	✓	✓									25
Particle size distribution							✓						8
Form of the substance	✓	✓	✓	✓			✓	✓	✓			✓	67
Crystalline structure (phase)	✓	✓	✓	✓	✓	✓		✓	✓	✓		✓	83
Colour	✓	✓	✓	✓	✓								42
Colour Index		✓	✓	✓	✓								33
*Group-specific element**	✓	✓	✓	✓	✓								42
*Common characteriser***											✓	✓	17
*Other characteriser****	✓	✓				✓	✓	✓	✓	✓	✓		67
No. of applied SID elements per substance	9	11	10	10	8	5	7	7	7	3	6	7	Avg. = 58
Average no. of applied SID elmts. per sub-group	9.6 ± 1.1					6 ± 1.4		6 ± 1.7					
Average no. of applied SID elmts. per group	7.5 ± 2.3												

* SID element specific to a certain group/sub-group of substances, in particular: Inorganic pigment (5078, 9439, 9636, 10344, 11694).

** Common group-specific jargon, in particular: Dust (457), Glass (9390-9391).

*** Reaction product (reaction mass) (5078, 9439, 45-47), Concentrate (9617, 10056), Salt (41, 45-47, 175), Flue dust (457), By-product (457)

Comments to Table 27:

- 13 SID elements were used by registrants of the screened substances for identification of substances in this group;

- 6 of the 12 substances were identified with 6 – 8 SID elements, 4 substances with 9 – 11 SID elements, one substance with SID elements and one with 3 SID elements, the average number of SID elements used for identification of a substance in this group is 7.5 ± 2.3;

- Besides composition, source, manufacturing process and its parameters (conditions), registrants of substances in this group report also crystalline structure (reported for identification of 83 % of the screened substances) and form of the substance (67 %), e.g. powder or fibres.

- Registrants of substances in the sub-group "Inorganic pigments" used on average a significantly higher number of SID elements (9.6 ± 1.1). Additional SID elements used in most cases by registrants of inorganic pigments are crystalline structure, colour, colour index number, form of the substance (powder) and state (solid).

- One of the screened substances (175 - Silicic acid, titanium salt) lacks information on the process and source due to the fact that the substance was registered by only a single registrant based outside the EU, therefore without the obligation of providing this information. These facts (single registrant based outside the EU) are likely the reasons why this substance was identified using only 3 SID elements as opposed to the related substance "Silicic acid, calcium salt" (ID 45-7) identified with 7 SID elements and registered in a joint submission by 7 EU-based registrants (and by additional 2 in individual submissions) which needed to assess the sameness of their substances, likely inducing the need for more complex identification.

Composition

The registrants of the substances subject to the screening most frequently specified composition of the substances providing concentration ranges of individual constituents together with their typical concentrations in vast majority of cases. In cases where only one of these two values was provided, frequency of use of concentration ranges and of typical concentrations was similar.

The data from the screened registration dossiers document the following specifics of substances originating from calcination and smelting processes:

- The composition of the substances in the sub-group of Inorganic pigments always included a constituent with concentration of ≥ 80%. This main constituent always includes in its name different chemical elements and the specification of a crystalline structure (e.g. spinel, hematite), indicating that the registrants consider the crystalline structure as the key substance identity element. A contributing factor to this observation can be that all substances screened in this sub-group were covered by a single consortium.
- All screened substances in the sub-group of Silicates sub-group with the exceptions of "Flue dust, portland cement" and "glass, oxide, chemicals" share the common feature that the reported composition always includes generic constituent, a salt of silicic acid in ≥ 93%. Only in a few cases the reported compositional data are further broken down to report contents of individual silicates represented by this generic constituent.

Unlike substances originating from combustion processes or metallurgical processes, the screened registration dossiers of substances originating from calcination and smelting processes rarely include multiple compositions. In the few cases where a single dossier included multiple compositions, the following contributing factors were identified:

a) provided compositions were describing different samples (registrant-specific representative sample vs. typical consortium/SIEF/SIP-defined values or different grades of the substance)

b) one of the provided compositions is claimed to be covered by the registration of the individual constituents

The following table summarises the number of compositions specified in registration dossiers by registrants of substances originating from calcination and smelting processes.

Table 28 Number of compositions specified in registration dossiers by registrants of substances originating from calcination and smelting processes.

ID	Name (as registered)	% of No. of compositions		
		1	2	3
9439	Hematite, chromium green black	100		
9636	iron cobalt chromite black spinel	100		
10344	nickel iron chromite black spinel	100		
11694	zinc iron chromite brown spinel	100		
9617	Ilmenite (FeTiO3), conc.	100		
10056	Molybdenum sulfide (MoS2), roasted	100		
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel	100		
457	Flue dust, portland cement	85	5	10
9390-1	glass, oxide, chemicals	100		
41	Silicic acid, aluminum sodium salt	91	9	
45-47	Silicic acid, calcium salt	89	11	
175	Silicic acid, titanium salt	100		

75 % of the screened substances included only a single composition reported by the registrants. Reasons for reporting multiple compositions in a single dossier are already discussed above.

Table 29 Number of constituents specified in registration dossiers by registrants of substances originating from calcination and smelting processes.

ID	Name (as registered)	Composition & No. of constituents	
9439	Hematite, chromium green black		6[a]
9636	iron cobalt chromite black spinel		10[b]
10344	nickel iron chromite black spinel		9[c]
11694	zinc iron chromite brown spinel		10[b]
9617	Ilmenite (FeTiO3), conc.		7[d]
10056	Molybdenum sulfide (MoS2), roasted		16
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel		2
457	Flue dust, portland cement	#1	32
		#2	27
		#3	27
9390-1	glass, oxide, chemicals		1[e] 3[f]
41	Silicic acid, aluminum sodium salt	#1	3[g]
		#2	9
45-47	Silicic acid, calcium salt	#1	4[h,i] 3[f]
		#2	3[h] 6[f]
175	Silicic acid, titanium salt		2[j]

[a] 5 constituents were specified as impurities
[b] 9 constituents were specified as impurities
[c] 8 constituents were specified as impurities
[d] 6 constituents were specified as impurities
[e] Joint submission (2 dossiers)
[f] Individual submission (1 dossier)
[g] 2 constituents were specified as impurities
[h] Joint submission (7 dossiers)
[i] 3 constituents were specified as impurities
j 1 constituent was specified as an impurity

As documented in the table above, registrants reported some constituents as impurities in more than 60 % of specified compositions. **Out of the 19 reported compositions 15 included less than or equal to 10 constituents, one reported 16 constituents and three, referring to the same substance (flue dust, Portland cement) reported 27 – 32 constituents.**

Table 30 Consistency of compositional data provided in the registration dossiers for substances originating from calcination and smelting processes.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
9439	Hematite, chromium green black						100
9636	iron cobalt chromite black spinel						100
10344	nickel iron chromite black spinel						100
11694	zinc iron chromite brown spinel						100
9617	Ilmenite (FeTiO3), conc.				100		
10056	Molybdenum sulfide (MoS2), roasted				14		86
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel			100			
457	Flue dust, portland cement				100		
9390-1	glass, oxide, chemicals	33[a]					67[b]
41	Silicic acid, aluminum sodium salt					9%	100%
45-47	Silicic acid, calcium salt			67%		22%	78%
175	Silicic acid, titanium salt						100%

Notes: * Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

[a] Individual submission (1 dossier)
[b] Joint submission (2 dossiers)

There is a significant variability in approaches taken by registrants of the substance "Silicic acid, calcium salt" in reporting compositional information. The joint submission specifies a constituent (silicic acid, calcium salt) **in the concentration of 96 – 100** % and another three constituents reported as impurities (sodium chloride, aluminium oxide and diiron trioxide), whereas one of the dossiers submitted in an individual submission specifies two constituents (hypothetical oxides: silicon dioxide and calcium oxide) accounting for 39 % - 100 % (considering reported minimum and maximum concentrations) **with < 1 %** of quartz. The other individual submission lists the constituents as minerals (Tobermorite, Xonotlite, Calcite) accounting for 0 % – 100 % of the composition with also Quartz / silicon dioxide and X-ray amorphous phase **reported and accounting for another 0** % **- 73 % of the composition**.

Table 31 Typical constituents specified in registration dossiers by registrants of substances originating from calcination and smelting processes.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
9439	Hematite, chromium green black	Hematite, chromium green black / C.I. Pigment Green 17	272-713-7	80 – 100
		Silicon dioxide	231-545-4	0 – 10
		Calcium oxide	215-138-9	0 – 3
9636	iron cobalt chromite black spinel	Iron cobalt chromite black spinel / C.I. Pigment Black 27	269-060-5	80 – 100
		Aluminium oxide	215-691-6	0 – 2
		Calcium oxide	215-138-9	0 – 1
10344	nickel iron chromite black spinel	Nickel iron chromite black spinel / C.I. Pigment Black 30	275-738-1	80 – 100
		Aluminium oxide	215-691-6	0 – 3
		Silicon dioxide	231-545-4	0 – 4
11694	zinc iron chromite brown spinel	Zinc iron chromite brown spinel / C.I. Pigment Brown 33	269-050-0	80 – 100
		Silicon dioxide	231-545-4	0 – 1
		Calcium oxide	215-138-9	0 – 0.6
9617	Ilmenite (FeTiO3), conc.	Ilmenite (FeTiO3), conc.	308-551-1	80 – 96
		Aluminium oxide	215-691-6	0 – 3
		Quartz (SiO2)	238-878-4	0 – 3
		Diiron trioxide	215-168-2	2 – 9
		Manganese oxide	215-695-8	0 – 2
10056	Molybdenum sulfide (MoS2), roasted	Molybdenum sulfide (MoS2), roasted	289-178-0	100
		Molybdenum trioxide	215-204-7	45 – 96
		Mo suboxides	N/A	2 – 30
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel	Zinc iron chromite brown spinel / C.I. Pigment Brown 33	269-050-0	45 – 79
		Willemite, white	305-410-6	20 – 70
457	Flue dust, portland cement	Tricalcium silicate / Tricalcium silicon pentaoxide	235-336-9	0 – 55
		Dicalcium silicate / Dicalcium silicon tetraoxide	233-107-8	0 – 50
		Tricalcium aluminate / Dialuminium tricalcium hexaoxide	234-932-6	0 – 10
		Calcium oxide	215-138-9	0 – 65
		Calcium hydroxide	215-137-3	0 – 35
		Calcium carbonate	207-439-9	0 – 95
		Calcium sulfate	231-900-3	0 – 40
		Potassium sulfate	231-915-5	0 – 60
9390-1	glass, oxide, chemicals	E-glass special purpose fibres [Man-made vitreous (silicate) fibres with random orientation with	266-046-0	100

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
		the following composition (% given by weight): SiO2 50.0-56.0%, Al2O3 13.0-16.0%, B2O3 5.8-10.0%, Na2O <0.6%, K2O <0.4%, CaO 15.0-24.0%, MgO <5.5%, F2O3 …		
41	Silicic acid, aluminum sodium salt	Silicic acid, aluminum sodium salt / Sodium aluminosilicate	215-684-8	93 – 99.9
45-47	Silicic acid, calcium salt	Silicic acid, calcium salt / calcium oxosilanediolate	215-710-8	96 – 99.9
		Sodium chloride	231-598-3	0 – 2
		Aluminium oxide (Al2O3)	215-691-6	0.01 – 0.6
		Diiron trioxide	215-168-2	0.005 – 0.8
175	Silicic acid, titanium salt	Silicic acid, titanium salt / titanium(4+) oxosilanediolate	255-911-8	99 – 100
		Inorganic impurities	N/A	0 – 1

Note: Concentration ranges presented in the table are derived from the screened registration dossiers, where the lowest reported concentration and the highest reported concentration was extracted to the table. It shall be noted that the constituents presented in the table are those most frequently reported by the registrants of the screened substances, the list of constituents reported by the registrants is not exhaustive.

In the previous table, there are clear patterns in reporting compositional information in relation to individual substances or sub-groups of substances. Registrants of inorganic pigments, which are covered by a consortium always reported one constituent in concentrations equal to or more than 80 % referring to a generic constituent covered by a colour index number and several other constituents in concentrations of less than or equal to 10 %.

Another substance (Molybdenum sulfide (MoS2), roasted) is an illustration of two different approaches in reporting compositional information – some registrants reported a single generic constituent (Molybdenum sulfide (MoS2), roasted), while others provided further compositional breakdown reporting the contents of Molybdenum trioxide, Molybdenum suboxides and other constituents.

Most of the constituents reported by registrants of Portland cement, flue dust have very wide concentration ranges (spanning over an interval of more than 50 % in some cases).

Three salts of silicic acid (calcium salt, aluminium sodium salt and titanium salt) encountered in the study appear to be well-defined monoconstituent substances not regarded as complex in the sense of this study.

Source

Similarly to substances originating from combustion processes and metallurgical processes, source is one of the key elements contributing to the variability in composition of substances originating from calcination and smelting processes.

From the screened registration dossiers, two main types of sources specific to individual sub-groups of substances can be identified:

a) Mixtures of oxides in solid state are the raw materials used in the manufacture of inorganic pigments and mixed metal oxides

b) Solutions of silicates, suspended silica or silicic acid together with metallic salt(s) are sources of the substances screened within the group of silicates (with the exception of "Flue dust, portland cement", where the specified source is flue gas from the manufacture of Portland cement, and with the exception of "glass, oxide, chemicals", where the source is unspecified).

The group of inorganic pigments is a typical example of a group of substances where it is evident from the screened registration dossiers that registrants considered that different sources can lead to substances eligible for a single joint registration.

Table 32 Sources of substances originating from calcination and smelting processes as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
9439	Hematite, chromium green black	Chromium (III)oxide
9636	iron cobalt chromite black spinel	mixture of oxides of ferrous iron, cobalt, ferric iron and chromium (Raw materials in solid state)
10344	nickel iron chromite black spinel	Nickel, ferrous and ferric iron and chromium in varying amounts
11694	zinc iron chromite brown spinel	zinc, ferrous and ferric iron and chromium in varying amount
9617	Ilmenite (FeTiO3), conc.	Natural ilmenite ore
10056	Molybdenum sulfide (MoS2), roasted	Molybdenum sulfide concentrate (MoS2)
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel	Zinc oxide, iron oxides, silicon dioxide, and chromium(III) oxide in varying amounts (Raw material in solid state)
457	Flue dust, portland cement	Gases from manufacture of Portland cement clincer
9390-1	glass, oxide, chemicals	Molten glass
41	Silicic acid, aluminum sodium salt	Sodium silicate solutions (e.g. water glass, CAS-No. 1344-09-8; Na2O*nSiO2, n = 2 to 4) and metal salts, generally aluminum sulfate
45-47	Silicic acid, calcium salt	Calcium chloride or hydroxide with sodium silicate or suspended silica
175	Silicic acid, titanium salt	Not reported (substance registered by a non-EU entity)

Sources reported by registrants of substances in this group include mainly individual chemicals , more complex sources are also reported in some cases (e.g. molten glass or natural ilmenite ore).

Manufacturing process and its parameters (conditions)

Similarly to the substances originating from combustion processes, each sub-group of calcination process products shares typical manufacturing processes specified by registrants in general (calcination, grinding, roasting in the case of inorganic pigments and mixed metal oxides and precipitation, filtration, filter cake treatment, drying, milling and granulation in relation to silicates). Manufacturing conditions, including the ratios of reactants and combinations of different processing steps and treatment methods are the key factors determining the composition of the final products.

The level of detail of the manufacturing process description provided by the registrants is variable. Most registrants of inorganic pigments provided information on individual processing steps and temperature of the calcination process, which was not specified in dossiers to some of the other substances, but on the other hand some included detailed information on individual processing steps, ratio of reaction agents, temperature. pH and other conditions of the manufacturing process.

Table 33 Manufacturing processes of substances originating from calcination and smelting processes as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
9439	Hematite, chromium green black	Calcination, grinding
9636	iron cobalt chromite black spinel	Calcination, grinding
10344	nickel iron chromite black spinel	Calcination, grinding
11694	zinc iron chromite brown spinel	Calcination, grinding
9617	Ilmenite (FeTiO3), conc.	Oxidative roast, reductive roasting stage, an acidic leaching stage and washing and drying. Alternatively the process consists of selectively chlorinating the iron oxide present in the reduced ore.
10056	Molybdenum sulfide (MoS2), roasted	Roasting
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel	Calcination
457	Flue dust, portland cement	"Portland cement production (calcination) (thermal processing)" Separation from the exit gases
9390-1	glass, oxide, chemicals	Drawing or spinning the molten mix from nozzles.
41	Silicic acid, aluminum sodium salt	Precipitation, Filtration, Filter Cake Treatment, Drying Process Milling, Granulation (optionally)
45-47	Silicic acid, calcium salt	Precipitation, Filtration, Filter Cake Treatment, Drying Process Milling, Granulation (optionally)
175	Silicic acid, titanium salt	No description (importer)

Screened dossiers to inorganic pigments contained very consistent information on the manufacturing process, describing individual processing steps and specifying the temperature of the calcination. Even more detailed description of individual processing steps was encountered in the screened registration dossiers to the salts of silicic acid (with the exception of the titanium salt as justified in the table above).

Together with source and manufacturing process in general, parameters (conditions) of the manufacturing process are the key elements determining the chemical composition of substances originating from calcination and smelting processes.

As presented in Table 27, the only substances subject to the screening without information on the parameters of the manufacturing process in any of the screened dossiers were "Ilmenite (FeTiO3), conc." and "Silicic acid, titanium salt" The other screened substances, typically included information on the processing temperature and in liquid state processing also pH.

It has not been observed that different parameters (conditions) of a single manufacturing process with a single source would lead to different substance registration submissions.

Additional substance identity elements

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Substance identity element	Value	Substance identified with the SID element
State	Solid	Hematite, chromium green black (9439), iron cobalt chromite black spinel (9636), nickel iron chromite black spinel (10344)
Particle size distribution	Provided in analytical protocols in dossiers	Reaction mass of Willemite, white and zinc iron chromite brown spinel (5078), Molybdenum sulfide (MoS2), roasted (10056)
Form of the substance	Powder	Hematite, chromium green black (9439), iron cobalt chromite black spinel (9636), nickel iron chromite black spinel (10344), Reaction mass of Willemite, white and zinc iron chromite brown spinel (5078)
	Fibres (microfibres)	glass, oxide, chemicals (9390 – 9391)
Crystalline structure (phase)	Crystalline hematite	Hematite, chromium green black (9439)
	Amorphous	glass, oxide, chemicals (9390 – 9391), Silicic acid, aluminum sodium salt (41), Silicic acid, calcium salt (45-47), Silicic acid, titanium salt (175)
	Spinel	Reaction mass of Willemite, white and zinc iron chromite brown spinel (5078), iron cobalt chromite black spinel (9636), nickel iron chromite black spinel (10344), zinc iron chromite brown spinel (11694)
	White willemite	Reaction mass of Willemite, white and zinc iron chromite brown spinel (5078)
	Ilmenite	Ilmenite (FeTiO3), conc. (9617)
Colour	Green black	Hematite, chromium green black (9439)
	Brown	Reaction mass of Willemite, white and zinc iron chromite brown spinel (5078), zinc iron chromite brown spinel (11694)
	White	Reaction mass of Willemite, white and zinc iron chromite brown spinel (5078)
	Black	iron cobalt chromite black spinel (9636), nickel iron chromite black spinel (10344)
Colour Index	C.I. 77288	Hematite, chromium green black (9439)
	C.I. 77502	iron cobalt chromite black spinel (9636)
	C.I. 77504	nickel iron chromite black spinel (10344)
	C.I. 77503	zinc iron chromite brown spinel (11694)

It can be observed that especially the registrants of inorganic pigments used additional substance identity elements to characterise their substances, in particular form of the substance (powder), colour and Colour Index (C.I.) and crystalline structure.

As mentioned in the preceding sections, crystalline structure is one of the key substance identity elements determining the properties of the substances in this group. Crystalline structure (e.g. spinel, hematite, willemite, ilmenite) was specified in registration dossiers for all screened inorganic pigments, whereas all silicates with the exception of "Flue dust, Portland cement" were described by some registrants as amorphous.

c) Analytical methods

The following Table 34 and Table 35 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 34 REACH Annex VI analytical methods used by registrants of substances originating from calcination and smelting processes.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
9439	Hematite, chromium green black						
9636	iron cobalt chromite black spinel						
10344	nickel iron chromite black spinel						
11694	zinc iron chromite brown spinel						
9617	Ilmenite (FeTiO3), conc.						
10056	Molybdenum sulfide (MoS2), roasted	Y					
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel						
457	Flue dust, portland cement		Y				
9390-1	glass, oxide, chemicals						
41	Silicic acid, aluminum sodium salt		Y	Y			
45-47	Silicic acid, calcium salt	Y	Y	Y			
175	Silicic acid, titanium salt	Y	Y	Y			

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 35 Other analytical methods used by registrants of substances originating from calcination and smelting processes in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements				
		XRD	XRF	ICP-OES	AAS	Other
9439	Hematite, chromium green black	Y	Y			
9636	iron cobalt chromite black spinel	Y	Y			
10344	nickel iron chromite black spinel	Y	Y			
11694	zinc iron chromite brown spinel	Y	Y			
9617	Ilmenite (FeTiO3), conc.	Y	Y	Y		
10056	Molybdenum sulfide (MoS2), roasted	Y	Y	Y	Y	Gravimetry, Titration, LECO Combustion analysis, Wet chemistry, Particle size distribution
5078	Reaction mass of Willemite, white and zinc iron chromite brown spinel	Y	Y			
457	Flue dust, portland cement	Y	Y			Wet chemistry
9390-1	glass, oxide, chemicals		Y			Volumetric analysis, Titration (compelsometric, neutralization), Gravimetric analysis, Flame photometer
41	Silicic acid, aluminum sodium salt	Y				FTIR, ICP-AES
45-47	Silicic acid, calcium salt	Y	Y	Y		Drying (water content), Heating (loss on ignition)
175	Silicic acid, titanium salt	Y	Y	Y		Gravimetry, XANES

It can be observed that analytical methods explicitly mentioned in Annex VI of REACH are of limited relevance for this group of substances with predominantly inorganic constituents, only in the case of silicates a frequent use of ultraviolet-visible spectroscopy, infrared spectroscopy and nuclear magnetic resonance can be observed.

In accordance with common analytical practices, X-ray diffraction and X-ray fluorescence are the main analytical methods used by registrants for determination of chemical composition of substances of originating from calcination processes and in some cases also inductively coupled plasma optical emission spectrometry. Other analytical methods and techniques used by registrants of the screened substances originating from calcination processes are summarised in the table above.

The set of analytical methods and techniques used for determination of chemical composition of individual substances subject to the screening reflects the nature of the substances.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressed by the following operating consortia and associations:

- Inorganic Pigments Consortium – http://www.ipconsortium.eu/
- Molybdenum Consortium – http://www.molybdenumconsortium.org/
- SAS for REACH – http://www.reach-sas.org/
- Cimeurope – http://www.cimeur.com/Consortium.htm
- Verband der Mineralfarbenindustrie e. V. (Eurocolour) – http://www.vdmi.de/englisch/home.html

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 36 for direct links (where available).

Table 36 Publicly available substance identity profiles of substances originating from calcination and smelting processes.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
10056	Molybdenum sulfide (MoS2), roasted	http://www.molybdenumconsortium.org/assets/files/RMC/MoCon%20RMC%20Substance%20Identification%20doc%20for%20SIEF-V10F2-10July2015.pdf	Concentrations of molybdenum oxides and suboxides, molybdates, silicon dioxide and arsenic oxide
45-47	Silicic acid, calcium salt	http://www.reach-sas.org/index_htm_files/SIEF%20Info%20Letter%20CaSiO4%20EC%20215-710-8%20No%202.pdf	This substance is likely mono-constituent, the SIP defines maximum typical concentrations of selected impurities

3.1.4. Other Inorganic substances

Other registered complex inorganic substances registered include reaction masses and reaction products (often salts) of various inorganic compounds, as well as a group of zeolites and other inorganic substances of various nature – see the following Table 37 listing complex inorganic chemicals not falling into any of the groups described in previous sections. As this group is rather diverse, the following table presents all inorganic substances regarded as complex in this project and not falling into any of the groups already discussed above.

Table 37 Identified complex inorganic substances not falling in any of the previously described groups (other complex inorganic substances).

ID	EC/List No.	Name (as registered)
8118	232-989-1	Ammonium sulfide ((NH4)2(Sx))
10709	915-673-4	Polysulfides, bis[3-(triethoxysilyl)propyl]
10710	273-103-3	Polysulfides, di-tert-Bu
10711	270-335-7	Polysulfides, di-tert-dodecyl
10712	270-336-2	Polysulfides, di-tert-nonyl
10734	286-925-2	potassium difluorodihydroxyborate(1-)
5022	932-162-1	Reaction mass of ammonium hydrogensulphite, ammonium sulphite and sulphur dioxide
5033	932-280-3	Reaction mass of selenious acid and sulphuric acid
5050	934-716-8	Reaction mass of sodium hydrogensulfide and sodium carbonate
5032	932-279-8	Reaction mass of sodium selenite and sodium sulphate
5002	931-722-2	Reaction product of lead chloride or lead sulphate with alkaline solution
4722	914-103-1	SEL BINAIRE 6/0/15 Reaction mass of ammonium sulphate and potassium sulfate and sodium sulphate
11206	232-379-5	Superphosphates
11207	266-030-3	Superphosphates, concd.
4921	931-125-7	Zeolite, cuboidal, crystalline, synthetic, non fibrous, thermally produced_x000D_
11668	930-915-9	Zeolite, cuboidal, crystalline, synthetic, non-fibrous
4907	930-989-2	Zeolite, phosphor containing, crystalline, synthetic, non fibrous
4908	930-991-3	Zeolite, silica and titanium based, crystalline, synthetic, non fibrous
4905	930-985-0	Zeolite, silica rich, crystalline, synthetic, non-fibrous
4906	930-986-6	Zeolite, silica rich, without aluminium, crystalline,synthetic, nonfibrous
4909	930-993-4	Zeolite, synthetic, crystalline, non fibrous, silica and titanium based
10412	614-074-2	Aluminium chloride, basic, reaction products with silica
8185	274-324-8	Bentonite, acid-leached
8534	215-609-9	Carbon black
4816	922-642-9	Cement, purification of copper electrolyte
9210	273-752-2	Electrolytes, copper-manufg., spent
4964	931-319-1	Feropur
5047	933-944-5	Gold electrolyte
9428	291-367-8	Graphite, acid-treated
4826	923-511-9	Inorganic residual from kraft or soda pulping separated from green liquor in the chemical recovery cycle.
4994	931-663-2	Materials for reclaim, precious metal production by-products
4998	931-674-2	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.
943	297-648-1	Oil shale, thermal processing waste
10707	232-417-0	Polyphosphoric acids
5018	932-084-8	reaction mass of calcium carbonate and calcium dihydroxide and silicon dioxide
4686	910-663-6	Reaction mass of cobalt sulphide and nickel sulphide and trinickel disulphide
4981	931-506-8	Silver electrolyte
386	268-612-2	Sulfite liquors and Cooking liquors, green
387	268-615-9	Sulfite liquors and Cooking liquors, white
108	235-819-4	sulphuric acid, compound with graphite
5363	not available	TexFRon AG (flame retardant)

a) Substances screened in this group

The following Table 38 lists substances selected for substance identity screening from this group.

Table 38 Other complex inorganic substances – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed*
		Joint	Indiv.	Total	
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]	7	0	7	100
5002	Reaction product of lead chloride or lead sulphate with alkaline solution	3	0	3	100
11206	Superphosphates	33	0	33	61
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous	42	0	42	48
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous	15	0	15	100
4994	Materials for reclaim, precious metal production by-products	7	0	7	100
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	6	0	6	100
943	Oil shale, thermal processing waste	4	0	4	100
4981	Silver electrolyte	4	0	4	100
386	Sulfite liquors and Cooking liquors, green	57	0	57	35

* 20 dossiers per substance were analysed as a maximum.

Out of the 10 screened substances, one contained 57 dossiers, one contained 42 dossiers, one contained 33 dossiers, another one 15 dossiers and the remaining 6 substances contained at most 7 dossiers.

For the purposes of this project, substances in this group have been further divided into the following sub-groups:

1. Inorganic salts
2. Zeolites
3. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 39 Substance identity elements used by registrants in identification of other complex inorganic substances.

	Inorganic salts			Zeolites		Others					
	10709	5002	11206	11668	4905	4994	4998	943	4981	386	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓			✓	✓	✓	80
Parameters of process			✓	✓	✓			✓	✓		50
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
State	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Density		✓	✓					✓		✓	40
Solubility		✓		✓	✓			✓		✓	50
Viscosity										✓	10
Particle size distribution		✓	✓	✓	✓			✓			50
Form of the substance		✓	✓	✓	✓	✓	✓	✓	✓	✓	90
Crystalline structure (phase)				✓	✓						20
Colour		✓	✓	✓	✓					✓	50
*Group-specific element**	✓		✓	✓	✓						40
*Common characteriser***		✓	✓	✓	✓	✓	✓	✓	✓	✓	90
*Other characteriser****	✓		✓	✓	✓	✓		✓	✓		70
No. of applied SID elements per substance	6	10	12	13	13	6	5	11	8	11	Average = 63
Average no. of applied SID elmts. per subgroup	9.3 ± 3.1			13 ± 0		8.2 ± 2.8					
Average no. of applied SID elmts. per group	9.5 ± 3										

* SID element specific to a certain group/sub-group of substances, in particular: Polysulfides (10709), Mixture of inorganic salts (11206), Zeolite (11668, 4905).

** Common group-specific jargon, in particular: Lead carbonate (5002), Fertilizer (11206), Aluminosilicate (11668, 4905), Materials for reclaim (4994, 4998), Thermal processing waste (943), Silver electrolyte (4981), Cooking liquor (386).

*** Reaction product (10709, 11206), melting point > 400 °C (11668, 4905), By-product (4994), Residue (943), Inorganic intermediate (4981)

Comments to Table 39:

- 15 SID elements were used by registrants of the screened substances for identification of substances in this group;

- 6 out of the 10 substances in this group were identified with 10 – 13 SID elements, 1 substance with 8 SID elements, 2 substances with 6 SID elements and 1 substance with 5 SID elements. The average number of SID elements used by registrants in this group is 9.5±3 (standard deviation is the highest observed among all groups of substances screened in this study). The highest number of 13 SID elements was used for identification of two substances grouped together into the sub-group of zeolites. The set of SID elements used for identification of both zeolites was identical. From the other side, the two substances with the lowest number of SID elements used for identification are both materials for reclaim.

- Besides composition, source and manufacturing process, the most frequently used SID elements are form of the substance (e.g. powder, slurry), "common characteriser" (Common group-specific jargon, e.g. cooking liquor) and "other characteriser" (e.g. residue, by-product, reaction-product) used for identification of over 70 % of substances in this group, followed by parameters (conditions) of the manufacturing process (50 %), solubility (50 %), colour (50 %), particle size distribution (50 %) and density (40 %). Other SID elements were used for characterisation of less than 20 % of substances in this group.

Composition

The registrants of the substances subject to the screening most frequently specified composition of the substances providing concentration ranges of individual constituents, together with their typical concentrations of individual constituents/additives/impurities. In cases where only one of these two values was provided, concentration ranges were predominant over typical concentrations.

Some registration dossiers include several compositions, due to the following factors:

a) describing different registrant' products, typically representative registrant-specific composition values vs. typical consortium/SIEF/SIP-defined composition values

b) describing either mineralogical composition or complementary elemental composition with trace constituents

c) different concentrations of constituents with relevance for classification and labelling and therefore different classification and labelling of the substance

d) describing samples from different locations (production sites)

e) describing compositions derived from different sources of recovered raw materials

In general, compared to other groups of substances, registrants of substances in this group specified multiple compositions in their dossiers much more frequently and often the number of provided compositions was high in comparison with other groups of substances, as documented in the following table. This is particularly true for the sub-group of "Others" including several substances originating from wastes or reclaimed materials.

Table 40 Number of compositions specified in registration dossiers by registrants of other complex inorganic substances.

ID	Name (as registered)	% of No. of compositions							
		1	2	3	4	5	6	9	10
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]	100							
5002	Reaction product of lead chloride or lead sulphate with alkaline solution		100						
11206	Superphosphates	90	10	0	0	0	0	0	0
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous	100	0	0	0	0	0	0	0
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous	100	0	0	0	0	0	0	0
4994	Materials for reclaim, precious metal production by-products	0	0	0	0	0	75	25	0
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	0	0	0	0	75	0	0	25
943	Oil shale, thermal processing waste	50	50	0	0	0	0	0	0
4981	Silver electrolyte	33			33	33	0	0	0
386	Sulfite liquors and Cooking liquors, green	30	5	20	0	40	5	0	0

Out of the 10 substances screened in this group, 7 included dossiers, where some of the registrants reported multiple compositional data. One of the screened dossiers reported 10 different compositions, reflecting identity of various grades of the substance with different concentrations of certain constituents relevant for hazard classification. This is the highest number of compositions observed in a single registration dossier for inorganic substances.

Table 41 Number of constituents specified in registration dossiers by registrants of other complex inorganic substances.

ID	Name (as registered)	Composition & No. of constituents	
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]		17[a]
5002	Reaction product of lead chloride or lead sulphate with alkaline solution	#1	6
		#2	14
11206	Superphosphates	#1	20[b]
		#2	8[c]
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous		6
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous		2[d]
4994	Materials for reclaim, precious metal production by-products	#1	34
		#2	32
		#3	8
		#4	7
		#5	7
		#6	7
		#7	6
		#8	7
		#9	5
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	#1	34
		#2	32
		#3	7
		#4	7
		#5	7
		#6	1
		#7	1
		#8	1
		#9	2
		#10	2
943	Oil shale, thermal processing waste	#1	8
		#2	6
4981	Silver electrolyte	#1	6
		#2	6
		#3	6
		#4	10
		#5	5
386	Sulfite liquors and Cooking liquors, green	#1	12
		#2	10
		#3	8
		#4	8
		#5	8
		#6	8

[a] 14 constituents were specified as impurities
[b] 18 constituents were specified as impurities
[c] 6 constituents were specified as impurities
[d] 1 constituent was specified as an impurity

There are several cases where 30 or more substances were reported in by registrants in a single composition, the highest number being 34. Despite that, nearly 80 % of the screened compositions included less than or equal to 10 substances, In two cases where 9 or more compositions were provided in a single dossier, 2 of these specified over 30 constituents, while the remaining compositions reported less than 10 constituents. In these two cases, the registrants reported contents of similar constituents as these substances are similar in nature (both being metallic materials for reclaim).

Table 42 Typical constituents specified in registration dossiers by registrants of other complex inorganic substances.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]	4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecane	260-350-7	15 – 25
		4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	254-896-5	20 – 30
		4,4,14,14-tetraethoxy-3,15-dioxa-8,9,10-trithia-4,14-disilaheptadecane	260-351-2	30 – 35
5002	Reaction product of lead chloride or lead sulphate with alkaline solution	Lead carbonate	209-943-4	50 – 95
		Calcium carbonate	207-439-9	0 – 20
		Lead sulphate	231-198-9	0 – 20
		Lead	231-100-4	48
		Oxygen	231-956-9	21.5
11206	Superphosphates	Calcium sulfate	231-900-3	30 – 65
		Calcium bis(dihydrogen orthophosphate)	231-837-1	23 – 45
		Calcium Hydrogen orthophosphate	231-826-1	0 – 15
		Fluorapatite	215-144-1	0 – 15
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous	Zeolite, synthetic, crystalline, non-fibrous, silica and titanium based	930-993-4	99 – 100
		Aluminium oxide	215-691-6	31.47
		Sodium oxide	215-208-9	18.63
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous	Zeolite, silica rich, crystalline, synthetic, non-fibrous	930-985-0	99 – 100
		Aluminium oxide	215-691-6	4 – 6
4994	Materials for reclaim, precious metal production by-products	Silver	231-131-3	0 – 85
		Aluminium	231-072-3	0 – 35
		Palladium	231-115-6	0.1 – 8
		Platinum	231-116-1	0 – 15
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	Carbon	231-153-3	0 – 38
		Chromium(2+) (Refers to % element. Element is present as Cr2O3.)	231-157-5	0 – 13
		Iron (Refers to % element. Element is present as Fe2O3.)	231-096-4	0 – 22
		Lead (Refers to % element. Element is present as PbO.)	231-100-4	0.15 – 85
943	Oil shale, thermal processing waste	Calcite / calcium carbonate	215-279-6	1 – 25
		XRD-Amorphous Fraction	N/A	5 – 80
		Quartz / dioxosilane	238-878-4	1 – 25
4981	Silver electrolyte	Silver nitrate	231-853-9	5 – 21
		Nitric acid	231-714-2	0.5 – 3
		Silver (Refers to % element. Element is present as AgNO3)	231-131-3	7.5 – 21
386	Sulfite liquors and Cooking liquors, green	Disodium sulphide	215-211-5	0 – 15
		Sodium carbonate	207-838-8	2 – 21
		Sodium hydroxide	215-185-5	0 – 16.669

As illustrated in the table above, there are different ways how the registrants of the screened substances reported compositional information. There are some examples where the registrants reported compositions in the form of elemental content. Others provided mineralogical information and in the case of zeolites, most substances reported only a single constituent referring to the zeolite itself, while one of the registrants reported contents of various oxides.

Source

As documented in the following table, the sources of substances in this group are variable.

Table 43 Sources of other complex inorganic substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]	trichlorsilane / allylchloride, ethanol, sodiumsulfide sodium sulfide / sulfur / 3-Chloropropyltriethoxysilane
5002	Reaction product of lead chloride or lead sulphate with alkaline solution	Pb salts (lead chloride, lead sulphate) - waste materials produced by Pb battery recycling process or by-products of the hydrometallurgical upgrading of PGM rich lead bullion.
11206	Superphosphates	Phosphate rock
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous	Sodium silicate and sodium aluminate solution (prepared out of sodium hydroxide and aluminium hydroxide)
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous	Hydrogel obtained by the reaction of alumina hydrate, silicon dioxide or silicate, and optionally some other substances
4994	Materials for reclaim, precious metal production by-products	Materials for reclaim Materials that are non-intentional products of the production and refining of precious metals
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	The production and refining of precious metals
943	Oil shale, thermal processing waste	Oil shale
4981	Silver electrolyte	Silver (The primary or secondary raw material from which silver is recovered.)
386	Sulfite liquors and Cooking liquors, green	Chemicals used in the process of the chemical recovery cycle of pulp mills.

Some sources as reported by the registrants are rather generic. The sources reported in the dossiers screened for this group of substances include individual chemicals (substances) as well as more complex sources (e.g. phosphate rock) and in many cases recovered or reclaimed materials.

Manufacturing process and its parameters (conditions)

Similarly to the source, manufacturing processes described by the registrants of substances in this group are very variable and specific to each substance. Some descriptions of the manufacturing processes indicate that substances with different manufacturing processes may have been registered within a single joint registration submission in some cases (e.g. products of reclaimed metals).

The level of detail of the manufacturing process description is highly variable. Some registrants provide just a general description of the manufacturing process, while others report also the conditions (e.g. temperature or pH) and the technology (e.g. fluidized bed reactor).

Table 44 Manufacturing processes of other complex inorganic substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]	Catalysed reaction, separation processes - (filtering), destillation - (drying) – purification
5002	Reaction product of lead chloride or lead sulphate with alkaline solution	Neutralization, separation step – filtering
11206	Superphosphates	• Milling the phosphate rock - mixing with acids (reaction) - solidification - transport (curing) – granulation • Treating raw materials (phosphate rock) with sulfuric acid. • Acidification of ground phosphate rock with dilute 70% sulphuric acid • Treating phosphate rock with sulfuric acid, or a mixture of sulfuric acid and hexafluorosilicic acid, or a mixture of sulfuric, hexafluorosilicic and phosphoric acids.
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous	Selection of starting materials - mixing - hydro-thermall crystallization - (drying) - surface treatment – dealumination
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous	Hydrogel obtained by the reaction of alumina hydrate, silicon dioxide or silicate , optionally other substances
4994	Materials for reclaim, precious metal production by-products	Materials will either undergo hydrometallurgical processes to leach the precious metal content or be smelted to recover the precious metals.
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	Materials are crushed to varying degrees and added to smelting furnaces where they act as both flux and precious metal source.
943	Oil shale, thermal processing waste	Thermal processing (combustion) in a thermal reactor - heat production
4981	Silver electrolyte	Electrolytic refining of silver
386	Sulfite liquors and Cooking liquors, green	The chemical recovery cycle of pulp mills, sodium based on sulphite and sulphate process. Dissolving the melt from the recovery boiler in water or diluted white liquor.

Manufacturing processes described by the registrants of substances in this group include general chemical reactions and processes (e.g. neutralization, acidification), sometimes catalysed, as well as technological processing steps (e.g. separation, distillation, drying, purification). In some cases registrants of the same substance described a different process of manufacturing the substance (or possibly the same process described in a different way).Conditions of the manufacturing process are sometimes also provided as documented in the following table.

Substance	Conditions of the manufacturing process as reported in the screened registration dossiers
Superphosphates (11206)	90 - 100 °C, atmospheric pressure
Zeolite, cuboidal, crystalline, synthetic, non-fibrous (11668)	• Crystallization at 35 –95 °C at atmospheric pressure, pH 10 –14 • Crystallization at 35 –105 °C at atmospheric pressure,pH 10–14 • X- and A-Zeolit: crystallization at 70 – 100 °, pH 10 – 14; • Y-Zeolit: 85 - 100°C, crystallization time 12 / 48 h.
Zeolite, silica rich, crystalline, synthetic, non-fibrous (4905)	Crystallization: 105–200 °C, 1.5-70 bars, pH 10 - 14, crystallisation time 0.5 - 240 h
Oil shale, thermal processing waste (943)	above 650 °C (e.g. at ~800 °C in a fluidized bed reactor, at ~1300 °C in pulverized combustion boilers) "Galoter process : Oil shale is mixed with hot ash of 800 °C, The temperature of pyrolysis is kept at 520 °. Kiviter process: the lower section of the retort is heated to about 900 °C"
Silver electrolyte (4981)	The electrolyte is heated up to 55 °C

Additional substance identity elements

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Substance identity element	Value	Substance identified with the SID element
State	solid	Reaction product of lead chloride or lead sulphate with alkaline solution (5002), Superphosphates (11206), Materials for reclaim, precious metal production by-products (4994), Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc. (4998), Oil shale, thermal processing waste (943)
	liquid	Polysulfides, bis[3-(triethoxysilyl)propyl] (10709), Silver electrolyte (4981), Sulfite liquors and Cooking liquors, green (386)
Density	approx. 7.6 g/cm3	Reaction product of lead chloride or lead sulphate with alkaline solution (5002)
	approx. 2.41 g/cm3	Superphosphates (11206)
	approx. 2.8 g/cm3	Oil shale, thermal processing waste (943)
	1.505	Sulfite liquors and Cooking liquors, green (386)
Solubility	various values in wide ranges	Superphosphates (11206)
	water solubility approx. 1.4 mg/L	Zeolite, cuboidal, crystalline, synthetic, non-fibrous (11668), Zeolite, silica rich, crystalline, synthetic, non-fibrous (4905)
	water solubility: < 1 g/L	Oil shale, thermal processing waste (943)
Particle size distribution (PSD)	PSD depends on sources and process conditions. Results by the enclosed protocol: D80: 147 - 1568 µm, D50 = 5.16 - 441 µm	Reaction product of lead chloride or lead sulphate with alkaline solution (5002)
	"SSP powder: Particle size (µm) < 1 µm: 0.93%, < 10 µm: 27.3%, < 100 µm: 61.3%, < 1000 µm: 100.0%" "Granulated SSP Granular size (mm) > 5 mm: 3 % max, 1 – 5 mm: 94 %, < 1 mm: 3 % max"	Superphosphates (11206)
	D10 = 1.745 µm, D50 = 6.668 µm and D90 = 19.17 µm	Zeolite, cuboidal, crystalline, synthetic, non-fibrous (11668)
	Typical particle size distribution: D10 = 3.18 µm, D50 = 12.14 µm and D90 = 30.94 µm	Zeolite, silica rich, crystalline, synthetic, non-fibrous (4905)
	"Characteristic values of Sief Reference Samples: d10 value: 0.6 - 0.8 µm; d50 value: 6.5 - 9.4 µm; d90 value: 41.6 - 49.1 µm"	Oil shale, thermal processing waste (943)
Form of the substance	solid powder or slurry	Reaction product of lead chloride or lead sulphate with alkaline solution (5002)
	powder with lumps	Superphosphates (11206), Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc. (4998)
	powder or slurry	Zeolite, cuboidal, crystalline, synthetic, non-fibrous (11668), Zeolite, silica rich, crystalline, synthetic, non-fibrous (4905)
	powder	Materials for reclaim, precious metal production by-products (4994)
	powder or granular	Oil shale, thermal processing waste (943)
	solution	Silver electrolyte (4981)

Substance identity element	Value	Substance identified with the SID element
Crystalline structure	LTA/FAU/SOD/GIS/ANA/KFI/ LTN/PAU/RHO	Zeolite, cuboidal, crystalline, synthetic, non-fibrous (11668)
	MFI/MOR/BEA/CHA/FER/OFF /NES/MEL/EUO/MTT/MTW/M AZ/LOS/TON/LTL	Zeolite, silica rich, crystalline, synthetic, non-fibrous (4905)
Colour	white	Reaction product of lead chloride or lead sulphate with alkaline solution (5002)
	grey	Superphosphates (11206)
	colourless	Zeolite, cuboidal, crystalline, synthetic, non-fibrous (11668), Zeolite, silica rich, crystalline, synthetic, non-fibrous (4905)
	yellowish	Sulfite liquors and Cooking liquors, green (386)

It can be observed, that in addition to the basic substance identity elements (composition, source and manufacturing process), registrants often specified also other substance identity elements to characterise the substances. Especially parameters (conditions) of the manufacturing process, state and form of the substance and particle size distributions were often provided by the registrants, in some cases (rather seldom) registrants also provide information regarding ratios of reactants.

Particularly zeolites were characterised with a high number of substance identity elements, namely parameters (conditions) of the manufacturing process, state and form, particle size distribution, crystalline structure, solubility, colour and melting point.

c) Analytical methods

The following Table 45 and Table 46 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 45 REACH Annex VI analytical methods used by registrants of other complex inorganic substances.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]	Y	Y	Y	Y	Y	Y
5002	Reaction product of lead chloride or lead sulphate with alkaline solution						
11206	Superphosphates	Y	Y	Y			
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous		Y	Y	Y		
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous		Y	Y			
4994	Materials for reclaim, precious metal production by-products						
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.						
943	Oil shale, thermal processing waste		Y				
4981	Silver electrolyte						
386	Sulfite liquors and Cooking liquors, green						

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 46 Other analytical methods used by registrants of other complex inorganic substances in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements				
		XRD	XRF	ICP-OES	AAS	Other
10709	Polysulfides, bis[3-(triethoxysilyl)propyl]					LC-MS
5002	Reaction product of lead chloride or lead sulphate with alkaline solution	Y		Y		Particle size distribution, Specific surface area
11206	Superphosphates	Y	Y	Y		ICP-AES, Elemental chemical analysis, Gravimetry, Granulometry, Differential scanning calorimetry, Calculation of crystalline silica in single superphosphate
11668	Zeolite, cuboidal, crystalline, synthetic, non-fibrous	Y	Y	Y		Scanning electron microscopy
4905	Zeolite, silica rich, crystalline, synthetic, non-fibrous	Y	Y			Gravimetry
4994	Materials for reclaim, precious metal production by-products	Y	Y	Y		
4998	Materials for reclaim, Precious Metals in Bricks, Pots, Crucibles and trays, etc.	Y	Y	Y		Particle size distribution, Specific surface area, Moisture content, Precious metal content determined by fire assay
943	Oil shale, thermal processing waste	Y	Y			Elemental chemical analysis, Loss on ignition
4981	Silver electrolyte			Y		Potentiometric titration
386	Sulfite liquors and Cooking liquors, green			Y		Variable methods not specified in detail

It can be observed that analytical methods explicitly mentioned in Annex VI of REACH are of limited relevance for this group of substances with predominantly inorganic constituents. Only for the substance "Polysulfides, bis[3-(triethoxysilyl)propyl]", the complete set of REACH Annex VI tests was performed by the registrants. Infrared spectroscopy and nuclear magnetic resonance was also used in the cases of superphosphates and zeolites.

For analysis of other substances, X-ray diffraction and X-ray fluorescence together with inductively coupled plasma optical emission spectrometry are the main analytical methods used by registrants for determination of chemical composition of substances in this group.

The set of analytical methods and techniques used for determination of chemical composition of individual substances subject to the screening reflects the nature of the substances.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressed by the following operating consortia and associations:

- FARM REACH consortium – http://www.reachcentrum.eu/consortium/farm-reach-consortium-112.html
- Reconsile REACH Consortium – http://www.reachcentrum.eu/consortium/reconsile-reach-consortium-updated-section-42.html
- Synthetic Zeolites Consortium – http://www.zeolites.be/

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 47 for direct links (where available).

Table 47 Publicly available substance identity profiles of other complex inorganic substances.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
11206	Superphosphates	http://www.reachcentrum.eu/Consortia%20Documents/P-I240/Substance%20Identification%20Profile/P-I240_EC232-379-5_SIP-21_SSP.pdf	Concentrations of main constituents (calcium sulphate and calcium bis(dihydrogenorthophosphate)) and impurities (calcium hydrogenorthophosphate, phosphate rock and orthophosphoric acid)

3.2. Substance identity of complex organic substances

3.2.1. Substances with variability in alkyl chain length

As the title suggests, this is a very broad group of substances including all different types of synthesised or refined chemicals with variability in alkyl chain length and nature (i.e. saturated/unsaturated, branched/linear/cyclic).

It shall be noted that whenever appropriate, substances were assigned to other more specific groups (e.g. petroleum-derived products, oligomers or other suitable groups in each single case). This group of substances therefore includes only substances which do not belong to any other more specific group. Nevertheless, this group of substances remains the most numerous one – with 741 substances, accounting for over 30% of all identified complex substances.

a) Substances screened in this group

The following Table 48 lists substances with variability in alkyl chain length selected for substance identity screening.

Table 48 Substances with variability in alkyl chain length – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed*
		Joint	Indiv.	Total	
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	4	5	9	100
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	20	0	20	100
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	7	0	7	100
353	Fatty acids, C12-18	9	0	9	100
850	Fatty acids, C16-18, zinc salts	22	0	22	91
797-8	Fatty acids, C18-unsatd.	3	1	4	100
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	3	0	3	100
623	Soaps, stocks, vegetable-oil, acidulated	3	0	3	100
7916-7	Acid chlorides, coco	2	1	3	100
7938	Alcohols, C12-14(even numbered), ethoxylated	25	0	25	80
4953	Alcohols, C14-15-branched and linear	3	0	3	100
7954	Alcohols, lanolin	4	0	4	100
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	5	0	5	100
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	15	0	15	100
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	5	0	5	100
745	Fatty acids, C16-18 and C18-unsatd., Et esters	1	0	1	100
366	Fatty acids, C16-18 and C18-unsatd., Me esters	142	0	142	14
437-9	Fatty acids, C5-10, esters with pentaerythritol	5	1	6	100
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. residues	16	0	16	100
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	11	0	11	100
5000	Amides, C16-C18 (even numbered)	4	0	4	100
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	11	0	11	100
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	4	0	4	100
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	2	11	13	100
2682	KOMPLEXSEIFE TH 17[1]	1	2	3	100

* 20 dossiers per substance were analysed as a maximum.

[1] Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide

6 of the screened substances contain besides dossiers from joint submissions also individual submission dossier(s). One of the screened substances was registered by 142 registrants, two substances by more than 20 registrants and the rest by up to 20 registrants.

For the purposes of this project, substances with variability in alkyl chain length have been further divided into the following sub-groups:

1. Acid alkyl derivates
2. Acids and salts
3. Alcohols and chlorides
4. Alkyl derivates
5. Esters
6. Nitrogen derivates
7. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

As presented **in** Table 49, 13 SID elements were used in studied registration dossiers for this group of substances. Substances with variability in alkyl chain length is a group where a low number of SID elements is typically used by registrants to characterise substances (average: 5.2 ± 1.2).

Table 49 Substance identity elements used by registrants in identification of substances with variability in alkyl chain length.

	Acid alkyl derivates			Acids and salts					Alcohols and chlorides				Alkyl derivates		
	1375-8,8448	774	629	353	850	797-8	4260	623	7916-7	7938	4953	7954	578	730	4955
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Parameters of process	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓		✓	✓	✓
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Alkyl chain length	✓	✓	✓	✓	✓	✓				✓	✓		✓	✓	✓
State													✓		
Density		✓	✓											✓	
Viscosity															
Boiling point														✓	
Flash point														✓	
Colour									✓						
*Common characteriser**															
*Other characteriser***						✓	✓							✓	
No. of applied SID elements per substance	5	6	6	5	5	6	5	3	5	5	5	3	6	9	5
Average no. of applied SID elmts. per subgroup	5.7 ± 0.6			4.8 ± 1.1					4.5 ± 1				6.7 ± 2.1		

Table 49 continued

	Esters			Nitrogen derivates				Others		
	366	437-9	1056	4959	5000	4358	5179	1415-25	2682	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process	✓	✓	✓	✓	✓	✓	✓	✓		88
Composition	✓	✓	✓	✓	✓	✓	✓	✓		96
Alkyl chain length	✓	✓		✓	✓	✓	✓			71
State										4
Density										13
Viscosity			✓							4
Boiling point										4
Flash point										4
Colour										4
*Common characteriser**	✓									4
*Other characteriser***			✓			✓		✓	✓	29
No. of applied SID elements per substance	6	5	6	5	5	6	5	5	3	Average = 40
Average no. of applied SID elmts. per subgroup	5.7 ± 0.6			5.3 ± 0.5				4 ± 1.4		

Average no. of applied SID elmts. per group	5.2 ± 1.2

* Common group-specific jargon, in particular: Soaps & Detergent Association Reporting Number (SDA Number) (366).

** Unsaturated fatty acids (797-798), Reaction products (4260, 4358), Residual co-products (730), Residues (1056), Mixture, reaction mass (1415-1425), Reaction mixture (2682)

Note: 25 substances were selected for the substance identity screening, however, the dossier(s) to the substance No. 745 has not been provided.

Comments to Table 49:

- 13 SID elements were used by registrants of the screened substances for identification of substances in this group;

- 13 substances were identified with 5 SID elements, 7 substances with 6 SID elements. Therefore 20 out of the 24 screened substance are rather homogeneous in terms of the number of SID elements used for their identification (5 or 6 SID elements);

- standard deviation linked to the average number of SID elements used by registrants of substances in this group is rather low (1.2) compared to other groups, and the set SID elements used by registrants of different substances in this group is very consistent, indicating that there is a wide consensus among registrants on the way of appropriate identification of substances with variability in alkyl chain length;

- Alkyl chain length is a SID element used for identification of 71 % of the screened substances in this group and furthermore, this SID element is not used in identification of other groups of substances;

- 6 SID elements were only used once for identification of the screened substances, these SID elements are state, viscosity, boiling point, flash point, colour and Soaps & Detergent Association Reporting Number (SDA Number);

Composition

The registrants of the substances subject to the screening most frequently specified composition of the substances providing concentration ranges of individual constituents, together with their typical concentrations. In cases where only one of these two values was provided, concentration ranges were predominant over typical concentrations.

Some registration dossiers include several compositions, due to the following factors:

a) presence of a constituent with relevance for classification and labelling detected in some of the tested samples (and not detected in other samples)

b) different concentrations/ratios of individual constituents in general (without relevance for classification and labelling)

c) describing samples manufactured under different conditions (pressure, distillation temperature, etc.)

Opposed to inorganic substances or coal-derived substances, where multiple compositions were often described in a single registration dossier, studied dossiers of registrants of substances with variability in alkyl chain length included multiple compositions very rarely.

Table 50 Number of compositions specified in registration dossiers by registrants of substances with variability in alkyl chain length.

ID	Name (as registered)	% of No. of compositions		
		1	2	3
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	100		
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	100		
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	100		
353	Fatty acids, C12-18	100		
850	Fatty acids, C16-18, zinc salts	100		
797-8	Fatty acids, C18-unsatd.	100		
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	100		
623	Soaps, stocks, vegetable-oil, acidulated	100		
7916-7	Acid chlorides, coco	66	33	
7938	Alcohols, C12-14(even numbered), ethoxylated	100		
4953	Alcohols, C14-15-branched and linear	100		
7954	Alcohols, lanolin	100		
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	100		
730	Benzene, mono-C10-13-alkyl derivs., distn. residues	94	6	
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	80		20
745	Fatty acids, C16-18 and C18-unsatd., Et esters	Not available*		
366	Fatty acids, C16-18 and C18-unsatd., Me esters	100		
437-9	Fatty acids, C5-10, esters with pentaerythritol	100		
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	83	17	
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	100		
5000	Amides, C16-C18 (even numbered)	100		
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	100		
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	100		
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	100		
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide	100		

Note: Void cells mean zero.

* Registration dossiers have not been provided

Registration dossiers of substances with variability in alkyl chain length contain 1 composition in the vast majority of cases. This is a typical approach applied by registrants of UVCB substances, where the composition often includes constituents with wide concentration ranges, and the compositional variability can therefore be covered within a single composition.

One of the screened substances contained a dossier with 3 compositions. These compositions specified different typical concentrations of some constituents. Concentration ranges were identical in all three compositions. Reasoning for using three different compositions is not provided in the dossier.

Table 51 Number of constituents specified in registration dossiers by registrants of substances with variability in alkyl chain length.

ID	Name (as registered)	No. of constituents
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	11[a]
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	16
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	14
353	Fatty acids, C12-18	10
850	Fatty acids, C16-18, zinc salts	10
797-8	Fatty acids, C18-unsatd.	12
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	7
623	Soaps, stocks, vegetable-oil, acidulated	8
7916-7	Acid chlorides, coco	13[b]
7938	Alcohols, C12-14(even numbered), ethoxylated	31
4953	Alcohols, C14-15-branched and linear	16
7954	Alcohols, lanolin	10[b]
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	12
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	34
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	21
366	Fatty acids, C16-18 and C18-unsatd., Me esters	31
437-9	Fatty acids, C5-10, esters with pentaerythritol	27
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	65
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	20
5000	Amides, C16-C18 (even numbered)	13
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	11
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	14
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	27[c]
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide	3

[a] 3 constituents were specified as impurities
[b] 2 constituents were specified as impurities
[c] 25 constituents were specified as impurities

The highest number of constituents identified in the screened dossiers is 67. For two substances, 30-35 constituents were identified, another 4 substances contained 20 - 27 constituents and the remaining 16 substances contained between 3-16 constituents.

Table 52 Consistency of compositional data provided in the registration dossiers for substances with variability in alkyl chain length.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate				100		
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	50			85	10	
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	71	29				
353	Fatty acids, C12-18				100		
850	Fatty acids, C16-18, zinc salts					95	5
797-8	Fatty acids, C18-unsatd.				100		
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	33					67
623	Soaps, stocks, vegetable-oil, acidulated				100		
7916-7	Acid chlorides, coco				100		
7938	Alcohols, C12-14(even numbered), ethoxylated				100		
4953	Alcohols, C14-15-branched and linear				100		
7954	Alcohols, lanolin	75			25	25	25
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.				60		40
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues			13		13	74
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid				100		
366	Fatty acids, C16-18 and C18-unsatd., Me esters	15	25				60
437-9	Fatty acids, C5-10, esters with pentaerythritol	33				50	17
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	50	44			6	
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	70			10		20
5000	Amides, C16-C18 (even numbered)				100		
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	45		82	18		
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides				100		
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane			100[a]			
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide			100			

Note: void cells mean zero.

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: Numbers in the cells of the table are percentages of dossiers sharing the same composition consistency score. The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

[a] The compositions differ in impurities.

For 15 out of the 24 screened substances, most (but not all) constituents specified by the registrants a substance were identical (score 4). In 10 cases, composition consistency score was 4 for all screened dossiers. Next most frequent approaches were that all constituents specified in the screened dossiers for a single substance were identical with typical registrant-specific concentrations/concentration ranges provided (score 1) followed by the approach where the registrants specified only a single constituent with identical name as the registered substance (score 6).

Table 53 Typical constituents specified in registration dossiers by registrants of substances with variability in alkyl chain length.

ID	Name (as registered)	Typical constituent	
		Name	Concentration [%]
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	C7-9-(branched)-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoate	92 – 100
		C8-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	55 – 100
		C9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	0 – 35
		C7-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	0 – 35
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	Sodium dodecyl sulfate	45 – 80
		Sodium tetradecyl sulfate	15 – 55
		Sodium hexadecyl sulfate (CAS 1-Hexadecanol, 1-(hydrogen sulfate), sodium salt (1:1))	0 – 10
		Sodium sulfate	0 – 10
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	Sodium dodecyl sulfate	1 – 80
		Sodium tetradecyl sulfate	1 – 55
		Sodium hexadecyl sulfate (CAS 1-Hexadecanol, 1-(hydrogen sulfate), sodium salt (1:1))	0 – 60
		Sodium octadecyl sulfate	0 – 60
		Sodium sulfate	0 – 10
353	Fatty acids, C12-18	Lauric acid	45 – 65
		Myristic acid	5 – 30
		Palmitic acid	5 – 50
		Stearic acid	0 – 60
850	Fatty acids, C16-18, zinc salts	Zinc dipalmitate	22 – 80
		Zinc distearate	20 – 99
		Fatty Acids, <C16, zinc salts - Fatty Acids, zinc salts from natural origin with c chain length below C 16, e.g. C14 or C12	0 – 6
		Fatty Acids, >C18, zinc salts / Fatty Acids, >C18, zinc salts - Fatty Acids, zinc salts from natural origin with c chain length above C 18, e.g. C20 or C22	0 – 5
797-8	Fatty acids, C18-unsatd.	Palmitic acid	0 – 9
		Stearic acid	0 – 20
		Oleic acid	70 – 10
		Linoleic acid	0 – 20
		Linolenic acid	0 – 5

ID	Name (as registered)	Typical constituent	
		Name	Concentration [%]
		Icosanoic acid	0 – 5
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	Fatty acids, tall-oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts	0 – 100
		Rosin, maleated	30 – 35
		Rosin	35 – 40
		Fatty acids, tall oil	20 – 25
623	Soaps, stocks, vegetable-oil, acidulated	Glycerides, vegetable-oil	20 – 80
		Fatty acids, vegetable-oil	20 – 80
		Fatty acids, vegetable-oil, Me esters	1 – 5
		Fatty acids, vegetable-oil, esters with sterols, mixed with vegetable-oil glycerides (Plantsterol esters)	0 – 3
		Unsaponifiable matter, vegetable-oil	0 – 10
7916-7	Acid chlorides, coco	dodecanoyl chloride	30 – 70
		tetradecanoyl chloride	10 – 30
		hexadecanoyl chloride	0 – 20
		octadecanoyl chloride	0 – 25
		octadec-9-enoyl chloride	0 – 25
		octanoyl chloride	0 – 15
		decanoyl chloride	1 – 15
7938	Alcohols, C12-14(even numbered), ethoxylated	Dodecanol, 1EO /Dodecan-1-ol, ethoxylated	35 – 65
		Dodecanol 2EO /2-(2-(dodecyloxy)ethoxy)ethanol	11.4 – 16.9
		Docecanol 3EO / 2-(2-(2-(dodecyloxy)ethoxy)ethoxy)ethanol	5 – 10.2
		dodecan-1-ol	10 – 40
		tetradecan-1-ol	0 – 18
		Tetradecanol 2EO /Tetradecan-1-ol, ethoxylated	10 – 40
		hexadecan-1-ol	0 – 5
4953	Alcohols, C14-15-branched and linear	tetradecan-1-ol	3 – 52
		Pentadecanol, branched and linear	25 – 55
		2-methyltridecan-1-ol	4 – 17
		2-ethyldodecan-1-ol	0 – 9
		2-propyldodecan-1-ol	0 – 5
7954	Alcohols, lanolin	cholesterol/ cholest-5-en-3-ol	0 – 40
		(20R)-cholesta-3,5-dien-7-one	0 – 20
		Dihydrolanosterol/ (3β)-lanost-8-en-3-ol / 4,4,14-Trimethyl-5α-cholesta-8-ene-3β-ol	0 – 10
		Lanosterol/ (3β, 20R)-lanosta-8,24-dien-3-ol/ lanosta-8,24-dien-3-ol	3 – 20
		Unidentified long chain and sterol alcohols	38 – 95
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	3-hexadec-1-en-1-yldihydrofuran-2,5-dione	3 – 97
		3-octadec-1-en-1-yldihydrofuran-2,5-dione	3 – 97
		IUPAC Not applicable (UVCB substance, mixture of numerous isomers)/ 2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	100
		IUPAC Not applicable - UVCB substance, mixture of numerous isomers / Iso C15-20 Alkenyl Succinic Anhydrides	80 – 98
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	Benzene, mono-C10-13-alkyl derivs., distn. residues / Benzene, mono-C10-13-alkyl derivs., distn. Residues	97 – 100
		Dialkyl benzenes	80 – 95
		alkyl-benzene isomers	82.6 – 93.9
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	Group of constituents (alkyl derivatives) in Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	55 – 81
		Sodium glycolate	0 – 15
		sodium chloride	10 – 30
		Water	0 – 10
		Unknown impurities	0 – 5

ID	Name (as registered)	Typical constituent	
		Name	Concentration [%]
366	Fatty acids, C16-18 and C18-unsatd., Me esters	UVCB substance, no IUPAC name avalilable / Fatty acids, C16-18 and C18-unsatd., Me esters	99
		Esters	99.52 – 99.82
		Mehtyl Hexadecanoate / methyl palmitate	0 – 62
		Methyl (Z)-octadec-9-enoate / Methyl Oleate	13 – 95
		methyl (9Z,12Z)-octadeca-9,12-dienoate / Methyl Linoleate	1 – 40
		Other constituents	14.7
437-9	Fatty acids, C5-10, esters with pentaerythritol	Reaction products of fatty acids C5-C10 linear saturated and pentaerythritol	84 – 99
		Reaction products of fatty acids C5-C10 linear saturated and pentaerythritol (minor constituent)	1 – 16
		2,2-bis[[(1-oxoheptyl)oxy]methyl]propane-1,3-diyl bisheptanoate	4 – 12
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	not available UVCB / Fatty acids, C6-C24 and C6-C24 Unsatd. , Me esters	2 – 60
		Not applicable / Free fatty acids	0 – 60
		Polymers	0 – 15
		Glycerides	0 – 95
		glycerides, C16-18 and C18 unsatd. mono and di-	0 – 60
		Fatty acids, vegetable-oil, Me esters	0 – 50
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	N-(carboxymethyl)-3-(dodecanoylamino)-N,N-dimethylpropan-1-aminium hydroxide	35 – 65
		N-(carboxymethyl)-N,N-dimethyl-3-(tetradecanoylamino)propan-1-aminium hydroxide	10 – 26
		{dimethyl[3-(palmitoylamino)propyl]ammonio}acetate	3 – 16
		N-(carboxymethyl)-N,N-dimethyl-3-(stearoylamino)propan-1-aminium hydroxide	2 – 24
		sodium chloride	5 – 20
5000	Amides, C16-C18 (even numbered)	stearamide / Octadecanamide	40 – 100
		palmitamide / Hexadecanamide	19.4 – 60
		myristamide / tetradecanamide	0 – 2.5
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	DETA I / 2-{2-[(8Z)-heptadec-8-en-1-yl]-4,5-dihydro-1H-imidazol-1-yl}ethanamine	0 – 70
		DETA AI / (9Z)-N-(2-{2-[(8Z)-heptadec-8-en-1-yl]-4,5-dihydro-1H-imidazol-1-yl}ethyl)octadec-9-enamide	0 – 80
		DETA A / (9Z)-N-{2-[(2-aminoethyl)amino]ethyl}octadec-9-enamide	0 – 30
		DETA AA - C18unsat / N,N'-(iminodiethane-2,1-diyl)di-C18 unsaturated-alkylamide	0 – 60
		N-(2-aminoethyl)ethane-1,2-diamine //2,2'-iminodi(ethylamine)	0 – 10
		Fatty acid / Undefined, group of substances	0 – 10
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	N-Benzyl-N,N-dimethyl-1-hexadecanaminium chloride / cetalkonium chloride / benzenemethanaminium, N-hexadecyl-N,N-dimethyl-, chloride	10 – 75
		benzyldimethyl(octadecyl)ammonium chloride / benzenemethanaminium, N,N-dimethyl-N-octadecyl-, chloride	10 – 75
		miristalkonium chloride/ benzenemethanaminium, N,N-dimethyl-N-tetradecyl-, chloride	0 – 10
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-	Bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate // Decanedioic acid, 1,10-bis[2,2,6,6-tetramethyl-1-(octyloxy)-4-piperidinyl] ester	65 – 85
		1,8-Bis((2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)decane-1,10-dioyl)piperidin-1-yl)oxy)octane	5 – 25
		non-specified impurities	0 – 5
		tert-butyl hydroperoxide	0 – 5
		Octane	0 – 5
		2-methylpropan-2-ol	0 – 8
		bis(2,2,6,6-tetramethylpiperidin-4-yl) sebacate // bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate	0 – 8

ID	Name (as registered)	Typical constituent	
		Name	Concentration [%]
	yl)oxy]octane		
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide	Dibariumsebacate // Decanoic acid, barium salt (1:1)	51.5 – 53.5
		Barium salt of sebacic acid stearylamide	38.7 – 40.7
		Sebacic acid distearylamide // Decanediamide, N,N'-dioctadecyl-	6.8 – 8.8

In some cases registrants use an approach of specifying a generic constituent which is then broken down into several more specific constituents. Concentration ranges specified in the screened dossiers were often very wide (often intervals of tens of percent), indicating high compositional variability among dossiers for a single substance. This variability is likely to be closely linked to the nature of the processes used for manufacturing of these substances for which separation of individual substances with a single alkyl chain length and constitution is an issue.

Source

Substances in this group include mostly chemically modified products of various natural sources. Sources provided by the registrants in the registration dossiers include vegetable oils, fatty acids, fatty alcohols, biodiesel, etc.

Dossiers submitted by registrants of the screened substances always included very similar information on the source of each substance (only described in more general/specific manner in some cases, e.g. "fat" vs. "triglycerides" vs. "oils and fats (triglycerides)", the only exception being the substance "reaction mass of isomers of C7-9-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate"), where it is not quite clear whether the submitted dossiers described different sources in the submitted separate joint/individual submissions

The information in the studied dossiers indicate that source is closely linked to manufacturing process, i.e. different sources require different processing steps.

Since there is an indication that different sources typically require different processing, source is unlikely to provide unambiguous characterisation of substances in this group without information on the manufacturing process.

Table 54 Sources of substances with variability in alkyl chain length as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	• 3-(3,5-Di-tert-butyl-4-hydroxy phenyl)-propionic acid-methylester (Metilox, CAS 6386-38-5) and isooctanol • PP-base, iso-octanol, zinc octanoate
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	• Fatty alcohols
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	• Fatty alcohols
353	Fatty acids, C12-18	• Triglycerides, Fat, Oils and fats, Oleochemicals, Vegetable oils
850	Fatty acids, C16-18, zinc salts	• Fatty acids
797-8	Fatty acids, C18-unsatd.	• Oils and fats (triglycerides) • Fractionated rape fatty acids
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	• Tall oil fatty acids and Rosin
623	Soaps, stocks, vegetable-oil, acidulated	• Vegetable oil
7916-7	Acid chlorides, coco	• Fatty acids/Organic acids • Cocoyl alcohol
7938	Alcohols, C12-14(even numbered), ethoxylated	• (Fatty) alcohols C12-C14
4953	Alcohols, C14-15-branched and linear	• Olefins (alkenes) • Syngas
7954	Alcohols, lanolin	• Wool grease/Lanolin
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	• Linear Alpha Olefin (LAO)/Linear internal olefins (LIO)
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	• Olefin, Chloroparaffin
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	• 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-17 odd-numbered, C17-unsatd. alkyl) derivs., aminoamide
366	Fatty acids, C16-18 and C18-unsatd., Me esters	• natural oils
437-9	Fatty acids, C5-10, esters with pentaerythritol	• linear C5, branched C5, linear C7, linear C8 and linear C10 fatty acids • fatty acids (C7, C8/10 and 2-ethylhexanoic acid (heptanoic, octanoic, decanoic and 2 ethylhexanoic acids) • n-decanoic, n-heptanoic, n-octanoic and n-valeric acids
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	• FAME/biodiesel
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	• Coconut oil, Amides
5000	Amides, C16-C18 (even numbered)	• C18-C18, even Fatty acids/Fatty acid
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	• fatty acids/tall oil fatty acid (TOFA)/C18 unsatd. fatty acids • Acids (not specified)
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	• Dimethylalkylamines
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	• Bis(2,2,6,6,-tetramethyl-4-piperidinyl) decanedioate
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide	• Oils

Manufacturing process and its parameters (conditions)

As indicated in the previous section, the information from the studied dossiers document that the manufacturing process is closely related to the particular source of the substance. Together with source, manufacturing process (and the conditions of the manufacturing process) is therefore one of the key substance identity elements necessary for characterisation of substances with variability in alkyl chain length.

It has not been observed that different manufacturing processes could be applied to a single source leading to a substance allowing registration in a single joint submission, i.e. no cases of substances with the same source where part of the dossiers described a different manufacturing process than other dossiers for that substance.

Parameters (conditions) of the manufacturing process have been provided in by registrants of substances with variability in alkyl chain length in a majority of cases, indicating that together with process and source, conditions of the manufacturing process are the key elements determining the composition of resulting substances and therefore also vital for assessment of substance sameness. The level of detail of the manufacturing process description was highly variable in the studied dossiers. Some registrants provided only information regarding identity of the reaction agents, while others specify also their molar rations, reaction times and temperatures, used catalysts and other information describing the manufacturing process.

Most frequently, the registrants specified the reaction/process temperature. Other process conditions specified in some of the studied registration dossiers include reaction pressure, specification of the reaction agents (sometimes also with their molar ratio), specification of catalysts, reaction time and pH.

Many manufacturing process descriptions in this group report a chemical reaction (e.g. esterification, neutralisation, saponification).

It has not been observed that different parameters (conditions) of a single manufacturing process with a single source would lead to different substance registration submissions, there were no cases where a single source specified in dossiers for a single substance would include

Table 55 Manufacturing processes of substances with variability in alkyl chain length as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	• trans esterification
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	• Sulphation, Neutralisation
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	• Sulphation, Neutralisation
353	Fatty acids, C12-18	• Splitting – hydrolysis, Hydrogenation, Distillation, Fractionation
850	Fatty acids, C16-18, zinc salts	• Reaction with ZnO, Reaction with NaOH and reaction with zinc salts
797-8	Fatty acids, C18-unsatd.	• Hydrolysis (splliting), hydrogenation, fractionation
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	• Diels-Alder reaction with maleic anhydride • Salification (Ca(OH)2, ZnO, MgO)
623	Soaps, stocks, vegetable-oil, acidulated	• Treatment with alkali and water, acidulation and subsequent separation of the aqueous fraction
7916-7	Acid chlorides, coco	• Phosgenation, Chlorination by PCl3
7938	Alcohols, C12-14(even numbered), ethoxylated	• Ethoxylation
4953	Alcohols, C14-15-branched and linear	• Hydroformylation
7954	Alcohols, lanolin	• Saponification

ID	Name (as registered)	Manufacturing process
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	• "ene" reaction - reaction with Maleic Anhydride (MA)
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	• Alkylation
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	• Reaction with chloroacetic acid
366	Fatty acids, C16-18 and C18-unsatd., Me esters	• Transesterification
437-9	Fatty acids, C5-10, esters with pentaerythritol	• Esterification
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	• vacuum distillation
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	• 1. reaction with DMAPA • 2. reaction with monochloroacetic acid/sodium chloroacetate
5000	Amides, C16-C18 (even numbered)	• reaction with ammonia
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	• 1a. reaction with DETA (condensation, amidation) • 1b. reaction with amine(s) - (not specified) • 2. dehydratation
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	• reaction with benzylchloride
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	• Bis(2,2,6,6,-tetramethyl-4-piperidinyl) decanedioate
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide	• neutralisation reaction

Additional substance identity elements

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Table 56 Additional substance identity elements used by the registrants of the screened substances.

Substance identity element	Value	Substance identified with the SID element
State	Liquid	• 2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.
Density	≥ 400 g/L < 400 g/L (different classification)	• Sulfuric acid, mono-C12-14-alkyl esters, sodium salts • Sulfuric acid, mono-C12-18-alkyl esters, sodium salts
	0.865	• Benzene, mono-C10-13-alkyl derivs., distn. residues
Viscosity	503,2 mm2/s	• Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. residues
Boiling point	370-420°C	• Benzene, mono-C10-13-alkyl derivs., distn. Residues
Flash point	186°C	• Benzene, mono-C10-13-alkyl derivs., distn. Residues
Colour	American Public Health Association (APHA) color standard 15	• Acid chlorides, coco

Another key element in identification of substances with variability in alkyl chain length is the description of the alkyl chain length and nature. In accordance with the

Guidance for identification and naming of substances under REACH and CLP published by ECHA as well as the OECD Guidance for characterising oleochemical substances for assessment purposes[21], many of the registered substances include alkyl descriptors, functionality descriptors and salt descriptors already in their registered name or in the names of individual constituents.

These descriptors characterise the length of the carbon chain (e.g. C12 - 14, optionally further specified as even numbered or odd numbered), saturation (saturated or unsaturated), structure (linear or branched), identity of a functional group (e.g. fatty acids, amides, acidulated, ethoxylated, Me esters, etc.), position of the functional group and identity of a cation/anion of any salt present in the substance (e.g. sodium salt, zinc salt, etc.).

c) Analytical methods

Table 57 and Table 58 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 57 REACH Annex VI analytical methods used by registrants of substances with variability in alkyl chain length.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	Y	Y	Y		Y	Y
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	Y	Y	Y		Y	Y
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	Y	Y	Y	Y	Y	Y
353	Fatty acids, C12-18	Y	Y	Y			Y
850	Fatty acids, C16-18, zinc salts	Y	Y	Y			Y
797-8	Fatty acids, C18-unsatd.	Y	Y	Y			Y
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	Y	Y	Y		Y	
623	Soaps, stocks, vegetable-oil, acidulated	Y	Y	Y			Y
7916-7	Acid chlorides, coco	Y	Y	Y			Y
7938	Alcohols, C12-14(even numbered), ethoxylated	Y	Y	Y		Y	Y
4953	Alcohols, C14-15-branched and linear	Y	Y	Y			Y
7954	Alcohols, lanolin	Y	Y	Y			Y
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	Y	Y	Y		Y	Y
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	Y	Y	Y		Y	Y
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	Y	Y	Y	Y	Y	Y
366	Fatty acids, C16-18 and C18-unsatd., Me esters	Y	Y	Y			Y
437-9	Fatty acids, C5-10, esters with pentaerythritol	Y	Y	Y			Y
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	Y	Y	Y			Y
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	Y	Y	Y	Y	Y	Y

[21] http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)6&doclanguage=en

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
5000	Amides, C16-C18 (even numbered)	Y	Y	Y		Y	Y
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	Y	Y	Y		Y	Y
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	Y	Y	Y	Y	Y	Y
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	Y	Y	Y	Y	Y	Y
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide		Y				Y
	Percentage of use of analytical methods (%)	96	100	96	21	54	96

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 58 Other analytical methods used by registrants of substances with alkyl chain length in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements
1375-8, 8448	Reaction mass of C7-9-alkyl 3-(3,5-di-trans-butyl-4-hydroxyphenyl)propionate	
774	Sulfuric acid, mono-C12-14-alkyl esters, sodium salts	KF titration, Titration, ICP-AES, Ion exchange chromatography
629	Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	KF titration, Titration, ICP-AES, Ion exchange chromatography, Unsulfated part PE-extraction
353	Fatty acids, C12-18	
850	Fatty acids, C16-18, zinc salts	XRD, AAS, ICP-AES, KF titration, Loss on drying, Content of free fatty acids, Titration, Differential scanning calorimetry
797-8	Fatty acids, C18-unsatd.	GPC/SEC, Elemental analysis
4260	Fatty acids, tall oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts, consisting of mainly calcium, magnesium, zinc salts of maleated rosin, fatty acids and rosin.	
623	Soaps, stocks, vegetable-oil, acidulated	KF titration, HPSEG (High Performance Size Exclusion Chromatography), Free Fatty Acid content, FAME analysis, Unsaponifiable matter analysis
7916-7	Acid chlorides, coco	AAS
7938	Alcohols, C12-14(even numbered), ethoxylated	Water content, Titration - OH value, PEG (Polyethylene glycol) content, Head space ethylene oxide + Dioxane, C-Distribution and ethylene oxide-degree
4953	Alcohols, C14-15-branched and linear	
7954	Alcohols, lanolin	
578	2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	GPC
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	
4955	Reaction products of 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-(C7-C17 odd-numbered, C17-unsatd. alkyl) derivs. and sodium hydroxide and chloroacetic acid	KF Titration
366	Fatty acids, C16-18 and C18-unsatd., Me esters	
437-9	Fatty acids, C5-10, esters with pentaerythritol	
1056	Fatty acids, C6-24 and C6-24-unsatd., Me esters, distn. Residues	GPC, Determination of heavy metals, Sulphur content, Chlorine conten, CHNO content, Dynamic viscosity, Kinematic viscosity, Saponification value, Simulated distillation
4959	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-C8-18(even numbered) acyl derivs., hydroxides, inner salts	Titration – water, Titration - sodium chloride, Titration – glycerol, Thin Layer Chromatography

ID	Name (as registered)	Additional analytical techniques and measurements
5000	Amides, C16-C18 (even numbered)	Potenziometric titration, Alkalimetric titration
4358	Fatty acids, C18 unsat, reaction products with diethylenetriamine	GPC, Titration
5179	Quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides	Titration
1415-25	A mixture of: bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate; 1,8-bis[(2,2,6,6-tetramethyl-4-((2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-decan-1,10-dioyl)piperidin-1-yl)oxy]octane	KF Titration
2682	Reaction mixture of hydrogenated tallow alkyl amines with sebacic acid and barium hydroxide	

It can be observed that analytical methods explicitly mentioned in Annex VI of REACH are essential for this group of substances. Among these, Ultraviolet-visible spectroscopy, Infrared spectroscopy, Nuclear magnetic resonance spectroscopy and gas chromatography have been used in identification of a vast majority of the studied substances. High-performance liquid chromatography was used to determine composition of ca. 50 % of the studied substances, while mass spectrometry was performed to characterise the substances in only a few cases.

In addition to the analytical methods explicitly mentioned in Annex VI of REACH, the registrants often used also other analytical methods and techniques to determine the composition of the registered substances, especially various titration methods (Karl Fischer titration most frequently). Other methods used by the registrants of the studied substances are summarised in the table above.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressed by the following operating consortia and associations:

- Fatty Acids Consortium (FATAC) – http://www.fatac.co.uk/
- Zinc salts of fatty acids Consortium – https://chemicalwatch.com/4283/zinc-salts-of-fatty-acids-consortium
- EBB Biodiesel REACH Consortium – http://www.ebb-eu.org/reach/
- Linear Alkyl Benzene (LAB) & Derivatives REACH Consortium – http://www.reachcentrum.eu/consortium/linear-alkyl-benzene-lab-derivatives-reach-consortium-131.html
- APAG - The European Oleochemicals and Allied Products Group - http://www.apag.org/
- Higher Olefins and Poly Alpha Olefins REACH Consortium (HOPA) - http://www.hopaconsortium.com/
- Hydrocarbon Solvents Producers Association (HSPA) - http://www.reachcentrum.eu/consortium/hydrocarbon-solvents-reach-consortium-122.html

It shall also be noted that some of the substances in this group fall under the scope of OECD guidance for characterising oleochemical substances for assessment purposes publicly available at http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)6&doclanguage=en

Some substances in this group fall under the scope of a guidance prepared by the Hydrocarbon Solvent Producers Association and OECD in collaboration with ECHA for hydrocarbon solvents publicly available at http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2015)52&doclanguage=en.

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 25 for direct links (where available).

Table 59 Publicly available substance identity profiles of substances with variability in alkyl chain length.

ID	Name (as registered)	Link to SIP(s)	Identity /sameness based on
730	Benzene, mono-C10-13-alkyl derivs., distn. Residues	http://www.reachcentrum.eu/Consortia%20Documents/P-I268/Substance%20Identification%20Profile/P-I268_EC284-660-7_SIP.pdf	Carbon ranges C10, C11, C12, C13, C14, C15 ranges

3.2.2. Petroleum-derived substances

This large group of substances includes various products from processing of petroleum. There were 517 complex petroleum-derived substances identified in this study, accounting for ca. 21% of all identified complex substances.

Substances in this group often have variability in alkyl chain lengths, however, as mentioned in section 3.2.1, substances clearly derived from petroleum based on publicly available information were assigned to this group of substances rather than a more generic group of substances with variability in alkyl chain length.

Besides being variable, chemical composition of petroleum-derived substances often remains unknown to some extent, mainly determined by the source and origin of raw materials.

a) Substances screened in this group

The following Table 60 lists petroleum-derived substances selected for substance identity screening.

Table 60 Petroleum-derived substances – 59 substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% of dossiers analysed
		Joint	Indiv.	Total	
770	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	38	0	38	53
432	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	58	0	58	34
197	Sulfonic acids, petroleum, calcium salts	8	0	8	100
8155	Asphalt	79	0	79	25
8156	Asphalt, oxidized	67	0	67	30
229	Residues (petroleum), vacuum	64	0	64	31
4213-4	Butene, homopolymer (products derived from butene)	2	1	3	100
9193-4	Dodecene, branched	2	1	3	100
569-570	Extracts (petroleum), solvent-refined heavy paraffinic distillate solvent	9	1	10	100
415-420	Fuels, diesel	249	2	251	8
234-7	Gas oils (petroleum), light vacuum	66	0	66	30
466-9	Fuel oil, residual	180	0	180	11
230-3	Gas oils (petroleum), heavy vacuum	89	0	89	22
250	Residues (petroleum), hydrocracked	37	0	37	54
506-7	Residues (petroleum), light vacuum	8	1	9	100
73-4	Kerosine (petroleum)	169	0	169	12
314-7	Solvent naphtha (petroleum), heavy arom.	15	0	15	100
476-480	Hydrocarbons, C5-rich	27	1	28	71
634	Naphtha (petroleum), catalytic reformed	60	0	60	33
214	Naphtha (petroleum), full-range straight-run	114	0	114	18
251	Distillates (petroleum), heavy hydrocracked	13	0	13	100
287	Distillates (petroleum), hydrotreated heavy paraffinic	67	0	67	30
693	Lubricating oils	33	0	33	61
670	Lubricating oils, used	7	0	7	100
4983-4	Alkenes, C11-12	2	1	3	100
4560	Alkenes, C20-24 alpha	1	0	1	100
7973	Alkenes, C20-24 α-	6	0	6	100

ID	Name (as registered)	No. of registrants			% of dossiers analysed
		Joint	Indiv.	Total	
7979-80	Alkenes, C8-10-branched, C9-rich	10	0	10	100
7959	Alkanes, C12-26-branched and linear	2	0	2	100
4794	Hydrocarbons, C10-14 (even numbered), n-alkanes, isoalkanes, <2% aromatic	3	0	3	100
4780	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	7	0	7	100
4859	Hydrocarbons, C11-C14, isoalkanes, cyclics, <2% aromatics	3	0	3	100
4835	Hydrocarbons, C11-C14, n-alkanes, <2% aromatics	3	0	3	100
4766	Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	2	0	2	100
4872	Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	1	0	1	100
4768	Hydrocarbons, C14-C17, n-alkanes, <2% aromatics	4	0	4	100
4864	Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	5	0	5	100
4790	Hydrocarbons, C14-C19, isoalkanes, cyclics, <2% aromatics	2	0	2	100
4945	Hydrocarbons, C14-C20 (even numbered), n-alkanes, isoalkanes, <2% aromatics	1	0	1	100
4779	Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, <2% aromatics	6	0	6	100
4892	Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	5	0	5	100
4839	Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich	17	0	17	100
4783	Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	12	0	12	100
4342	Renewable hydrocarbons (diesel type fraction)	3	0	3	100
284	Paraffin waxes (petroleum), hydrotreated	24	0	24	83
68-9	Paraffin waxes and Hydrocarbon waxes	55	0	55	36
632	Gases (petroleum), light steam-cracked, butadiene conc.	23	0	23	87
473	Hydrocarbons, C2-4, C3-rich	6	0	6	100
475	Hydrocarbons, C4, ethylene-manuf.-by-product	27	0	27	74
891-2	Hydrocarbons, C4, steam-cracker distillate	31	0	31	65
495-6	Distillates (petroleum), steam-cracked, C8-12 fraction	26	0	26	77
224	Distillates (petroleum), heavy paraffinic	20	0	20	100
297	Foots oil (petroleum)	16	0	16	100
7961	Alkanes, C14-17, chloro	12	0	12	100
605	Distillates (petroleum), heavy straight-run	20	0	20	100
4438	Hydrogenated dimerization products of 1-decene, 1-dodecene and 1-octene	2	0	2	100
10300	Naphthenic acids	3	0	3	100
5348*	*Not Applicable (petroleum product)*	12	0	12	0
4289	Reaction products of 1-decene and 1-dodecene, hydrogenated	2	0	2	100

* Registration dossiers have not been provided

For the purposes of this project, petroleum-derived substances have been further divided into the following sub-groups, based on the grouping introduced by CONCAWE (European Petroleum Refiners Association):

1. Alkyl aryl sulphonic acids, sulphonates
2. Bitumen, modified asphalt
3. Butylene oligomers
4. Distillate and residual aromatic extracts (untreated/treated)
5. Gas oils and distillate fuels
6. Fuel oils and heavy residues
7. Kerosines
8. Low boiling point naphthas (gasolines)
9. Lubricating oils, greases, base oils, petrolatums
10. Olefins
11. Other hydrocarbons (aliphatics, cyclic, aromatics)
12. Paraffin and hydrocarbon waxes, slack waxes
13. Petroleum gases
14. Resin Oils & alkenes
15. Foot oils
16. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

Seven substances contain dossiers from individual registration submissions. One of the screened substances is registered by 251 registrants, which is the highest number among all substances screened in this study. 4 substances in this group are registered by more than 100 registrants, 9 substances by 50-100 registrants and 26 substances by less than 10 registrants. 65% of substances with less than 10 registrants were registered with a provisional List number (i.e. not with an EC number).

Twenty-two substances contain more than 20 dossiers and therefore not all of them were screened in the study.

b) Substance identity elements

Table 61 Substance identity elements used by registrants in identification of petroleum-derived substances.

	Alkyl aryl sulphonic acids, sulphonates			Bitumen, modified asphalt			Butylene oligomers		Distillate and residual aromatic extracts	Gas oils and distillate fuels		Fuel oils and heavy residues			
	770	432	197	8155	8156	229	4213-4	9193-4	569-70	415-20	234-7	466-9	230-3	250	506-7
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Parameters of process	✓	✓					✓								
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Alkyl chain length	✓	✓													
Carbon number range				✓	✓	✓									
State			✓		✓										
Density					✓	✓			✓	✓	✓	✓		✓	✓
Viscosity			✓	✓	✓	✓			✓	✓	✓	✓	✓	✓	✓
Boiling point					✓	✓			✓	✓	✓	✓	✓	✓	✓
Flash point				✓	✓	✓			✓	✓		✓	✓		✓
Colour					✓										
*Other characteriser**							✓								
No. of applied SID elements per substance	5	5	5	6	10	8	5	3	7	7	6	7	6	6	7
Average no. of applied SID elmts. per subgroup	5 ± 0			8 ± 2			4 ± 1.4		7	6.5 ± 0.7		6.5 ± 0.6			

Table 61 continued

	Kerosines		Low boiling point naphthas (gasolines)			Lubricating oils, greases, base oils, petrolatums				Olefins			
	73-74	314-7	476-80	634	214	251	287	693	670	4983-4	4560	7973	7979-80
Source	✓	✓	✓	✓		✓	✓			✓	✓	✓	✓
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Parameters of process		✓				✓				✓	✓	✓	✓
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Alkyl chain length													
Carbon number range		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
State													
Density	✓		✓		✓	✓	✓	✓					
Viscosity	✓				✓	✓		✓					
Boiling point	✓	✓	✓		✓	✓	✓	✓					✓
Flash point		✓			✓	✓	✓	✓					
Colour													
*Other characteriser**													
No. of applied SID elements per substance	6	7	6	4	7	9	7	7	3	5	5	4	5
Average no. of applied SID elmts. per subgroup	6.5 ± 0.7		5.7 ± 1.5			6.5 ± 2.5				4.8 ± 0.5			

Table 61 continued

	Other hydrocarbons (aliphatics, cyclic, aromatics)														
	4794	4780	4859	4835	4766	4872	4768	4864	4790	4945	4779	4892	4839	4783	4342
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Parameters of process	✓	✓	✓	✓	✓		✓	✓			✓		✓	✓	✓
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Alkyl chain length															
Carbon number range	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
State															
Density													✓		
Viscosity															
Boiling point	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	
Flash point															
Colour															
*Other characteriser**															
No. of applied SID elements per substance	6	6	6	6	6	5	6	6	5	5	6	4	7	6	5
Average no. of applied SID elmts. per subgroup	5.7 ± 0.7														

Table 61 continued

	Paraffin and hydrocarbon waxes, slack waxes		Petroleum gases				Resin oils & alkenes	Foot oils		Others					
	284	68-69	632	473	475	891-2	495-6	224	297	7961	605	4438	10300	4289	% availability
Source	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	93
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process	✓		✓		✓		✓			✓		✓	✓		47
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Alkyl chain length										✓					5
Carbon number range	✓	✓			✓	✓	✓	✓	✓		✓		✓		65
State															4
Density	✓							✓	✓	✓	✓				35
Viscosity	✓								✓	✓	✓				33
Boiling point	✓	✓					✓	✓	✓		✓		✓		65
Flash point	✓	✓						✓		✓					30
Colour															2
*Other characteriser**												✓		✓	5
No. of applied SID elements per substance	9	5	4	3	5	4	6	7	7	8	7	5	6	4	Average = 45
Average no. of applied SID elmts. per subgroup	7 ± 2.8		4 ± 0.8				6	7 ± 0		6 ± 1.6					

Average no. of applied SID elmts. per group	5.8 ± 1.4

* homopolymer (4213 – 4214), hydrogenated dimerization products (4438), reaction products (4289)

Comments to Table 61:

- 13 SID elements were used by registrants of the screened substances for identification of substances in this group;

- For 17 substances, more than 7 SID elements were specified. The highest number of SID elements used for identification of a single substance was 10, the lowest number being 3.

- some SID elements often specified for petroleum-derived substances are vital for hazard classification (e.g. flash point, boiling point, viscosity)

Composition

Unlike in other groups of substances, the registrants of the petroleum-derived substances subject to the screening most frequently specified composition of the substances providing typical concentrations of individual constituents, without specifying concentration ranges. This observation applies especially to heavy distillation fractions. Registrants of light distillation fractions (low boiling point naphthas (gasolines), petroleum gases, etc.) typically provided both values, i.e. typical concentrations of individual constituents as well as concentration ranges of individual constituents.

The following tables document the number of identified constituents in the screened registration dossiers and the consistency of compositional data provided therein.

Table 62 Number of constituents specified in registration dossiers by registrants of petroleum-derived substances.

ID	Name (as registered)	No. of constituents
770	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	31
432	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	30
197	Sulfonic acids, petroleum, calcium salts	5
8155	Asphalt	7
8156	Asphalt, oxidized	8
229	Residues (petroleum), vacuum	9
4213-4	Butene, homopolymer (products derived from butene)	9
9193-4	Dodecene, branched	2
569-570	Extracts (petroleum), solvent-refined heavy paraffinic distillate solvent	12
415-420	Fuels, diesel	9
234-7	Gas oils (petroleum), light vacuum	8
466-9	Fuel oil, residual	5
230-3	Gas oils (petroleum), heavy vacuum	9
250	Residues (petroleum), hydrocracked	9
506-7	Residues (petroleum), light vacuum	12
73-4	Kerosine (petroleum)	9
314-7	Solvent naphtha (petroleum), heavy arom.	54
476-480	Hydrocarbons, C5-rich	27
634	Naphtha (petroleum), catalytic reformed	20
214	Naphtha (petroleum), full-range straight-run	14
251	Distillates (petroleum), heavy hydrocracked	7
287	Distillates (petroleum), hydrotreated heavy paraffinic	12[a]
693	Lubricating oils	20
670	Lubricating oils, used	2[a]
4983-4	Alkenes, C11-12	6
4560	Alkenes, C20-24 alpha	4
7973	Alkenes, C20-24 α-	9[b]
7979-80	Alkenes, C8-10-branched, C9-rich	11[a]
7959	Alkanes, C12-26-branched and linear	N/A[c]

ID	Name (as registered)	No. of constituents
4794	Hydrocarbons, C10-14 (even numbered), n-alkanes, isoalkanes, <2% aromatic	9
4780	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	14
4859	Hydrocarbons, C11-C14, isoalkanes, cyclics, <2% aromatics	4
4835	Hydrocarbons, C11-C14, n-alkanes, <2% aromatics	7
4766	Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	7
4872	Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	3
4768	Hydrocarbons, C14-C17, n-alkanes, <2% aromatics	11
4864	Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	6
4790	Hydrocarbons, C14-C19, isoalkanes, cyclics, <2% aromatics	4
4945	Hydrocarbons, C14-C20 (even numbered), n-alkanes, isoalkanes, <2% aromatics	13
4779	Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, <2% aromatics	7
4892	Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	4
4839	Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich	13
4783	Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	14
4342	Renewable hydrocarbons (diesel type fraction)	4
284	Paraffin waxes (petroleum), hydrotreated	61
68-9	Paraffin waxes and Hydrocarbon waxes	7
632	Gases (petroleum), light steam-cracked, butadiene conc.	8
473	Hydrocarbons, C2-4, C3-rich	10
475	Hydrocarbons, C4, ethylene-manuf.-by-product	24
891-2	Hydrocarbons, C4, steam-cracker distillate	18
495-6	Distillates (petroleum), steam-cracked, C8-12 fraction	41
224	Distillates (petroleum), heavy paraffinic	7
297	Foots oil (petroleum)	7
7961	Alkanes, C14-17, chloro	1
605	Distillates (petroleum), heavy straight-run	13[d]
4438	Hydrogenated dimerization products of 1-decene, 1-dodecene and 1-octene	7
10300	Naphthenic acids	14
5348	*Not Applicable (petroleum product)*	N/A[c]
4289	Reaction products of 1-decene and 1-dodecene, hydrogenated	3
	Average number of constituents:	13 ± 12

[a] 1 constituent was specified as an impurity
[b] 2 constituents were specified as impurities
[c] information from the registration dossiers were not provided
[d] a dossier which includes 178 identified constituents is excluded from the count in the table

Despite being the largest group of substances screened in the study, the number of constituents reported by registrants is comparable to other substance groups. There are two substances for which 61, respectively 54 constituents were reported, but in general, substances in this group included on average 13 ± 12 substances.

Table 63 Consistency of compositional data provided in the registration dossiers for petroleum-derived substances.

ID	Name (as registered)	Composition consistency score*					
		1	2	3	4	5	6
770	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	79			84		16
432	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	37%	0%	58%	74%	0%	26%
197	Sulfonic acids, petroleum, calcium salts	50%	0%	0%	0%	0%	50%
8155	Asphalt	0%	0%	85%	0%	5%	10%
8156	Asphalt, oxidized	0%	0%	80%	0%	15%	5%
229	Residues (petroleum), vacuum	0%	0%	0%	94%	6%	0%
4213-4	Butene, homopolymer (products derived from butene)	0%	0%	0%	0%	25%	75%
9193-4	Dodecene, branched	67%	0%	0%	100%	0%	100%
569-570	Extracts (petroleum), solvent-refined heavy paraffinic distillate solvent	0%	0%	0%	100%	0%	0%
415-420	Fuels, diesel	0%	0%	0%	100%	0%	0%
234-7	Gas oils (petroleum), light vacuum	0%	0%	89%	0%	11%	0%
466-9	Fuel oil, residual	0%	0%	77%	100%	0%	0%
230-3	Gas oils (petroleum), heavy vacuum	47%	0%	0%	68%	0%	0%
250	Residues (petroleum), hydrocracked	0%	0%	0%	95%	0%	5%
506-7	Residues (petroleum), light vacuum	0%	0%	0%	75%	13%	13%
73-4	Kerosine (petroleum)	0%	0%	0%	95%	5%	0%
314-7	Solvent naphtha (petroleum), heavy arom.	0%	0%	0%	43%	57%	7%
476-480	Hydrocarbons, C5-rich	0%	0%	21%	95%	0%	5%
634	Naphtha (petroleum), catalytic reformed	0%	0%	0%	100%	0%	0%
214	Naphtha (petroleum), full-range straight-run	0%	0%	0%	100%	0%	0%
251	Distillates (petroleum), heavy hydrocracked	0%	0%	0%	100%	0%	0%
287	Distillates (petroleum), hydrotreated heavy paraffinic	0%	0%	0%	90%	0%	10%
693	Lubricating oils	0%	0%	0%	95%	5%	0%
670	Lubricating oils, used	0%	0%	0%	0%	0%	100%
4983-4	Alkenes, C11-12	33%	0%	0%	0%	0%	67%
4560	Alkenes, C20-24 alpha	100%	0%	0%	0%	0%	0%
7973	Alkenes, C20-24 α-	17%	0%	0%	0%	0%	83%
7979-80	Alkenes, C8-10-branched, C9-rich	0%	18%	0%	18%	0%	64%
4794	Hydrocarbons, C10-14 (even numbered), n-alkanes, isoalkanes, <2% aromatic	33%	0%	0%	0%	0%	67%
4780	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	0%	0%	33%	0%	17%	50%
4859	Hydrocarbons, C11-C14, isoalkanes, cyclics, <2% aromatics	33%	0%	0%	0%	0%	67%
4835	Hydrocarbons, C11-C14, n-alkanes, <2% aromatics	0%	0%	0%	67%	0%	33%
4766	Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	0%	0%	0%	0%	100%	0%
4872	Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	100%	0%	0%	0%	0%	0%
4768	Hydrocarbons, C14-C17, n-alkanes, <2% aromatics	0%	0%	0%	75%	25%	25%
4864	Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	0%	0%	60%	60%	0%	40%
4790	Hydrocarbons, C14-C19, isoalkanes, cyclics, <2% aromatics	50%	0%	0%	0%	0%	50%
4945	Hydrocarbons, C14-C20 (even numbered), n-alkanes, isoalkanes, <2% aromatics	100%	0%	0%	0%	0%	0%
4779	Hydrocarbons, C16-C20, n-alkanes,	0%	0%	0%	40%	0%	60%

ID	Name (as registered)	Composition consistency score*					
		1	2	3	4	5	6
	isoalkanes, cyclics, <2% aromatics						
4892	Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	20%	0%	0%	0%	0%	80%
4839	Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich	0%	0%	0%	31%	0%	67%
4783	Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	0%	0%	0%	20%	20%	60%
4342	Renewable hydrocarbons (diesel type fraction)	0%	100%	0%	0%	0%	0%
284	Paraffin waxes (petroleum), hydrotreated	0%	0%	79%	0%	16%	5%
68-9	Paraffin waxes and Hydrocarbon waxes	0%	0%	85%	0%	5%	10%
632	Gases (petroleum), light steam-cracked, butadiene conc.	0%	0%	0%	63%	0%	37%
473	Hydrocarbons, C2-4, C3-rich	0%	50%	100%	100%	0%	0%
475	Hydrocarbons, C4, ethylene-manuf.-by-product	0%	0%	0%	0%	95%	5%
891-2	Hydrocarbons, C4, steam-cracker distillate	0%	0%	0%	100%	0%	0%
495-6	Distillates (petroleum), steam-cracked, C8-12 fraction	0%	0%	0%	78%	0%	22%
224	Distillates (petroleum), heavy paraffinic	0%	0%	0%	89%	0%	11%
297	Foots oil (petroleum)	0%	0%	0%	100%	0%	0%
7961	Alkanes, C14-17, chloro	0%	0%	0%	0%	0%	100%
605	Distillates (petroleum), heavy straight-run	0%	0%	52%	26%	11%	11%
4438	Hydrogenated dimerization products of 1-decene, 1-dodecene and 1-octene	100%	0%	0%	0%	0%	0%
10300	Naphthenic acids	0%	0%	0%	0%	100%	33%
4289	Reaction products of 1-decene and 1-dodecene, hydrogenated	0%	0%	0%	0%	0%	100%

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

In comparison with other groups of substances, registrants of petroleum-derived products often use the approach of specifying only a single constituent with identical name as the registered substance (there was at least one registrant using this approach in 65% of the screened substances).

It can be observed, that composition of petroleum-derived substances is often specified as contents of general groups of substances (e.g. aromatic hydrocarbons, non-aromatic hydrocarbons, saturated hydrocarbons) rather than chemical individua (e.g. benzene, toluene, xylene). This applies especially to heavy distillation fractions. The vast majority of substances in this group is covered by well-established long-term operating REACH consortia, which can be a factor contributing to this observation. It appears that the approach applied by most registrants aims at identification of substances critical for hazard characterisation and classification, grouping together substances sharing similar or identical hazardous properties (e.g. di-aromatic hydrocarbons), rarely trying to identify each single chemical individuum.

Despite the fact that constituents are often specified as groups of substances, it can also be observed that the consistency of compositional data provided by registrants is high in the sense that the registrants usually specify identical groups of substances, as documented in the following table.

Table 64 Sub-groups of petroleum-derived products sharing identical set of specified constituents in most of the studied dossiers.

Constituents typically specified in registration dossiers	Applicable sub-groups of petroleum-derived substances
- Non-aromatic hydrocarbons	- Bitumen, modified asphalt - Distillate and residual aromatic extracts (untreated/treated) - Gas oils and distillate fuels - Fuel oils and heavy residues - Kerosines - Lubricating oils, greases, base oils, petrolatums - Paraffin and hydrocarbon waxes, slack waxes - Foot oils
- Mono-aromatic hydrocarbons	
- Di-aromatic hydrocarbons	
- Tri-aromatic hydrocarbons and higher	
- Saturated hydrocarbons	
- Polar hydrocarbons	
- Aromatic hydrocarbons	
- Asphaltenes	
- DMSO extract	
- n-paraffins - isoparaffins - Benzene - Toluene - Hexane	- Low boiling point naphthas (gasolines)
- Various alkenes	- Olefins
- Various hydrocarbons or groups of hydrocarbons within the scope of the registered name (e.g. dodecane, isododecane, tetradecane, isotetradecane, C10-C13 cycloalkanes, C10-C13 isoalkanes, C10-C13 n-alkanes, etc.)	- Other hydrocarbons (aliphatics, cyclic, aromatics)
- Various alkanes and alkenes within the scope of the registered name of the substance (e.g. ethane, propane, butane, but-1-ene, but-2-ene, 2-methylprop-1-ene, etc.)	- Petroleum gases

Registrants of petroleum-derived substances often follow an approach presented by CONCAWE (a division of the European Petroleum Refiners Association carrying out research on environmental issues relevant to the oil industry), which covers a significant number of registered petroleum-derived substances. The approach presented by CONCAWE aims at reporting classification markers (e.g. benzene), hydrocarbon classes (e.g. non-aromatic hydrocarbons, mono-aromatic hydrocarbons, di-aromatic hydrocarbons, etc.), and individual constituents present at concentrations of 10 % or higher. This approach was observed in a notable number of screened registration dossiers.

In the group of "other hydrocarbons (aliphatics, cyclic, aromatics)", comprising mostly hydrocarbon solvents, another two general approaches in reporting composition can be observed. Typically, the registrants report the compositional data using general groups of constituents characterised by carbon number descriptors (e.g. C9-C11) and hydrocarbon structure descriptors (e.g. branched alkanes, linear alkanes, cycloalkanes, aromatics, etc.) or they report concentrations of individual substances (e.g. tetradecane, pentadecane, hexadecane, etc.).

Source

Besides crude oil as the primary source of petroleum-derived products, products of various processing streams of crude oil are typical sources of substances in this group as documented in the following table.

Table 65 Typical sources of individual sub-groups of petroleum-derived substances as specified by registrants of the screened substances.

ID	Sub-group of petroleum-derived substances	Typical source
1	Alkyl aryl sulphonic acids, sulphonates	Sulphonic acids Linear alkylbenzenes
2	Bitumen, modified asphalt	Crude oil or residual oil
3	Butylene oligomers	Butene and its isoforms
4	Distillate and residual aromatic extracts (untreated/treated)	Solvent-refined heavy paraffinic distillate
5	Gas oils and distillate fuels	Residuum from atmospheric distillation of crude oil
6	Fuel oils and heavy residues	Residuum from atmospheric distillation of crude oil
7	Kerosines	Crude oil
8	Low boiling point naphthas (gasolines)	Pyrolysis gasoline Piperylene-rich petroleum distillates
9	Lubricating oils, greases, base oils, petrolatums	Products from a hydrocracking process
10	Olefins	Ethylene
11	Other hydrocarbons (aliphatics, cyclic, aromatics)	Kerosene
12	Paraffin and hydrocarbon waxes, slack waxes	Petroleum
13	Petroleum gases	Naphtha
14	Resin Oils & alkenes	Hydrocarbons - heavy/feedstock Products from a steam cracking process Pyrolysis gasoline
15	Foot oils	Residuum from atmospheric distillation of crude oil
16	Others	Variable

The table above presents aggregated information provided by registrants of the screened substances on sources of these substances. The table is structured according to the sub-grouping of petroleum-derived substances as used in this study, division of the substances into individual sub-groups is provided in Table 60.

Since many sources of petroleum-derived substances are already products of processing crude oil, various manufacturing processes together with corresponding sources are the basic substance identity elements of petroleum-derived substances by which the registrants distinguish and group individual substances (together with other substance identity elements described in the following sections).

Compositional variability of petroleum-derived substances is also greatly influenced by inherent variability in the composition of crude oil, based on its origin.

In some cases, different sources were specified by registrants of a single substance (e.g. butane or a mixture of but-1-ene and but-2-ene in the manufacture of "dodecene, branched" (from the sub-group of butylene oligomers) or natural gas, coal, biomass animal fats or vegetable oils (triglycerides) in the manufacture of "Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich" (from the sub-group of other hydrocarbons)).

The description of the source provided by registrants is often based on the description of the source in the EC Inventory.

Manufacturing process and its parameters (conditions)

As mentioned in the previous section, manufacturing process and its conditions, are (together with source) the basic substance identity elements by which registrants distinguish and group individual petroleum-derived substances. The manufacturing process, its conditions and used source determine to a great extent other basic substance identity elements used frequently for identification of substances with variability in alkyl chain length (e.g. the carbon number range and boiling point range) and ultimately composition of these substances.

The description of the manufacturing process is often identical in all dossiers of a substance covered by an operating REACH consortium, indicating a high level of harmonisation within the consortium. Furthermore, the description of the manufacturing process is sometimes identical to the description specified in the EC Inventory or is often based on the EC Inventory description. An aspect possibly contributing to this observation can be that the refinery processes are very well known and described in various sources.

The following table lists manufacturing processes typical for individual sub-groups of substances as specified by the registrants of the screened substances.

Table 66 Typical manufacturing processes of individual sub-groups of petroleum-derived substances as specified by registrants of the screened substances.

ID	Sub-group of petroleum-derived substances	Typical manufacturing process
1	Alkyl aryl sulphonic acids, sulphonates	Sulphonation Neutralisation
2	Bitumen, modified asphalt	Distillation
3	Butylene oligomers	Oligo-/poly-merisation
4	Distillate and residual aromatic extracts (untreated/treated)	Re-extraction
5	Gas oils and distillate fuels	Vacuum distillation
6	Fuel oils and heavy residues	Vacuum distillation
7	Kerosines	Distillation
8	Low boiling point naphthas (gasolines)	Distillation
9	Lubricating oils, greases, base oils, petrolatums	Distillation
10	Olefins	Oligomerisation, distillation
11	Other hydrocarbons (aliphatics, cyclic, aromatics)	Distillation, hydrogenation, desulphurisation (hydrogenation), dearomatisation (hydrogenation), dearomatisation
12	Paraffin and hydrocarbon waxes, slack waxes	Hydrogenation
13	Petroleum gases	Distillation, cracking, extraction, hydrogenation
14	Resin Oils & alkenes	Distillation, steamcracking
15	Foot oils	Variable (e.g. wax deoiling, vacuum distillation)
16	Others	Variable (e.g. atmospheric distillation of crude oil, catalytic oligomerization of alpha olefin feed streams, chlorination of alkanes, caustic (sodium hydroxide) extraction of petroleum distillates and acidification)

Additional substance identity elements

Registrants of petroleum-derived products in general use a low number of substance identity elements to characterise the registered substances (on average 5.8 ± 1.4 substance identity elements to characterise a substance, including composition, source and manufacturing process). The most frequently used substance elements in addition to composition, source and manufacturing process are:

- Carbon number range
- Boiling point (boiling point range)
- Flash point
- Density
- Viscosity

Boiling point (or boiling point range) was used for identification of substances in some dossiers for 65% of substances and so was the carbon number range. Density, flash point and viscosity were specified for 30 – 30 % of the screened substances.

The average number of substance identity elements used by registrants is higher for heavy distillation fractions, where the registrants typically specify the carbon number range, density, viscosity, boiling point and flash point.

c) Analytical methods

The following Table 67 summarises the use of analytical methods and techniques in identification of the screened substances.

Table 67 REACH Annex VI analytical methods used by registrants of petroleum-derived products.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
770	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	Y	Y	Y	Y	Y	Y
432	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	Y	Y	Y	Y	Y	Y
197	Sulfonic acids, petroleum, calcium salts	Y	Y	Y	Y	Y	Y
8155	Asphalt	Y	Y	Y	-	Y	Y
8156	Asphalt, oxidized	Y	Y	Y	-	Y	Y
229	Residues (petroleum), vacuum	Y	Y	Y	-	Y	Y
4213-4	Butene, homopolymer (products derived from butene)	Y	Y	Y	-	-	Y
9193-4	Dodecene, branched	Y	Y	Y	-	-	Y
569-570	Extracts (petroleum), solvent-refined heavy paraffinic distillate solvent	Y	Y	Y	Y	Y	Y
415-420	Fuels, diesel	Y	Y	Y	-	Y	Y
234-7	Gas oils (petroleum), light vacuum	Y	Y	Y	-	Y	Y
466-9	Fuel oil, residual	-	-	Y	-	Y	Y
230-3	Gas oils (petroleum), heavy vacuum	-	-	Y	-	Y	Y
250	Residues (petroleum), hydrocracked	Y	Y	Y	-	Y	Y
506-7	Residues (petroleum), light vacuum	Y	Y	Y	-	Y	Y
73-4	Kerosine (petroleum)	-	Y	-	-	Y	Y
314-7	Solvent naphtha (petroleum), heavy arom.	Y	Y	Y	-	Y	Y
476-480	Hydrocarbons, C5-rich	Y	Y	Y	-	-	Y
634	Naphtha (petroleum), catalytic reformed	Y	Y	Y	-	-	Y
214	Naphtha (petroleum), full-range straight-run	Y	Y	Y	-	-	Y
251	Distillates (petroleum), heavy hydrocracked	Y	Y	Y	-	Y	Y
287	Distillates (petroleum), hydrotreated heavy paraffinic	Y	Y	Y	-	Y	Y
693	Lubricating oils	Y	Y	Y	Y	Y	Y
670	Lubricating oils, used	-	-	-	-	Y	Y
4983-4	Alkenes, C11-12	Y	Y	Y	-	-	Y

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
4560	Alkenes, C20-24 alpha	Y	Y	Y	-	-	Y
7973	Alkenes, C20-24 α-	Y	Y	Y	-	-	Y
7979-80	Alkenes, C8-10-branched, C9-rich	Y	Y	Y	-	-	Y
4794	Hydrocarbons, C10-14 (even numbered), n-alkanes, isoalkanes, <2% aromatic	Y	Y	Y	-	-	Y
4780	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	Y	Y	Y	-	Y	Y
4859	Hydrocarbons, C11-C14, isoalkanes, cyclics, <2% aromatics	Y	Y	Y	-	-	Y
4835	Hydrocarbons, C11-C14, n-alkanes, <2% aromatics	Y	Y	Y	-	-	Y
4766	Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	Y	Y	Y	-	Y	Y
4872	Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	Y	Y	Y	-	-	Y
4768	Hydrocarbons, C14-C17, n-alkanes, <2% aromatics	Y	Y	Y	-	Y	Y
4864	Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	Y	Y	Y	-	Y	Y
4790	Hydrocarbons, C14-C19, isoalkanes, cyclics, <2% aromatics	Y	Y	Y	-	-	Y
4945	Hydrocarbons, C14-C20 (even numbered), n-alkanes, isoalkanes, <2% aromatics	Y	Y	Y	-	-	Y
4779	Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, <2% aromatics	Y	Y	Y	-	Y	Y
4892	Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	Y	-	-	-	-	Y
4839	Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich	Y	Y	Y	-	-	Y
4783	Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	Y	Y	Y	-	Y	Y
4342	Renewable hydrocarbons (diesel type fraction)	Y	Y	Y	Y	Y	Y
284	Paraffin waxes (petroleum), hydrotreated	Y	Y	Y	Y	Y	Y
68-9	Paraffin waxes and Hydrocarbon waxes	Y	Y	Y	-	Y	Y
632	Gases (petroleum), light steam-cracked, butadiene conc.	Y	Y	Y	-	-	Y
473	Hydrocarbons, C2-4, C3-rich	-	Y	-	-	-	Y
475	Hydrocarbons, C4, ethylene-manuf.-by-product	Y	Y	Y	-	-	Y
891-2	Hydrocarbons, C4, steam-cracker distillate	Y	Y	Y	-	-	Y
495-6	Distillates (petroleum), steam-cracked, C8-12 fraction	Y	Y	Y	-	-	Y
224	Distillates (petroleum), heavy paraffinic	Y	Y	Y	-	Y	Y
297	Foots oil (petroleum)	Y	Y	Y	-	Y	Y
7961	Alkanes, C14-17, chloro	Y	Y	Y	-	Y	Y
605	Distillates (petroleum), heavy straight-run	Y	Y	Y	-	Y	Y
4438	Hydrogenated dimerization products of 1-decene, 1-dodecene and 1-octene	Y	Y	Y	-	-	Y
10300	Naphthenic acids	Y	Y	Y	-	Y	Y
4289	Reaction products of 1-decene and 1-dodecene, hydrogenated	Y	Y	Y	-	Y	-
	Percentage of use of analytical methods (%)	91	93	93	12	60	98

Note: Information in the table is based on analytical methods as reported by the registrants in IUCLID section 1.4. It shall be noted that certain specific analytical methods can be reported under more generic entries (e.g. the PIONA method for determination of aromatic content combines GC and MS).

Analytical methods explicitly mentioned in Annex VI of REACH are of key importance in determination of composition of petroleum-derived substances. Among these, Ultraviolet-visible spectroscopy, Infrared spectroscopy, Nuclear magnetic resonance spectroscopy and gas chromatography have been used in identification of a vast majority of the studied substances. High-performance liquid chromatography was used to determine composition of ca. 60 % of the studied substances, while mass spectrometry was performed to characterise the substances in only a few cases. These

observations are very similar to the ones made for substances with variability in alkyl chain length.

In addition to the analytical methods explicitly mentioned in Annex VI of REACH, the registrants often used also other analytical methods and techniques to determine the composition of the registered substances, in particular:

Analytical method	% of substances where the method was used
Determination of boiling point range	47
Determination of carbon number range	37
Clay-Gel Absorption Chromatographic Method	25
Elution chromatography (e.g. TLC-FID)	11
DMSO extract	9
Determination of water content (titration)	7
Supercritical Fluid Chromatography	7
ICP (ICP-AES)	4
Determination of active matter content	2
Determination of alkylbenzenesulfonates content	2
Determination of aromatic content (method PIONA)	2
Determination of content of CHN	2
Determination of heptane insoluble asphaltenes	2
Determination of chlorine content	2
Determination of Ni (Filtration test)	2
Determination of oil content	2
Determination of PAH content	2
Determination of PCB content	2
Determination of sodium sulfate content	2
Determination of sulfuric acid content	2
Determination of sulphur, PAH, BTEX	2
ESI-MS	2
Gravimetry	2
Hydrocarbon analysis	2
Ion chromatography	2
Microgravimetric Method	2
X-ray microfluorescence	2

Note: It shall be noted that certain specific analytical methods can be reported under more generic entries (e.g. the SIMDIST method used for determination of boiling point range can be reported within the entry "determination of boiling point range").

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressesd by the following operating consortia and associations:

- Linear Alkyl Benzene (LAB) & Derivatives REACH consortium - http://www.reachcentrum.eu/consortium/linear-alkyl-benzene-lab-derivatives-reach-consortium-131.html
- Environmental Science for European Refining Industry (CONCAWE) - https://www.concawe.eu/
- Lower Olefins and Aromatics (LOA) REACH Consortium - http://www.loa-reach.com/
- Higher Olefins and Poly Alpha Olefins (HOPA) REACH consortium - http://hopaconsortium.com/
- Medium-Chain Chlorinated Paraffin (MCCP) Consortium - https://chemicalwatch.com/4225/mccp-reach-consortium

It shall also be noted that some of the substances in this group fall under the scope of OECD guidance for characterising hydrocarbon solvent substances for assessment purposes publicly available at http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2015)52&doclanguage=en.
A sector-specific supporting document for substance identification is also being prepared by CONCAWE in collaboration with ECHA for petroleum products such as gasoline, kerosene (jet-fuel), diesel fuel, lubricants, paraffin wax or bitumen.

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 68 for direct links (where available).

Table 68 Publicly available substance identity profiles of petroleum-derived products.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
770	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs.	http://www.reachcentrum.eu/Consortia%20Documents/P-I268/Substance%20Identification%20Profile/P-I268_EC287-494-3_SIP.pdf	- empirical formula - character of isomers - purity and linear alkyl chain distribution
432	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	http://www.reachcentrum.eu/Consortia%20Documents/P-I268/Substance%20Identification%20Profile/P-I268_EC270-115-0_SIP.pdf	- representational structure - alkyl chain distribution

3.2.3. Coal-derived substances

Coal-derived substances registered in accordance with REACH include complex organic products, by-products and residues derived from the processing of materials extracted from coal (e.g. coal tar). Typical representatives of this group of substances are anthracene oils, naphthalene oils, tar acids and pitches as well as crude tar bases.

Coal-derived substances are often used (and therefore also registered) as intermediates.

Chemical composition of coal-derived substances is highly variable, mainly because of the origin of the raw materials (coal).

a) Substances screened in this group

The following Table 69 lists the eight coal-derived substances selected for substance identity screening.

Table 69 Coal-derived substances – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed*
		Joint	Indiv.	Total	
821	Distillates (coal tar), heavy oils	15	0	15	100
721	Distillates (coal tar), light oils	8	0	8	100
343	Pitch, coal tar, high-temp.	29	0	29	69
341	Tar, coal, high-temp.	56	0	56	36
334	Light oil (coal), coke-oven	44	0	44	45
820	Creosote oil, acenaphthene fraction	9	0	9	100
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	2	0	2	100
67	Montan wax	2	0	2	100

* 20 dossiers per substance were analysed as maximum.

All screened dossiers were submitted in joint submissions, none of the screened substances contains individual submissions (and furthermore, none of all identified complex coal-derived substances with 2 or more co-registrants contains individual submissions).

3 of the screened substances were each registered by more than 25 registrants, the rest of the screened substances were each registered by less than 15 registrants.

For the purposes of this project, substances with variability in alkyl chain length have been further divided into the following sub-groups:

1. Anthracene Oils
2. Tar acids
3. Coal Tar, Coal Tar Bases, Pitches
4. Light Oils and naphthas
5. Naphthalene Oils, Wash Oils
6. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 70 Substance identity elements used by registrants in identification of coal-derived substances.

	Anthracene Oils	Tar acids	Coal Tar, Coal Tar Bases, Pitches		Light Oils and naphthas	Naphthalene Oils, Wash Oils		Others	
	821	721	343	341	334	820	882	67	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process	✓	✓	✓		✓	✓		✓	75
Composition	✓	✓	✓	✓	✓	✓	✓	✓	100
State					✓			✓	25
Softening point			✓						13
Density	✓	✓	✓	✓	✓	✓	✓		88
Boiling point	✓	✓	✓	✓	✓	✓	✓		88
Flash point	✓	✓	✓	✓	✓	✓	✓		88
*Common characteriser**	✓								13
*Other characteriser***	✓	✓		✓	✓	✓	✓		75
No. of applied SID elements per substance	9	8	8	7	9	8	7	5	Average = 69
Average no. of applied SID elmts. per sub-group	9	8	7.5 ± 0.7		9	7.5 ± 0.7		5	
Average no. of applied SID elmts. per group	7.6 ± 1.3								

* Common group-specific jargon, in particular: Anthracene Oil > 50 ppm (821)

** heavy oil, distillate (821), light oil (721), by-product (341), volatile liquid (334), wash oil (820), filtrate (882)

Comments to Table 70:

- 11 SID elements were used by registrants of the screened substances for identification of substances in this group;

- 7 out of the 8 screened substances were identified with 7 – 9 SID elements, while the remaining substance was identified with 5 SID elements;

- standard deviation linked to the average number of SID elements used by registrants of substances in this group is rather low (1.3) compared to other groups, and the set SID elements used by registrants of different substances in this group is very consistent, indicating that there is a wide consensus among registrants on the way of appropriate identification of coal-derived substances;

- source, process and composition was used for identification of substances in this group in all cases (specified by at least one registrant of each substance);

- parameters (conditions) of the process, density, boiling point, flash point and other characteriser (e.g. heavy oil, light oil, wash oil, distillate, filtrate, by-product, volatile liquid) were also used for identification of the substances screened in this group in most cases (for 75 % of the screened substances or more);

Composition

Coal-derived substances usually have a very high number of constituents. It is a common practice, that registrants identify and determine well-defined constituents (or groups of) resulting from a particular controlled manufacturing process and substances which are relevant for classification and labelling (especially various polyaromatic hydrocarbons), while other constituents of the substance remain unreported (the sum of concentrations / concentration ranges is less than 100 %). There is high variability in the number of constituents reported by individual registrants within a single joint submission, where some of them report only a few constituents (5 – 10), whereas some report a significantly higher number of constituents, reporting even those present in very low concentrations (e.g. < 1 %).

The registrants of the substances subject to the screening most frequently specified composition of the substances specifying concentration ranges of individual constituents together with their typical concentrations in vast majority of cases. In cases where only one of these two values was provided, frequency of use of concentration ranges and of typical concentrations was similar.

Some registration dossiers include several compositions, due to the following factors:

a) describing different grades of a substance (e.g. coal tar with or without benzene content or naphthalene-rich creosote oil and naphthalene-depleted creosote oil)
b) different content of constituents relevant for classification and labelling

Table 71 Number of compositions specified in registration dossiers by registrants of coal-derived substances.

ID	Name (as registered)	% of No. of compositions		
		1	2	3
821	Distillates (coal tar), heavy oils	87	13[a]	0
721	Distillates (coal tar), light oils	50	50[b]	0
343	Pitch, coal tar, high-temp.	100	0	0
341	Tar, coal, high-temp.	100	0	0
334	Light oil (coal), coke-oven	100	0	0
820	Creosote oil, acenaphthene fraction	78	11[a]	11[c]
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	100	0	0
67	Montan wax	100	0	0

[a] 2 grades of the substance were specified
[b] content of benzene 0 – 0.1% (opposed to other dossiers with 0 – 5%)
[c] 3 grades of the substance were specified

Table 72 Number of constituents specified in registration dossiers by registrants of coal-derived substances.

ID	Name (as registered)	No. of constituents
821	Distillates (coal tar), heavy oils	18
721	Distillates (coal tar), light oils	33
343	Pitch, coal tar, high-temp.	1
341	Tar, coal, high-temp.	25
334	Light oil (coal), coke-oven	7
820	Creosote oil, acenaphthene fraction	15
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	5
67	Montan wax	1

Table 73 Consistency of compositional data provided in the registration dossiers for coal-derived substances.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
821	Distillates (coal tar), heavy oils			7	87		7
721	Distillates (coal tar), light oils			13	100		
343	Pitch, coal tar, high-temp.						100
341	Tar, coal, high-temp.		26		100		
334	Light oil (coal), coke-oven			100			
820	Creosote oil, acenaphthene fraction			56	100		
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	100					
67	Montan wax						100

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

Table 74 Typical constituents specified in registration dossiers by registrants of coal-derived substances.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
821	Distillates (coal tar), heavy oils	Phenanthrene	201-581-5	0 – 21.2
		Fluoranthene	205-912-4	0 – 30
		Pyrene	204-927-3	2.5 – 30
		Anthracene	204-371-1	0 – 10
		Benzo[pqr]tetraphene	200-028-5	0.005 – 3
721	Distillates (coal tar), light oils	Indane	207-814-7	0 – 30
		1H-indene	202-393-6	0 – 50
		Naphthalene	202-049-5	0 – 30
		Phenol	203-632-7	0 – 40
		Benzene	200-753-7	0 – 5
343	Pitch, coal tar, high-temp.	Benzo[a]pyrene	200-028-5	0 – 5
341	Tar, coal, high-temp.	Macromolecular organic compounds	N/A	60 – 100
		Naphthalene	202-049-5	0 – 20
		Anthracene	204-371-1	0 – 3
		Benzo[def]chrysene / Benzo[pqr]tetraphene / Benzo[a]pyrene	200-028-5	0 – 2
		Benzene	200-753-7	0 – 2
334	Light oil (coal), coke-oven	Benzene	200-753-7	50 – 90
		Toluene	203-625-9	0 – 30
		Xylene	215-535-7	0 – 30
		Naphthalene	202-049-5	0 – 15
820	Creosote oil, acenaphthene fraction	1-methylnaphthalene	201-966-8	0 – 25
		2-methylnaphthalene	202-078-3	0 – 50
		acenaphthene / 1,2-dihydroacenaphthylene	201-469-6	0 – 30
		Naphthalene	202-049-5	0 – 25
		Quinolone	202-051-6	0 – 10
		9H-fluorene	201-695-5	0 – 15
		Anthracene	204-371-1	0 – 5
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	Naphthalene	202-049-5	10 – 80
		2-methylnaphthalene	202-078-3	1 – 20
		Quinolone	202-051-6	1 – 10
		3,5-dimethylphenol	203-606-5	0 – 5
		1-benzothiophene	202-395-7	1 – 25
67	Montan wax	Montan wax	232-313-5	100

Source

Similarly to petroleum-derived substances, source is one of the key elements bringing variability to coal-derived substances, originating from various materials extracted from coal.

Table 75 Sources of coal-derived substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
821	Distillates (coal tar), heavy oils	Coal tar
721	Distillates (coal tar), light oils	Coal tar
343	Pitch, coal tar, high-temp.	Coal tar
341	Tar, coal, high-temp.	Hard coal
334	Light oil (coal), coke-oven	Coal, gas envolved
820	Creosote oil, acenaphthene fraction	Coal tar
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	Naphthalene oil from coal tar
67	Montan wax	Lignite

Since a number of substances in this group shares a single source (coal tar), source alone is not the key element for identification of coal-derived substances. Furthermore, coal as the primary source has intrinsically variable composition

depending on its origin and the manufacturing process and the conditions of the manufacturing process are therefore critical elements determining the final identity of coal-derived substances. Nevertheless, the importance of source is documented by the fact that it has not been observed in the screened registration dossiers that two different sources could lead to a single substance, each of the screened registered substances had a single source specified by the registrants (e.g. coal tar, hard coal, naphthalene oil).

Manufacturing process and its parameters (conditions)

Distillation is the central manufacturing process specified by registrants of the screened substances.

Table 76 Manufacturing processes of coal-derived substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
821	Distillates (coal tar), heavy oils	Distillation
721	Distillates (coal tar), light oils	Distillation
343	Pitch, coal tar, high-temp.	Distillation
341	Tar, coal, high-temp.	Destructive distillation
334	Light oil (coal), coke-oven	Destructive distillation, extraction
820	Creosote oil, acenaphthene fraction	Distillation
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	Crystallization
67	Montan wax	Extraction

The level of detail of the manufacturing process description is highly variable. Some registrants provide only a general description of the process and of the processed material (e.g. "fraction produced during the distillation of coal tar"), while some registrants provide a rather detailed description of individual processing steps, conditions of the process and specification of the starting materials.

The manufacturing process together with the source are the key substance elements determining resulting composition of the substances in this group. It was not observed that a single source processed in different ways would lead to a single substance.

Additional substance identity elements

With the exception of montan wax (which is sometimes extracted from brown coal, but more commonly from lignite), the following substance identity elements were used by the registrants in identification of substances in this group:

- Density
- Boiling point
- Flash point

These substance identity elements are closely related to the parameters (conditions) of the manufacturing process, another key substance identity element for clear characterisation of coal-derived substances.

It can be observed that the set of substance identity elements used by registrants of coal-derived substances is very similar to the set of substance identity elements used for identification of petroleum-derived substances.

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Substance identity element	Value	Substance identified with the SID element
State	Liquid	Light oil (coal), coke-oven (334)
	Wax (solid)	Montan wax (67)

Softening point	> 65°C	Pitch, coal tar, high-temp. (343)

c) Analytical methods

The following Table 77 and Table 78 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 77 REACH Annex VI analytical methods used by registrants of coal-derived substances.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
821	Distillates (coal tar), heavy oils		Y				Y
721	Distillates (coal tar), light oils		Y				Y
343	Pitch, coal tar, high-temp.	Y	Y				Y
341	Tar, coal, high-temp.		Y				Y
334	Light oil (coal), coke-oven	Y	Y				Y
820	Creosote oil, acenaphthene fraction		Y				Y
882	Distillates (coal tar), naphthalene oil crystn. mother liquor						Y
67	Montan wax	Y	Y				Y
Percentage of use of analytical methods (%)		38	88	0	0	0	100

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 78 Other analytical methods used by registrants of coal-derived substances in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements
821	Distillates (coal tar), heavy oils	
721	Distillates (coal tar), light oils	
343	Pitch, coal tar, high-temp.	XRF
341	Tar, coal, high-temp.	
334	Light oil (coal), coke-oven	
820	Creosote oil, acenaphthene fraction	
882	Distillates (coal tar), naphthalene oil crystn. mother liquor	
67	Montan wax	

All of the screened substances were analysed using gas chromatography and all but one (Distillates (coal tar), naphthalene oil crystn. mother liquor) were analysed also using infrared spectroscopy. Ultraviolet-visible spectroscopy was also used in some cases. From additional analytical methods, only X-ray fluorescence was used in a single case (Pitch, coal tar, high-temp.).

Analytical methods used for identification of coal-derived substances aim at identifying constituents critical for hazard characterisation and classification, especially polyaromatic hydrocarbons. Some of the substances critical for assessment of substance sameness are specified in the SIP published by the REACH for Coal Chemicals (R4CC) consortium. It can be observed that the registrants aim primarily at determination of the contents of these chemicals. The compositional data provided by the registrants as determined by the set of performed analyses do not always account for identification of 100 % of constituents.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressesd by the REACH for Coal Chemicals (R4CC) consortium (http://www.r4cc.org/).

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 79 for direct links (where available).

Table 79 Publicly available substance identity profiles of coal-derived substances.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
821	Distillates (coal tar), heavy oils	http://www.boenigk.homepage.t-online.de/r4ccorg/index-Dateien/R4CC_UVCB.pdf	- flash point range (EN ISO 2719) - boiling point range (EN ISO 3405) - density (ASTM D4052) - potential main constituents (determined by GC)
821	Distillates (coal tar), heavy oils		
721	Distillates (coal tar), light oils		
343	Pitch, coal tar, high-temp.		
341	Tar, coal, high-temp.		
334	Light oil (coal), coke-oven		
820	Creosote oil, acenaphthene fraction		

3.2.4. Other organic substances

Other complex organic substances outside the scope of the aforementioned groups of substances include organic oligomers, organic pigments and dY, synthetic resins and their derivates and other specific complex substances.

a) Substances screened in this group

The following Table 80 lists other complex organic substances selected for substance identity screening.

Table 80 Other complex organic substances – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed
		Joint	Indiv.	Total	
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	8	0	8	100
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	8	1	9	100
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	1	0	1	100
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	10	0	10	100
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	5	0	5	100
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016	1	2	3	100
10705	polychloro copper phthalocyanine	12	0	12	100
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	16	0	16	100
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	4	0	4	100
525-6	Dodecene, hydroformylation products, high-boiling	1	1	2	100
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	2	0	2	100
625-6	Oxirane, reaction products with ammonia, distn. Residues	2	1	3	100
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	10	0	10	100
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters	9	0	9	100
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	5	0	5	100
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	14	0	14	100
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	5	0	5	100
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	0	1	1	100
10522	oxybis(methyl-2,1-ethanediyl) diacrylate	9	0	9	100
10617	Phenol, dodecyl-, branched, sulfurized	2	0	2	100
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	7	0	7	100
10852	Propylidynetrimethanol, ethoxylated	9	0	9	100
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	10	0	10	100
10854	Propylidynetrimethanol, propoxylated	6	0	6	100
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	7	0	7	100
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	1	0	1	100

ID	Name (as registered)	No. of registrants			% dossiers analysed
		Joint	Indiv.	Total	
202	Resin acids and Rosin acids, sodium salts	8	0	8	100
346	Rosin, fumarated	9	0	9	100
975	Rosin, fumarated, reaction products with formaldehyde	1	0	1*	100
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	3	0	3	100
860	Rosin, reaction products with formaldehyde	9	0	9	100
5899	1,2-Diaminotoluene, propoxylated	5	0	5	100
6665	2-aminoethanol, monoester with boric acid	3	0	3	100
6308	2,2',2''-Nitrilotriethanol, propoxylated	5	0	5	100
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	19	0	19	100
8731	D-Glucitol, propoxylated	11	0	11	100
4426-31	Inositol phosphates	0	6	6	100
384-5	Naphthenic acids, reaction products with diethylenetriamine	1	1	2	100
10615-6	Phenol, dodecyl-, branched	7	1	8	100
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	7	0	7	100
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene	1	4	5	100
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	0	1	1	100
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	2	5	7	100

* The dossier was not provided.

11 of the screened substances contain besides dossiers from joint submissions also individual submission dossier(s). None of the substances screened in this group was registered by more than 20 registrants.

The preceding table documents generally low harmonisation of the registration approaches taken by registrants of the substances in this group, where 25% of the substances were registered in multiple submissions, either in a joint and one or more individual, or in multiple individual submissions.

For the purposes of this project, substances with variability in alkyl chain length have been further divided into the following sub-groups:

1. Oligomers
2. Pigments/DY
3. Residues
4. Resins (synthetic) and polymers
5. Rosin Resin Derivates
6. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 81 Substance identity elements used by registrants in identification of other complex organic substances.

	Oligomers				Pigments/DY			Residues				
	5857	5904-5	4215	4223	8634	1528 - 30	10705	5126	414	525-6	599	625-6
Source	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓
Process	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓
Parameters of process	✓	✓	✓	✓	✓		✓	✓				
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Alkyl chain length								✓				
State												
Softening point												
Density												
Viscosity												
pH												
Boiling point												
Flash point												
Optical activity												
Refractive index												
Colour						✓	✓					
Colour index							✓					
*Other characteriser**			✓								✓	✓
No. of applied SID elements per substance	4	4	5	4	4	4	6	5	1	3	4	4
Average no. of applied SID elmts. per sub-group	4.3 ± 0.5				4.7 ± 1.2			3.4 ± 1.5				

Table 81 continued

	Resins (synthetic) and polymers												Rosin Resin Derivates					
	5418	6986	4962	4225	433	2458	10522	10617	10816	10852	10853	10854	969	212	202	346	924	860
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Parameters of process				✓	✓	✓	✓	✓			✓		✓	✓	✓	✓	✓	✓
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Alkyl chain length		✓				✓												
State																		✓
Softening point													✓			✓	✓	
Density							✓											
Viscosity							✓											
pH															✓			
Boiling point																		
Flash point																		
Optical activity																		
Refractive index							✓											
Colour													✓			✓	✓	
Colour index																		
*Other characteriser**			✓	✓		✓												
No. of applied SID elements per substance	3	4	4	5	4	6	7	4	3	3	4	3	6	4	5	6	6	5
Average no. of applied SID elmts. per sub-group	4.2 ± 1.3												5.3 ± 0.8					

Table 81 continued

	Others												
	5899	6665	6308	7997	8731	4426-31	384-5	10615-6	581	4117-21	4471	10906-10	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		95
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		95
Parameters of process	✓	✓	✓					✓		✓			57
Composition	✓	✓	✓	✓	✓	✓		✓	✓	✓	✓	✓	98
Alkyl chain length													7
State													2
Softening point													7
Density									✓				5
Viscosity													2
pH													2
Boiling point									✓		✓		5
Flash point									✓				2
Optical activity					✓								2
Refractive index													2
Colour													12
Colour index													2
*Other characteriser**										✓			17
No. of applied SID elements per substance	4	4	4	3	4	3	2	4	6	5	4	1	Average = 24
Average no. of applied SID elmts. per sub-group	3.7 ± 1.3												

Average no. of applied SID elmts. per group	4.1 ± 1.3

* Oligomeric reaction products (4215, 4225), complex residuum (599), by-product (625-626), homopolymer (4962), condensation products (2458), reaction products (4117-4121)

Comments to Table 81:

- 17 SID elements were used by registrants of the screened substances for identification of substances in this group;

- Number of used SID elements varies between 1 and 6 for each substance, with 4.1 being the average number of SID elements used by registrants for identification of substances in this group. The average number of applied SID elements is the lowest among all studied groups of substances;

- Standard deviation linked to the average number of SID elements used by registrants of substances in this group is 1.3.;

- One of the substances was identified only with a single SID element (composition).

Composition

In general, three different approaches in specifying compositional data can be observed in the screened registration dossiers:

a) Only a single constituent with identical name as the registered substance is specified (this approach was frequently observed in substances within the sub-groups of "resins (synthetic) and polymers" and "others")

b) Composition is specified through general groups of substances

c) Composition is specified as concentration ranges and typical concentrations of particular chemical individua

The compositional data on substances in this group are very variable as indicated in the following tables.

Table 82 Number of compositions specified in registration dossiers by registrants of other complex organic substances.

ID	Name (as registered)	% of No. of compositions		
		1	3	≥4
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	76	12	12
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	100		
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	100		
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	100		
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	100		
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016	100		
10705	polychloro copper phthalocyanine	100		
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	100		
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	100		
525-6	Dodecene, hydroformylation products, high-boiling	100		
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	100		
625-6	Oxirane, reaction products with ammonia, distn. Residues	100		
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	100		
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters	100		
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	100		

4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	100		
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	100		
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	100		
10522	oxybis(methyl-2,1-ethanediyl) diacrylate	100		
10617	Phenol, dodecyl-, branched, sulfurized	100		
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	86		14[a]
10852	Propylidynetrimethanol, ethoxylated	100		
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	100		
10854	Propylidynetrimethanol, propoxylated	100		
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	100		
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	100		
202	Resin acids and Rosin acids, sodium salts	100		
346	Rosin, fumarated	100		
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	100		
860	Rosin, reaction products with formaldehyde	100		
5899	1,2-Diaminotoluene, propoxylated	100		
6665	2-aminoethanol, monoester with boric acid	100		
6308	2,2',2''-Nitrilotriethanol, propoxylated	100		
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	100		
8731	D-Glucitol, propoxylated	100		
4426-31	Inositol phosphates	100		
384-5	Naphthenic acids, reaction products with diethylenetriamine	100		
10615-6	Phenol, dodecyl-, branched	100		
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	100		
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene	100		
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	100		
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	100		

[a] 6 grades of the substance were specified

All but two of the screened substances had only a single composition specified by the registrants.

Table 83 Number of constituents specified in registration dossiers by registrants of other complex organic substances.

ID	Name (as registered)	No. of constituents	
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	Composition #1	4
		Composition #2	5
		Composition #3	5
		Composition #4	5
		Composition #5	5
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers		26
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol		24[a]
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane		11
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated		7[b]
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016		6[b]
10705	polychloro copper phthalocyanine		44[c]
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts		5[d]
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues		6[a]
525-6	Dodecene, hydroformylation products, high-boiling		1
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from		12
625-6	Oxirane, reaction products with ammonia, distn. Residues		6
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate		18[e]
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters		15[d]
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type		7
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid		12[f]
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene		8
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)		5
10522	oxybis(methyl-2,1-ethanediyl) diacrylate		16[g]
10617	Phenol, dodecyl-, branched, sulfurized		3
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	Composition #1	9[d]
		Composition #2	4
		Composition #3	4
		Composition #4	4
		Composition #5	4
		Composition #6	4
		Composition #7	4
10852	Propylidynetrimethanol, ethoxylated		9
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid		32[d]
10854	Propylidynetrimethanol, propoxylated		9
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol		12
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol		4
202	Resin acids and Rosin acids, sodium salts		21
346	Rosin, fumarated		23
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol		6
860	Rosin, reaction products with formaldehyde		22
5899	1,2-Diaminotoluene, propoxylated		1
6665	2-aminoethanol, monoester with boric acid		1
6308	2,2',2''-Nitrilotriethanol, propoxylated		3
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]		1
8731	D-Glucitol, propoxylated		1

4426-31	Inositol phosphates		8
384-5	Naphthenic acids, reaction products with diethylenetriamine		1
10615-6	Phenol, dodecyl-, branched		25
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased		28[d]
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene		4
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment		17
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate		16[h]

[a] 5 constituents were specified as impurities
[b] 3 constituents were specified as impurities
[c] 38 constituents were specified as impurities
[d] 1 constituent was specified as impurity
[e] 11 constituents were specified as impurities
[f] 2 constituents were specified as impurities
[g] 6 constituents were specified as impurities
[h] 7 constituents were specified as impurities

6 substances included only a single constituent with identical name as the registered substance. The highest number of constituents reported by the registrants of the screened dossiers is 44.

Table 84 Consistency of compositional data provided in the registration dossiers for other complex organic substances.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	100					
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers				78		22
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol			50		12	38
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane		80			20	
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated						100
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016			100			
10705	polychloro copper phthalocyanine						100
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	100					
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues						100
525-6	Dodecene, hydroformylation products, high-boiling						100
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	100					
625-6	Oxirane, reaction products with ammonia, distn. Residues	67			33		
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	30			70		100
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters			77	44		11
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	100			20		
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-		64		14		21

	epoxypropane, esters with acrylic acid						
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	20					80
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	100					
10522	oxybis(methyl-2,1-ethanediyl) diacrylate		22	56	100		100
10617	Phenol, dodecyl-, branched, sulfurized					50	60
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene			86	100		
10852	Propylidynetrimethanol, ethoxylated					11	89
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid				30	40	30
10854	Propylidynetrimethanol, propoxylated				17		83
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	50			63		25
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	100					
202	Resin acids and Rosin acids, sodium salts		25			63	13
346	Rosin, fumarated			25	38		50
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol			67		33	
860	Rosin, reaction products with formaldehyde				22	22	56
5899	1,2-Diaminotoluene, propoxylated						100
6665	2-aminoethanol, monoester with boric acid						100
6308	2,2',2''-Nitrilotriethanol, propoxylated	100					
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]						100
8731	D-Glucitol, propoxylated						100
4426-31	Inositol phosphates	100					
384-5	Naphthenic acids, reaction products with diethylenetriamine						100
10615-6	Phenol, dodecyl-, branched				38	12	50
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	43				14	43
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene						100
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	100					
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	86					14

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

Table 85 Typical constituents specified in registration dossiers by registrants of other complex organic substances.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	1,1'-methylenebis(4-isocyanatobenzene) /4,4'-methylenediphenyl diisocyanate	202-966-0	5 – 85
		1-isocyanato-2-(4-isocyanatobenzyl)benzene / o-(p-isocyanatobenzyl)phenyl isocyanate	227-534-9	0 – 65
		1,1'-methylenebis(2-isocyanatobenzene) / 2,2'-methylenediphenyl diisocyanate	219-799-4	0 – 5
		Higher oligomers of MDI homopolymer	N/A	5 – 60
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	2,2,4-Trimethyl-1H-quinoline // 1,2-Dihydro-2,2,4-trimethylquinoline, Monomer	205-688-8	0 – 3
		2,2,4-Trimethyl-1H-quinoline, dipolymer // 1,2-dihydro-2,2,4-trimethylquinoline, dipolymer	N/A	12 – 50
		2,2,4-Trimethyl-1H-quinoline, trimer //1,2-dihydro-2,2,4-trimethylquinoline, trimer	N/A	5 – 40
		2,2,4-Trimethyl-1H-quinoline, tetramer // 1,2-dihydro-2,2,4-trimethylquinoline, tetramer	N/A	4 – 20
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	Phenol, polymer with formaldehyde, oxiranylmethyl ether	500-006-8	80 – 100
		[[2-[p-(oxiranylmethoxy)benzyl]phenoxy]methyl]oxirane	260-750-1	25 – 51
		2,2'-[methylenebis(p-phenyleneoxymethylene)]bisoxirane	218-257-4	16 – 50
		2,2'-[methylenebis(o-phenyleneoxymethylene)]bisoxirane	259-026-8	8.5 – 18
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	3-(aminomethyl)-3,5,5-trimethylcyclohexanamine	220-666-8	20 – 80
		Poly(Bisphenol A-co-epichlorohydrin-co-isophoronediamine) with Mw < 700 g/mol	N/A	15 – 60
		Poly(Bisphenol A-co-epichlorohydrin-co-isophoronediamine) with Mw >= 700 g/mol	N/A	10 – 25
		Unspecified species each below 1% w/w	N/A	0 - 15
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	[29H,31H-phthalocyaninato(2-)-kappa-2N-29~,N-31~]copper, brominated chlorinated	270-958-4	94 – 100
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016	4-{2-[(E)-2-(2-chloro-4-{3-chloro-4-[(E)-2-[2-oxo-1-(phenylcarbamoyl)propyl]diazen-1-yl]phenyl}phenyl)diazen-1-yl]-3-oxobutanamido}benzene-1-sulfonate;dimethyldioctadecylazanium (1:1)	N/A	50 – 60
		4-{2-[(E)-2-(2-chloro-4-{3-chloro-4-[(E)-2-{oxo-1-[(4-sulfonatophenyl)carbomoyl]propyl}diazen-1-yl]phenyl}phenyl)diazen-1-yl]-3-oxobutanamido}benzene-1-sulfonate;bis(dimethyldioctadecylazanium)(1:2)	N/A	15 – 30
		2-[(E)-2-(2-chloro-4-{3-chloro-4-[(E)-2-[2-oxo-1-(phenylcarbmoyl)propyl]diazen-1-yl]phenyl}phenyl)diazen-1-yl]-3-oxo-	228-787-8	15 – 25

		N-phenylbutanamide		
10705	polychloro copper phthalocyanine	29H,31H-phthalocyaninato(2-)-kappa~2~N~29~,N~31~]copper, chlorinated // polychloro copper phthalocyanine	215-524-7	78 – 100
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	Alkenes, C11-14, hydroformylation products, distn. residues, sulfosuccinated, sodium salt	N/A	30 – 60
		Alkenes, C11-14, hydroformylation products, distn. residues, maleated, sodium salt	N/A	20 – 45
		disodium sulfate	231-820-9	0 – 2
		Water	231-791-2	5 – 30
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	269-798-8	40 – 80
525-6	Dodecene, hydroformylation products, high-boiling	Phenol	203-632-7	0.0001 – 10
		1-phenylethanone // acetophenone	202-708-7	0.0001 – 25
		isopropylbenzene // cumene	202-704-5	0.0001 – 10
		4-(1-methyl-1-phenylethyl)phenol // 4-(α,α-dimethylbenzyl)phenol	209-968-0	0.0001 – 25
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	2-[(2-aminoethyl)amino]ethanol	203-867-5	10 – 80
		N,N'-bis(2-aminoethyl)ethane-1,2-diamine // trientine	203-950-6	5 – 50
		non-specified impurities	N/A	0 – 20
		2-({2-[(2-aminoethyl)amino]ethyl}amino)ethane	217-811-2	0 – 15
625-6	Oxirane, reaction products with ammonia, distn. Residues	2,2',2''-nitrilotriethanol	203-049-8	60 – 90
		2,2'-{[2-(2-hydroxyethoxy)ethyl]imino}diethanol	241-604-6	0 – 30
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	2-{2-[2-(acryloyloxy)-1-methylethoxy]-1-methylethoxy}-1-methylethyl acrylate // (1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	256-032-2	70 – 100
		2-Propenoic acid, 2-[2-(2-hydroxymethylethoxy)methylethoxy]methylethyl ester	N/A	0 – 14
		2-Propenoic acid (1 or 2), (4 or 5), (7 or 8)-trimethyl-10,14-dioxo-3,6,9,13-tetraoxahexadec-15-en-1-yl ester	N/A	0 – 8
		acrylic acid	201-177-9	0 – 0.1
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters	dodecyl methacrylate	205-570-6	20 – 30
		tridecyl methacrylate	219-671-8	25 – 35
		tetradecyl methacrylate	219-835-9	20 – 30
		pentadecyl methacrylate	228-126-3	20 – 30
		2-Propenoic acid, 2-methyl-, dodecyl ester, branched and linear	N/A	15 – 30
		2-Propenoic acid, 2-methyl-, tridecyl ester, branched and linear	N/A	25 – 35
		2-Propenoic acid, 2-methyl-, tetradecyl ester, branched and linear	N/A	20 – 30
		2-Propenoic acid, 2-methyl-, pentadecyl ester, branched and linear	N/A	10 – 30
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	3,3',3''-[(1H,3H,5H)-2,4,6-trioxo-1,3,5-triazine-1,3,5-triyltris(methylene)]tris[3,5,5-trimethylcyclohexyl] triisocyanate	267-445-2	40 – 75
		1-[3-({3,5-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-2,4,6-trioxo-1,3,5-triazinan-1-yl}methyl)-3,5,5-trimethylcyclohexyl]-3,5-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-1,3,5-triazinane-2,4,6-trione /// Isophorone diisocyanate, oligomerization product, isocyanurate type, n = 5	N/A	15 – 25
		1-[3-({3,5-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-2,4,6-	N/A	5 – 20

		trioxo-1,3,5-triazinan-1-yl}methyl)-3,5,5-trimethylcyclohexyl]-3-[(5-{3,5-bis[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-2,4,6-trioxo-1,3,5-triazinan-1-yl}-1,3,3-trimethylcyclohexyl)methyl]-5-[(5-isocyanato-1,3,3-trimethylcyclohexyl)methyl]-1,3,5-triazinane-2,4,6-trione /// Isophorone diisocyanate, oligomerization product, isocyanurate type, n = 7		
		not applicable // Isophorone diisocyanate, oligomerization product, isocyanurate type, n >= 9	N/A	2 – 12
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane, esters with acrylic acid	500-130-2	0 – 100
		Reaction product of 3-(4-{1-methyl-1-[4-(oxiran-2-ylmethoxy) phenyl]ethyl}phenoxy) propane-1,2-diol and 2-propenoic acid (molar ratio 1:1)	N/A	0 – 10.69
		Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-, 2-propenoate // Reaction product of 2,2'-[propane-2,2-diylbis(4,1-phenyleneoxymethylene)] dioxirane and 2-propenoic acid (molar ratio 1:2)		46.99 - 79
		Reaction product of 2,2'-[propane-2,2-diylbis(4,1-phenyleneoxymethylene)] dioxirane and 2-propenoic acid (molar ratio 1:3)	N/A	0 – 11
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	N/A	99.9 – 100
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	Condensation products of m-phenylenebis(methylamine) with Dodecan-1-yl(3-isocyanato-4-methylphenyl)carbamate and Dodecan-1-yl(5-isocyanato-2-methylphenyl)carbamate and Tetradecan-1-yl(3-isocyanato-4-methylphenyl)carbamate and Tetradecan-1-yl(5-isocyanato-2-methylphenyl)carbamate	N/A	25 – 35
		Condensation products of m-phenylenebis(methylamine) with Dodecan-1-yl(3-isocyanato-4-methylphenyl)carbamate and Dodecan-1-yl(5-isocyanato-2-methylphenyl)carbamate and condensation products of m-phenylenebis(methylamine) with Decan-1-yl(3-isocyanato-4-methylphenyl)carbamate and Decan-1-yl(5-isocyanato-2-methylphenyl)carbamate and Tetradecan-1-yl(3-isocyanato-4-methylphenyl)carbamate and Tetradecan-1-yl(5-isocyanato-2-methylphenyl)carbamate	N/A	29 – 39
		Condensation products of m-phenylenebis(methylamine) with Decan-1-yl(3-isocyanato-4-methylphenyl)carbamate and Decan-1-yl(5-isocyanato-2-methylphenyl)carbamate and Dodecan-1-yl(3-isocyanato-4-methylphenyl)carbamate and	N/A	15 – 25

		Dodecan-1-yl(5-isocyanato-2-methylphenyl)carbamate		
10522	oxybis(methyl-2,1-ethanediyl) diacrylate	oxydipropane-1,2-diyl bisacrylate	260-754-3	74 – 100
		2-Propenoic acid (1 or 2), (4 or 5), (11 or 12), (14 or 15)-tetramethyl-7,17-dioxo-3,6,10,13,16-pentaoxanonadec-18-en-1-yl ester	N/A	2 – 8
		2-Propenoic acid 3-{(1 or 2)-methyl-2-[(1 or 2)-methyl-2-(2-propenoyloxy)-ethoxy]-ethoxy}-3-oxopropyl ester	N/A	2 – 8
		2-Propenoic acid, monoester with oxybis[propanol]	N/A	2 – 10
10617	Phenol, dodecyl-, branched, sulfurized	Phenol, dodecyl-, branched, sulfurized	306-115-5	100
		Unknown constituents	N/A	85 – 90
		Phenol, alkylation products with C10 - 15 branched olefins derived from propene oligomerization	N/A	5 – 20
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	1,1'-methylenebis(4-isocyanatobenzene)	202-966-0	10 – 98
		1-isocyanato-2-(4-isocyanatobenzyl)benzene	227-534-9	0 – 70
		1,1'-methylenebis(2-isocyanatobenzene)	219-799-4	0 – 5
		Higher oligomers of MDI/DPG	N/A	1 – 60
10852	Propylidynetrimethanol, ethoxylated	Propylidynetrimethanol, ethoxylated // Propylidynetrimethanol, ethoxylated, (>1 - <6.5 mol, EO)	500-110-3	99 – 100
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-[(1-oxo-2-propenyl)oxy]-, ether with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1)	500-066-5	80 – 100
		2-Propenoic acid 2-ethyl-2-[({2-[(1-oxo-2-propenyl)oxy]ethyl}oxy)methyl]-1,3-propanediyl ester	N/A	0.8 – 17
		2-Propenoic acid 2-ethyl-3-({2-[(1-oxo-2-propenyl)oxy]ethyl}oxy)-2-[({2-[(1-oxo-2-propenyl)oxy]ethyl}oxy)methyl]-propyl ester	N/A	24 – 34
		2-Propenoic acid 8-ethyl-8-{[(1-oxo-2-propenyl)oxy]methyl}-3,6,10-trioxadodecane-1,12-diyl ester	N/A	17 – 36
10854	Propylidynetrimethanol, propoxylated	Propylidynetrimethanol, propoxylated (>1 - <6.5 mol PO) // Poly[oxy(methyl-1,2-ethanediyl)], .alpha.-hydro-.omega.-hydroxy-, ether with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1)	500-041-9	99 – 100
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	Resin acids and Rosin acids, fumarated, Tri esters with pentaerythritol	N/A	15 – 30
		Tetraester of rosin with pentaerythritol, as the reactor is charged with rosin and pentaerythritol and reacted until a low 'acid value' is achieved, indicating that most of the –COOH groups of the parent rosin have been esterified	N/A	5 – 35
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	Resin Acids, Hydrogenated, Tri-Esters with Pentaerythritol	N/A	25 – 45
		Resin Acids, Hyrogenated, Tetra-Esters with Pentaerythritol	N/A	25 – 50
		(Heavy Ends)-Complex mixture of dimerized esters, acids and polyol	N/A	2 – 20
		Hydrogenated resin acids	N/A	6 – 10
202	Resin acids and Rosin acids, sodium salts	sodium abietate // sodium abieta-7,13-dien-18-oate // 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-,	238-313-1	0 – 70

		sodium salt (1:1), (1R,4aR,4bR,10aR)-		
		Sodium salt of dehydroabietic acid // sodium abieta-8,11,13-trien-18-oate	248-873-9	0 – 70
		Sandaracopimaric acid, sodium salts / 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, sodium salt (1:1), (1R,4aR,4bS,7R,10aR)-	N/A	0.3 – 64
		Levopimaric acid, sodium salts / 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, sodium salt (1:1), (1R,4aR,4bS,10aR)-	N/A	0.3 – 64
346	Rosin, fumarated	ROSIN, FUMARATED	266-040-8	100
		Resin acids and rosin acids	277-299-1	15 – 90
		abieta-8,11,13-trien-18-oic acid // [1R-(1α,4aβ,10aα)]-1,2,3,4,4a,9,10,10a-octahydro-7-isopropyl-1,4a-dimethylphenanthren-1-carboxylic acid	217-102-8	15 – 40
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	Pentaerythritol, triester with rosin acids	N/A	10 – 55
		Pentaerythritol, tetraester with rosin acids	N/A	10 – 40
		Pentaerythritol, polYters with rosin acids	N/A	20 – 45
860	Rosin, reaction products with formaldehyde	Rosin, reaction products with formaldehyde	293-659-0	100
5899	1,2-Diaminotoluene, propoxylated	1,2-Diaminotoluene, propoxylated	918-139-9	99 – 100
6665	2-aminoethanol, monoester with boric acid	MEA Polyborate	233-829-3	99.5 – 100
6308	2,2',2''-Nitrilotriethanol, propoxylated	2, 2', 2'' - Nitriloethanol, propoxylated	500-094-8	80 – 100
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-(methyl-1,2-ethanediyl)]	500-044-5	80 – 100
8731	D-Glucitol, propoxylated	D-Glucitol, propoxylated (>1<12.5 mol PO)// Poly[oxy(methyl-1,2-ethanediyl)],.alpha.-hydro-.omega.-hydroxy-,ether with D-glucitol (6:1)	500-118-7	99.95 – 100
4426-31	Inositol phosphates	phosphoric acid	231-633-2	23.8 - 26
		tetrahydroxycyclohexanediyl bis(dihydrogen phosphate)	N/A	14 – 19
		trihydroxycyclohexanetriyl tris(dihydrogen phosphate)	N/A	6 – 9
384-5	Naphthenic acids, reaction products with diethylenetriamine	Naphthenic acids, reaction products with diethylenetriamine	268-610-1	100
10615-6	Phenol, dodecyl-, branched	Phenol, dodecyl-, branched// phenol, alkyl branched (species comprising decyl, undecyl, dodecyl, tridecyl, tetradecyl, pentadecyl, substituents)	310-154-3	57 – 100
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	Phenol, dodecyl-(tetrapropenyl), sulfurized, carbonates, calcium salts, overbased / Phenol, tetrapropylene-, sulfurized, carbonates, calcium salts, overbased / 122384-87-6	N/A	52 – 62
		Distillates (petroleum), hydrotreated heavy paraffinic	265-157-1	30 – 40
		Phenol, dodecyl-, branched	310-154-3	3.5 – 9
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-	1-[(4Z,8Z)-4,9-dimethyl-12-methylidenecyclododeca-4,8-dien-1-yl]ethanone	N/A	18 – 35

	1,5,9-cyclodecatriene	1-[(2Z,5Z,9Z)-2,5,10-trimethylcyclododeca-2,5,9-trien-1-yl)ethanone	N/A	12 – 22
		1-[(1E,5Z,9Z)-2,5,10-trimethylcyclododeca-1,5,9-trien-1-yl)ethanone	N/A	10 – 24
		unknown constituents	N/A	35 – 60
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	benzene	200-753-7	0 – 5
		Toluene	203-625-9	0 – 5
		xylene (mixed isomers)	215-535-7	0 – 2.5
		Phenol	203-632-7	0 – 3
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	S-(tricyclo[5.2.1.02,6]deca-3-en-8(or 9)-yl)-O-isopropyl-O'-isobutylphosphorodithioate	N/A	30 – 40
		S-(tricyclo[5.2.1.02,6]deca-3-en-8(or 9)-yl)-O-isobutyl-O'-isobutylphosphorodithioate	N/A	12 – 25
		S-(tricyclo[5.2.1.02,6]deca-3-en-8(or 9)-yl)-O-isopropyl-O'-2-ethylhexylphosphorodithioate	N/A	8 – 13
		S-(tricyclo[5.2.1.02,6]deca-3-en-8(or 9)-yl)-O-isobutyl-O'-2-ethylhexylphosphorodithioate	N/A	10 – 17

In a few cases the registrants reported only a single constituent with identical name as the name of the registered substance. There are also cases where the concentration ranges of reported constituents are very wide (e.g. 10 – 98 %).

Source

Due to the heterogeneity of substances in this group, observations on typical sources are presented in relation to individual sub-groups of substances.

Oligomers
All substances in this sub-group are on the No-Longer Polymers (NLP) List. Source of these substances specified by registrants therefore corresponds to individual reaction agents undergoing, typically well-defined organic substances.

Organic pigments and dY
Copper phthalocyanine is specified as the source of two of the three screened substances, with diazotized 3, 3'-Dichlorobenzidine dihydrochloride (DCB) and coupling component being specified as the source of the third screened substance within this sub-group.

Residues
No general observations in relation to the source of the substances can be made for this sub-group. Substances in this sub-group include distillation residues or residues from various chemical processes, e.g. hydroformylation products, or by-products of various reactions. It is usually described already in the substance name that it is a residue, but there are some cases where it is not so.

Resins (synthetic) and polymers
Typical reaction agents used in syntheses of resins are specified by registrants as sources of these substances, including e.g. acrylic acid, bisphenol A, epichlorhydrine as well as various alcohols and polyols. Curing agents are also present among the sources of resins specified by the registrants, e.g. amines.

Rosin/resin derivates
Rosin is the only source specified by the registrants of the substances screened in this sub-group.

Others
No general observations in relation to the source of the substances can be made for this sub-group.

The following table summarises the sources of substances in this group specified by the registrants of the screened substances.

Table 86 Sources of other complex organic substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	4,4'-methylenediphenyl diisocyanate methylenediphenyl diisocyanates (EC 500-079-6 or 905-806-4 or 247-714-0 or 202-966-0 or 227-534-9)
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	aniline and acetone
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	Bisphenol F and Epichlorohydrin
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	bisphenol-A-diglycidylether/oligomeric bi-functional bisphenol A-based liquid Epoxy Resin
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	copper phthalocyanine
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016	diazotized 3, 3'-Dichlorobenzidine dihydrochloride (DCB) and coupling component
10705	polychloro copper phthalocyanine	copper phthalocyanine
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	Alkenes, C11-14, hydroformylation products, distn. residues mixture of Alkenes, C11-12, hydroformylation products, distn. residues (90622-29-0) and Alkenes, C13-14, hydroformylation products, distn. residues (90622-29-0)
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	a byproduct in the phenol production process (the oxidation of cumene (Hock process))
525-6	Dodecene, hydroformylation products, high-boiling	Dodecene
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	reaction products of ethanolamine and ammonia
625-6	Oxirane, reaction products with ammonia, distn. Residues	reaction products of ethylenoxide with ammonia
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	tripropylene glycol and acrylic acid
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters	metacrylic acid fatty alcohols
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate (IPDI)
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	BADGE(diglycidyl ether of bisphenol A) epoxy resin (4,4'-isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane with an average molecular weight between 350 and 390 g/mole / oligomeric bi-functional bisphenol A-based Epoxy Resin (BPADGE) bisphenol A, epichlorohydrin and trimethylamine
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	diisobutylene and diphenylamine
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	m-phenylenebis(methylamine) and condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)
10522	oxybis(methyl-2,1-ethanediyl) diacrylate	oxydipropanol and acrylic acid
10617	Phenol, dodecyl-, branched, sulfurized	Dodecylphenol
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-	MDIs

	isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	
10852	Propylidynetrimethanol, ethoxylated	Propylidynetrimethanol
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	acrylic acid and propylidynetrimethanol, ethoxylated (ethoxylate trimethylolpropane)
10854	Propylidynetrimethanol, propoxylated	Propylidynetrimethanol
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	Rosin
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	Rosin
202	Resin acids and Rosin acids, sodium salts	Rosin
346	Rosin, fumarated	Rosin
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	Rosin
860	Rosin, reaction products with formaldehyde	Rosin
5899	1,2-Diaminotoluene, propoxylated	o-diaminotoluene as starter and propylene oxide (PO) as monomer
6665	2-aminoethanol, monoester with boric acid	Monoethanolamine
6308	2,2',2''-Nitrilotriethanol, propoxylated	Triethanolamine
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	Glycerin
8731	D-Glucitol, propoxylated	D-Glucitol (sorbitol)
4426-31	Inositol phosphates	Inositol
384-5	Naphthenic acids, reaction products with diethylenetriamine	naphtenic acids and diethylenetriamine
10615-6	Phenol, dodecyl-, branched	phenol + olefins
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	Alkylphenol
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene	unsaturated terpene and aliphatic anhydride
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	organic liquid phase (called: Aromatic hydrocarbons, >C5, reclaimed, waste water treatment
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	-

Manufacturing process and its parameters (conditions)

Due to the heterogeneity of substances in this group, observations on typical manufacturing processes are presented in relation to individual sub-groups of substances.

Oligomers
Various oligomerisation (e.g. condensation, addition) reactions are typical manufacturing processes specified by registrants of the substances in this sub-group. In some cases the description of the manufacturing process is identical to the description linked to the reference substance and the descriptions are therefore sometimes identical in several dossiers.

Organic pigments and dY
Halogenation is the process specified in registration dossiers for two of the three screened substances, with coupling being the process of manufacture of the third one.

Residues
Substances in this sub-group are residues or by-products from various chemical reactions (often hydroformylation) separated in the process from the main reaction product, most frequently through distillation..

Resins (synthetic) and polymers
The most frequently encountered manufacturing process of synthetic resins and polymers is catalytic oligomerisation or polymerisation (often esterification or alkoxylation) of alcohols in reaction with acrylic or methacrylic acid. Catalysed polymerisation of polyols was alse encountered as the manufacturing process reported in the screened registration dossiers and in one case the manufacturing process specified by the registrants was catalysed reaction between dodecylphenol and elemental sulphur, alternatively between tetrapropenyl phenol and sulphur monochloride. *Rosin/resin derivates*
Esterification is the most typical process specified in the screened dossiers. Descriptions of the manufacturing processes are often very detailed in this sub-group of substances, giving information on reaction agents and their molar ratios, catalysts, conditions of the process (reaction temperature) and descriptions of individual processing steps.

Others
No general observations.

Compared to other groups of substances, the description of the manufacturing processes of substances in this group focuses mainly on describing corresponding chemical reactions rather than describing various separation processes (e.g. distillation), which is typical for some of the other groups of studied substances (e.g. petroleum-derived products or coal-derived products).

The following table summarises the manufacturing process of the substances in this group specified by the registrants of the screened substances.

Table 87 Manufacturing processes of other complex organic substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	reaction of 4,4'-methylenediphenyl diisocyanate with itself reaction of MDIs (methylenediphenyl diisocyanate) with themselves or with hydroxy or amino compounds
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	condensation and simultaneous polymerisation
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	1. condensation (strong base) 2. dehydrohalogenation
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	addition reaction with isophorone diamine (IPD)
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	direct halogenation
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016	Coupling
10705	polychloro copper phthalocyanine	Chlorination
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	Reaction of distillation residues from hydroformylation of alkenes C11-14 with maleic anhydride and subsequent sulfitation.
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	-
525-6	Dodecene, hydroformylation products, high-boiling	Hydroformylation and subsequent distillation
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	Distillation
625-6	Oxirane, reaction products with ammonia, distn. residues	Distillation
5418	(1-methyl-1,2-	Esterification

	ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters	Esterification
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	catalytic oligomerization
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	reaction with acrylic acid
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	cracking and alkylation processes catalytic reaction
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	Condensation
10522	oxybis(methyl-2,1-ethanediyl) diacrylate	Esterification
10617	Phenol, dodecyl-, branched, sulfurized	sulphurization by sulphur sulphurization by sulphur monochloride
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	catalyzed partial reaction with themselves or with hydroxy or amino compounds reaction with oxydipropanol and the polymer of oxydipropanol having an average molecular weight of 450 g/Mol reaction with oxydipropanol
10852	Propylidynetrimethanol, ethoxylated	alkoxylation reaction with ethylene oxide
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	Esterification
10854	Propylidynetrimethanol, propoxylated	alkoxylation reaction with propylene oxide
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	1. Reaction with fumaric acid 2. Esterification
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	Esterification
202	Resin acids and Rosin acids, sodium salts	Saponification
346	Rosin, fumarated	Diels-Alder reaction (reaction with fumaric acid)
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	1. Reaction with fumaric acid 2. Esterification
860	Rosin, reaction products with formaldehyde	Reaction with formaldehyde
5899	1,2-Diaminotoluene, propoxylated	alkoxylation reaction
6665	2-aminoethanol, monoester with boric acid	reaction with boric acid
6308	2,2',2''-Nitrilotriethanol, propoxylated	reaction with propylene oxide alkoxylation reaction with propylene oxide
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	alkoxylation reaction with propylene oxide
8731	D-Glucitol, propoxylated	alkoxylation reaction with propylene oxide
4426-31	Inositol phosphates	phosphorylation reaction (reaction with phosphorus pentoxide and phosphoric acid)
384-5	Naphthenic acids, reaction products with diethylenetriamine	Condensation
10615-6	Phenol, dodecyl-, branched	exothermic catalytic reaction
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	reaction with calcium oxide/hydroxide, sulphur, carbon dioxide
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene	Acetylation
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	static separation of process water coming from the tar distillation plant
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	-

Additional substance identity elements

Despite the heterogeneity of substances in this group, a common feature is a low number of substance identity elements used to characterise the registered substances (on average 4.1 ± 1.3 substance identity elements to characterise a substance, including composition, source and manufacturing process).

Besides specifying the parameters (conditions) of the manufacturing process, registrants of the substances screened in this group used additional substance identity elements rarely.

c) Analytical methods

The following Table 88 and **Table 89**summarise the use of analytical methods and techniques in identification of the screened substances.

Table 88 REACH Annex VI analytical methods used by registrants of other complex organic substances.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	Y	Y	Y		Y	Y
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	Y	Y	Y		Y	
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	Y	Y	Y	Y	Y	Y
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	Y	Y	Y	Y	Y	Y
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated	Y	Y	Y	Y	Y	
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016	Y	Y	Y		Y	
10705	polychloro copper phthalocyanine	Y	Y	Y	Y	Y	Y
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts	Y	Y	Y		Y	
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues	Y	Y	Y		Y	
525-6	Dodecene, hydroformylation products, high-boiling	Y	Y	Y		Y	
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from	Y	Y	Y		Y	
625-6	Oxirane, reaction products with ammonia, distn. residues	Y	Y	Y		Y	
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate	Y	Y	Y		Y	Y
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters	Y	Y	Y		Y	
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	Y	Y	Y	Y	Y	
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	Y	Y	Y	Y	Y	Y
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	Y	Y	Y	Y	Y	Y
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)	Y	Y	Y	Y	Y	
10522	oxybis(methyl-2,1-ethanediyl) diacrylate	Y	Y	Y	Y	Y	Y
10617	Phenol, dodecyl-, branched, sulfurized	Y	Y	Y	Y	Y	Y
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-	Y	Y	Y	Y	Y	Y

	isocyanatophenyl)methyl]benzene						
10852	Propylidynetrimethanol, ethoxylated	Y	Y	Y	Y		Y
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	Y	Y	Y	Y	Y	Y
10854	Propylidynetrimethanol, propoxylated	Y	Y	Y	Y		Y
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	Y	Y	Y	Y	Y	Y
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	Y	Y	Y	Y	Y	Y
202	Resin acids and Rosin acids, sodium salts	Y	Y	Y	Y		Y
346	Rosin, fumarated	Y	Y	Y	Y		Y
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	Y	Y	Y	Y		Y
860	Rosin, reaction products with formaldehyde	Y	Y	Y	Y	Y	Y
5899	1,2-Diaminotoluene, propoxylated	Y	Y	Y	Y	Y	Y
6665	2-aminoethanol, monoester with boric acid	Y	Y	Y			
6308	2,2',2''-Nitrilotriethanol, propoxylated	Y	Y	Y	Y		
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	Y	Y	Y	Y		Y
8731	D-Glucitol, propoxylated	Y	Y	Y	Y	Y	Y
4426-31	Inositol phosphates	Y	Y	Y	Y	Y	
384-5	Naphthenic acids, reaction products with diethylenetriamine	Y	Y	Y			Y
10615-6	Phenol, dodecyl-, branched	Y	Y	Y	Y	Y	Y
581	Phenol, dodecyl-, sulfurized, carbonates, calcium salts, overbased	Y	Y	Y	Y	Y	Y
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene	Y	Y	Y			Y
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment	Y	Y	Y			Y
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate	Y	Y	Y			Y
Percentage of use of analytical methods (%)		100	100	100	64	71	67

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 89 Other analytical methods used by registrants of other complex organic substances in addition to REACH Annex VI methods.

ID	Name (as registered)	GPC	Additional analytical techniques and measurements
5857	1,1'-methylenebis(4-isocyanatobenzene) homopolymer	Y	Determination of CHN (carbon, hydrogen, nitrogen), Oxygen; Sulfated ash; NCO titration (determination of isocyanate content)
5904-5	1,2-Dihydro-2,2,4-trimethylquinoline, oligomers	Y	
4215	Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol	Y	Size exclusion chromatography
4223	Reaction product of 3-aminomethyl-3,5,5-trimethylcyclohexanamine with oligomerisation products of 4,4'-propane-2,2-diyldiphenol with 2-(chloromethyl)oxirane	Y	Size exclusion chromatography
8634	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, brominated chlorinated		XRD, ICP-OES, Determination of C, N, Determination of Br, Cl, Headspace capillary gas chromatography
1528-30	H 109368; HYPERSOL SYNERGIST L 4722; YELLOW PD4016		
10705	polychloro copper phthalocyanine		XRD, AAS, ICP-OES, KF titration, Elemental analysis, Determination of Polychlorinated Dibenzodioxins (PCDDs) and Dibenzofurans (PCDFs), Determination of PCB, HCB, Determination of tetra- to octa-chlorinated dioxines and furanes, Determination of Primary Aromatic Amines, Determination of Cl and Cl-, Determination of Tetrachlorophthalicacidanhydride, Tetrachlorophthalamidacid and

			Tetrachlorophthalimid, Determination of 2,3,7,8-substituted PBDFs and PBDDs, Determination of p-xylene
5126	Alkenes, C11-14, hydroformylation products, distn. residues, reaction products with maleic anhydride and sodium bisulfite, sodium salts		KF titration, Hyamine method, Acidic and saponification values, Ionic chromatography
414	Benzene, (1-methylethyl)-, oxidized, polyphenyl residues		
525-6	Dodecene, hydroformylation products, high-boiling		
599	Ethanol, 2-amino-, reaction products with ammonia, by-products from		
625-6	Oxirane, reaction products with ammonia, distn. Residues		
5418	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate		KF titration, Acrylic acid determination
6986	2-Propenoic acid, 2-methyl-, C12-15-branched and linear alkyl esters		
4962	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer, isocyanurate type	Y	
4225	4,4'-Isopropylidenediphenol, oligomeric reactionproducts with 1-chloro-2,3-epoxypropane, esters with acrylic acid	Y	Titration, Colorimetry
433	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene		thermogravimetric analysis
2458	Condensation products of m-phenylenebis(methylamine) with condensation products of 4-methyl-m-phenylene diisocyanate with alcohols, C10-14 (even numbered)		KF titration, Titration
10522	oxybis(methyl-2,1-ethanediyl) diacrylate		
10617	Phenol, dodecyl-, branched, sulfurized		ICP
10816	propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	Y	
10852	Propylidynetrimethanol, ethoxylated	Y	KF titration, Determination of TMP (trimethoprim)
10853	Propylidynetrimethanol, ethoxylated, esters with acrylic acid	Y	KF titration, Elemental analysis CHN O, Sulfated ash determination
10854	Propylidynetrimethanol, propoxylated	Y	KF titration, Determination of TMP (trimethoprim), Elemental analysis CNH O, Sulfated ash determination
969	Resin acids and Rosin acids, fumarated, esters with pentaerythritol	Y	MALDI-TOF, Titration
212	Resin acids and Rosin acids, hydrogenated, esters with pentaerythritol	Y	
202	Resin acids and Rosin acids, sodium salts	Y	ICP
346	Rosin, fumarated	Y	
924	Rosin, fumarated, reaction products with glycerol and pentaerythritol	Y (GPC/ SEC)	Titration
860	Rosin, reaction products with formaldehyde	Y (GPC/ SEC)	
5899	1,2-Diaminotoluene, propoxylated	Y	KF titration, Determination of sulfated ash, Elemental analysis (CHNO)
6665	2-aminoethanol, monoester with boric acid		Analysis of C N B (H), ICP-OES, Nitrogen Kjeldahl
6308	2,2',2''-Nitrilotriethanol, propoxylated	Y	Elemental analysis CHN, O, Sulfated ash determination, KF titration
7997	alpha, alpha', alpha''-1,2,3-propanetriyltris[w-hydroxypoly(oxy-methyl-1,2-ethanediyl)]	Y	Sulfated ash determination, KF titration, Elemental analysis CHN, O
8731	D-Glucitol, propoxylated	Y	GLC, SEC, Optical activity
4426-31	Inositol phosphates		Raman spectra, KF titration, Analysis & calculation of phosphorylation ratio & % inositol (free orthophosphate, Analysis- total orthophosphate, Inositol)
384-5	Naphthenic acids, reaction products with diethylenetriamine		Determination of amine nitrogen content, Acid number, Elemental analysis
10615-6	Phenol, dodecyl-, branched		KF Titration
581	Phenol, dodecyl-, sulfurized, carbonates,		ICP-OES, Field Ionisation Mass Spectrometry

	calcium salts, overbased		
4117-21	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene		
4471	Reclaimed >C5 aromatic compounds from tar oils manufacturing wastewater treatment		
10906-10	S-(tricyclo(5.2.1.0'2,6)deca-3-en-8(or 9)-yl O-(isopropyl or isobutyl or 2-ethylhexyl) O-(isopropyl or isobutyl or 2-ethylhexyl) phosphorodithioate		

Despite (and maybe thanks to) the heterogeneity of the substances in this group, a very high use of analytical methods explicitly mentioned in Annex VI of REACH as well as of additional analytical methods and techniques was observed in the screened registration dossiers. Use of the complete set of methods explicitly mentioned in Annex VI of REACH (i.e. ultraviolet-visible spectroscopy, infrared spectroscopy, nuclear magnetic resonance spectroscopy, mass spectrometry, high-performance liquid chromatography and gas chromatography) was observed for 38% of the substances screened in this group.

As documented in the table above, numerous analytical methods not explicitly mentioned in Annex VI of REACH were also often used by the registrants of the screened substances.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressesd by the following operating consortia and associations:

- MDI/MDA REACH Consortium - http://www.reachcentrum.eu/consortium/mdi-mda-reach-consortium-135.html
- Phenol & Derivatives REACH consortium - http://www.reachcentrum.eu/consortium/phenol-derivatives-reach-consortium-149.html
- Ethylene Amines Consortium - https://chemicalwatch.com/4151/ethylene-aminesconsortium
- IPDI Trimer REACH consortium - http://www.reachcentrum.eu/consortium/oligomerization-product-isocyanurate-type-of-isophorone-diisocyanate-reach-consortium-128.html
- Polymerisable Acrylate Resins and Derivatives PARAD REACH Consortium - http://www.reachcentrum.eu/consortium/polymerisable-acrylate-resins-and-derivatives-reach-consortium-151.html
- NLP Polyols Consortium - http://www.reachcentrum.eu/consortium/nlp-polyols-reach-consortium-145.html
- Hydrocarbon Resins & Rosin Resins (H4R) REACH Consortium - http://www.h4rconsortium.com/
- Alkanolamine Borates Consortium - http://www.alkanolamineborates.eu/
- ATC Consortium - https://chemicalwatch.com/4228/atc-consortium

e) Substance identity profiles

Not found for the substances in this group.

3.3. Substance identity of complex substances of biological origin

3.3.1. Substances originating from fermentation process

Substances originating from fermentation process registered in accordance with REACH include complex substances such as enzymes, vinasses and other products of fermentation processes, e.g. amino acids (L-ornithine, L-threonine) and high molecular weight biopolymers (Biozan, Diutan).

As documented further below, composition of these substances is unknown to a large extent and due to the complexity of the fermentation process also highly variable.

a) substances screened in this group

The following Table 90 lists substances originating from fermentation processes selected for substance identity screening.

Table 90 Substances originating from fermentation processes – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed
		Joint	Indiv.	Total	
90	Amylase, α-	5	0	5	100
93	Cellulase	6	0	6	100
858	Peptones, casein	4	0	4	100
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	1	0	1	100
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	0	1	1	100
5027	Vinasses, residue of fermentation	19	0	19	100
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	15	0	15	100
5085	Vinasses, residue of fermentation, depotassified	3	0	3	100

None of the substances screened in this group was registered by more than 20 registrants. For the purposes of this project, substances originating from fermentation processes have been further divided into the following sub-groups:

1. Enzymes
2. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 91 Substance identity elements used by registrants in identification of substances originating from fermentation processes.

	Enzymes			Others					
	90	93	858	4788	4524	5027	5021	5085	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process			✓	✓	✓				38
Composition	✓	✓	✓	✓	✓	✓	✓	✓	100
State	✓	✓	✓			✓	✓	✓	75
Solubility			✓						13
pH			✓			✓	✓	✓	50
Form of the substance			✓		✓				25
Colour			✓		✓	✓	✓	✓	63
*Group-specific element**	✓	✓	✓						38
Odour						✓	✓		25
*Common characteriser***	✓	✓	✓			✓			50
*Other characteriser****	✓	✓	✓	✓	✓	✓	✓	✓	100
No. of applied SID elements per substance	7	7	12	5	7	9	8	7	Average = 60
Average no. of applied SID elmts. per sub-group	8.7 ± 2.9			7.2 ± 1.5					
Average no. of applied SID elmts. per group	7.8 ± 2.1								

* SID element specific to a certain group/sub-group of substances, in particular: Enzyme Commission number (90, 93, 858), Active enzyme protein (90, 93), Enzymatic digestion products (858).

** Enzyme (90, 93), Peptone (858), Vinasses (5027).

*** Product of a microbial fermentation process (90, 93), Products of biochemical processes (858), Biomass residue (4788), Fermentation products (4524), Residue of fermentation (5027, 5021, 5085), By-product (5085).

Comments to Table 91:

- 13 SID elements were used by registrants of the screened substances for identification of substances in this group;

- Number of used SID elements varies between 5 and 12 for each substance, with 7.8 being the average number of SID elements used by registrants for identification of substances in this group;

- Standard deviation linked to the average number of SID elements used by registrants of substances in this group is 2.1;

- Besides composition, source and manufacturing process, most substances (50 % or more)were identified using the following SID elements: state (e.g. liquid), pH, colour and other characteriser (e.g. fermentation product, residue of fermentation, product of a microbial fermentation process, products of biochemical processes, biomass residue).

Composition

The registrants of the substances subject to the screening specified composition of the substances providing concentration ranges of individual constituents together with their typical concentrations in all screened registration dossiers (unless a single constituent in the concentration of 100% was specified, which was the case of all the three vinasses as titled in the registered substance name).

The following tables provide further information on compositional data provided by registrants of the screened substances.

Table 92 Number of compositions specified in registration dossiers by registrants of substances originating from fermentation processes.

ID	Name (as registered)	% of No. of compositions	
		1	2
90	Amylase, α-	100%	
93	Cellulase	100%	
858	Peptones, casein	100%	
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	100%[a]	
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	100%[a]	
5027	Vinasses, residue of fermentation	95%	5%
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	100%	
5085	Vinasses, residue of fermentation, depotassified	100%	

[a] Only a single registration dossier

All but one of the screened registration dossiers included a single composition. The only case where a single registrant specified multiple compositions was describing besides the substance itself also a marketed product with 50% water content.

Table 93 Number of constituents specified in registration dossiers by registrants of substances originating from fermentation processes.

ID	Name (as registered)	Composition & No. of constituents	
90	Amylase, α-		5
93	Cellulase		5
858	Peptones, casein		8
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis		1
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola		8
5027	Vinasses, residue of fermentation	Composition #1	1
		Composition #2	2
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)		1
5085	Vinasses, residue of fermentation, depotassified		1

In comparison with other groups of complex organic substances, the number of constituents identified by the registrants is rather low. The registrants either specify only a single constituent (with identical name to the name of the registered substance) in 100% concentration or even in cases where 5 – 8 constituents are specified, these have wide concentration ranges.

Table 94 Consistency of compositional data provided in the registration dossiers for substances originating from fermentation processes.

ID	Name (as registered)	Composition consistency score*					
		1	2	3	4	5	6
90	Amylase, α-	0%	100%	0%	0%	0%	0%
93	Cellulase	0%	83%	17%	0%	0%	0%
858	Peptones, casein	0%	0%	0%	100%	0%	0%
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	0%	0%	0%	0%	0%	100%
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	100%	0%	0%	0%	0%	0%
5027	Vinasses, residue of fermentation	0%	0%	0%	5%	0%	100%
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	0%	0%	0%	0%	0%	100%
5085	Vinasses, residue of fermentation, depotassified	0%	0%	0%	0%	0%	100%

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

Table 95 Typical constituents specified in registration dossiers by registrants of substances originating from fermentation processes.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
90	Amylase, α-	alpha-amylase (active enzyme protein)	N/A	10 – 80
		Protein as a constituent of enzyme deriving from the fermentation or extraction process	N/A	5 – 55
		Carbohydrates constituent of enzyme deriving from the fermentation or extraction process	N/A	3 – 40
		Inorganic salts as a constituent of enzyme deriving from the fermentation or extraction process	N/A	1 – 45
		Lipids as a constituent of enzyme deriving from the fermentation or extraction process	N/A	0 – 5
93	Cellulase	Cellulase (active enzyme protein)	N/A	10 – 80
		Protein as a constituent of enzyme deriving from the fermentation or extraction process	N/A	5 – 55
		Carbohydrates constituent of	N/A	3 – 40

		enzyme deriving from the fermentation or extraction process		
		Lipids as a constituent of enzyme deriving from the fermentation or extraction process	N/A	0 – 5
		Inorganic salts as a constituent of enzyme deriving from the fermentation or extraction process	N/A	1 – 45
858	Peptones, casein	Peptones, Casein	293-428-4	70 – 100
		Lactose	200-559-2	0 – 8
		disodium hydrogenorthophosphate	231-448-7	0 – 22.1
		sodium chloride	231-598-3	0 – 22.1
		sodium sulphate	231-820-9	0 – 22.1
		potassium sulphate	231-915-5	0 – 22.1
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	Biomass residue ex B2	920-031-1	99.9 – 100
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	17-([2'O-β-D-glucopyranosyl-β-D-glucopyranosyl]-oxy)-9-octadecenoate-1,4''-lactone-6',6''-diacetate / 17-([2'O-β-D-glucopyranosyl-β-D-glucopyranosyl]-oxy)-9-octadecenoate-1,4''-lactone-6',6''-diacetate	N/A	15 – 40
		17-([2'-O-b-D-glucopyranosyl-b-D-glucopyranosyl]-oxy)-9,12-octadecadienoic acid 1,4''-lactone-6',6''-diacetate / 17-([2'-O-b-D-glucopyranosyl-b-D-glucopyranosyl]-oxy)-9,12-octadecadienoic acid 1,4''-lactone-6',6''-diacetate	N/A	0 – 10
		Methyl 17-([2'O-β-D-glucopyranosyl-β-D-glucopyranosyl]-oxy)-9-octadecenoate-6',6''-diacetate / Methyl 17-([2'O-β-D-glucopyranosyl-β-D-glucopyranosyl]-oxy)-9-octadecenoate-6',6''-diacetate	N/A	10 – 40
5027	Vinasses, residue of fermentation	Vinasses, residue of fermentation	N/A	100
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	N/A	100
5085	Vinasses, residue of fermentation, depotassified	Vinasses, residue of fermentation, depotassified	N/A	100

In a few cases the registrants reported only a single constituent with identical name as the name of the registered substance. For one of **the substances (peptones, casein), one of the registrants reported four different constituents (disodium hydroge**northophosphate, sodium chloride, sodium sulphate and potassium sulphate) with identical concentration ranges (0 – 22.1 %). There is no reasoning provided in the dossier explaining this anomaly.

Source

Sources specified by the registrants of the screened substances originating from fermentation process are mainly microbial cultures and culture media. Since microbial cultures – microorganisms drive the fermentation process, it can be concluded that source and process are the key elements determining the composition of the resulting substance.

In some cases the description of the source includes the name of the microbial species responsible for the fermentation process.

The following table summarises sources specified by the registrants of the screened substances.

Table 96 Sources of substances originating from fermentation processes as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
90	Amylase, α-	microbial culture, biomass
93	Cellulase	microbial culture / biomass
858	Peptones, casein	Casein
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	Sugar solution (glucose, saccharose), Bacillus subtilis. Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	Yeast extract, urea, glucose, Candida bombicola, citric acid, (NH4)2SO4, 4 H2O , Ca(NO3)2,4 H2O, MgSO4, 7H2O, NaCl , K2HPO4 , KH2PO4, Strucktol
5027	Vinasses, residue of fermentation	Water, sugar, yeast, benzaldehyde Culture medium consisting of substrates, mineral nutrients and vitamins Aerobic culture of Yeast (Saccharomyces Cerevisiae)
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	Biomass of bakers yeast (Saccharomyces cerevisiae)
5085	Vinasses, residue of fermentation, depotassified	Culture medium consisting of substrates, mineral nutrients and vitamins

Manufacturing process and its parameters (conditions)

The central process for this group of substances is microbial fermentation, followed by a number of different processing steps, typically concentration (evaporation, drying, ultra-filtration), separation, purification (filtration), etc.

Table 97 Manufacturing processes of substances originating from fermentation processes as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
90	Amylase, α-	Microbial fermentation - recovery process (separation, purification)
93	Cellulase	Microbial fermentation - recovery process: separation, purification (filtration), concentration (evaporation, ultra-filtration), stabilization
858	Peptones, casein	Controlled enzymatic hydrolysis of casein
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	Fermentation
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	Aerobic fermentation and then bioconversion, dilution, heating
5027	Vinasses, residue of fermentation	Fermentation
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	Fermentaion Product is concentrated by centrifugation, evaporation or drying
5085	Vinasses, residue of fermentation, depotassified	Fermentation Concentration (evaporation, centrifugation…) Depotassification

Registrants usually provide detailed description of the manufacturing process, specifyingindividual processing steps (e.g. the individual recovery process steps after fermentation in the case of enzymes and description of the fermentation process and its conditions such as ratios of fermentation reactants, temperature, agitation speed, aeration, cover pressure or intial pH for other fermentation process products).

Example of a description of the conditions of the manufacturing process conditions as reported in one of the screened dossiers: “The fermentation conditions are: T 30°C, agitation speed 130 rpm, aeration 10.5 m3/h, cover pressure 0.5 bar, initial pH 5.5 for 30h. The development is controlled by the optic density.”

Additional substance identity elements

Of the additional substance identity elements, pH appears to be of high importance for characterisation of substances in this group. Due to the fact that the activity and viability of microorganisms driving the fermentation processes is highly dependent on pH, variability in pH brings variability also to the composition of the fermentation products.

In addition to the aforementioned substance identity elements, registrants used the following additional substance identity elements in some of the screened dossiers:

Substance identity element	Value	Substance identified with the SID element
State	Liquid	Amylase, α- (90), Cellulase (93), Vinasses, residue of fermentation (5027), Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae) (5021), Vinasses, residue of fermentation, depotassified (5085)
	Solid	Peptones, casein (858)
Solubility	Different components show different solubility in water.	Peptones, casein (858)
pH	pH (5 % solution): 6.5 - 7.5	Peptones, casein (858)
	3 – 9	Vinasses, residue of fermentation (5027), Vinasses, residue of fermentation, depotassified (5085)
	3.5 - 6.5	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae) (5021)
Form of the substance	Powder	Peptones, casein (858)
	Paste	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola (4524)
Colour	from white to light brown	Peptones, casein (858)
Enzyme Commission number	3.2.1.1	Amylase, α- (90)
	3.2.1.4	Cellulase (93)

c) Analytical methods

The following Table 98 and Table 99 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 98 REACH Annex VI analytical methods used by registrants of substances originating from fermentation processes.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
90	Amylase, α-						Y
93	Cellulase				Y		Y
858	Peptones, casein	Y	Y	Y		Y	
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis		Y				
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	Y	Y	Y	Y	Y	Y
5027	Vinasses, residue of fermentation						
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)						
5085	Vinasses, residue of fermentation, depotassified		Y				

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 99 Other analytical methods used by registrants of substances originating from fermentation processes in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements
90	Amylase, α-	Enzyme activity assay - Electrophoresis and Spectrophotometry Kjeldahl method (nitrogen determination) Antron methods (total carbohydrate content) Ignition - gravimetric method (Ash - inorganic salts content) Lipids content - extraction or hydrolysis/GC method
93	Cellulase	Enzyme activity assay - Electrophoresis and Spectrophotometry Kjeldahl method (nitrogen determination) Antron method (total carbohydrate content) Ignition - gravimetric method (Ash - inorganic salts content) Lipids content - extraction or hydrolysis/GC method ICP-MS Röse-Gottliebs/Schmid-Bondzynski-Rattzlaffs method (lipids content]
858	Peptones, casein	Gravimetry
4788	Biomass residue ex B2, fermentation residues of molasses, yeast extract, sucrose and ammonia with bacillus subtilis	LECO Combustion Analysis Determination dry matter - DIN ISO 11465 Total Phosphate as P2O5, Total Potassium as K2O, Total Calcium as CaO, Total Magnesium as MgO - DIN EN ISO 11885 Total Nitrogen - DIN ISO 11281 Total Sulphur - DIN EN ISO 10304 Sum Nitrate and Ammonium Nitrogen - VDLUFA (CaCl2)
4524	Sophorolipids: fermentation products of glucose and rapeseed-oil fatty acids methyl esters with yeast Candida Bombicola	
5027	Vinasses, residue of fermentation	Determination of dry matter - according to EN 12880 Determination of total organic carbon (TOC) -according to DIN EN 13137 Determination of total nitrogen - titrimetric methods according to ISO 11261 Elemental analysis - AAS and photometric determination Elemental analysis - ICP-OES according to DIN EN ISO 11885, decomposition method and EN 1483 Determination of ash residue - according to EN 12879 Determination of main sugar, protein and lipid compositions - according to VDLUFA-Methode, Methodenbuch III (1993) Determination of phosphor (P) - NMKL No 139 1991, Determination of potassium (K) - EN13657 mod;ICP-AES, Determinatin of sulphur (S) -EN13657 mod; ICP-AES, Determination of sodium (Na) - NMKL No 139 1991
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)	Determination of dry matter - according to EN 12880 Determination of total organic carbon (TOC) -according to DIN EN 13137 Determination of total nitrogen and ammonium ion - titrimetric methods according to ISO 11261 and DIN 38406-5-2 Determination of main sugar, protein and lipid compositions - according to VDLUFA-Methode, Methodenbuch III (1993) Elemental analysis - ICP-OES according to DIN EN ISO 11885, decomposition method and EN 1483 Determination of ash residue - according to EN 12879
5085	Vinasses, residue of fermentation, depotassified	Determination of total organic carbon (TOC) according to DIN EN 13137 Determination of ash residue according to EN 12879 Determination of total nitrogen titrimetric methods according to ISO 11261 Elemental analysis ICP-OES according to DIN EN ISO 11885, decomposition method and EN 1483 pH, loss of ignition Dry metter on Mud NF EN 12880

Despite being organic substances, it can be observed that the analytical methods explicitly mentioned in Annex VI of REACH were rarely used by registrants of substances in this group.

The following note encountered in one of the registration dossiers can give an indication for the reasoning of this observation.

"Because of the complexity of this UVCB substance, information from IR, UV/VIS, NMR and GC spectra is not helpful identifying the substance identity of Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae); although it may be useful for fingerprinting of individual batches. In addition test techniques applied provided sufficient information for identification of this substance, therefore there is no need for other techniques to be used as no useful information is added."

The spectral data and chromatograms attached to some of the screened dossiers indeed show very high complexity of the substances making identification of individual constituents hardly possible.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressed by the following operating consortia and associations:

- Association of Manufacturers and Formulators of Enzyme Products – http://www.amfep.org/
- Ethanol REACH Association - http://www.etoh-reach.com/

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 100 for direct links (where available).

Table 100 Publicly available substance identity profiles of substances originating from fermentation processes.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
5027	Vinasses, residue of fermentation	http://www.etoh-reach.com/uploads/Substance%20Sameness%20Statement%20of%20the%20Vinasses%20Consortium%20101110.pdf	Ratio (concentration ranges) of ash residue (dry matter content of vinasses), total organic carbon, N, P, K, S, Na and pH of the material. Identity/sameness criteria specified for 5 sub-groups of vinasses.
5021	Vinasses, residue of fermentation containing biomass of bakers yeast (Saccharomyces cerevisiae)		
5085	Vinasses, residue of fermentation, depotassified		

3.3.2. Substances originating from plants and animals

Substances originating from plants and animals include a variety of substances from processed natural oils, saccharides and proteins, plant extracts and essential oils to wood-derived products.

Some of the substances originating from plants and animals are regarded as being registered, but this study focuses only on those actually registered to provide observations on substance identity in relation to REACH.

Composition of substances in this group is often unknown as well as variable due to intrinsic variability in composition of their sources (most frequently botanicals), as a consequence of the origin (region of growth), annual variations in climate within the region and part of processed source material in the case of plants as sources.

a) Substances screened in this group

The following Table 101 lists substances originating from plants and animals selected for substance identity screening.

Table 101 Substances originating from plants and animals – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed
		Joint	Indiv.	Total	
72	Cashew, nutshell liq.	5	1	6	100
65	Castor oil, hydrogenated	18	0	18	100
399-400	Castor oil, sulfated, sodium salt	7	1	8	100
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	1	1	2	100
965	Oils, animal, sulfated, sodium salts	5	0	5	100
976-7	Rape oil, oxidized	7	1	8	100
78	Soybean oil, epoxidized	18	0	18	100
718	Cinnamomum zeylanicum, ext.	17	0	17	100
719	Cocoa, ext.	5	0	5	100
729	Lemon, ext.	11	0	11	100
715	Saccharomyces cerevisiae, ext.	8	0	8	100
700	Myristica fragrans, ext.	24	0	24	83
82	Orange, sweet, ext.	30	0	30	67
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry. It is a dark brown viscous liquid extracted and processed from softwoods and hardwoods. CTO has a complex composition of fatty acids, resin acids, and neutrals.	49	0	49	41
84	Rosin (Colophony)	54	0	54	37
4989	Spent liquor from alkaline pulping and bleaching containing spent inorganic process chemicals and dissolved organic substances originating from the cellulosic raw material.	64	0	64	31
66	Tall oil	7	0	7	100
344	Tall oil, sodium salt	25	0	25	80
565-6	Charcoal, coconut shell	3	1	4	100
350	Corn, steep liquor	11	0	11	100

* 20 dossiers per substance were analysed as a maximum.

25 % of the screened substances contain besides dossiers from joint submissions also an individual submission dossier. One of the screened substances was registered by 64 registrants, another one by 54 registrants, 4 substances by 20 – 50 registrants, 5 substances by 10 – 20 registrants and the remaining 9 by up to 10 registrants. The substance with the lowest number of dossiers was registered by 2 registrants.

For the purposes of this project, substances originating from fermentation processes have been further divided into the following sub-groups:

1. Derivates
2. Extracts
3. Vegetable oils
4. Wood-derived products
5. Others

Where appropriate, observations on substance identity are presented in relation to these sub-groups of substances.

b) Substance identity elements

Table 102 SID elements used by registrants in identification of substances originating from plants and animals.

	Derivates							Extracts				Vegeta-ble oils		Wood-derived products					Others		
	72	65	399 - 400	4404-5	965	976-7	78	718	719	729	715	700	82	4973	84	4989	66	344	565-6	350	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓	✓	✓		✓		✓	✓	✓	✓	85
Composition	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
State	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓			✓		✓				✓	70
Softening point															✓						5
Density	✓	✓				✓		✓		✓			✓								30
Solubility		✓				✓					✓										15
Viscosity										✓											5
pH			✓		✓													✓		✓	20
Boiling point										✓						✓					10
Flash point						✓															5
Particle size distribution									✓												5
Form of the substance		✓		✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓		✓			70
Optical activity					✓			✓		✓		✓	✓								25
Refractive index								✓					✓								10
Colour	✓				✓	✓	✓	✓	✓	✓	✓			✓	✓	✓					55
*Group-specific element**	✓	✓	✓		✓	✓	✓	✓	✓	✓	✓			✓	✓	✓			✓		70
Odour									✓	✓	✓					✓					20
*Common characteriser***	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓		✓		✓		✓	80
*Other characteriser****	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓	✓		✓		✓	85
No. of applied SID elements per substance	10	11	9	8	12	13	10	12	12	15	12	7	8	9	9	11	4	8	5	8	Average = 46
Average no. of applied SID elmts. per sub-group	10.4 ± 1.7							12.8 ± 1.5				7.5 ± 0.7		8.2 ± 2.6					6.5 ± 2.1		
Average no. of applied SID elmts. per group	9.7 ± 2.7																				

* SID element specific to a certain group/sub-group of substances, in particular: Plant extractives and their physically modified derivatives (72), modified plant extract (65), triglycerides, sulphated, neutralized (399-400), animal oil derivates (965), Rape oil, modified (976-977), Epoxidized Oils (78), Extractives obtained from plants (718, 729), Protein extracts from yeast (715), Complex mixture of fatty acids, resin acids, andneutrals (4973), Acid number (84), Sulfite spent liquor (4989), Charcoal (565-566).

** Plant product (72), Triglyceride (65), oil of plant origin, modified (399-400), esterification product (4404-4405), Sulphated oil derivatives substances (965), oil of natural origin, modified (976-977), Substances of biological nature, chemically modified (78), Extract (718, 729, 715), wood extractives (4973), spent liquor (4989), Crude tall oil soap (344), Liquor (350).

*** Plant extract, by-product (72), Blend of triglycerides (65), natural oil, modified (399-400), Polymer (4404-4405), Reaction product (965, 976-977, 78), essential oil (718), by-product (729, 4973), Residue (715, 4989, 82), By-product from the wood pulping industry (344), By-product of the initial stages of wet milling of corn (350).

Comments to Table 102:

- 21 SID elements were used by registrants of the screened substances for identification of substances in this group, which is the highest number of SID elements used among all studied groups of substances;

- 17 out of the 20 screened substances were identified with 7 – 13 SID elements, 2 substances were identified with 4 – 5 SID elements and 1 was identified with 15 SID elements, the average number of SID elements used for identification of a substance within this group is 9.7, which is the highest average observed in this study;

- standard deviation linked to the average number of SID elements used by registrants of substances in this group is 2.7 (second highest observed within this study just after the group "other inorganic substances"). The sets of SID elements used by registrants are different for different substances in this group, indicating either that there is high variability regarding identity of the substances in this group or that the level of harmonisation of information reported by the registrants is generally low (or both). Within the sub-group of "Extracts", the set of SID elements is significantly more harmonised, most of the SID elements (e.g. composition, source, manufacturing process, state, form of the substance, colour and several group-specific SID elements, e.g. indication that these substances are extracts) are used for identification of all four screened substances in this sub-group.

Composition

The registrants of the substances subject to the screening most frequently specified composition of the substances providing concentration ranges of individual constituents together with their typical concentrations in vast majority of cases. In cases where only one of these two values was provided, frequency of use of concentration ranges and of typical concentrations was similar.

The registrants usually specify a very high number of constituents, even those in very small concentrations (0 – 1%). The guidelines on substance identification and sameness of natural complex substances under REACH and CLP published by the European Federation of Essential oils (EFEO) and International Fragrance Association (IFRA)[22] mention that the number of constituents of natural complex substances ranges from very few to over a hundred.

The guidelines published by EFEO and IFRA also indicate that composition ranges set by ISO (International Standards Organisation) standards for characterisation and identification of essential oils may be used for assessing sameness of essential oils when considering joint registration under REACH.

The following tables summarise the information on compositional data provided in the screened registration dossiers.

Table 103 Number of compositions specified in registration dossiers by registrants of substances originating from plants and animals.

ID	Name (as registered)	No. of compositions				
		1	2	3	4	11
72	Cashew, nutshell liq.	100				
65	Castor oil, hydrogenated	100				
399-400	Castor oil, sulfated, sodium salt	100				
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	100				
965	Oils, animal, sulfated, sodium salts	100				
976-7	Rape oil, oxidized	100				
78	Soybean oil, epoxidized	100				
718	Cinnamomum zeylanicum, ext.	100				
719	Cocoa, ext.	100				
729	Lemon, ext.	91				9
715	Saccharomyces cerevisiae, ext.	100				
700	Myristica fragrans, ext.	100				
82	Orange, sweet, ext.	100				
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry.	90	5	5		
84	Rosin (Colophony)	90	10			
4989	Spent liquor from alkaline pulping and bleaching	41		53	6	
66	Tall oil	100				
344	Tall oil, sodium salt	80	15	5		
565-6	Charcoal, coconut shell	100				
350	Corn, steep liquor	100				

25 % of substances screened in this group include dossiers reporting multiple compositions. 4 out of 5 of these substances belong to the sub-group of wood-derived products. In one of the dossiers (for the substance "Lemon, ext."), 11 different compositions were reported, which is the highest number observed in this study. These compositions specified different phases of the extracted product, e.g. a product of cold pressed extraction, concentrated product from cold pressed extraction,

[22] Available at http://efeo-org.org/wp-content/uploads/2015/08/EFEO-IFRA-Guidelines-NCS-SID-REACH-CLP-Version-5-August-2015.pdf

terpenes from cold pressed extraction, furocoumarinefree / decoulorized phase from cold pressed extraction, product from oil phase extraction or essence oil, and several other phases.

Table 104 Number of constituents specified in registration dossiers by registrants of substances originating from plants and animals.

ID	Name (as registered)	No. of constituents	
72	Cashew, nutshell liq.		20
65	Castor oil, hydrogenated		20
399-400	Castor oil, sulfated, sodium salt		8
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione		1
965	Oils, animal, sulfated, sodium salts		1
976-7	Rape oil, oxidized		18
78	Soybean oil, epoxidized		2
718	Cinnamomum zeylanicum, ext.		34
719	Cocoa, ext.		17
729	Lemon, ext.	#1 - #11	16
715	Saccharomyces cerevisiae, ext.		6
700	Myristica fragrans, ext.		38
82	Orange, sweet, ext.		10
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry.	#1	7
		#2	3
		#3	3
84	Rosin (Colophony)		34
4989	Spent liquor from alkaline pulping and bleaching	#1 - #3	10
66	Tall oil		10
344	Tall oil, sodium salt		8
565-6	Charcoal, coconut shell		21
350	Corn, steep liquor		4

3 of the screened substances included over 30 constituents (38 being the highest number of reported constituents), another 3 comprised of 20 – 21 reported constituents, 6 substances included 10 – 20 constituents and for the remaining 10 substances, less than 10 constituents were reported (with 2 substances having just a single constituents specified).

Table 105 Consistency of compositional data provided in the registration dossiers for substances originating from plants and animals.

ID	Name (as registered)	Composition consistency score*					
		1	2	3	4	5	6
72	Cashew, nutshell liq.				100		
65	Castor oil, hydrogenated			28	44	6	22
399-400	Castor oil, sulfated, sodium salt				37		63
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione						100
965	Oils, animal, sulfated, sodium salts						100
976-7	Rape oil, oxidized				37		63
78	Soybean oil, epoxidized				5		95
718	Cinnamomum zeylanicum, ext.	94			6		
719	Cocoa, ext.	40			60		
729	Lemon, ext.	100					
715	Saccharomyces cerevisiae, ext.		25	50	25		
700	Myristica fragrans, ext.	45		70	100		
82	Orange, sweet, ext.	100					
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry. It is a dark brown viscous liquid extracted and processed from softwoods and hardwoods. CTO has a complex composition of fatty acids, resin acids, and neutrals.		50		50		
84	Rosin (Colophony)				60		40
4989	Spent liquor from alkaline pulping and bleaching containing spent inorganic process chemicals and dissolved organic substances originating from the cellulosic raw material.	85			15		
66	Tall oil				67		33
344	Tall oil, sodium salt				95	5	
565-6	Charcoal, coconut shell	75[a]					25[b]
350	Corn, steep liquor			100			

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

[a] Joint submission
[b] Individual submission

Table 106 Typical constituents specified in registration dossiers by registrants of substances originating from animals and plants.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
72	Cashew, nutshell liq.	Cardanol	N/A	20 – 99.5
		C13 and unidentified phenolics (meta-triadecenyl and unidentified phenols)	N/A	0.01 – 12
		C17 phenolic (meta-heptadecenyl phenols)	N/A	0.01 – 10
		Cardol (saturated side chain, monoene, diene and triene)	221-599-7	0 – 70
65	Castor oil, hydrogenated	Castor oil, hydrogenated	232-292-2	80 – 100
		1,2,3-propanetriyl tris(12-hydroxyoctadecanoate)	205-364-6	50 – 100
		distearic acid, diester with glycerol	215-359-0	1 – 15
		stearic acid	200-313-4	1 – 15
399-400	Castor oil, sulfated, sodium salt	Castor Oil, sulphated, sodium salt	269-123-7	80 – 100
		sodium sulphate	231-820-9	0 – 10
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	700-064-6	80 – 100
		tetrahydromethylphthalic anhydride	234-290-7	0 – 4
965	Oils, animal, sulfated, sodium salts	Oils, animal, sulfated, sodium salts	304-835-4	80 – 100
976-7	Rape oil, oxidized	Rape oil, oxidized	305-871-3	98 – 100
78	Soybean oil, epoxidized	Soybean oil, epoxidized	232-391-0	99 – 100
718	Cinnamomum zeylanicum, ext.	Eugenol	202-589-1	70 – 97
		Caryophyllene	201-746-1	1.5 – 7
		Linalool	201-134-4	1 – 4
		benzyl benzoate	204-402-9	1 – 4
		Eugenol Acetate	202-235-6	0.5 – 4.25
		Unknown Substances less than 1%	N/A	0 – 8
719	Cocoa, ext.	Protein, cocoa	N/A	16 – 31
		Cocoa fat glycerides	295-412-2	9 – 25
		Starch	232-679-6	5 – 24
		Cellulose	232-674-9	15 – 40
		Pectin	232-553-0	0.3 – 10
729	Lemon, ext.	beta-pinene	204-872-5	0 – 25
		Citral	226-394-6	0.1 – 35
		gamma-terpinene	202-794-6	1 – 35
		Limonene, D-	227-813-5	25 – 89
		Unknown constituents	N/A	0 – 10
715	Saccharomyces cerevisiae, ext.	Proteins from Yeast	N/A	40 – 80
		Carbohydrates from Yeast	N/A	0 – 25
		Minerals from yeast	N/A	0 – 20
		Food-grade salts	N/A	0 – 5
		Lipids from Yeast	N/A	0 – 5
700	Myristica fragrans, ext.	pin-2(3)-ene	201-291-9	9 – 29
		pin-2(10)-ene	204-872-5	8 – 28
		thuj-4(10)-ene	222-212-4	11 – 45
		6-allyl-4-methoxy-1,3-benzodioxole	210-146-9	1 – 15
		p-menth-1-en-4-ol	209-235-5	2 – 10
		p-mentha-1,4-diene	202-794-6	1 – 10

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
82	Orange, sweet, ext.	D-Limonene	227-813-5	60 – 99
		Linalool	201-134-4	0 – 9
		Decanal	203-957-4	0 – 6
		Unknown constituents	N/A	0 – 10
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry. It is a dark brown viscous liquid extracted and processed from softwoods and hardwoods. CTO has a complex composition of fatty acids, resin acids, and neutrals.	linoleic acid	200-470-9	0 – 60
		oleic acid	204-007-1	0 – 65
		abietic acid	208-178-3	0 – 65
		Fatty acids, other, typically constituents of Crude Tall Oil	N/A	0 – 30
		Resin acids, other, typically constituents of Crude Tall Oil	N/A	0 – 50
		Neutrals, polymeric acids and other minor constituents, typically constituents of Crude Tall Oil	N/A	1 – 50
84	Rosin (Colophony)	Rosin	232-475-7	99 – 100
		Pimaric Acid / (1R, 4aR, 4bS, 7S, 10aR)-1, 4a, 7-trimethyl-7-vinyl-3,4,4b,5,6,9,10, 10a-octahydro-2H-phenanthrene-1carboxylic acid	N/A	0 – 80
		abieta-7,13-dien-18-oic acid // abietic acid // 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R,4aR,4bR,10aR)-	208-178-3	0 – 90
		1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-1,4a,7-trimethyl-, (1theta-(1alpha,4abeta,4balpha,7alpha,10a alpha))- // Isopimaric acid	N/A	0 – 25
4989	Spent liquor from alkaline pulping and bleaching containing spent inorganic process chemicals and dissolved organic substances originating from the cellulosic raw material.	abieta-8,11,13-trien-18-oic acid // [1R-(1α,4aβ,10aα)]-1,2,3,4,4a,9,10,10a-octahydro-7-isopropyl-1,4a-dimethylphenanthren-1-carboxylic acid // Dehydroabietic acid	217-102-8	0 – 70
		Lignin	N/A	5 – 60
		Polysaccharides	N/A	0 – 28
		Volatile carboxylic acids	N/A	0 – 28
		Sodium carbonate	207-838-8	0 – 48
		sodium sulphate	231-820-9	0 – 19.2
66	Tall oil	Distilled Tall Oil (DTO)	N/A	99.9 – 100
		(9Z)-Octadec-9-enoic acid //oleic acid	204-007-1	3 – 30
		octadeca-9,12-dienoic acid // linoleic acid	200-470-9	0 – 40
		abieta-7,13-dien-18-oic acid // abietic acid	208-178-3	1 – 15
344	Tall oil, sodium salt	(9Z)-Octadec-9-enoic acid //oleic acid	204-007-1	1 – 30
		octadeca-9,12-dienoic acid // linoleic acid	200-470-9	0 – 20
		abieta-7,13-dien-18-oic acid //	208-178-3	2 – 30

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
		abietic acid		
		Mix of volatile constituents	N/A	20 – 45
		Mix of other organic constituents	N/A	0.5 – 15
565-6	Charcoal, coconut shell	Carbon	231-153-3	73
		Nitrogen	231-783-9	1
		Hydrogen	215-605-7	1.5 – 4.5
		Oxygen	231-956-9	5 – 26
350	Corn, steep liquor	Protein hydrolyzates, corn	309-349-6	15.75 – 26.25
		lactic acid	200-018-0	5.25 – 15.75
		Water	231-791-2	40 – 55
		Unknown constituents of Corn Steep Liquor	N/A	0 – 10

There is significant variability in concentration ranges of individual constituents reported by the registrants of substances in this group. Out of the 80 constituents presented in the above table (please note that the list of constituents presented in the table is not an exhaustive list including all substances reported by the registrants of the screened substances), 10 constituents have a 50 % or higher difference between the lower and upper concentration range, 8 have a range spanning 30 – 50 % reported, 38 span 10 – 30 % difference in concentration and 24 are reported within the range of less than 10 %.

Source

Source, together with manufacturing process is the key element in identification of the substances originating from plants and animals. According to the ECHA guidance on identification and naming of substances under REACH and CLP, the source should be identified by the plant or animal genus, species and family (and strain or genetic type, if relevant) and part of the plant/animal from which the substance is derived.

The following table demonstrates how these principles were reflected in the screened dossiers.

Table 107 Sources of substances originating from plants and animals as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
72	Cashew, nutshell liq.	the shell of the cashew nut
65	Castor oil, hydrogenated	Castor Oil extracted from the seeds of Ricinus Comunis L.
399-400	Castor oil, sulfated, sodium salt	Castor oil
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	Castor oil
965	Oils, animal, sulfated, sodium salts	animal oils
976-7	Rape oil, oxidized	Rapeseed oil
78	Soybean oil, epoxidized	Soybean oil
718	Cinnamomum zeylanicum, ext.	leaves of cinnamomum zeylanicum
719	Cocoa, ext.	Cocoa beans
729	Lemon, ext.	Lemon fruits
715	Saccharomyces cerevisiae, ext.	Yeast
700	Myristica fragrans, ext.	Myristica Fragans, Nutmeg oil, Crushed nutmeg
82	Orange, sweet, ext.	peel of Citrus sinensis (L.), fruits pericarps, fruits
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry.	crude tall oil soap from the pulping processes
84	Rosin (Colophony)	Oleoresin from pine trees Family: Pinaceae; Genus: Pinus. Rosin, sodium hydroxide solution Crude rosin + turpentine crude gum from trees Pine trees Pine gum Pine gum which contains crude oleoresin, plus a variable amount of water and solid materials like bark, needles, sand and other trash Oleoresin collected by tapping softwoods (gum collection) The oleo-resin exuded by various species of pine(crude turpentine); other source: Crude Tall Oil or aged pine stumps - terated with solvent Crude Tall-oil Natural Pine Resin (country Portugal) Row gum resin
4989	Spent liquor from alkaline pulping and bleaching	cellulosic raw material - softwood / hardwood / agricultural fibres and white liquor
66	Tall oil	a) crude tall oil (CTO) b) tall oil rosin and tall oil fatty acid
344	Tall oil, sodium salt	Extractives in the pulp wood, primarily fatty and resin acids
565-6	Charcoal, coconut shell	Coconut shell
350	Corn, steep liquor	Corn, water, sulphur dioxide

As presented in the table above, registrants often did not follow the guidance of ECHA regarding the identification of the source (advising to define substances of biological origin by the genus, species and the family), however, the source was sometimes identified in accordance with ECHA guidance in the description of the manufacturing process.

It can be observed that botanicals and/or parts of botanicals are sources for a majority of substances in this group, with tall oil and its derivates being the most frequently specified source in the sub-group of wood-derived products.

There were no cases where different botanical sources were covered within a single joint registration.

Manufacturing process and its parameters (conditions)

Manufacturing process, together with source, is the key substance identity element determining the composition of substances originating from plants and animals.

Separation methods are the most frequently described processes in the manufacture of substances originating from plants and animals, e.g. extraction, distillation, filtration, fractionation, flaking.

The fact that the manufacturing process plays a vital role in identification of substances is supported in the screened dossiers where a detailed description of the manufacturing process was often provided, specifying individual reaction agents and conditions of the process(es) (e.g. temperature, reaction time, pressure, evaporation temperature, ratios of reaction agents and other key factors).

A simplified summary of manufacturing processes specified by the registrants of the screened substances is presented in the following table.

Table 108 Manufacturing processes of substances originating from plants and animals as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
72	Cashew, nutshell liq.	Initial extraction - Heat treatment - Fractionation - Purification The process of removing the cashew kernel from the nut: Hot-oil and roasting of the shell (descarboxylation) Heat processing of whole seeds - isolation, washing and roasting of cashew nuts - cutting the shell - mechanically crushing the shells and heating to speed up extraction
65	Castor oil, hydrogenated	hydrgenation at high temperature and pressure - Filtration - Flaking crushing and / or solvent extracting beans from the Castor Oil plant (Ricinus Communis) - hydrogenation at high temperature and pressure - filtration - drying under vacuum
399-400	Castor oil, sulfated, sodium salt	Sulfation with sulfuric acid and neutralization with caustic soda
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	PolYterification
965	Oils, animal, sulfated, sodium salts	sulfonation - neutralization - (purification)
976-7	Rape oil, oxidized	Oxidation with air under ambient pressure at high temperature Catalytic oxidation with air at high temperature Catalytic oxidation with oxygen at high temperature
78	Soybean oil, epoxidized	epoxidation - separation - purification
718	Cinnamomum zeylanicum, ext.	steam distillation
719	Cocoa, ext.	Pasteurisation (steam application) – roasting in hot air dryers – multi-stage milling – hydraulic pressing – pulverization
729	Lemon, ext.	Extraction - Separation processes - Vacuum distillation
715	Saccharomyces cerevisiae, ext.	Autolyses of Yeast biomass through the action of its own enzymes followed by the application of physical methods
700	Myristica fragrans, ext.	distillation extraction
82	Orange, sweet, ext.	mainly cold pressing and/or distillation (extraction, centrifugation etc.)
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry. It is a dark brown viscous liquid extracted and processed from softwoods and hardwoods. CTO has a complex composition of fatty acids, resin acids, and neutrals.	acidulation - gravity separation - (ultra-filtration, flotation and decanting)
84	Rosin (Colophony)	Distilation Disproportionation reaction Refinement Filtration Stripping
4989	Spent liquor from alkaline pulping and bleaching containing spent inorganic process chemicals and dissolved organic substances originating from the cellulosic raw material.	alkaline cooking processes - washing - evaporation
66	Tall oil	a) vacuum distillation b) blending
344	Tall oil, sodium salt	"kraft or soda pulping processes -> alkaline conditions -> saponification -> Crude tall oil soap (TOS) alkaline bleaching stages in some sulfite pulping processes -> Crude tall oil soap (TOS) separation from the water phase by decanting"
565-6	Charcoal, coconut shell	Carbonisation (thermal decomposition of coconut shells in the absence of air)
350	Corn, steep liquor	Steeping of corn

It is indicated in the guidelines published by EFEO and IFRA that different manufacturing processes (different steps in the same generic process) can lead to substances similar enough to allow registration in a single joint submission. This approach was observed in some of the screened dossiers where some of the dossiers included several similar compositions as a result of different separation steps in the processing of the same raw materials.

Additional substance identity elements

Registrants of the screened substances originating from plants and animals used various substance identity elements to characterise the registered substances. The average number of elements used in identification of the substances is 9.7 ± 2.7 – the highest average among all studies groups of substances. However, besides the description of composition, source, manufacturing process and parameters (conditions) of the manufacturing process, only state and form of the substance were used in the description of a majority of the screened substances.

In the sub-group of extracts the average number of elements used in identification of the substances is particularly high (12.8 ± 1.5). Some registrants of the substances in this sub-groups used the following substance identity elements to characterise the substances:

Substance identity element	Value	Substance identified with the SID element
State	solid	Castor oil, hydrogenated (65), Cashew, nutshell liq. (72), Cocoa, ext. (719)
	liquid	Soybean oil, epoxidized (78), Castor oil, sulfated, sodium salt (399-400), Oils, animal, sulfated, sodium salts (965), Rape oil, oxidized (976-977), Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione (4404-5), Cinnamomum zeylanicum, ext. (718), Lemon, ext. (729), Crude Tall Oil (CTO) (4973), Spent liquor from alkaline pulping and bleaching (4989), Corn, steep liquor (350)
	liquid or paste	Tall oil, sodium salt (344)
	liquid, paste, powder, or granular substance	Saccharomyces cerevisiae, ext. (715)
Density	970 kg/m^3	Castor oil, hydrogenated (65)
	0.956 g/cm^3	Cashew, nutshell liq. (72)
	0.963 at 20 ^{0} C	Rape oil, oxidized (976-977)
	1.06 g/cm^3	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione (4404-5)
	1.037 - 1.053g/ml	Cinnamomum zeylanicum, ext. (718)
	0.8512 g/ml at 20 ^{0} C	Lemon, ext. (729)
	0.8413 – 0.8770 g/cm^3	Orange, sweet, ext. (82)
Solubility	water solubility < 0.05mg/L	Castor oil, hydrogenated (65)
	<1 mg/L at 20 °C	Rape oil, oxidized (976-977)
	highly water soluble	Saccharomyces cerevisiae, ext. (715)
	Components have different solubilities, 70 - 80 % of components are insoluble in water.	Cocoa, ext. (719)
Viscosity	243 cSt at 50 ^{0} C	Castor oil, sulfated, sodium salt (399-400)
	1.09 mPa*s at 20 ^{0} C	Lemon, ext. (729)
	different viscosities, from just below 100 mPa*s, up to a viscosity of 9 Pa*s	Rape oil, oxidized (976-977)
Boiling point	The substance decomposes prior to boiling at atmospheric pressure	Soybean oil, epoxidized (78)
	107 ^{0} C	Castor oil, sulfated, sodium salt (399-400)
	Boiling was not observed below the temperature at which reaction and/or decomposition started	Rape oil, oxidized (976-977)
	160 +/-20 ^{0} C at 1016 hPa	Lemon, ext. (729)
Flash point	188 °C at 1013 hPa	Rape oil, oxidized (976-977)
	148 ^{0} C	Esterification product of castor oil and tetrahydromethyl-

Substance identity element	Value	Substance identified with the SID element
		1,3-isobenzofuranedione (4404-5)
pH	6 – 8	Castor oil, sulfated, sodium salt (399-400), Oils, animal, sulfated, sodium salts (965)
	high pH - pH of ≥ 11.5 (80 %), low pH - pH of < 11.5 (10 %), low pH - pH between ≥9 and <11.5 (10 %)	Tall oil, sodium salt (344)
Particle size distribution	1- 100 microns	Cocoa, ext. (719)
Form of the substance	powder/flakes	Castor oil, hydrogenated (65)
	powder	Cocoa, ext. (719)
Optical activity	Most of the components may have optical activity. However due to the high complexity of the substance and unspecific method of manufacturing the final substance can be considered with no optical activity.	Castor oil, sulfated, sodium salt (399-400)
	not optically active	Saccharomyces cerevisiae, ext. (715), Crude Tall Oil (CTO) (4973), Spent liquor from alkaline pulping and bleaching (4989)
	Optically active, the determined optical rotation of the sample of = 0.44° complies with the range of -2,5° to +2°	Cinnamomum zeylanicum, ext. (718)
	Optically active, typically lemon oil should record an optical rotation between +54.0° and +76.0°	Lemon, ext. (729)
	+8° to +18°, resp. +6° to +18°	Myristica fragrans, ext. (700)
	66.9 - 100.8°	Orange, sweet, ext. (82)
Refractive index	1.5270 - 1.5400	Cinnamomum zeylanicum, ext. (718)
	1.4702 – 1.4822	Orange, sweet, ext. (82)
Colour	dark brown	Cashew, nutshell liq. (72), Tall oil, sodium salt (344), Crude Tall Oil (CTO) (4973)
	yellow	Soybean oil, epoxidized (78), Rape oil, oxidized (976-977), Lemon, ext. (729)
	from light beige to dark brown	Saccharomyces cerevisiae, ext. (715)
	light to dark brown	Cinnamomum zeylanicum, ext. (718)
	mid to dark brown	Cocoa, ext. (719)
	black	Spent liquor from alkaline pulping and bleaching (4989)
Group-specific element or other common characteriser	modified plant extract	Castor oil, hydrogenated (65)
	plant extractive	Cashew, nutshell liq. (72), Cinnamomum zeylanicum, ext. (718), Cocoa, ext. (719), Lemon, ext. (729)
	substance of biological nature, chemically modified	Soybean oil, epoxidized (78)
	oil of plant origin, modified	Castor oil, sulfated, sodium salt (399-400)
	sulphated oil derivatives substances	Oils, animal, sulfated, sodium salts (965)
	protein extracts from yeast	Saccharomyces cerevisiae, ext. (715)
	rosin	Rosin (Colophony) (84)
	crude tall oil soap	Tall oil, sodium salt (344)
	wood extractive	Crude Tall Oil (CTO) (4973)
Other characteriser	by-product	Cashew, nutshell liq. (72), Lemon, ext. (729), Tall oil, sodium salt (344), Crude Tall Oil (CTO) (4973), Corn, steep liquor (350)
	reaction product	Soybean oil, epoxidized (78), Oils, animal, sulfated, sodium salts (965), Rape oil, oxidized (976-977)
	esterification product (polymer)	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione (4404-5)
	residue	Saccharomyces cerevisiae, ext. (715), Cocoa, ext. (719), Spent liquor from alkaline pulping and bleaching (4989)

There is no indication that any of the substance identity elements would be of similar importance in identification of substances in this group as the ones mentioned earlier (composition, source, manufacturing process and parameters (conditions) of the manufacturing process).

c) Analytical methods

The following Table 109 and Table 110summarise the use of analytical methods and techniques in identification of the screened substances.

Table 109 REACH Annex VI analytical methods used by registrants of substances originating from plants and animals.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
72	Cashew, nutshell liq.	Y	Y	Y		Y	Y
65	Castor oil, hydrogenated	Y	Y	Y		Y	Y
399-400	Castor oil, sulfated, sodium salt	Y	Y	Y		Y	Y
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	Y	Y	Y			Y
965	Oils, animal, sulfated, sodium salts	Y	Y	Y	Y		Y
976-7	Rape oil, oxidized	Y	Y	Y	Y	Y	Y
78	Soybean oil, epoxidized	Y	Y	Y	Y	Y	Y
718	Cinnamomum zeylanicum, ext.	Y	Y	Y			Y
719	Cocoa, ext.	Y	Y	Y		Y	Y
729	Lemon, ext.	Y	Y			Y	Y
715	Saccharomyces cerevisiae, ext.	Y	Y	Y	Y	Y	Y
700	Myristica fragrans, ext.						Y
82	Orange, sweet, ext.	Y	Y	Y	Y		Y
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry.	Y	Y	Y			Y
84	Rosin (Colophony)	Y	Y	Y	Y		Y
4989	Spent liquor from alkaline pulping and						
66	Tall oil	Y	Y	Y			Y
344	Tall oil, sodium salt		Y				Y
565-6	Charcoal, coconut shell						
350	Corn, steep liquor		Y				Y
Percentage of use of analytical methods (%)		75	85	70	30	40	90

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

Table 110 Other analytical methods used by registrants of substances orignating from plants and animals in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements
72	Cashew, nutshell liq.	
65	Castor oil, hydrogenated	
399-400	Castor oil, sulfated, sodium salt	Panzer – Niebuer Test, Hyamine Test, Karl Fischer test, Other titration methods
4404-5	Esterification product of castor oil and tetrahydromethyl-1,3-isobenzofuranedione	GPC
965	Oils, animal, sulfated, sodium salts	ICP-OES, LC-MS, Hyamine method, Karl Fischer titration; Panzer Niebuer test, other titration methods
976-7	Rape oil, oxidized	GPC, Thermogravimetric Analysis (TGA), Titration methods (KF)
78	Soybean oil, epoxidized	AAS, Titration methods (Iodine value, Oxirane Oxygen), LC-MS
718	Cinnamomum zeylanicum, ext.	Polarimetry - optical rotation, Refractive index, Relative density, solubility in alcohol
719	Cocoa, ext.	gravimetric analysis, titration methods
729	Lemon, ext.	Polarimetry - Optical Rotation
715	Saccharomyces cerevisiae, ext.	Total nitrogen content - Kjeldahl method, Carbohydrates content - Anthrone method, minerals content - ignition test, Lipids = fat content - extraction/GC (AOAC official method 996.06), Protein content - combustion method (AOAC Official Method 990.03)
700	Myristica fragrans, ext.	Optical rotation
82	Orange, sweet, ext.	Optical rotation
4973	Crude Tall Oil (CTO) is obtained from the wood pulping industry.	Various standard methods (ASTM, SCAN)
84	Rosin (Colophony)	Gel permeation chromatography (GPC), GC-MS, Acid number, Softneing Point
4989	Spent liquor from alkaline pulping and bleaching	Gravimetry, ICP, AES, AAS, titration methods, IC, HPEC
66	Tall oil	
344	Tall oil, sodium salt	ICP-OES
565-6	Charcoal, coconut shell	XRF, Determination of the total moisture content and the moisture content, Determination of carbon, hydrogen, and nitrogen Determination of oxygen
350	Corn, steep liquor	Kjeldahl digestion (Proteins contents), Combustion method (Proteins contents), Weight loss on drying under reduced pressure (Water content determination), pH metry (Total acidity determination), Titration method (Aminated nitrogen contents), Karl Fisher titration (+ HPLC)

Similarly to other groups of organic substances screened within this study, substances originating from plants and animals were typically analysed by methods explicitly mentioned in Annex VI of REACH, most frequently with ultraviolet-visible spectroscopy, infrared spectroscopy, nuclear magnetic resonance and gas chromatography, sometimes supported also with high-performance liquid chromatography and/or mass spectrometry.

In addition, certain analytical methods were typically used in relation to individual sub-groups of substances:

- Derivates: various titration methods were often used
- Extracts and vegetable oils: Polarimetry was often used

To the date of compilation of this report, a decision on a compliance check of a registration by ECHA has been issued to three of the substances in this group. One of these decisions was concerning substance identity, where the registrant who initially determined composition of the registered substance using GC-MS (but with omitting the mass spectra corresponding to analysed peaks) was requested to provide also ultraviolet-visible, infrared and nuclear magnetic resonance spectra and the missing mass spectra from the GC-MS determination for all identified constituents.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressesd by the following operating consortia and associations:

- Cashew Nutshell Liquid consortium – https://chemicalwatch.com/4116/cashew-nutshell-liquid-consortium-cnsl
- European Federation of Essential Oils (EFEO) - http://efeo-org.org/
- EURASYP (European Association for Speciality Yeast Products) - http://www.yeastextract.info/
- CTO-TOS-TOPP REACH Consortium - https://reach.poyry.se/sites/public/default.aspx
- H4R Consortium (Hydrocarbon Resins & Rosin Resins REACH Consortium) - http://www.h4rconsortium.com/
- The Activated Carbon Consortium - http://www.reachactivatedcarbon.eu/
- ACPA (Activated Carbon Producers Association) - http://www.cefic.org/About-us/How-Cefic-is-organised/Fine-Speciality-and-Consumer-Chemicals/Activated-Carbon-Producers-Association-ACPA/
- WGS&CSL REACH consortium - http://www.reachcentrum.eu/consortium/wgs-csl-consortium-174.html

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 111 for direct links (where available).

Table 111 Publicly available substance identity profiles of substances originating from animals and plants.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
350	Corn, steep liquor	http://www.reachcentrum.eu/consortium/wgs-csl-consortium-174.html#	concentration ranges of the following constituents: Protein hydrolyzates, corn, lactic acid, water, other (unknown) constituents

3.4. Substance identity of other complex substances

a) Substances screened in this group

Substances in this group have been further divided into the following sub-groups:

1. Chemicals with organic and inorganic part
2. Organic-inorganic salts
3. Others

The following Table 112 lists substances selected for substance identity screening.

Table 112 Other complex substances – substances selected for substance identity screening.

ID	Name (as registered)	No. of registrants			% dossiers analysed*
		Joint	Indiv.	Total	
957	Boric acid (H3BO3), reaction products with ethanolamine	2	0	2	100
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	43	0	43	47
157	orthoboric acid, compound with 2-aminoethanol	20	0	20	100
373	orthoboric acid, compound with 2,2'-iminodiethanol	1	0	1	100
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	3	0	3	100
9044	dioxobis(stearato)trilead	6	0	6	100
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	8	0	8	100
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	4	0	4	100
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	7	0	7	100
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	6	0	6	100
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	2	0	2	100
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	2	0	2	100
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	0	1	1	100

* 20 dossiers per substance were analysed as a maximum.

One of the screened substances was registered by 43 registrants, another one by 20 registrants, and the remaining 11 by up to 10 registrants. There are 2 substances registered only by a single registrant.

b) Substance identity elements

Table 113 Substance identity elements used by registrants in identification of other complex substances.

	Chemicals with organic and inorganic part					Organic-inorganic salts					Others			
	957	5020	157	373	10817	9044	716	787	455	11683	4379	4380	4891	% availability
Source	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Process	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	100
Parameters of process	✓		✓		✓	✓	✓	✓	✓					54
Composition	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓	✓	92
State											✓	✓		15
pH	✓		✓											15
Form of the substance						✓					✓	✓		23
Optical activity											✓	✓		15
Colour						✓								8
*Other characteriser**	✓			✓	✓		✓	✓	✓	✓	✓	✓	✓	77
No. of applied SID elements per substance	6	3	5	4	5	6	5	5	4	4	7	7	4	Average = 50
Average no. of applied SID elmts. per sub-group	4.7 ± 1.5					5.5 ± 0.7					6 ± 1.7			
Average no. of applied SID elmts. per group	5 ± 1.2													

* Reaction product (373, 957, 10817), Zinc complex (455, 11683), Zinc salt (716, 787), Reaction mass (4379, 4380, 4891).

Comments to Table 113:

- 10 SID elements were used by registrants of the screened substances for identification of substances in this group;

- Number of used SID elements varies between 3 and 7 for each substance, with 5 being the average number of SID elements used by registrants for identification of substances in this group;

- Standard deviation linked to the average number of SID elements used by registrants of substances in this group is 1.2;

- Besides composition, source and manufacturing process, parameters (conditions) of the manufacturing process was the only SID element used for identification of at least 50 % of substances in this group, 77 % of the screened substances were also identified by SID elements specific to individual sub-groups of substances including reaction products, reaction masses, complexes or salts.

Composition

Compositional data of the screened substances indicate that substances in this group are often borderline cases between UVCB and well-defined substances. Composition of the screened substances is often specified by a limited number of well-defined chemical individua, e.g. optical isomers. Compositional variability of some of the other substances in this group is determined by the nature of the manufacturing process – oligo-/poly-merisation.

Table 114 Number of compositions specified in registration dossiers by registrants of other complex substances.

ID	Name (as registered)	% of No. of compositions		
		1	2	3
957	Boric acid (H3BO3), reaction products with ethanolamine	100	0	0
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	100	0	0
157	orthoboric acid, compound with 2-aminoethanol	100	0	0
373	orthoboric acid, compound with 2,2'-iminodiethanol	100	0	0
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	67	33	0
9044	dioxobis(stearato)trilead	100	0	0
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	100	0	0
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	0	0	25
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	88	0	12
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	100	0	0
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	100	0	0
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	100	0	0
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	100	0	0

23 % of substances screened in this group include dossiers reporting multiple compositions.

Table 115 Number of constituents specified in registration dossiers by registrants of other complex substances.

ID	Name (as registered)	No. of constituents	
957	Boric acid (H3BO3), reaction products with ethanolamine		1
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification		8
157	orthoboric acid, compound with 2-aminoethanol		8
373	orthoboric acid, compound with 2,2'-iminodiethanol		1
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	#1	6
		#2	4
9044	dioxobis(stearato)trilead		8
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts		5[a]
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	#1	14
		#2	6
		#3	6
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	#1	7
		#2	6
		#3	6
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)		6[b]
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate		5
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid		8[c]
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol		3[b]

[a] 2 constituents were specified as impurities
[b] 1 constituent was specified as an impurity
[c] 4 constituents were specified as impurities

Only one of the screened substances included over 10 constituents (14 constituents). For the remaining 13 substances, less than 10 constituents were reported (with 2 substances having just a single constituents specified). This relatively low number of reported constituents in comparison with other groups of substances screened within this study can be attributed to the nature of the substances in this group, which are mostly reaction products and reaction masses of a limited number of well-defined substances.

Table 116 Consistency of compositional data provided in the registration dossiers for other complex substances.

ID	Name (as registered)	Composition consistency score [%]*					
		1	2	3	4	5	6
957	Boric acid (H3BO3), reaction products with ethanolamine	0	0	0	0	0	100
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	0	0	0	100	0	0
157	orthoboric acid, compound with 2-aminoethanol	0	0	0	40	0	60
373	orthoboric acid, compound with 2,2'-iminodiethanol	0	0	0	0	0	100
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	67	0	0	0	33	0
9044	dioxobis(stearato)trilead	17	0	0	83	0	0
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	63	0	0	13	24	0
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	0	0	0	0	50	50
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	0	63	0	12	25	0
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	0	0	0	0	17	83
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difl…	0	0	0	100	0	0
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-…	0	0	0	100	0	0
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	100[a]	0	0	0	0	0

* Composition consistency scoring scale:

1: all constituents specified in the dossiers are identical, typical registrant-specific concentration/concentration range is provided
2: all constituents, typical concentrations and concentration ranges are identical in the dossiers
3: all constituents are identical in the dossiers
4: most of the constituents are identical, some are different or missing in the dossiers
5: constituents in the dossiers are completely different
6: only a single constituent is defined (identical with the registered substance)

Note: The number of possible combinations is so great that in order to fully cover all possible combinations, the scoring scale would necessarily have tens of scoring grades. As a result, the sum based on this simplified scoring scale can be greater than 100%.

[a] Only a single registration dossier

Table 117 Typical constituents specified in registration dossiers by registrants of other complex substances.

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
957	Boric acid (H3BO3), reaction products with ethanolamine	MEA Polyborate / Orthoboric acid, compound with 2-aminoethanol	302-207-4	100
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	Calcium carbonate	207-439-9	60 – 95.6
		Calcium oxalate	209-260-1	0 – 11.1
		Silicon dioxide (amorphous)	231-545-4	0.5 – 22
		Organic matter derived from sugar beet fragments	N/A	1.8 – 18.3
		Sand / Naturally occurring substances	310-127-6	0.5 – 22
157	orthoboric acid, compound with 2-aminoethanol	orthoboric acid, compound with 2-aminoethanol	247-421-8	40 – 100
		2-aminoethanol	205-483-3	10 – 30
		boric acid Trihydroxidoboron / boric acid	233-139-2	0 – 0.1 in three dossiers 60 – 65 in one dossier
373	orthoboric acid, compound with 2,2'-iminodiethanol	orthoboric acid, compound with 2,2'-iminodiethanol	267-886-0	100
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	methylenediphenyl diisocyanate	247-714-0	1 – 98
		4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with butane- 1,3-diol, 2,4'-diisocyanatodiphenylmethane, 2,2'-oxydiethanol and propane-1,2-diol	500-415-1	5 – 99
		ureylenebis(p-phenylenemethylene-p-phenylene)diisocyanate	298-531-8	0 – 5
9044	dioxobis(stearato)trilead	Hexadecanoic acid, lead(2+) salt, basic	291-389-8	22 – 65
		Octadecanoic acid, lead(2+) salt, basic	291-696-7	35 – 80
		Fatty acids <C16, lead salt (+2), basic	N/A	1 – 6
		Fatty acids >C18, lead salt (2+) basic	N/A	0 – 5
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	283-392-8	80 – 100
		Zinc dialkyl dithiophosphate ZDDP neutral salt / Phosphorodithioic acid, mixed 0,0-bis(4-methylpentan-2-yl and iso Pr) esters, zinc salts	N/A	60 – 85
		Zinc dialkyl dithiophosphate ZDDP basic salt / Zinc dialkyl dithiophosphate ZDDP basic salt	N/A	10 – 35
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts / Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	288-917-4	100
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts / Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	270-608-0	80 – 100
11683	zinc bis[O,O-bis(2-ethylhexyl)]	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate) / 1-	224-235-5	80 – 100

ID	Name (as registered)	Typical constituent		
		Name	EC/List No.	Concentration [%]
	bis(dithiophosphate)	Hexanol, 2-ethyl-, O,O-diester with phosphorodithioic acid, zinc salt / Zinc, bis[O,O-bis(2-ethylhexyl) phosphorodithioato-kS,kS']-, (T-4)-		
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	Ammonium difluoro{[(4S,5S)2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate / Ammonium difluoro{[(4S,5S)2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	N/A	17 – 26
		Ammonium difluoro{[(4R,5R)2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate / Ammonium difluoro{[(4R,5R)2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	N/A	17 – 26
		Ammonium difluoro{[(4S,5R)2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate / Ammonium difluoro{[(4S,5R)2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	N/A	22 - 31
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	Difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid / difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	N/A	15 – 27
		Difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid / difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	N/A	15 – 27
		Difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid / difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	N/A	15 – 25
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	cis-4-(3-methylbutyl) cyclohexanol / cis 4-(3-methylbutyl)cyclohexanol / Cyclohexanol, 4-(3-methylbutyl)-, cis-	N/A	40 – 79
		trans-4-(3-methylbutyl) cyclohexanol / trans-4-(3-methylbutyl) cyclohexanol / Cyclohexanol, 4-(3-methylbutyl)-, trans-	N/A	21 – 60

Source

Any similarities in the sources of individual sub-groups of substances within this group can be attributed to the selection of substances rather than any actual common substance identity feature.

However, in the contrast with groups of substances where the sources are intrinsically highly variable and complex (e.g. substances of biological origin, petroleum-derived products, substances originating from combustion processes, etc.), sources of substances in this group are usually well-defined chemical individua.

Table 118 Sources of other complex substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Source
957	Boric acid (H3BO3), reaction products with ethanolamine	• Monoethanolamine • boric acid • water
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	Calcium dihydroxide
157	orthoboric acid, compound with 2-aminoethanol	• Mono ethanol amine(MEA) • boric acid (BOA) • water
373	orthoboric acid, compound with 2,2'-iminodiethanol	Boric acid, diethanolamin
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	• A mixture of butane-1,3-diol, propane-1,2-diol and 2,2'-oxydiethanol • 4,4'-MDI with a diol mixture
9044	dioxobis(stearato)trilead	• Lead oxide (PbO) , water, stearic acid • Lead oxide with Stearine • Aqueous solution of stearic acid (fatty acids, C16-18) with an aqueous suspension of lead monoxide
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	• Dialkyl dithiophosphoric acid (DDPA), phosphorus pentasulfide (P4S10), zinc salts • Mixed alcohols (isopropyl alcohol and 4-methylpentan-2-ol , phosphoris pentasulphide , zinc oxide • Alcohol with phosphorus pentasulfide, zinc oxide and oil
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	• Alcohol, phosphorus penta-sulphide, zinc oxide • Phosphorus pentasulfide, alcohols (mixture of 2-ethylhexanol, isobutanol and isopropanol), zinc oxide
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	• Alcohol and phosphorus pentasulfur • Phosphorus pentasulfide with a mixture of two alcohols of a similar class - branched alcohols containing C4 and C5 carbons, zinc oxide • Phosphorus pentasulfide, mixture of isobutanol and 1-pentanol, zinc oxide
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	• Phosphorus pentasulfide is reacted with 2-Ethylhexanol, zinc oxide • Alcohol and phosphorus penta-sulfur, zinc oxide • Mixed alcohols (isopropyl alcohol and 4-methylpentan-2-ol are reacted with phosphoris pentasulphide, zinc oxide
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-	• KOH, aqueous solution of 2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-oxadifluoroacetic acid, potassium salt • cC6O4 acid and a water solution of ammonia

ID	Name (as registered)	Source
	(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	KOH solution, Acetic acid, 2,2-difluoro-2-((2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxalan-4-yl)oxyl) potassium salt, sulfuric acid solution F-DIOX potassium salt, chloridric acid, carbonate salt and potassium fluoride
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	cis-4-(3-methylbutyl) cyclohexanol and trans-4-(3-methylbutyl) cyclohexanol

Manufacturing process and its parameters (conditions)

As stated in the case of source, similarities in the manufacturing process can be attributed to the selection of the screened substances rather than to any actual common substance identity features.

Table 119 Manufacturing processes of other complex substances as specified by registrants in registration dossiers.

ID	Name (as registered)	Manufacturing process
957	Boric acid (H3BO3), reaction products with ethanolamine	Chemical reaction (mixing, heating, dissolution, reaction)
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	Precipitation with CO2 during sugar juice purification
157	orthoboric acid, compound with 2-aminoethanol	Dissolution, homogenization, chemical reaction
373	orthoboric acid, compound with 2,2'-iminodiethanol	Chemical reaction (mixing, heating, dissolution, reaction)
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	Chemical reaction
9044	dioxobis(stearato)trilead	Chemical reaction, drying Grinding, sieving
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	Acidification, Neutralisation Stripping and Filtration Distillation
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	Reaction, neutralization Stripping and Filtration Vacuum distillation
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	Chemical reaction Evaporation Neutralization Drying Acidification Stripping Filtration
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	reaction of ethylhexanol with phosphorous pentasulphide and subsequent neutralization with zinc oxide
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-	Multi-stage process: Concentration, Purification, Washing in a reactor, Azeotropic distillation and separation,

ID	Name (as registered)	Manufacturing process
	dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	Salification Multi-stage process The last step of the process is the reaction between cC6O4 acid and a water solution of ammonia.
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	Synthesis, purification
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	Two step manufacturing process (reaction agents not specified), decription of the conditions of the manufacturing process includes duration of production, pressure, temperature (first step: 170 °C; second step: 120°C) and solvents used.

Additional substance identity elements

Use of additional substance identity elements besides composition, source, manufacturing process and its parameters (conditions) is very limited. In the sub-group of "Others", where two of the screened substances are reaction masses of complex optical isomers, the registrants specified optical activity of the resulting substances, as well as state and form of the substances.

One of the key SID elements for some of the substances in this group is the ratio of reactants, which was specified in some dossiers to more than 50 % of the screened substances.

c) Analytical methods

The following Table 120 and Table 121 summarise the use of analytical methods and techniques in identification of the screened substances.

Table 120 REACH Annex VI analytical methods used by registrants of other complex substances.

ID	Name (as registered)	REACH Annex VI Analytical methods					
		UV-VIS	IR	NMR	MS	HPLC	GC
957	Boric acid (H3BO3), reaction products with ethanolamine	Y	Y	Y			
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification		Y				
157	orthoboric acid, compound with 2-aminoethanol		Y	Y		Y	
373	orthoboric acid, compound with 2,2'-iminodiethanol	Y	Y	Y		[a]	
10817	Propane-1,2-diol polymq+er with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	Y	Y	Y	Y		Y
9044	dioxobis(stearato)trilead		Y				
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	Y	Y	Y		Y	Y
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	Y	Y	Y		Y	Y
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts		Y	Y		Y	Y
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	Y	Y	Y			
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro …	Y	Y	Y	Y		Y
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and …		Y	Y	Y		Y
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	Y	Y	Y	Y		Y
Percentage of use of analytical methods (%)		62	100	85	31	31	54

Note: Void cell means that no information has been found and Y that use of the analytical method was reported in the screened dossiers

[a] Impossible to perform HPLC on this substance as it dissociates under the conditions of the test.

Table 121 Other analytical methods used by registrants of other complex substances in addition to REACH Annex VI methods.

ID	Name (as registered)	Additional analytical techniques and measurements
957	Boric acid (H3BO3), reaction products with ethanolamine	
5020	Calcium dihydroxide precipitated with carbon dioxide during sugar juice purification	XRD, XRF
157	orthoboric acid, compound with 2-aminoethanol	ICP, Coulometric Karl Fischer technique, Elemental analysis – LECO combustion method
373	orthoboric acid, compound with 2,2'-iminodiethanol	Determination of Carbon, Boron, Nitrogen content
10817	Propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene	Gel Permeation Chromatography Liquid chromatography exclusion chromatography (SEC) coupled to refraction index (RI) detection Electrospray-MS-detection
9044	dioxobis(stearato)trilead	XRD, ICP/OES, Differential scanning calorimetry (DSC)
716	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters, zinc salts	ICP
787	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and iso-Pr) esters, zinc salts	XRF, ICP
455	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters, zinc salts	XRF, ICP
11683	zinc bis[O,O-bis(2-ethylhexyl)] bis(dithiophosphate)	
4379	Reaction mass of ammonium difluoro {[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate, ammonium difluoro {[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate and ammonium difluoro {[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	Ion Chromatography, Polarimetry
4380	Reaction mass of difluoro{[(4S,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4R,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid, difluoro{[(4S,5S)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid and difluoro{[(4R,5R)-2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid	FTIR, Karl Fisher analysis, Mass spectrometry (GC-MS coupling)., Polarimetry
4891	Reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol	

It can be observed that analytical methods typically used for determination of composition of inorganic subtances as well as those suitable for determination of organic substances were used in this heterogeneous group of substances.

d) Consortia/associations

Identity of some of the substances screened within this group is systematically addressesd by the following operating consortia and associations:

- ALKANOLAMINE BORATES CONSORTIUM (ABC) - http://www.alkanolamineborates.eu/
- Lead REACH Consortium - http://www.reach-lead.eu/
- Additive Technical Committee (ATC) Consortium - http://www.atc-europe.org/

e) Substance identity profiles

There is a publicly available substance identity profile for some of the substances screened within this group, see the following Table 122 for direct links (where available).

Table 122 Publicly available substance identity profiles of other complex substances.

ID	Name (as registered)	Link to SIP(s)	Identity/sameness criteria based on
9044	Dioxobis(stearato)trilead	http://www.reach-lead.eu/substanceinfo/batch/Dioxobis(stearato)trilead.pdf.zip	Concentration ranges and typical concentrations of the following constituents: Hexadecanoic acid, lead(2+) salt, basic; Octadecanoic acid, lead(2+) salt, basic; Fatty acids <C16, lead salt (+2), basic; Fatty acids >C18, lead salt (2+) basic; Fatty acids, C16-18; Water

3.5. Overall analysis

The following Table 123 provides the statistics of use of individual substance identity elements by the registrants of the screened dossiers in relation to individual groups of substances.

Table 123 Frequency of use of identified substance identity elements by the registrants of the screened dossiers in relation to individual groups of substances.

		Groups of complex substances											
SID elements		1.1	1.2	1.3	1.4	2.1	2.2	2.3	2.4	3.1	3.2	4	Sum (max.=11)
Source	*Source***	1.00	1.00	0.92	1.00	1.00	0.91	1.00	0.95	1.00	1.00	1.00	10.78
Process	*Process***	1.00	1.00	0.92	0.80	1.00	1.00	1.00	0.95	1.00	1.00	1.00	10.67
	*Parameters of process***	0.75	0.41	0.83	0.50	0.88	0.47	0.75	0.57	0.38	0.85	0.54	6.93
Chemistry	*Composition**	1.00	1.00	1.00	1.00	0.96	1.00	1.00	0.98	1.00	1.00	0.92	10.86
	*Alkyl chain length***	0.00	0.00	0.00	0.00	0.71	0.05	0.00	0.07	0.00	0.00	0.00	0.83
	*Carbon number range***	0.00	0.00	0.00	0.00	0.00	0.65	0.00	0.00	0.00	0.00	0.00	0.65
	Crystalline structure (phase)	0.25	0.18	0.83	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.46
Physical	*State*	0.00	0.35	0.25	1.00	0.04	0.04	0.13	0.02	0.75	0.70	0.15	3.43
	Softening point	0.00	0.00	0.00	0.00	0.00	0.00	0.13	0.07	0.00	0.05	0.00	0.25
	Density	0.00	0.06	0.00	0.40	0.13	0.35	0.88	0.05	0.00	0.30	0.00	2.16
	Solubility	0.00	0.18	0.00	0.50	0.00	0.00	0.00	0.00	0.13	0.15	0.00	0.95
	*Viscosity***	0.00	0.00	0.00	0.10	0.04	0.33	0.00	0.02	0.00	0.05	0.00	0.55
	pH	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.50	0.20	0.15	0.88
	*Boiling point***	0.00	0.00	0.00	0.00	0.04	0.65	0.88	0.05	0.00	0.10	0.00	1.71
	Flash point	0.00	0.00	0.00	0.00	0.04	0.30	0.88	0.02	0.00	0.05	0.00	1.29
	Particle size distribution	0.25	0.12	0.08	0.50	0.00	0.00	0.00	0.00	0.00	0.05	0.00	1.00
Morphology	*Form of the substance*	0.50	0.41	0.67	0.90	0.00	0.00	0.13	0.00	0.25	0.70	0.23	3.78
Light properties	*Optical activity**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.25	0.15	0.43
	Refractive index	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.10	0.00	0.12
	Colour	0.00	0.18	0.42	0.50	0.04	0.02	0.00	0.10	0.63	0.55	0.08	2.50
Group-specific identifiers	*Colour Index***	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.36
	Group-specific element	0.50	0.12	0.42	0.40	0.00	0.00	0.00	0.00	0.38	0.70	0.00	2.51
Other	*Common characteriser*	0.50	0.71	0.17	0.90	0.04	0.00	0.13	0.00	0.50	0.80	0.00	3.74
	Other characteriser	0.50	0.71	0.67	0.70	0.29	0.05	0.75	0.17	1.00	0.85	0.77	6.45
		10	14	13	15	13	13	12	17	12	20	10	

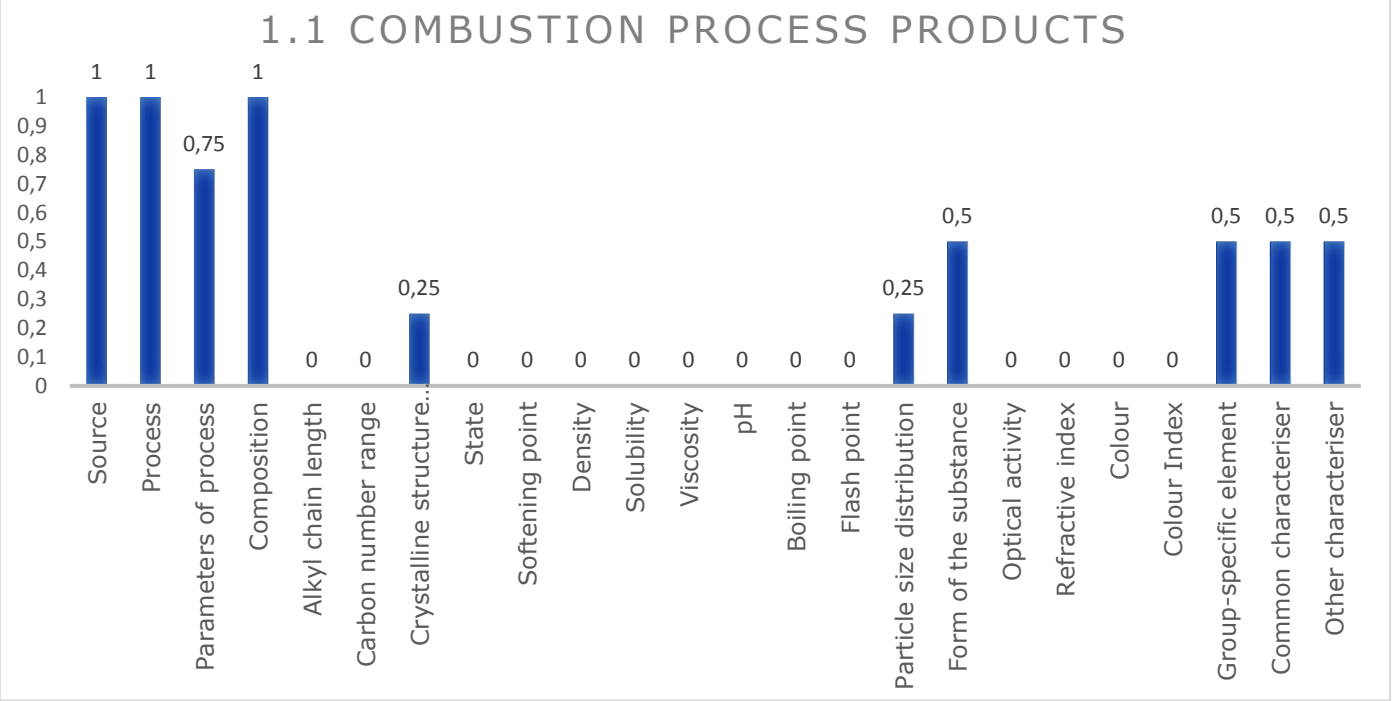
Notes: The **green fields** indicate frequency of use of individual SID elements on the scale of 0 – 1 (1 meaning that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)
The **blue fields** indicate overall frequency of use of individual SID elements across all groups of substances (numbers are sums of rows)
The **brownish fields** specify the total number of used substance elements in identification of a single group of substances
Numbering of the groups of complex substances in the header of the table corresponds to the numbering introduced in 2.1, group number 4 includes three (rather small) sub-groups which were merged together in this table.
* Required information according to REACH Annex VI
** Substance identity element mentioned in ECHA guidance for identification and naming of substances

The study identified 24 substance identity elements commonly used by registrants of complex substances. The highest number of substance identity elements used by registrants of a particular group of substances is 20 (substances originating from animals and plants), while the lowest is 10 (combustion process products and the group of other organic substances). The average number of substance identity elements used per group is 13.5 ± 2.9.

Among the substance identity elements, composition, source and manufacturing process (often with the conditions of the manufacturing process also reported) are by far the most frequently used ones, confirming their importance in identification of all different groups of complex substances. Other frequently used substance identity elements include state (e.g. solid), form of the substance (e.g. fibres), colour and density. Other substance identity elements are more group-specific (e.g. boiling point for petroleum-derived substances and coal-derived substances, crystalline structure for substances originating from calcination processes). Frequency of use of SID elements for identification of different groups of substances is further illustrated by figures on the following pages.

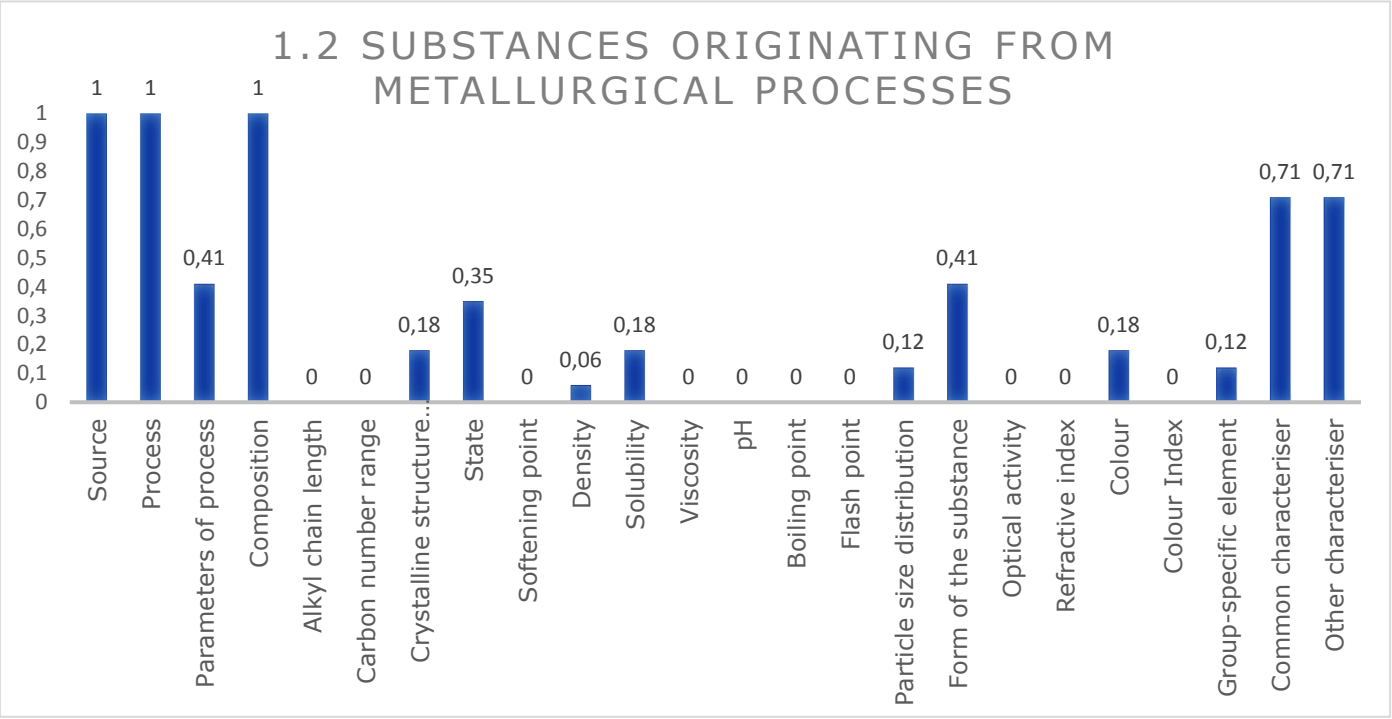
It shall be noted that identified SID elements include physicochemical properties required by Annex VII and Annex IX of REACH (e.g. boiling point, flash point, density) and therefore reported by registrants also in other IUCLID sections than those related to substance identification which were screened in this study. However, in numerous cases these substance identity elements were considered by the registrants as relevant for identification of the substances and were therefore reported also in IUCLID section 1.1 relating to substance identification.

Figure 2 Frequency of use of individual SID elements on the scale of 0 – 1: Combustion process products.



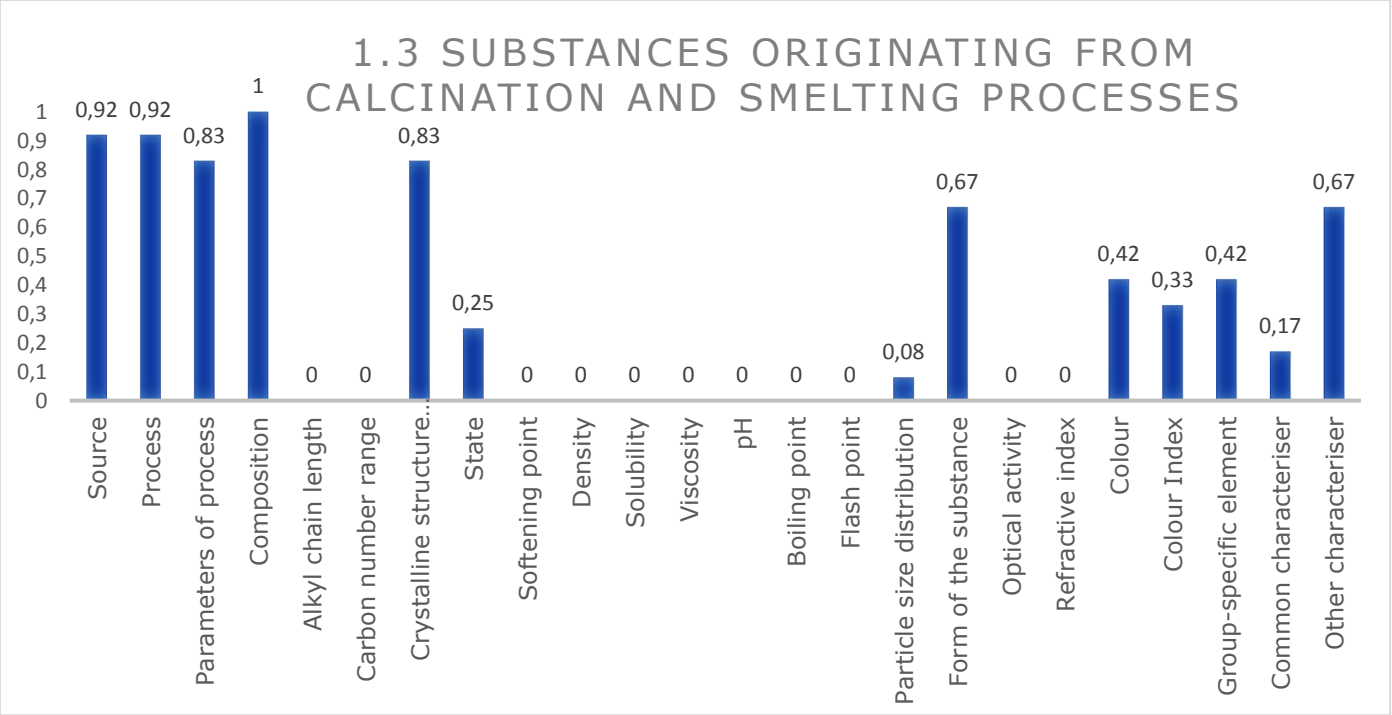
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 1 Frequency of use of individual SID elements on the scale of 0 – 1: Substances originating from metallurgical processes.



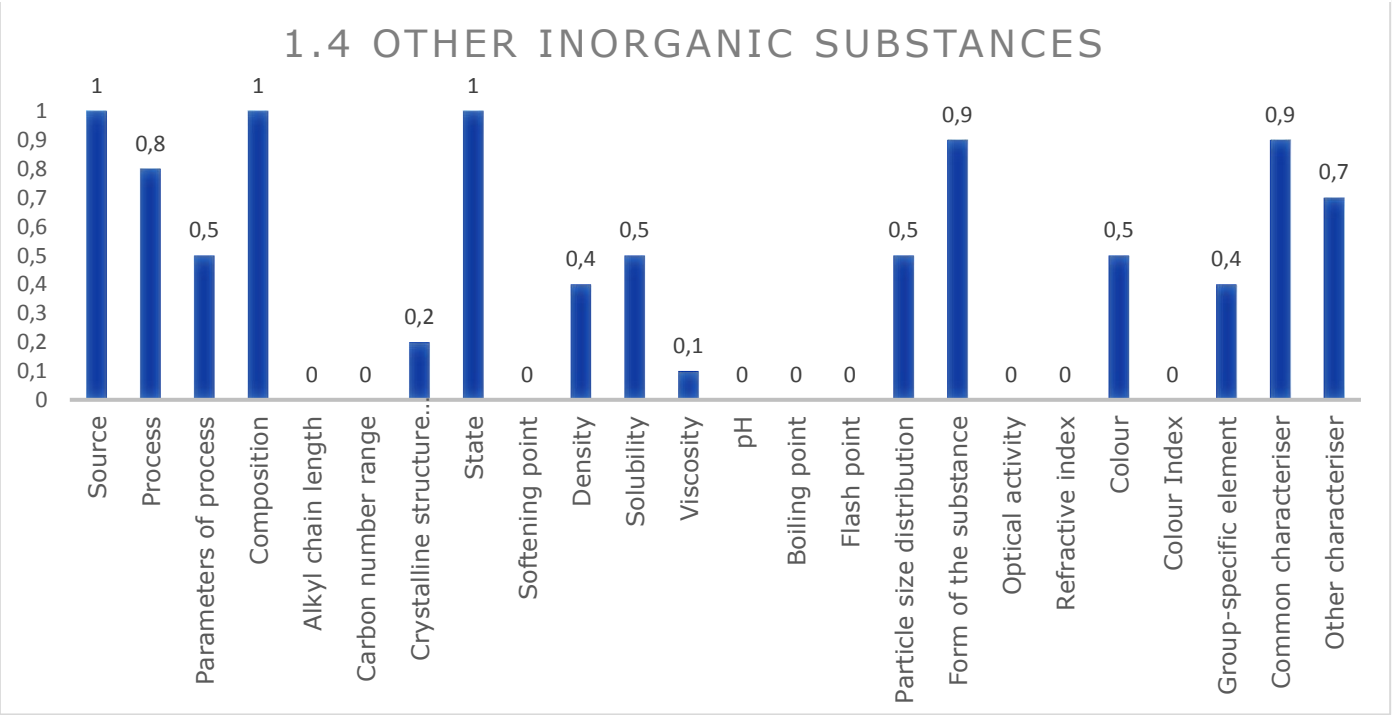
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 3 Frequency of use of individual SID elements on the scale of 0 – 1: Substances originating from calcination and smelting processes.



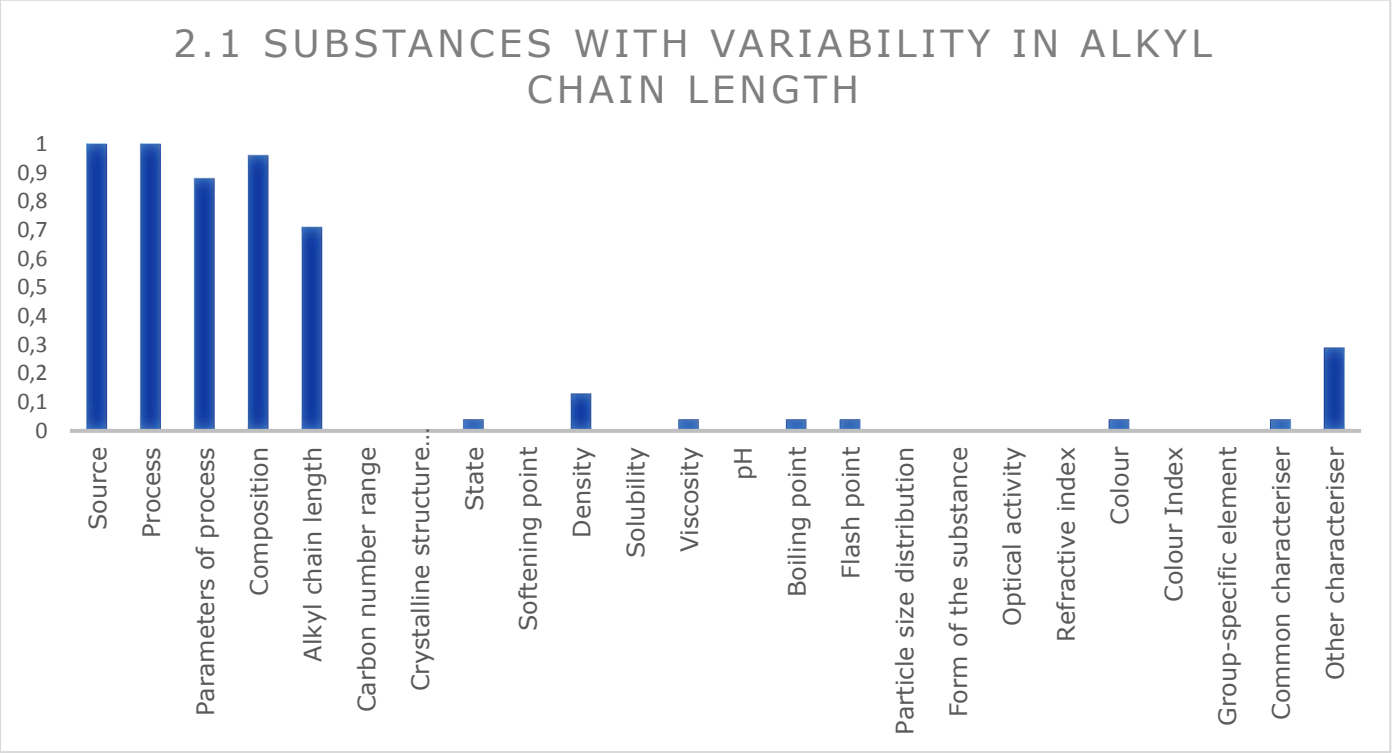
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 4 Frequency of use of individual SID elements on the scale of 0 – 1: Other inorganic substances.



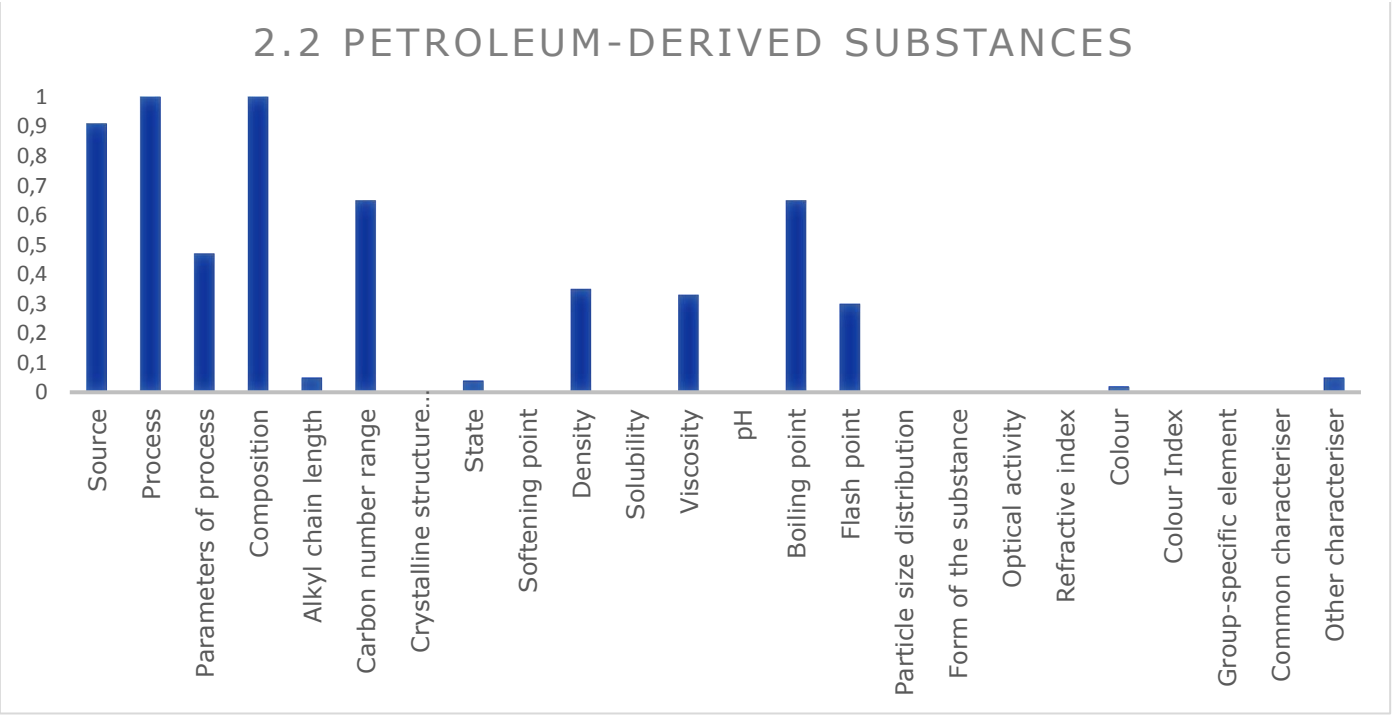
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 5 Frequency of use of individual SID elements on the scale of 0 – 1: Substances with variability in alkyl chain length.



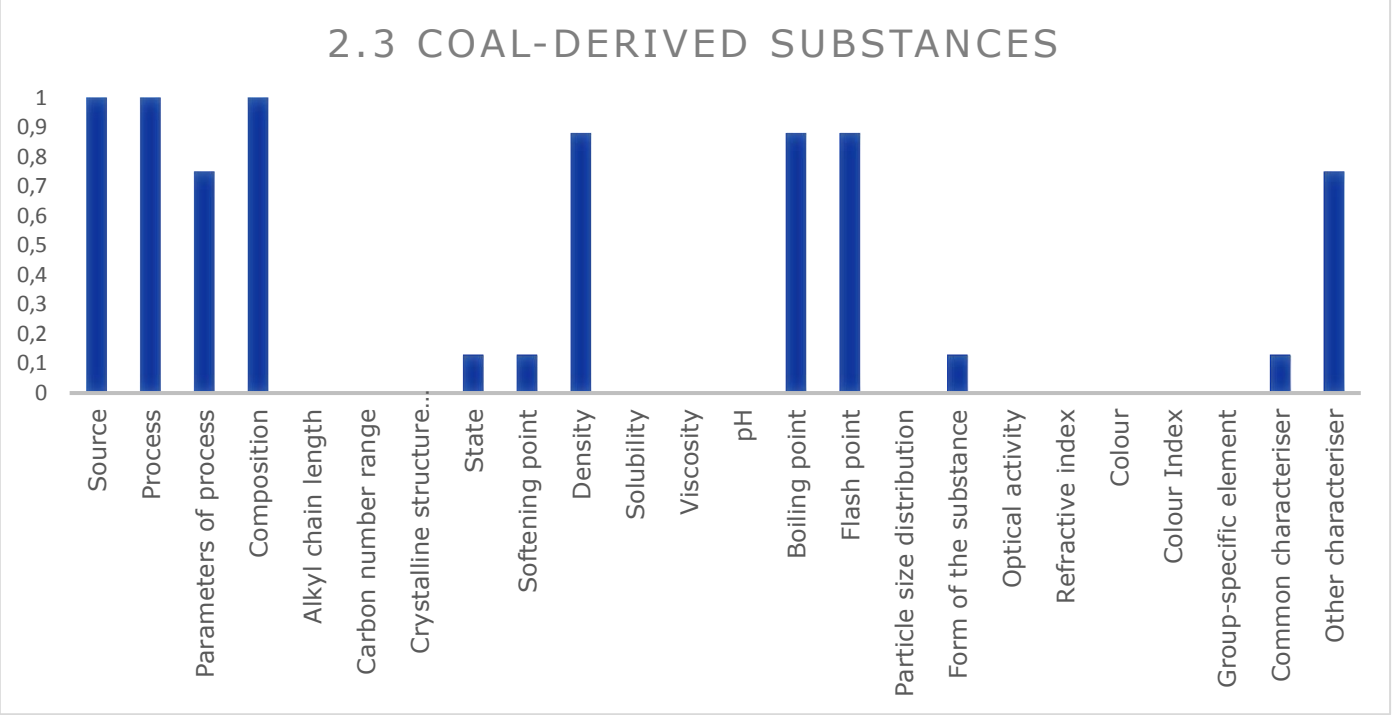
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 6 Frequency of use of individual SID elements on the scale of 0 – 1: Petroleum-derived substances.



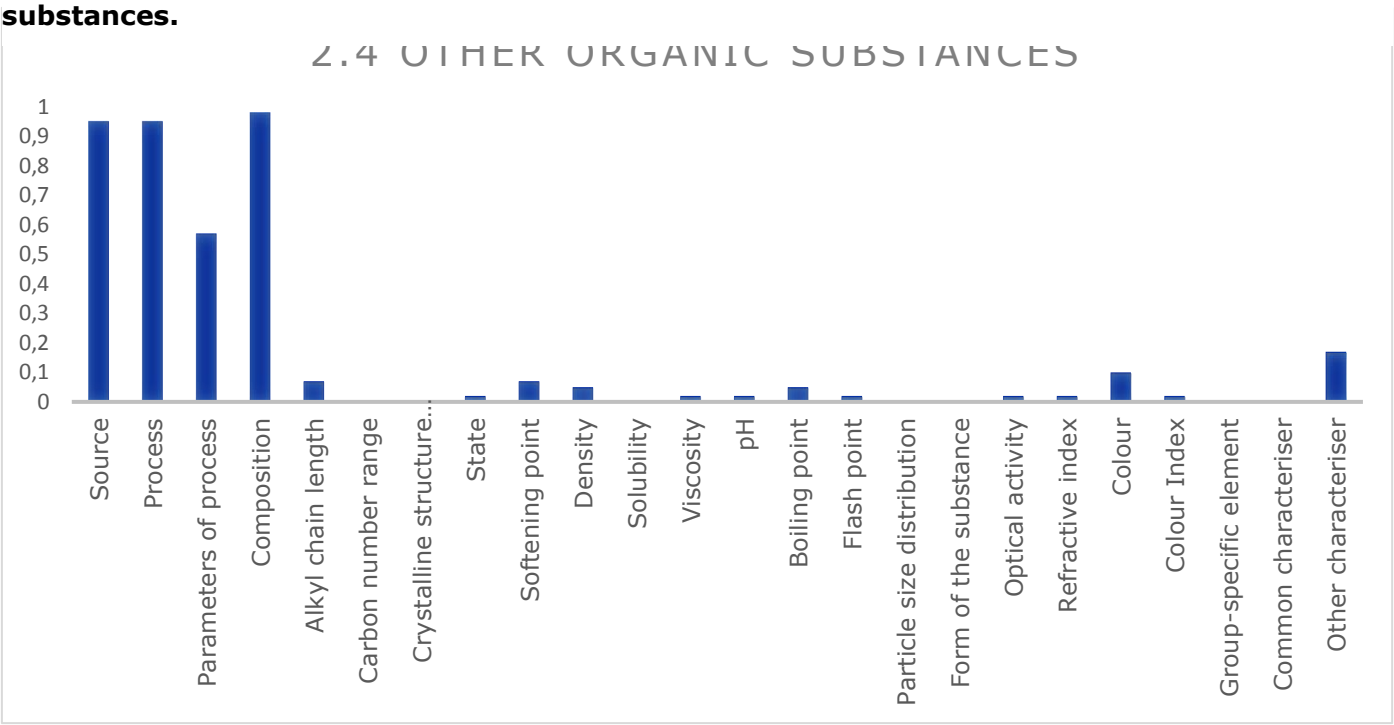
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 5 Frequency of use of individual SID elements on the scale of 0 – 1: Coal-derived substances.



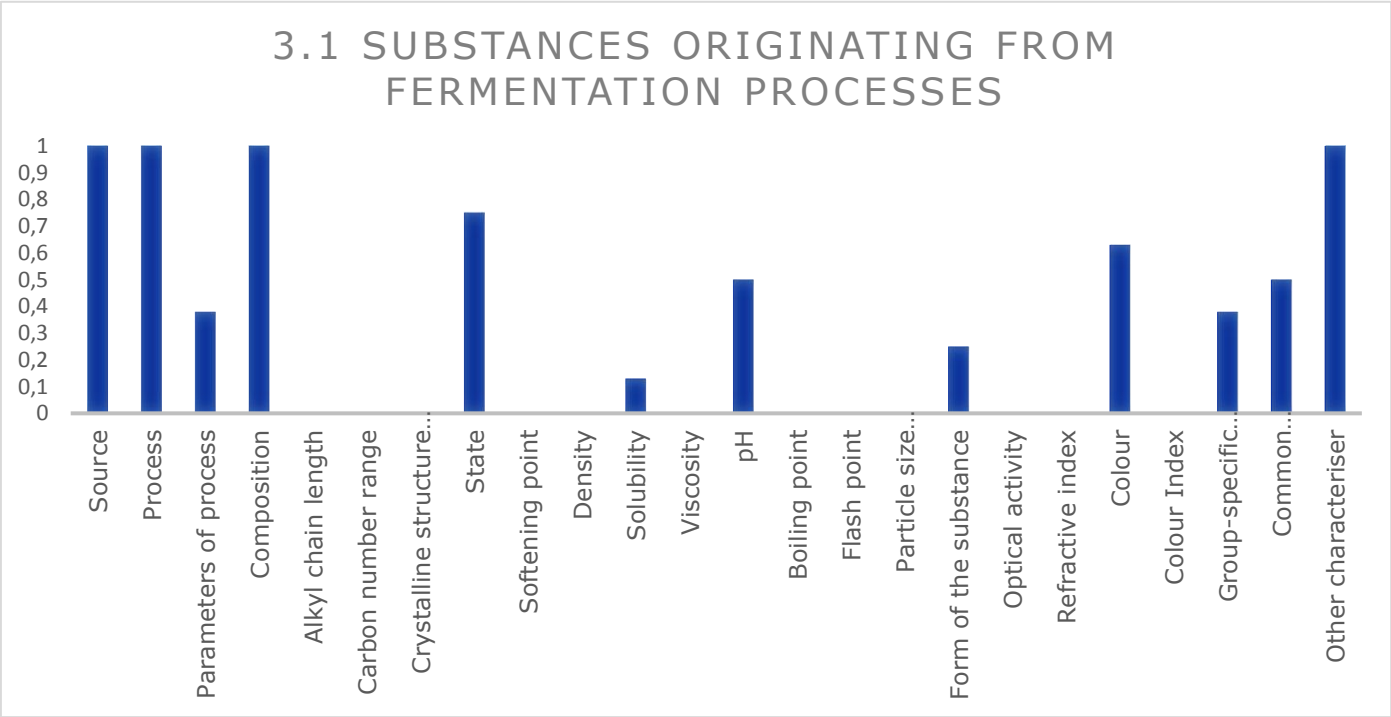
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 6 Frequency of use of individual SID elements on the scale of 0 – 1: Other organic substances.



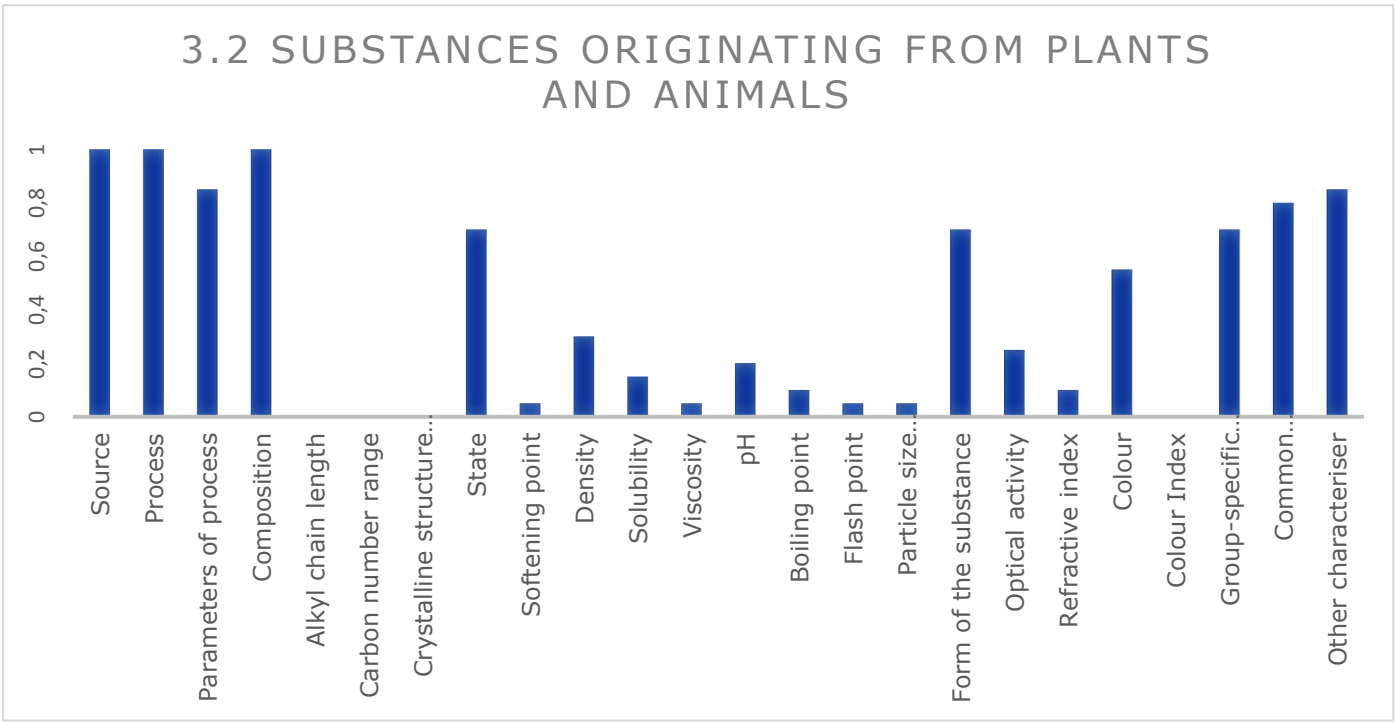
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 7 Frequency of use of individual SID elements on the scale of 0 – 1: Substances originating from fermentation processes.



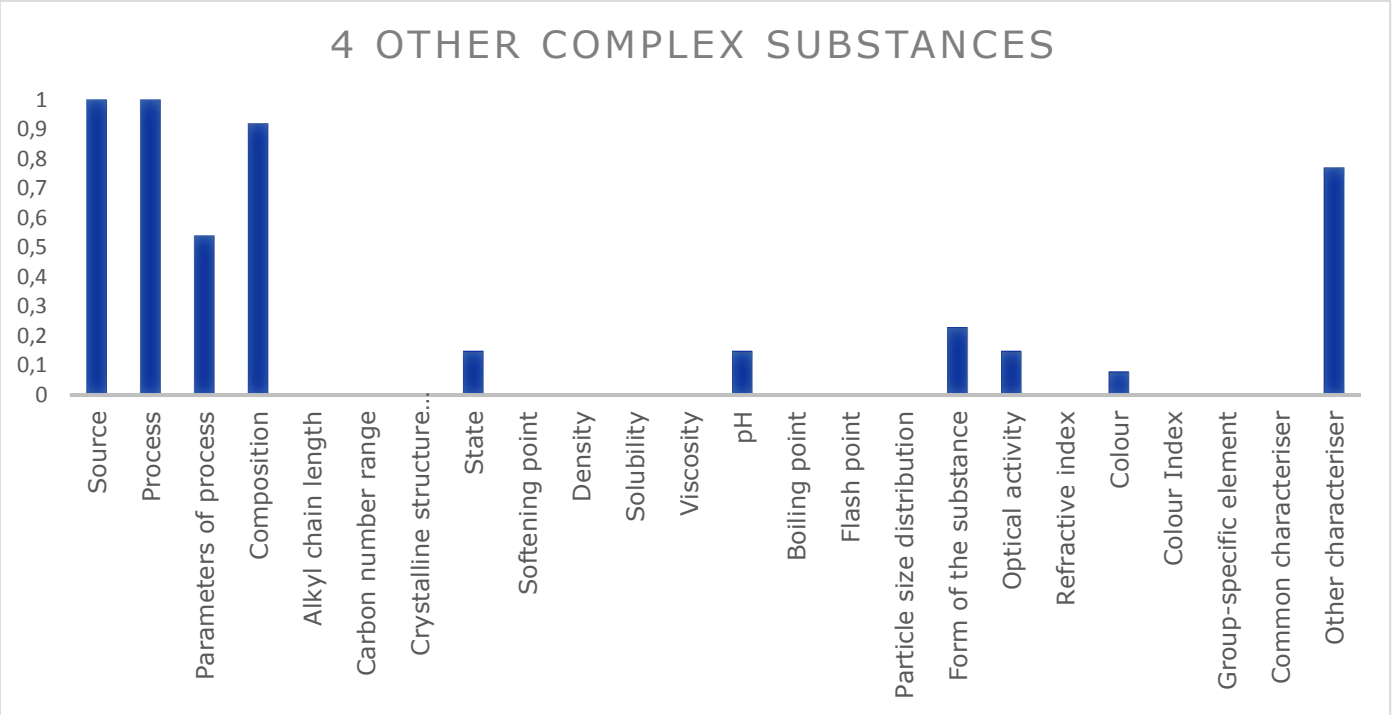
Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 8 Frequency of use of individual SID elements on the scale of 0 – 1: Substances originating from plants and animals.



Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

Figure 9 Frequency of use of individual SID elements on the scale of 0 – 1: Other complex substances.



Note: Score 1 means that the SID element was used in at least one dossier for all substances in the group, 0.5 that the SID element was used in at least one dossier for 50% substances in the group, etc.)

The statistics of use of individual SID elements clearly shows that the most composition, source and manufacturing process together with its parameters (conditions) play the key role in identification of UVCB substances.

In general, the following different approaches in specifying compositional data and describing the manufacturing process were observed across all groups of substances

Composition:

- There are numerous cases where only a single constituent with an identical name to the registered substance is specified – no breakdown to individual constituents are provided by the registrants.
- Some registrants specify multiple compositions describing different grades of the same substance.
- Another typical reason for specifying multiple compositions in a single registration dossier is the description of a general SIEF/SIP-defined composition and the registrant-specific sample.
- Particular attention in providing compositional data and determining sameness of substances is usually paid to substances relevant for hazard classification and labelling.

Manufacturing process:

- The level of detail of the manufacturing process description is generally highly variable. Generally higher level of detail of the manufacturing process description was observed in the dossiers of lead registrants, which were subjected to the compliance check on substance identity by ECHA.
- Information on the manufacturing process are sometimes identical to or based on the existing description in the EC Inventory. This approach was observed in the descriptions of some registered substances as well as the corresponding reference substances.

Approaches applied in identification of substances are rarely justified in registration dossiers, description or justification of applied SID approaches is more typically formulated at the level of SIEFs, REACH consortia or industry associations and usually publically available on the website of the SIEF or REACH consortium rather than included in the registration dossiers.

In defining typical, minimum and maximum concentrations of individual constituents, two approaches were identified:

a) Top-down approach: The lead registrant presents a proposal to the members of the SIEF (and optionally also of the pre-SIEF) on which they comment. Based on the comments, the composition for the joint submission is finalised and the defined concentration ranges present the substance identity profile for the determination of sameness for new registrants joining the SIEF.

b) Bottom-up approach: The SIEF manager collects information on the composition from the members of the SIEF (and optionally also of the pre-SIEF), the information is collated into a proposal for the composition of the SIEF on which the members can comment. As in the top-down approach, the composition for the joint submission is finalised and the defined concentration ranges present the

substance identity profile for the determination of sameness for new registrants joining the SIEF.

Both approaches sometimes include several re-iterations before an agreement on the composition for the joint submission is reached.

As a result, concentration ranges of individual constituents specified in the joint submission are often very wide, especially in cases of large SIEFs (SIEFs with a high number of co-registrants). Defining clear boundaries of concentration ranges to ensure that the data submitted jointly according to Annex VII – XI are relevant for all concentrations reported in the registration dossiers remains challenging.

Furthermore, it can be observed across all groups of substances that members of the SIEF sometimes specify these SIEF-derived concentration ranges of constituents without specifying their own typical compositional data.

General observations can also be formulated regarding the use of analytical methods in determination of composition of complex substances:

- Principal difference in the use of analytical methods was observed in determination of composition of inorganic substances (often in solid state) and organic substances.
    - Methods explicitly mentioned in Annex VI of REACH were usually used in determination of composition organic substances. These are ultraviolet-visible spectroscopy, infrared spectroscopy, nuclear magnetic resonance, mass spectrometry, high-performance liquid chromatography and gas chromatography.
    - Methods typically used for determination of composition of inorganic substances include X-ray diffraction, X-ray fluorescence, Inductively coupled plasma optical emission spectroscopy and atomic absorption spectroscopy.
- With growing number of constituents, spectra and chromatograms become less suitable for determination of substance sameness. Due to the growing compositional complexity and number of combinations of concentrations of the constituents, comparison of spectroscopic and chromatographic fingerprints is rendered more difficult. In such cases the importance of other substance identity elements is growing with the growing number of constituents (typically detailed description of the manufacturing process and its conditions is vital).

The following Table 124 presents summarising statistics regarding percentage of use of SID elements across substances in different groups and number of SID elements used by registrants in each group.

Table 124 Summarising statistics regarding percentage of use of SID elements across substances in different groups and number of SID elements used by registrants in each group

	Inorganic				Organic				Biological		Others
	1.1	**1.2**	**1.3**	**1.4**	**2.1**	**2.2**	**2.3**	**2.4**	**3.1**	**3.2**	**4**
Percentage of use of SID elements*	67	46	58	63	40	45	69	24	60	46	50
number of SID elements used in the group	9	14	13	15	13	13	11	17	13	21	10
Highest number of used SID elements for a single substance	9	12	11	13	9	10	9	7	12	15	7
Average number of SID elements used in a group	6 ± 2.2	6.4 ± 2.2	7.5 ± 2.3	9.5 ± 3	5.2 ± 1.2	5.8 ± 1.4	7.6 ± 1.3	4.1 ± 1.3	7.8 ± 2.1	9.7 ± 2.7	5 ± 1.2
Number of substances screened in a group/sub-group	4	17	12	10	24	57	8	42	8	20	13

* for a single substance a SID element is regarded as used if reported in at least one of the screened dossiers for that substance

Groups of substances reported in Table 124:

- 1.1: Substances originating from combustion processes
- 1.2: Substances originating from metallurgical processes
- 1.3: Substances originating from calcination and smelting processes
- 1.4: Other inorganic substances
- 2.1: Substances with variability in alkyl chain length
- 2.2: Petroleum-derived substances
- 2.3: Coal-derived substances
- 2.4: Other organic substances
- 3.1 Substances originating from fermentation processes
- 3.2 Substances originating from plants and animals
- 4: Other substances (including the following three sub-groups: Substances with organic and inorganic part, Organic-inorganic salts, Others)

Table 124 shows that in general, registrants of organic substances used on average less substance identity elements to identify their substances than registrants of inorganics and of substances of biological origin. Also the highest number of used SID elements for a single substance is in most cases higher for groups of inorganic substances and substances of biological origin than for groups of organics. The highest encountered number of SID elements used for identification of a single substance is 15 (a plant extract from the group of substances originating from plants and animals).

3.6. Information exchange with stakeholders (industry associations, REACH consortia, etc.)

3.6.1. Substance identity workshop

To support exchange of information and views on substance identity challenges and best practices among different stakeholders, a workshop was organised within the course of the project.

The workshop was organised as a two day event, taking place on 27 – 28 April 2015 in Brussels, Belgium. The event brought together over a hundred professionals dealing with substance identity from different positions – representatives of industry associations and of individual manufacturers of complex substances, testing facilities, REACH consultants as well as delegates of national competent authorities, ECHA and of the European Commission. The workshop was also web-streamed, with 144 online viewers on the first day of the workshop and 107 viewers on the second day of the workshop.

Over the two days, preliminary results of this study were presented and common cross-cutting as well as sector-specific issues were discussed in plenary sessions and especially in 4 break-out groups focusing on the following topics:

1. Good practices in developing Substance Identity Profiles (SIPs)
2. Elements of substance identity / characteristics of complex substances
3. Role of chemical analysis in identification of substances
4. Communication of substance identity elements within SIEFs / consortia

Presentations from the workshop and outcomes of the break-out groups have been published together with recordings of the workshop at the website of the European Commission – Directorate General for Internal Market, Industry, Entrepreneurship and SMEs[23].

3.6.2. Questionnaires and other feedback from stakeholders

Since the results of this study aim to support the activities of current and future registrants of complex substances, stakeholders were actively approached to share their experience and provide additional information on substance identity in their specific industry sectors.

Stakeholders were first approached with a request for data to support the selection of the representative set of substances for substance identity information assessment. The call for data was published at the website created specifically to disseminate information related to this project[24] on 27 March 2014, circulated to 163 e-mail addresses of relevant stakholders, published at the European Commission website, at the website of ECHA and circulated through ECHA newsletter. 25 responses to the call for data were received.

Another call for data was announced on 6 November, aiming at collection of additional information on substance identity from individual industry associations and REACH consortia. Since the call for data was targeted specifically to industry associations and REACH consortia, these were contacted through direct e-mails. A document with a set of questions targeted to industry associations and REACH consortia was sent to 67 e-mail addresses. 3 responses were received, presented in Annex 5.

[23] Recordings of the workshop and documents summarising the outcomes of the workshop are available at http://ec.europa.eu/growth/tools-databases/newsroom/cf/itemdetail.cfm?item_id=8162.

[24] http://sidc.reach-2018.eu/

4. CONCLUSIONS

The results and observations of this study confirmed that identification and especially determination of sameness of complex substances, typically UVCBs, remains a challenge.

In particular, the following typical challenges and issues were identified:

- Inconsistency of compositional data among dossiers submitted for a single substance (inconsistency in naming of the main constituent, constituents with identical names reported with different EC and CAS numbers or without EC and CAS numbers, compositional data provided as a result of incomparable analytical methods – e.g. elemental analysis vs. mineralogy). It is questionable how substance sameness was assessed in such cases. Studied information and feedback from stakeholders indicate that basis for such inconsistencies might be in poor or no communication of co-registrants. A particular group of substances where there is an indication of poor or no communication between co-registrants are substances on the ELINCS List (with EC numbers 4xx-xxx-x), i.e. substances that were notified in accordance with the Directive 67/548/EEC.

- Substance identification and comparability of compositional data for substances where registrants state that the constituents (or their concentrations) are to a significant extent unknown (e.g. substances of biological origin, petroleum-derived products, coal-derived products, substances originating from calcination processes and reclaimed substances). In such cases, using combinations of substance identity elements appears to be an efficient way of overcoming this challenge based on the information reported in the screened registration dossiers (e.g. specifying boiling point range in the case of petroleum-derived substances and coal-derived substances, detailed description of the processing steps and processing conditions in the case of plant extracts, description of the processing steps, conditions and technology in the case of coal-derived substances, etc.).

- Defining sameness criteria, especially concentration ranges of individual constituents and concentration thresholds when a substance can be regarded as eligible for a joint registration by multiple co-registrants.

- Defining sameness criteria and assessing sameness of substances (mostly inorganic) where compositional data resulting from chemical analyses are of limited relevance to capture chemical speciation of constituents and properties of the substance (e.g. substances originating from calcination processes, substances originating from metallurgical processes, combustion process products, zeolites, mixed metal oxides and in particular inorganic pigments, where mineralogy information is essential).

- In a significant number of cases, analytical data provided by registrants lack description or interpretation of the results.

- In a significant number of cases, co-registrants in a joint submission do not provide registrant-specific compositional and analytical data (and provide only data of the lead registrant or typical data determined within the SIEF/consortium instead).

- From the feedback from stakeholders collected within the study (in a workshop and questionnaires), it can be concluded that substance identity requirements imposed by REACH force registrants to carry out further analytical tests in addition to those traditionally performed by the industry where the need for analytical testing is market-driven (and therefore risk-driven only to limited extent in comparison with REACH). The study showed that substance identity is very sector-specific or even substance-specific and based on the information reported in the screened dossiers, no widely applicable sameness assessment

criteria can be developed. In some cases, registrants documented the applied sameness assessment criteria (e.g. boiling point range in the case of petroleum-derived substances and coal-derived substances, concentration of polyaromatic hydrocarbons in the case of coal-derived substances). Sameness assessment criteria are also sometimes described in additional documents developed by SIEFs, consortia and associations, typically in substance identity profiles or sector-specific guidances. While it may not be feasible to develop widely applicable sameness assessment criteria, particular examples presented by some registrants showed that these criteria can be defined at the level of individual substances and some generic criteria can in some cases be defined also at the level of groups of substances (e.g. crystalline structure of inorganic pigments, presence of crystalline structures in zeolites, definition of processing steps and process conditions for extracts from plants, etc.).

Sector-specific guidances developed by industry associations and consortia in collaboration with ECHA and other international bodies proved valuable, e.g. the OECD guidance for characterising oleochemicals publicly available at http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)6&doclanguage=en or a guidance prepared by the Hydrocarbon Solvent Producers Association and OECD in collaboration with ECHA for hydrocarbon solvents available at http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2015)52&doclanguage=en.

- Some stakeholders mentioned in questionnaires and in the workshop organised within the study an issue of changing EC numbers as a result of substance identity discussions within SIEFs or with ECHA (as a result of an inquiry process or in case of compliance checks aiming at substance identity). It was stated that change of an EC number of a substance within a marketed product has significant impacts regarding trading with countries where REACH is not in force and also regarding impacts in relation to other legislation (e.g. legislation regarding biocides, pesticides or non-EU legislation where different restrictions may apply).

Identified practices efficient for addressing challenges in identification of complex substances include:

- Ensuring harmonisation of the character of substance identity information specified by potential co-registrants (e.g. through substance identity profiles) to allow comparison of the data thus enhancing the process of determination of substance sameness (it was concluded from the feedback provided by registrants in the workshop and in responses to circulated questionnaires that assessment of substance sameness is particularly difficult if the registrants in a SIEF do not reach agreement on the substance identity elements to be determined and analytical methods to be used to allow comparison of substance identity information)

- Using combinations of substance identity elements and detailed descriptions of the manufacturing process and source in cases where analytical data provide limited information on the composition of the substance.

- Using combinations of analytical methods for identification of complex substances. Information from IR, UV/VIS, NMR and GC spectra is usually useful for fingerprinting, but often needs to be complemented with other analytical methods (depending on the nature of the analysed substance) for proper identification of complex substances.

- Providing detailed description of the manufacturing process and its conditions in cases where the source is highly variable.

Other conclusions and observations:

- 25 substance identity elements used by registrants of complex substances were identified. The number of substance identity elements used by the registrants varies from 10 to 20 for different groups of substances, with 13.5 being the average. At the level of individual substances, a few substances with only a single SID element used were encountered (only composition was provided by the registrants), while the highest number of SID elements used by registrants of a substance was 15.

- In accordance with the guidance for identification and naming of substances under REACH and CLP published by ECHA, information about composition, source and manufacturing (technological) process, often with specified conditions of the manufacturing process (e.g. temperature, pressure, pH, specification of catalysts) are the most frequently used substance identity elements.

- Registrants of inorganic substances often specify also state (predominantly solid), form (e.g. powder, fibres), crystalline structure and particle size distribution.

- Registrants of organic substances often use alkyl chain length or carbon number range as substance identity elements for substances with variability in alkyl chain length (including a large group of petroleum-derived products), combined with boiling point, flash point and density in the case of petroleum-derived products. Boiling point, flash point and density are frequently used as substance identity elements also by registrants of coal-derived substances.

- Registrants of substances of biological origin most frequently specified state (predominantly liquid) in addition to composition, source, manufacturing process and its conditions, followed by form (e.g. paste, viscous liquid, powder), colour and pH.

- In many cases, there is high variability in the composition (broad ranges of individual constituents – constituents with ranges broader than 50 % were encountered in some cases in all groups of the screened substances), indicating that the source and/or the manufacturing process might have been overly broadly defined in such cases.

- The set of analytical methods and techniques used for determination of chemical composition of individual substances subject to the screening reflects the nature of the substances in most cases. Analytical methods explicitly mentioned in Annex VI of REACH were used for identification of the vast majority of organic substances, with ultra violet-visible spectroscopy, infrared spectroscopy and nuclear magnetic resonance being the most frequently used ones, followed closely by gas chromatography, while high performance liquid chromatography and mass spectrometry are used less frequently. In addition, registrants of organic substances often use various titration methods to provide further substance identity information. In contrast, analytical methods explicitly mentioned in Anneex VI of REACH are of limited relevance for identification of inorganic substances (predominantly solid), where X-Ray diffraction and X-Ray fluorescence are the most frequently used analytical methods, often combined with inductively coupled plasma optical emission spectrometry and atomic absorption spectrometry.

- In cases where a SIP was developed, information in the registration dossiers usually reflected (or even copied) information defined in the SIP, especially regarding composition. In such cases, second composition was sometimes (but not always) specified, pertaining to registrant-specific compositional data.

Further conclusions regarding individual groups of substances are mentioned in the corresponding sections of this report.

Notes:

It shall be noted that the conclusions and observations presented in this report are based on the information from registration dossiers reported in the ECHA database of registered substances as of August 2014. The information in the registration dossiers may have been updated since then and the conclusions may not reflect the latest approaches applied by the registrants in identification of complexes.

It shall also be noted that the conclusions and observations presented in this report, summarising approaches of registrants in identification of complex substances, are in no way addressing whether these approaches are the correct way to meet the requirements for identification of substances laid down by REACH and whether the information provided in the screened registration dossiers as reported to ECHA is in accordance with the provisions of REACH.

5. RECOMMENDATIONS

The results and observations of the performed study support recent activities of certain sectoral organisations in collaboration with ECHA and other international bodies to harmonise the approaches in identification and determination of sameness of certain specific groups of complex substances.

The report presents the state of play in identification of complex substances under REACH, on which authorities and industry can build further work to enhance this key process in registration of substances. Presented conclusions and observations can serve ECHA in further development of the compliance check procedures, further development of the guidance for identification and naming of substances or in development of sector-specific substance identification guidances. Information in this report can also be taken into consideration by the European Commission in the next REACH review in 2017 or in further work to support efficient implementation of REACH.

Based on the conclusions and observations made within the study, the following recommendations are proposed:

- It is highly recommended to carry on with initiated collaborative activities of ECHA, industry associations and other international bodies to develop sector-specific guidances for identification of individual groups of substances and especially for assessment of substance sameness.

- To facilitate exchange of information between potential SIEF members in assessment of substance sameness, further development of substance identity profiles (SIPs) should be considered to address specifics in identification of UVCBs. The concept of substance identification profiles proved an efficient tool in substance identity and sameness discussions within SIEFs and pre-SIEFs for well-defined substances and the results of the study indicate that with further development, SIPs can be efficiently used also for UVCBs (with sector-specific modifications).

- Annex VI of REACH, sections 2.3.5 and 2.3.6 list analytical data which shall be sufficient to enable each substance to be identified. As confirmed by the results of this study, these data are appropriate and sufficient usually only for identification of some groups of substances, especially organics. For other groups of substances, other analytical data are more appropriate for identification (e.g. data from X-ray diffraction, X-ray fluorescence or Inductively coupled plasma optical emission spectroscopy for various inorganic substances). It is therefore recommended to consider updating Annex VI, section 2.3 of REACH or to compile a compendium of analytical methods appropriate for identification of different groups of substances.

- It is not currently regarded necessary to conduct a similar complex study addressing substance identity. Within this study, information from more than 2 000 registration dossiers of 223 substances were analysed. Encountered approaches, issues and challenges were highly repetitive and it is believed that extending the set of screened substances would be of limited value, bringing forward no further issues of notable significance. Furthermore, applicability of any eventual findings from such an extended study before the next registration deadline in 2018 would be questionable. It can be considered to perform a similar study after the 2018 registration deadline to assess development in the field and identify any outstanding issues which might arise with new registrants (especially SMEs) becoming involved. Such study could provide valuable information to new potential future registrants after the 2018 registration deadline.

- In designing an eventual future study on substance identity, it is recommended to narrow down the scope, i.e. to select only several groups of substances

(industry sectors) and to extend the depth of analyses or assessment (e.g. focusing on particular substance identity issues relevant to the selected groups of substances, developing substance identity profiles and substance sameness criteria, assessing in more detail whether the information in registration dossiers is in accordance with developed sector-specific guidances and materials).

- It is recommended to support exchange of information and experience on identification of substances between registrants via workshops, both general and sector-specific, organised by stakeholders from industry as well as authorities, especially before the upcoming registration deadline in 2018.

The study showed that identification of complex substances can be very demanding in terms of expert capacities, analytical testing requirements and costs and the level of detail required for appropriate identification of complex substances is questionable. It is therefore recommended that when considering any subsequent actions and measures further enhancing the current state of play, it should be carefully considered to what extend such measures contribute to the objectives of REACH.

List of Annexes

Annex I : List of complex substances organised by groups and sub-groups ("Complex Substances List")

Annex II : List of substances selected for substance identity analysis ("The Sample Set")

Annex III : Substance Identity Information Protocol Template

Annex IV : Substance Group Evaluation Protocol Template

Annex V : Responses of stakeholders to the first call for data

Annex VI : Responses of stakeholders to the second call for data

Annex VII : Sector-specific substance identity factsheets

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