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18/2024

Final Report

Intermediate uses of petroleum and coal substances - a regulatory issue?

Environmental emission assessment of substances of very high concern from petroleum and coal fractions in intermediates

German Environment Agency

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Intermediate uses of petroleum and coal substances - a regulatory issue?

Environmental emission assessment of substances of very high concern from petroleum and coal fractions in intermediates

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Abstract: Study on Intermediate Uses of PetCo Substances

The study describes the intermediate uses of 53 petroleum and coal stream (PetCo) substances and assesses the potential for their constituents with properties of concern to transfer within the supply chain and into the environment. The study focuses on 15 marker constituents that have been shortlisted based on a screening of CMR (carcinogenic, mutagenic, reprotoxic), PBT (persistent, bioaccumulative and toxic) and ED (endocrine disrupting) properties.

The study relies on a combination of five approaches. Approach 0 considers the reactivity of the relevant constituent groups to assess how likely they are to be converted in one of the relevant processes. Approach 1 relies on literature review to assess likelihood of the marker constituents being converted in the relevant process based on thermodynamic and other factors such as the presence of catalysts. Approach 2 modifies the results of Approach 1 by adding information collected through consultation for this study. Approach 3 further adds the dimension of supply chain interactions to screen out the products that are subject to high-temperature processes further downstream. Approach 4 takes an upstream perspective and includes a review of the literature on the presence of some of the relevant constituents in the relevant end-products. Each of these approaches has its advantages and disadvantages and, for this reason, the results of all five approaches are presented in the report.

In addition, the report provides an overview of the potential for the constituents that are not converted to be emitted into the environment.

Kurzbeschreibung: Zwischenprodukte aus Erdöl- und Kohlefraktionen

Die Studie beschreibt die Verwendung von 53 Erdöl- und Kohlenfraktionen (PetCo) als Zwischenprodukte und bewertet das Potenzial, dass ihre Konstituenten mit besorgniserregenden Eigenschaften innerhalb der Lieferkette und in die Umwelt übertragen werden. Die Studie konzentriert sich auf 15 Marker-Konstituenten, die auf der Grundlage eines Screenings der CMR- (krebserregend, erbgutverändernd, fortpflanzungsgefährdend), PBT- (persistent, bioakkumulierbar und toxisch) und ED-Eigenschaften (endokrinschädigend) in die engere Auswahl genommen wurden.

Die Studie verwendet eine Kombination aus fünf Ansätzen. Ansatz 0 berücksichtigt die Reaktivität der relevanten Konstituentengruppen, um zu beurteilen, wie wahrscheinlich es ist, dass sie in einem der relevanten Prozesse umgewandelt werden. Ansatz 1 stützt sich auf eine Literaturrecherche, um die Wahrscheinlichkeit zu bewerten, dass die Marker-Konstituenten in dem relevanten Prozess umgewandelt werden, und zwar auf der Grundlage thermodynamischer und anderer Faktoren wie dem Vorhandensein von Katalysatoren. Ansatz 2 modifiziert die Ergebnisse von Ansatz 1, indem er Informationen hinzufügt, die durch Befragung für diese Studie gesammelt wurden. Ansatz 3 fügt die Dimension der Interaktionen in der Lieferkette hinzu, um die Produkte herauszufiltern, die in nachgelagerten Prozessen hohen Temperaturen ausgesetzt sind. Ansatz 4 nimmt eine upstream Perspektive ein und umfasst eine Überprüfung der Literatur über das Vorhandensein einiger der relevanten Konstituenten in den jeweiligen Endprodukten. Jeder dieser Ansätze hat seine Vor- und Nachteile und aus diesem Grund werden die Ergebnisse aller fünf Ansätze in dem Bericht vorgestellt.

Darüber hinaus gibt der Bericht einen Überblick über das Potenzial der Konstituenten, die nicht umgewandelt werden, in die Umwelt freigesetzt zu werden.

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CMR	Carcinogenic, mutagenic, reprotoxic
COT	Tar, coal, high-temp
CTPHT	Coal tar pitch high temperature
ED	Endocrine disrupting
HFO	Heavy fuel oil component
LBO	Other Lubricant Base Oils
LOA	Lower Olefins and Aromatics REACH Consortium
R4CC	REACH for Coal Chemicals (R4CC) consortium
PAH	Polycyclic aromatic hydrocarbons
PBT	Persistent, bioaccumulative and toxic
PetCo	Petroleum and coal stream
PPE	Personal protection equipment
SMILES	Simplified molecular-input line-entry system
SPAC	Semi Polar Aromatic Compounds
SPERC	Specific Environmental Release Category
SRGO	Straight run gas oil
UATO	Unrefined / Acid Treated Oils
UVCBs	Substances of unknown and variable composition or biological origin
VHGO	Vacuum Gas Oils, Hydrocracked Gas Oils & Distillate Fuels
WWTP	Waste water treatment plant

Summary

Aims and objectives

The aims of the study are to describe the intermediate uses of substances from the petroleum and coal stream (PetCo) and assess the potential for their constituents with properties of concern to transfer within the supply chain and into the environment. This is particularly pertinent given that intermediate uses are exempt from many of the requirements of the REACH Regulation, being either onsite isolated intermediates or transported isolated intermediates.

PetCo substances typically consist of a variety of constituents and their precise composition can be unknown and variable. Under REACH, such substances are referred to as substances of unknown and variable composition or biological origin (UVCBs).

The study addresses the following key questions:

- whether PetCo constituents with potential properties of concern are formed, retained or converted during the relevant chemical reactions/processes;
- for the constituents with potential properties of concern that are not converted, whether they are still present in the final product(s) passed on within the supply chain and if there is a potential for their release to the environment; and
- whether information is provided down the supply chain for these constituents.

Study scope

The scope of this study comprises intermediate uses of 53 PetCo substances. A large number of constituents of these substances are reviewed in the study and the constituent groups and marker constituents of particular concern are shortlisted for further assessment (see Table S1). The selection is based on a screening of CMR (carcinogenic, mutagenic, reprotoxic), PBT (persistent, bioaccumulative and toxic) and ED (endocrine disrupting) properties.

Table S1: Shortlisted constituent groups and marker constituents

Constituent groups			Marker constituents	
Group	**Branched?**	**Carbon range**	**Name**	**CAS No.**
Polyaromatic	No	18-20	benzo[k]fluoranthene	207-08-9
			*benz[a]anthracene**	56-55-3
			*fluoranthene***	206-44-0
Triaromatic	No	14-16	*anthracene*	120-12-7
			*phenanthrene**	85-01-8
	Yes	15-16	1-methylphenanthrene	832-69-9
Biphenyls	Yes	16-18	diethylbiphenyl	28575-17-9
			*4-pentylbiphenyl**	7116-96-3

Constituent groups			Marker constituents	
Mono-aromatic	Yes	14-16	1,3,5-tripropylbenzene	15181-14-3
Naphthenic aromatics	Yes	14-17	2-methylfluorene	1430-97-3
	No	13-17	fluorene	86-73-7
Naphthenics (non aromatics)	Yes	18-21	2,4-dimethylheptyldecahydronaphthalene	N/A
Heavily branched Paraffins / Iso-Paraffins	Yes	12-14	2,3,4,5-Tetramethyldecane	N/A
			*3-methyltridecane**	6418-41-3
SPAC	No	13-16	dibenzofuran	132-64-9

Note: Ten marker constituents were shortlisted based on CMR (carcinogenic, mutagenic, reprotoxic), PBT (persistent, bioaccumulative and toxic) and ED (endocrine disrupting). Four further constituents (italicised and marked with an asterisk) were originally selected as back-up marker constituents for inclusion in the analysis should insufficient data be available for the ten main constituents. A further constituent (italicised and marked with two asterisks) was selected as a back-up in case insufficient data were available for the first back-up. Given that feedback was provided through consultation for this study for 15 constituents, five back-up constituents were included in the main analysis.

Assessment of the fate of the shortlisted constituents

In the first instance, this report carries out a high-level assessment of the fate of **the relevant constituent groups** (Approach 0), followed by four analytical approaches (three downstream and one upstream approach) that assess the fate of the shortlisted **marker constituents** (Approaches 1-4). The key features of these approaches are summarised below.

Table S2: Comparison of the key features of the five approaches

Approach	Focus	Direction	Data sources	Only intermediate uses?	Supply chain interactions considered?	Not only retention but also creation?
0	Groups	Downstream	Literature review	No	No	**Yes**
1	Markers	Downstream	Literature review	No	No	No
2	Markers	Downstream	Literature review & consultation	**Yes**	No	No
3	Markers	Downstream	Literature review & consultation	**Yes**	**Yes**	No
4	Markers	Upstream	Literature review	No	**Yes**	**Yes**

Each of these approaches has its advantages and disadvantages and, for this reason, the results of all five approaches are presented in this report and should be taken into account when drawing conclusions about the fate of the relevant constituents.

Approach 0: This approach provides a high-level assessment of the potential fate of the different constituent groups in the reaction unit by considering thermodynamic and kinetic reactivity of the relevant constituent groups. The presence of catalysts is not taken into account. The key advantage of Approach 0 is that it considers the potential for formation, not just pass-through.

Table S3: Approach 0 – fate of the different groups (thermodynamic/kinetic reactivity)

Constituent group	Conversion potential	Formation potential
Polyaromatic	No conversion likely	Potential of formation
Triaromatic branched	Conversion to non-branched form possible	Potential of formation
Triaromatic	No conversion likely	Potential of formation
Diaromatics branched	Conversion to non-branched form possible	Potential of formation
Mono-aromatic	Possible conversion	Potential of formation
Naphthenic aromatics, non-branched	Possible conversion	-
Naphthenic aromatics, branched	Conversion to non-branched form possible	-
Naphthenics (non aromatics)	Possible conversion	-
Heavily branched Paraffins/Iso-Paraffins	Conversion very likely	-
SPAC	Possible conversion	-

Under **Approach 1**, the likelihood of the constituents of potential concern being converted in the relevant process is assessed by comparing the characteristics of the marker constituents with the thermodynamic characteristics of the relevant process (temperature, pressure), whilst also taking into account other factors such as the presence of catalysts.

Under **Approach 2**, the results of Approach 1 are revised based on the information collected through consultation. First, uses not identified as intermediate by stakeholders and processes indicated as not currently in use are screened out. Second, conclusions made on the basis of literature review under Approach 1 are revised based on stakeholder input.

The interactions in the supply chain are considered in Approaches 3 and 4. **Approach 3** is a further development of Approach 2 that additionally screens out the products which are likely to be further processed by high-temperature processes such as combustion further downstream (e.g. in fuels, coke, metals and minerals production). **Approach 4** relies on an upstream assessment involving a literature review of the presence of the fifteen constituents of concern in key products.

Table S4 provides a comparison of the results of Approaches 1-4.

Table S4: Comparison of the results of Approaches 1-4

Approach	Substance-constituent-product-process combinations	Of which confirmed intermediate use	Likely present	Likely converted (at any stage in the supply chain)
Approach 1	689	Unknown	370	113
Approach 2	689	280	134	144
Approach 3	689	280	102	175
Approach 4	315 (potential constituent-product combinations)	Unknown	Excl. fuels and coke: 19 (present> 0.1 mg/kg) 43 (present) Incl. fuels and coke: 21 (present> 0.1 mg/kg) 52 (present)	240

Table S5 provides a comparison of the products in which constituents of concern were identified as potentially present under either Approach 3 or 4. Cells marked with ✓✓ show instances in which both Approaches 3 and 4 identified the potential presence of the constituent. Where only one approach identified the potential presence of the constituent, this is shown with a '✓2', '✓3' or '✓4' for the relevant approach – please note that all combinations identified under Approach 3 were also identified under Approach 2. Where neither approach identified the presence of a constituent, this is shown with a ✘. Please note that only product categories considered under Approach 4 are included in Table S5 and some additional product categories were considered under Approach 3 (e.g. anti-freeze, metal working fluids, heat transfer fluids, hydraulic fluids, substances, etc.).

Table S5: Results of Approaches 2, 3 and 4

	benzo[k]fluoranthene	benz[a]anthracene	Fluoranthene	Anthracene	Phenanthrene	1-methylphenanthrene	4-pentylbiphenyl	1,3,5-tripropylbenzene	2-methylfluorene	Fluorene	Dibenzofuran	2,4-dimethylheltyld	Diethylbiphenyl	2,3,4,5-tetramethyldec	3-methyldecane
Fuels	✓✓	✓✓	✓✓	✓✓	✓✓	✓4	✘	✓✓	✓4	✓✓	✓4	✘	✓ 2	✘	✘
Perfumes, fragrances, cosmetics & personal	✓4	✓4	✓4	✘	✓4	✘	✘	✘	✘	✘	✘	✘	✘	✘	✘

	benzo[k]fluoranthene	benz[a]anthracene	Fluoranthene	Anthracene	Phenanthrene	1-methylphenanthrene	4-pentylbiphenyl	1,3,5-tripropylbenzene	2-methylfluorene	Fluorene	Dibenzofuran	2,4-dimethylheltyldecane	Diethylbiphenyl	2,3,4,5-tetramethyldecane	3-methyldecane
care products															
Lubricants & Greases	✓4	✓4	✓4	✓4	✓4	✗	✗	✓3	✗	✓✓	✓4	✓3	✗	✓3	✓3
Adhesives & Sealants	✓4	✓4	✓4	✓4	✓✓	✗	✗	✗	✗	✓✓	✗	✓3	✗	✓3	✓3
Polishes & Waxes	✗	✗	✗	✗	✓✓	✗	✗	✗	✗	✓3	✗	✓3	✗	✓3	✓3
Coatings	✓4	✓4	✓4	✓4	✓✓	✗	✗	✗	✗	✓✓	✗	✓3	✗	✓3	✓3
Rubber Production & Processing	✓4	✓4	✓4	✓✓	✓✓	✗	✗	✓3	✗	✓✓	✗	✓3	✗	✗	✗
Plant Protection Products	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓4	✓3	✗	✗	✗
Agriculture, Forestry & Fishing	✓4	✓4	✓4	✓✓	✓✓	✓4	✗	✓3	✗	✓✓	✓4	✓3	✗	✗	✗
Coal tar fractions	✓✓	✓✓	✓✓	✓✓	✓✓	✓3	✗	✗	✓✓	✓✓	✓✓	✗	✗	✗	✗
Carbon black	✓✓	✓✓	✓4	✓4	✓4	✗	✗	✗	✗	✓4	✓3	✗	✗	✗	✗
Coke	✗	✗	✗	✗	✓4	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Graphite	✗	✗	✗	✓4	✗	✗	✓4	✗	✗	✓4	✗	✗	✗	✗	✗
Inks & Toners	✓4	✓4	✓4	✓✓	✓✓	✗	✗	✓3	✗	✓✓	✗	✓3	✗	✗	✗

There is some degree of agreement between the different approaches for some product categories, for example: fuels; coal tar fractions; agriculture, forestry and fishing; coal tar fractions; inks and toners, etc.. As regards specific constituents, the results of the approaches agree to the greatest degree for phenanthrene, fluorene, anthracene, benzo[k]fluoranthene and benz[a]anthracene. Interestingly, some of the information in the literature used for Approach 4 is not consistent with the predictions derived under Approaches 1-3 including for products which are derived using high temperature processes. However, the limitations of the literature used for Approach 4 (some older and non-EU studies and the fact that there is no indication that these are the result of intermediate use) should be borne in mind when comparing the results.

Zusammenfassung

Ziele und Aufgaben

Ziel der Studie ist es, die Verwendung als Zwischenprodukt von Stoffen aus Erdöl- und Kohlefraktionen (PetCo) zu beschreiben und das Potenzial zu bewerten, dass ihre Konstituenten mit besorgniserregenden Eigenschaften innerhalb der Lieferkette und in die Umwelt übertragen werden. Dies ist besonders wichtig, da Verwendungen als Zwischenprodukt (vor Ort isolierte oder transportierte isolierte Zwischenprodukte) von vielen Anforderungen der REACH-Verordnung ausgenommen sind.

PetCo-Stoffe bestehen in der Regel aus einer Vielzahl von Konstituenten und ihre genaue Zusammensetzung kann unbekannt und variabel sein. Unter REACH werden solche Stoffe als UVCBs bezeichnet (UVCB-Stoffe = substances of unknown and variable composition or biological origin).

Die Studie befasst sich mit den folgenden Schlüsselfragen:

- Werden PetCo-Konstituenten mit potenziell besorgniserregenden Eigenschaften während der relevanten chemischen Reaktionen/Prozesse gebildet, zurückgehalten oder umgewandelt?
- Sind die Konstituenten mit potenziell besorgniserregenden Eigenschaften, die nicht umgewandelt werden, in dem/den Endprodukt(en) vorhanden, die innerhalb der Lieferkette weitergegeben werden, und besteht die Möglichkeit, dass sie in die Umwelt gelangen?
- Werden den nachgeschalteten Akteuren Informationen zu diesen Konstituenten zur Verfügung gestellt?

Umfang der Studie

Der Umfang dieser Studie umfasst die Verwendung als Zwischenprodukte von 53 PetCo-Stoffen. Eine große Anzahl von Konstituenten dieser Stoffe wird in der Studie überprüft und die besorgniserregenden Gruppen von Bestandteilen und Marker-Konstituenten werden für die weitere Bewertung in die engere Auswahl genommen (siehe Tabelle S1). Die Auswahl basiert auf einem Screening der CMR- (krebserregend, mutagen, reproduktionstoxisch), PBT- (persistent, bioakkumulierbar und toxisch) und ED- (endokrinschädlich) Eigenschaften.

Tabelle Z1: Ausgewählte Gruppen und Marker-Konstituenten

Gruppen von Konstituenten			Marker-Konstituenten	
Gruppe	**Verzweigt?**	**Kohlenstoffe**	**Name**	**CAS Nummer**
Polyaromatisch	Nein	18-20	Benzo[k]fluoranthen	207-08-9
			*Benz[a]anthracen**	56-55-3
			*Fluoranthen***	206-44-0
Triaromatisch	Nein	14-16	Anthracen	120-12-7
			*Phenanthren**	85-01-8

Gruppen von Konstituenten			Marker-Konstituenten	
	Ja	15-16	1-Methylphenanthren	832-69-9
Biphenyle	Ja	16-18	Diethylbiphenyl	28575-17-9
			*4-Pentylbiphenyl**	7116-96-3
Monoaromatisch	Ja	14-16	1,3,5-Tripropylbenzol	15181-14-3
Naphthenische Aromaten	Ja	14-17	2-Methylfluoren	1430-97-3
	Nein	13-17	Fluoren	86-73-7
Naphthenische (nicht aromatische)	Ja	18-21	2,4-Dimethylheptyldecahydronaphthalin	N/A
Stark verzweigte Paraffine / Iso-Paraffine	Ja	12-14	2,3,4,5-Tetramethyldekan	N/A
			*3-Methyltridecan**	6418-41-3
SPAC	Nein	13-16	Dibenzofuran	132-64-9

Hinweis: Zehn Marker-Konstituenten wurden auf der Grundlage von CMR (krebserregend, erbgutverändernd, fortpflanzungsgefährdend), PBT (persistent, bioakkumulierbar und toxisch) und ED (endokrinschädigend) in die engere Auswahl genommen. Vier weitere Konstituenten (kursiv und mit einem Sternchen gekennzeichnet) wurden ursprünglich als Ersatzmarker ausgewählt, die in die Analyse aufgenommen werden sollten, falls für die zehn primär ausgewählten Konstituenten nicht genügend Daten zur Verfügung stehen. Ein weiterer Bestandteil (kursiv und mit zwei Sternchen markiert) wurde als Reserve ausgewählt, falls zudem nicht genügend Daten für die erste Reservekonstituenten zur Verfügung standen. Da im Rahmen der Konsultation für diese Studie Rückmeldungen zu allen 15 Konstituenten eingegangen sind, wurden die fünf Ersatzkonstituenten in die Hauptanalyse aufgenommen.

Bewertung des Umwandlungspotenzial ausgewählter Gruppen und Marker-Konstituenten

In diesem Bericht wird zunächst eine umfassende Bewertung des Verbleibs der relevanten **Konstituenten-Gruppen** vorgenommen (Ansatz 0), gefolgt von vier analytischen Ansätzen (drei ‚downstream' und ein ‚upstream' Ansatz), die den Verbleib der ausgewählten **Marker-Konstituenten** bewerten (Ansätze 1-4). Die wichtigsten Merkmale dieser Ansätze werden im Folgenden zusammengefasst.

Tabelle Z2: Vergleich der wichtigsten Merkmale der fünf Ansätze

Ansatz	Fokus	Richtung	Datenquellen	Nur Verwendung als Zwischen-produkte?	Lieferkette berücksichtigt?	Nicht nur Verbleib, sondern auch Bildung?
0	Gruppen	Downstream	Literatur-recherche	Nein	Nein	**Ja**
1	Marker	Downstream	Literatur-recherche	Nein	Nein	Nein
2	Marker	Downstream	Literatur-recherche & Konsuta-tionen	**Ja**	Nein	Nein

Ansatz	Fokus	Richtung	Datenquellen	Nur Verwendung als Zwischen-produkte?	Lieferkette berücksichtigt?	Nicht nur Verbleib, sondern auch Bildung?
3	Marker	Downstream	Literatur-recherche & Konsuta-tionen	**Ja**	**Ja**	Nein
4	Marker	Upstream	Literatur-recherche	Nein	**Ja**	**Ja**

Jeder dieser Ansätze hat seine Vor- und Nachteile. Aus diesem Grund werden in diesem Bericht die Ergebnisse aller fünf Ansätze vorgestellt und sollten berücksichtigt werden, wenn Schlüsse über das Verbleibspotenzial der relevanten Konstituenten gezogen werden.

Ansatz 0: Dieser Ansatz ermöglicht eine einfache Bewertung des potenziellen Verbleibs der verschiedenen Konstituenten-gruppen in der Reaktionseinheit, indem die thermodynamische und kinetische Reaktivität der relevanten Konstituenten-Gruppen berücksichtigt wird. Die mögliche Verwendung von Katalysatoren wird nicht in Betracht gezogen. Der Hauptvorteil von Ansatz 0 ist, dass er das Potenzial für die Bildung und nicht nur den Durchgang berücksichtigt..

Tabelle Z3: Ansatz 0 – Verbleib verschiedener Gruppen aufgrund thermodynamischer und kinetischer Reaktivität

Gruppe	Verbleibspotenzial	Bildungspotenzial
Polyaromatisch	Keine Umwandlung wahrscheinlich	Potenzial zur Bildung
Triaromatisch verzweigt	Umwandlung in eine nicht-verzweigte Form möglich	Potenzial zur Bildung
Triaromatisch	Umwandlung unwahrscheinlich	Potenzial zur Bildung
Diaromaten verzweigt	Umwandlung in eine nicht verzweigte Form möglich	Potenzial zur Bildung
Monoaromatisch	Umwandlung möglich	Potenzial zur Bildung
Naphthenische Aromaten, nicht verzweigt	Umwandlung möglich	-
Naphthenische Aromaten, verzweigt	Umwandlung in eine nicht verzweigte Form möglich	-
Naphthenische (nicht aromatische)	Umwandlung möglich	-
Stark verzweigte Paraffine/Iso-Paraffine	Umwandlung sehr wahrscheinlich	-
SPAC	Umwandlung möglich	-

Bei **Ansatz 1** wird die Wahrscheinlichkeit, dass die potenziell besorgniserregenden Marker-Konstituenten umgewandelt werden, bewertet, indem die Eigenschaften der Marker-Konstituenten mit den thermodynamischen Eigenschaften des betreffenden Prozesses (Temperatur, Druck) verglichen werden, wobei auch andere Faktoren wie die Verwendung von Katalysatoren berücksichtigt werden.

Bei **Ansatz 2** werden die Ergebnisse von Ansatz 1 auf der Grundlage der im Rahmen der Konsultation gesammelten Informationen überarbeitet. Erstens werden Verwendungen, die von den Interessenvertretern nicht als Zwischenprodukt-verwendungen eingestuft wurden, und Prozesse, die als derzeit nicht in Gebrauch befindlich angegeben wurden, ausgesondert. Zweitens werden die Schlussfolgerungen, die auf der Grundlage der Literaturrecherche unter Ansatz 1 gezogen wurden, auf der Grundlage der Beiträge der Interessengruppen überarbeitet.

Die nachgeschaltete Lieferketten werden in den Ansätzen 3 und 4 berücksichtigt. **Ansatz 3** ist eine Weiterentwicklung von Ansatz 2, bei der zusätzlich die Produkte herausgefiltert werden, die wahrscheinlich durch Hochtemperaturprozesse wie Verbrennung weiterverarbeitet werden (z.B. in Brennstoffen, Koks, Metallen und Mineralien). **Ansatz 4** stützt sich auf eine vorgelagerte Bewertung, die eine Literaturrecherche über das Vorhandensein der fünfzehn besorgniserregenden Konstituenten in den wichtigsten Produkten umfasst.

Tabelle Z4 enthält einen Vergleich der Ergebnisse der Ansätze 1-4.

Tabelle Z4: Vergleich der Ergebnisse der Ansätze 1-4

Ansatz	Kombinationen von Stoffen, Konstituenten, Produkten und Prozessen	Davon Verwendung als Zwischenprodukt	Verbleib wahrscheinlich	Wahrscheinlich umgewandelt (auch in der nachgeschalteten Lieferkette)
Ansatz 1	689	Nicht vorhanden	370	113
Ansatz 2	689	280	134	144
Ansatz 3	689	280	102	175
Ansatz 4	315 (mögliche Kombinationen von Konstituenten und Produkten)	Nicht vorhanden	Exkl. Brennstoffe und Koks: 19 (> 0.1 mg/kg) 43 (vorhanden) Inkl. Brennstoffe und Koks: 21 (> 0.1 mg/kg) 52 (vorhanden)	240

Tabelle Z5 enthält einen Vergleich der Produkte, in denen besorgniserregende Konstituenten entweder nach Ansatz 3 oder 4 als potenziell vorhanden eingestuft wurden. Die mit ✓✓ gekennzeichneten Zellen zeigen die Fälle, in denen sowohl bei Ansatz 3 als auch bei Ansatz 4 das potenzielle Vorhandensein des Konstituenten festgestellt wurde. Wenn nur ein Ansatz das potenzielle Vorhandensein des Konstituenten festgestellt hat, wird dies mit einer '✓2', '✓3' or '✓4' für den entsprechenden Ansatz angezeigt - bitte beachten Sie, dass alle unter Ansatz 3 identifizierten Kombinationen auch unter Ansatz 2 identifiziert wurden. Wenn keiner der beiden Ansätze das Vorhandensein eines Bestandteils identifiziert hat, ist dies mit einem ✘ gekennzeichnet. Bitte beachten Sie auch, dass in Tabelle Z5 nur Produktkategorien enthalten sind, die unter Ansatz 4 berücksichtigt wurden. Einige weitere Produktkategorien wurden unter Ansatz 3 berücksichtigt (z.B. Frostschutzmittel,

Metallbearbeitungsflüssigkeiten, Wärmeübertragungsflüssigkeiten, Hydraulikflüssigkeiten, Stoffe usw.).

Tabelle Z5: Ergebnisse der Ansätze 2, 3 und 4

	Benzo[k]fluoranthen	Benz[a]anthracen	Fluoranthen	Anthracen	Phenanthren	1-Methylphenanthren	4-Pentylbiphenyl	1,3,5-Tripropylbenzol	2-Methylfluoren	Fluoren	Dibenzofuran	2,4-Dimethylheltyldecan	Diethylbiphenyl	22,3,4,5-Tetramethyldekan	3-Methyldekan
Kraftstoffe	✓✓	✓✓	✓✓	✓✓	✓✓	✓4	✗	✓✓	✓4	✓✓	✓4	✗	✓ 2	✗	✗
Parfüms, Duftstoffe, Kosmetika und Körperpflegeprodukte	✓4	✓4	✓4	✗	✓4	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Schmierstoffe & Fette	✓4	✓4	✓4	✓4	✓4	✗	✗	✓ 3	✗	✓✓	✓4	✓ 3	✗	✓ 3	✓ 3
Klebstoffe & Dichtungsmittel	✓4	✓4	✓4	✓4	✓✓	✗	✗	✗	✗	✓✓	✗	✓ 3	✗	✓ 3	✓ 3
Polituren & Wachse	✗	✗	✗	✗	✓✓	✗	✗	✗	✗	✓ 3	✗	✓ 3	✗	✓ 3	✓ 3
Beschichtungen	✓4	✓4	✓4	✓4	✓✓	✗	✗	✗	✗	✓✓	✗	✓ 3	✗	✓ 3	✓ 3
Gummiherstellung und -verarbeitung	✓4	✓4	✓4	✓✓	✓✓	✗	✗	✓ 3	✗	✓✓	✗	✓ 3	✗	✗	✗
Pflanzenschutzmittel	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓4	✓ 3	✗	✗	✗
Landwirtschaft, Forstwirtschaft & Fischerei	✓4	✓4	✓4	✓✓	✓✓	✓4	✗	✓ 3	✗	✓✓	✓4	✓ 3	✗	✗	✗
Steinkohlenteer-Fraktionen	✓✓	✓✓	✓✓	✓✓	✓✓	✓ 3	✗	✗	✓✓	✓✓	✓✓	✗	✗	✗	✗
Ruß	✓✓	✓✓	✓4	✓4	✓4	✗	✗	✗	✗	✓4	✓ 3	✗	✗	✗	✗
Koks	✗	✗	✗	✗	✓4	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Graphit	✗	✗	✗	✓4	✗	✗	✓4	✗	✗	✓4	✗	✗	✗	✗	✗
Tinte & Toner	✓4	✓4	✓4	✓✓	✓✓	✗	✗	✓ 3	✗	✓✓	✗	✓ 3	✗	✗	✗

Bei einigen Produktkategorien besteht eine gewisse Übereinstimmung zwischen den verschiedenen Ansätzen, z.B. bei Kraftstoffen, Steinkohlenteerfraktionen, Land- und Forstwirtschaft und Fischerei, Tinten und Tonern usw. Was spezifische Konstituenten betrifft, so stimmen die Ergebnisse der Ansätze am stärksten bei Phenanthren, Fluoren,

Anthracen, Benzo[k]fluoranthen und Benz[a]anthracen überein. Interessanterweise stimmen einige der Informationen in der für Ansatz 4 verwendeten Literatur nicht mit den Ergebnissen der Ansätzen 1-3 überein, auch nicht für Produkte, die durch Hochtemperaturprozesse gewonnen werden. Die Einschränkungen der für Ansatz 4 verwendeten Literatur (einige ältere und nicht aus der EU stammende Studien und die Tatsache, dass es keinen Hinweis darauf gibt, dass das Vorhandensein der Konstituenten das Ergebnis der Verwendung als Zwischenprodukt von den 53 PetCo-Stoffen sind) sollten jedoch beim Vergleich der Ergebnisse berücksichtigt werden.

1 Introduction to the study

Background

Substances that are derived from Petroleum and Coal (PetCo) substances typically consist of a variety of constituents which can be unknown and vary in composition. These are referred to as substances of unknown and variable composition or biological origin (UVCBs). As UVCB substances are often not fully identifiable and therefore a description of the manufacturing process and other types of information, are used to identify them. For example, one such UVCB PetCo substance is Naphtha (petroleum), full-range straight-run (EC No: 4850-28-6; CAS No: 4850-28-6) which contains a variety of unknown substances such as tri-aromatic hydrocarbons and higher and Hydrocarbons, C56-60.

UVCB PetCo substances can consist of constituents that possess human health hazards (carcinogenic, mutagenic, reproductive) and/or possess hazards to the environment (Persistent, Bioaccumulate and Toxic (PBT) or very Persistent and very Bioaccumulative (vPvB)). Hydrocarbon constituents are typically of PBT concern. Parent Polycyclic Aromatic Hydrocarbons (PAHs) are confirmed PBT/vPvB, alkylated PAHs have potential PBT/vPvB properties, naphthenics are potential PBT/vPvB and iso-paraffins are also potential PBT/vPvB.

It is therefore important to understand the release of these constituents to both the environment and the supply chain. This is particularly relevant given that intermediates are exempt from many of the requirements under the REACH regulation.

Aims and objectives

The aims of the study are to describe the intermediate uses of substances from the petroleum and coal stream (PetCo) and assess the potential for their constituents with properties of concern to transfer within the supply chain and into the environment. This is particularly pertinent given that intermediate uses are exempt from many of the requirements of the REACH regulation, being either onsite isolated intermediates or transported isolated intermediates.

PetCo substances typically consist of a variety of constituents and their precise composition can be unknown and variable. Under REACH, such substances are referred to as substances of unknown and variable composition or biological origin (UVCBs).

The study addresses the following key questions:

- whether PetCo constituents with potential properties of concern are formed, retained or converted during the relevant chemical reactions/processes;
- for the constituents with potential properties of concern that are not converted, whether they are still present in the final product(s) passed on within the supply chain and if there is a potential for their release to the environment; and
- whether information is provided down the supply chain for these constituents.

Scope

The scope of this study comprises intermediate uses of 53 PetCo substances. A large number of constituents of these substances are reviewed in the study and the constituent groups and marker constituents of particular concern are shortlisted for further assessment. The

selection is based on a screening of CMR (carcinogenic, mutagenic, reprotoxic), PBT (persistent, bioaccumulative and toxic) and ED (endocrine disrupting) properties.

Approach

The study comprises three work packages: literature review, consultation via questionnaires and telephone interviews, and the mapping of the supply chain and life cycle of constituents of particular concern.

The analysis is divided into nine steps:

1. Step 0: Selection of 53 PetCo substances for assessment
2. Step 1: Determination of all the potential constituents of the 53 substances
3. Step 2: Determination of all the potentially relevant sectors/uses and processes
4. Step 3: Screening of the relevant constituents for potential properties of concern
5. Step 4: Prioritisation of constituent groups/marker constituents for detailed analysis
6. Step 5: Final shortlist of the relevant substance-constituent-process-product combinations
7. Step 6: Analysis of the fate of prioritised constituents (groups and markers) in the relevant processes (Approaches 1 and 2)
8. Step 7: Supply chain analysis and upstream analysis (Approaches 3 and 4)
9. Step 8: Overview of the potential for releases/environmental emissions

2 Step 0: Selection of substances within the scope of the study

Step 0 (preliminary step) involved selecting the substances analysed in the study. Originally, 50 substances were selected for the assessment and eight substances were designated as back-up substances that were to be included in the assessment should there be insufficient information for any of the 50 substances. Since most of the analysis has also been carried out for three of the additional eight substances, they have been included in this report. The 53 substances assessed in this study are listed in Table 1. This list, together with the remaining five back-up substances, is also provided in Annex 1. The substances have been put into general broad categories in the table based on their main grouping used by the various consortiums. The substances have been selected to cover a wide range of different PetCo substances with a high proportion of intermediate uses.

Table 1: Substances within the scope of the study

EC number	Substance name	Category	Consortium[1]
265-042-6	Naphtha (petroleum), full-range straight-run	Naphtha	Concawe
265-057-8	Residues (petroleum), vacuum	Bitumen	Concawe
265-058-3	Gas oils (petroleum), heavy vacuum	HFO	Concawe
265-059-9	Gas oils (petroleum), light vacuum	VHGO	Concawe
265-060-4	Distillates (petroleum), light catalytic cracked	Cracked GO	Concawe
265-064-6	Clarified oils (petroleum), catalytic cracked	HFO	Concawe
265-076-1	Residues (petroleum), hydrocracked	HFO	Concawe
272-341-5	Distillates (petroleum), full-range straight-run middle	SRGO	Concawe
265-055-7	Naphtha (petroleum), heavy catalytic cracked	Naphtha	Concawe
265-056-2	Naphtha (petroleum), light catalytic cracked	Naphtha	Concawe
265-183-3	Distillates (petroleum), hydrodesulfurized middle	Other GO	Concawe
269-777-3	Residues (petroleum), atmospheric	HFO	Concawe
271-267-0	Naphtha (petroleum), full-range alkylate, butane-contg.	Naphtha	Concawe
272-186-3	Naphtha (petroleum), unsweetened	Naphtha	Concawe
273-271-8	Naphtha (petroleum), catalytic reformed	Naphtha	Concawe
295-511-0	Residues (petroleum), catalytic cracking	HFO	Concawe
265-077-7	Distillates (petroleum), heavy hydrocracked	LBO	Concawe

[1] Consortium of companies for REACH compliance purposes.

EC number	Substance name	Category	Consortium[1]
270-675-6	Fuel oil, residual	HFO	Concawe
265-043-1	Gas oils (petroleum), straight-run	SRGO	Concawe
265-045-2	Residues (petroleum), atm. tower	HFO	Concawe
274-685-1	Distillates (petroleum), vacuum	HFO	Concawe
232-366-4	Kerosine (petroleum)	Kerosine	Concawe
265-184-9	Kerosine (petroleum), hydrodesulfurized	Kerosine	Concawe
265-084-5	Distillates (petroleum), light thermal cracked	Cracked GO	Concawe
265-096-0	Residual oils (petroleum), solvent deasphalted	LBO	Concawe
273-263-4	Distillates (petroleum), petroleum residues vacuum	HFO	Concawe
265-051-5	Distillates (petroleum), light paraffinic	UATO	Concawe
265-150-3	Naphtha (petroleum), hydrotreated heavy	Naphtha	Concawe
265-066-7	Naphtha (petroleum), full-range alkylate	Naphtha	Concawe
265-073-5	Naphtha (petroleum), isomerization	Naphtha	Concawe
265-071-4	Naphtha (petroleum), light hydrocracked	Naphtha	Concawe
265-193-8	Residues (petroleum), steam-cracked	G	LOA[2]
273-494-0	Benzene, ethylenated, residues	G	LOA
270-662-5	Distillates (petroleum), light steam-cracked naphtha	G	LOA
308-487-4	Aromatic hydrocarbons, dist. residues, naphthalene-rich	G	LOA
310-057-6	Residues (petroleum), steam-cracked light, arom.	H	LOA
295-311-3	Distillates (petroleum), naphtha steam cracking-derived, hydrotreated light arom.	H	LOA
271-726-5	Gasoline, pyrolysis, debutanizer bottoms	H	LOA
292-699-6	Aromatic hydrocarbons, C7-8, ethylene-manuf.-by-product	H	LOA
270-737-2	Distillates (petroleum), steam-cracked, C8-12 fraction	L	LOA
270-790-1	Naphtha (petroleum), light steam-cracked, debenzenized, C8-16-cycloalkadiene conc. (LOA Category L2-DCPD	L	LOA

[2] Lower Olefins and Aromatics REACH Consortium

EC number	Substance name	Category	Consortium[1]
265-099-7	Extracts (petroleum), heavy naphtha solvent	J	LOA
265-198-5	Solvent naphtha (petroleum), heavy arom.	J	LOA
266-028-2	Pitch, coal tar, high-temp.	-	R4CC3
266-024-0	Tar, coal, high-temp.	-	R4CC
266-027-7	Distillates (coal tar)	-	R4CC
283-483-2	Distillates (coal tar), light oils	-	R4CC
283-484-8	Distillates (coal tar), naphthalene oils	-	R4CC
292-607-4	Distillates (coal tar), heavy oils	-	R4CC
310-256-8	extract residues (coal tar), high-temperature, naphthalene oil alkaline, distn. overheads	-	R4CC
292-604-8	Anthracene oil, anthracene-low	-	R4CC
292-603-2	Anthracene oil, anthracene paste	-	R4CC
292-602-7	Anthracene oil	-	R4CC

HFO: Heavy fuel oil components, LBO: Other lubricants base oil, SRGO: Straight run gas oil, UATO: Unrefined/acid treated oils, VHGO: Vacuum Gas Oils, Hydrocracked Gas Oils & Distillate Fuels

[3] REACH for Coal Chemicals (R4CC) consortium

3 Step 1: Determination of all the potential constituents of the 53 substances

The next step involved the identification of all the potential constituents of the 53 substances. This was initially carried out on the basis of literature review that included the following sources:

- ECHA REACH registration dossiers and Annex XV dossiers[4];
- Concawe Substance Identification Group Analytical Program Report[5];
- LOA REACH Consortium Category Identity Profiles[6];
- 'REACH for Coal Chemicals (R4CC)' REACH UVCB Categories and Specifications[7]; and
- study team judgement/knowledge of the relevant substances/processes.

By analysing and extracting information from the information sources, the following tables were developed:

- Detailed information on the constituents of Concawe substances;
- Detailed information on the constituents of LOA substances;
- Detailed information on the constituents of R4CC substances; and
- Summary of Concawe substances, LOA substances, and R4CC substances: These tabs consist of the constituents of the substances (grouped), processes the substances undergo, uses (as per information available on the substances on the ECHA website) and products that these substances are used for. Three examples have been provided for Concawe substances, LOA substances, and R4CC substances.[8]

These tables are provided in Annex 2 (Constituents of the 53 substances).

A questionnaire-based consultation was carried out and the lists of the shortlisted constituents present in each of the substances (or potentially generated during intermediate use of each of the substances) were revised. The final list is presented in Section 6 (Step 5: Final shortlist of the relevant substance-constituent/process-product combinations).

[4] ECHA website, https://echa.europa.eu/information-on-chemicals (accessed in March and April 2020)
[5] Concawe (2019): Substance identification programme, available at https://www.concawe.eu/publication/concawe-substance-identification-group-analytical-program-report-abridged-version/ (accessed in March 2020)
[6] LOA REACH Consortium (undated): Categories, available at https://loa-reach.com/categories.html (accessed in March 2020)
[7] REACH for Coal Chemicals (R4CC) (undated): REACH UVCB Categories and Specifications, available at https://www.r4cc.org/index-Dateien/R4CC_UVCB.pdf (accessed in March 2020)
[8] The processes/uses/products in the report (and in the annexes) include both those resulting from intermediate and direct uses. Products resulting from direct use will be eliminated during the remainder of the study.

4 Step 2: Determination of all the potentially relevant sectors/uses and processes

Based on a review of the available literature, an overview was developed for the 53 substances agreed with UBA illustrating all potentially relevant uses, processes and products. Annex 3 (Uses, products and processes) provides tables for all identified uses, processes and products for the 53 substances.

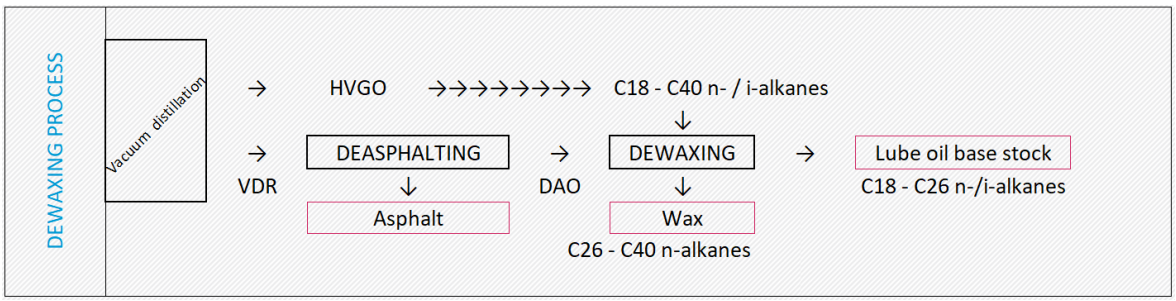
An example of the information on products and processes provided in Annex 3 is given in Table 2 for Naphtha (petroleum), full-range straight-run. The processes/uses/products in Annex 3 (and in the annexes) include both those resulting from intermediate and direct uses.

Table 2: Products and processes relevant to Naphtha (petroleum), full-range straight-run

EC number	Name	Products	Processes
265-042-6	Naphtha (petroleum), full-range straight-run	Fuels	Visbreaking
		Air care	Low octane number naphtha isomerisation
		Anti-freeze	Heavy low octane naphtha catalytic reforming
		Coating	Desulfurisation
		Lubricants & Greases	*Subject to various purification processes
		Washing & Cleaning	
		Welding & Soldering	

Annex 3 also provides an overview of the relevant process. An example is provided in Figure 1 for the dewaxing process.

Figure 1 Diagram of dewaxing



Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom (based on literature review)

The lists of potential uses and processes was further revised following consultation for this study, e.g. the products resulting from direct use were eliminated from further analysis. The revised lists are presented in Section 7 (Step 6).

5 Step 3: Screening of the relevant constituents for potential properties of concern

5.1 Screening of constituents for possible properties of concern

The SVHC criteria are given in Article 57 of the REACH Regulation. A substance or constituent may be proposed as an SVHC if it meets one or more of the following criteria:

- CMR properties: it is carcinogenic or mutagenic or toxic for reproduction;
- PBT properties: it is persistent, bio-accumulative and toxic according to the criteria set out in Annex XIII to the REACH Regulation;
- Mainly ED properties: there is "scientific evidence of probable serious effects to human health or the environment which give rise to an equivalent level of concern"; such substances are identified on a case-by-case basis. The "equivalent concern" criterion is significant because it is this classification which allows substances which are, for example, neurotoxic, endocrine-disrupting or otherwise present an unanticipated environmental health risk to be regulated under REACH.

The three criteria given above (CMR, PBT and ED) have been evaluated for the identified constituents. The main focus of the screening is the PBT criterion, however also the other criteria have been taken into account to identify priority constituents/constituent groups for more detailed fate and behavior analysis under this study.

5.1.1 Constituent identifiers/Constituent groups

The compositional data on the 53 substances from Section 2/Annex 2 resulted in an exhaustive and detailed list of constituents. Considering the complex chemistry of the PetCo substances, the compositional data was achieved by different analysis techniques, mostly in the area of GC analysis: PIONA analysis, DHA analysis, GCxGC analysis etc. This also has been described by Beens et al. (2000) and by CONCAWE in their substance identification analytical program (CONCAWE, 2019).

As a result of this, both direct (precise identification) and indirect (constituent group identification) information on the presence of the constituents is available:

- Direct **precise constituent identifier** information: a unique constituent identified by a CAS number, name or SMILES (**simplified molecular-input line-entry system**) notation; and
- Indirect constituent information, **constituent groups**: as a high number of specific constituents are present (typically >100 constituents) in one substance, the constituents are typically grouped during the reporting of the GC analyses. Examples of this are “C8 mono-aromatics” and “steranes”.

For the screening of the properties of concern via Quantitative Structure-Activity Relationship (QSAR)analysis, precise constituent information is required. For reporting purposes however, more high-level constituent group information is required to ensure readability. For assessment purposes, it is important to link the constituent specific

information with the more high-level information via the establishment of assessment groups and marker constituents.

5.1.1.1 Precise constituent identification determination

The GC analysis constituent group (such as "C8 mono-aromatics") provides an indication on the final constituent group and carbon number that will be used for the purposes of this report.

For QSAR, specific information up to the unique constituent level is required. To overcome this, two data sources have been consulted:

- the PETRORISK library (Redman et al., 2014): used to select specific marker constituents for each of the GC constituent groups; and
- Fingerprint biomarkers defined for crude oil and PetCo derivatives: used to select specific marker constituents for hopanes, steranes and asphaltenes.

Once precise constituent identification information has been derived, the following two activities were performed:

- Derivation of the corresponding constituent group (including presence of aromatics and/or branches) and carbon number (by analysis of the SMILES notation and expert judgement), see Chapter 4.1.1.2 below; and
- Identification of SMILES notation, CAS number (if available), IUPAC name and chemical structure by consulting the Pubchem library (NCBI, 2020), using the OECD QSAR Toolbox (OECD, 20215) and the "cirpy" Python script (NCI, 2015). The cirpy tool screens the US NCI (National Cancer Institute) database, which consolidates substance information from several US governmental departments.

5.1.1.2 Definition of constituent groups

In order to facilitate the screening of properties of concern, a number of constituent groups were defined and individual constituents were assigned to these groups. The following criteria were taken into account in the definition of constituent groups:

- The constituent group as indicated in the GC analysis;
- The constituent groups as used by CONCAWE in the HCB method (CONCAWE, 2019) and as indicated in the PETRORISK library. Those groups are similar to the groups as presented in the GC results; and
- The carbon number range: as detailed further below, the properties of concern can be directly linked to carbon number.

A refinement of constituent group identification was subsequently performed taking into account the following additional criteria:

- The presence of aromatics: constituents containing aromatic structure(s) typically show higher PBT potential
- The presence of branches: alkylated constituents show typically higher PBT potential

Following this exercise the following 13 constituent groups were defined:

- Polyaromatic: containing ≥ 4 aromatic rings
- Triaromatic: "branched" and "non branched" are reported separately.
- Diaromatic: "branched" and "non branched" are reported separately.
- Mono-aromatic
- Naphthenic aromatics: "branched" and "non branched" are reported separately.
- Naphthenic non aromatics: "branched" and "non branched" are reported separately.
- SPAC: Semi Polar Aromatic Compounds (containing N, O or S in the aromatic ring);
- Iso-Paraffins: saturated alkane containing 1 or 2 branches;
- Heavily branched paraffins: containing ≥ 3 branches;
- N-Paraffins;
- Olefins;
- Steranes; and
- Hopanes

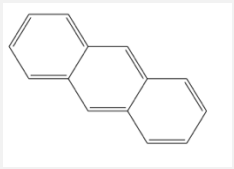
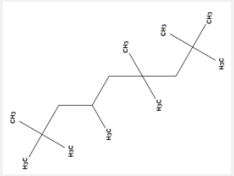
5.1.1.3 Specific considerations on iso-paraffins and heavily branched paraffins

In the results from the GC analysis of the substances, heavily branched paraffins have only been identified in a few cases as per Detailed Hydrocarbon Analysis (DHA), ASTM D6730-01 (ASTM, 2016). However, it should be noted that as of 3 to 4 branches, it typically becomes more difficult to separate heavily branched paraffins from aromatic constituents and less branched paraffins with similar carbon number due to very close retention times. It has indeed been observed that the total presence of alkylated paraffins can be underestimated by the DHA analysis (Kosal et al., 1990, Dunkle et al.,2019 and Santos et al., 2017). As such, as a worst-case assessment, the reported "ethyl/dimethyl" group in the GC results has been assumed as an indicator for the presence of heavily branched paraffins as well.

5.1.1.4 Final Constituent Library

The approaches described above have been combined, ensuring the data has been enriched to have both specific and grouping information available for each constituent. An example of the information available for both precise constituent identifiers and indirect constituent group identifiers is illustrated in Table 3 (Available data is indicated in underline/black. Enriched data is indicated in *italic/blue*).

Table 3: Example of the parameters per constituent as defined in the final constituent library

Parameter	Precise constituent identifier available	Constituent group identifier available
Name	**Anthracene**	***2,2,4,4,6,8,8-heptamethylnonane***
Chemical structure		
CAS Number	*120-12-7*	*4390-04-9*
SMILES	*c1ccc2cc3ccccc3cc2c1*	*CC(CC(C)(C)C)CC(C)(C)CC(C)(C)C*
Constituent Group	*Triaromatic, non branched*	Heavily branched paraffins
Carbon number	*14*	16

In total, 574 unique constituents (with carbon numbers in the range of C4-C32+) have been established, see Annex 4 (Constituents library) for a full overview. Figure 2 below summarises the presence of the constituents in the 50 substances per identified constituent group and carbon number range.

Figure 2 Maximum identified concentration (%w/w) of a constituent per carbon number / constituent group

Constituent Group	Branched	C nr																													
		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	#N/A	MAX
polyaromatic	NO												0.5	22.1	9.9	9.9		9.9		2.8		1.5									22.1
triaromatic	YES											15.0	1.9	5.0		3.8	2.4	1.2	0.5	1.3	0.4										15.0
triaromatic	NO											70.0		4.2																	70.0
diaromatic	YES					20.0			5.9	7.0	6.3	5.0	1.9	10.0	0.8	5.0	1.5	0.8	0.9	0.6	0.7	0.7	0.4								20.0
mono-aromatic	YES			40.0	40.0	20.0	24.0	15.0		5.0		1.1	1.2	1.2	1.3																40.0
naphthenic aromatics	YES						2.6	3.0	2.9	3.4	2.2	1.5	1.5	1.5	1.5	1.0	1.7	1.3	1.4	0.5		1.1	1.0	1.8	2.0	1.6	1.1	0.7			3.4
naphthenic aromatics	NO									9.9	45.0	15.0	4.0	3.0	0.7	0.7	0.5	0.7													45.0
naphthenics (non aromatics)	YES			7.8	13.7	15.0	2.9	5.9	2.1	4.6	1.4	1.5	1.1	1.0		0.7	1.6	1.5	1.8	1.2	1.4	3.6	4.6	5.9	5.3	3.4	3.6	2.9		18.4	18.4
SPAC	NO				19.9	0.0	0.1	0.1			30.0	0.0		0.0	4.9																30.0
heavily branched paraffin	YES					13.4	0.1	0.0					0.8	0.7	2.4	2.8		2.5				0.4	0.9	1.3	1.7	1.5	1.3	1.4			13.4
iso-Paraffins	YES			4.8	10.0	6.8	42.5	0.1					1.9	2.9			2.8		1.3	1.0	1.1	0.6		1.9	2.0	1.8	1.2	0.7			42.5
n-Paraffins	NO		20.0	10.0	5.0	5.0	8.9	6.8	7.6	4.9	2.6	1.7	2.2	2.3	2.2	1.8	1.4	1.4	65.0												65.0
olefins		5.0	10.0	1.0	0.4		0.0	40.0		5.0																					40.0
steranes																														2.0	2.0
hopanes																														2.0	2.0
MAX		5.0	20.0	40.0	40.0	20.0	42.5	40.0	7.6	9.9	45.0	70.0	4.0	22.1	9.9	9.9	2.8	9.9	65.0	2.8	1.4	3.6	4.6	5.9	5.3	3.4	3.6	2.9		18.4	70.0

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

The whole constituent library was screened for PBT, CMR and ED properties.

5.1.2 PBT screening

The constituents in the final constituent library have been screened on their PBT properties by reviewing inclusion in the REACH Annex XIV list and performing QSAR modelling by PROMETHEUS and PBT screening based on PETRORISK data. Results of PROMETHEUS and PETRORISK have been compared for further validation.

5.1.2.1 Inclusion in REACH Annex XIV list because of PBT properties

The constituent library (Annex 4) has been screened for their potential presence in the REACH Annex XIV list. The constituents that have been identified as relevant due to their PBT properties are discussed in Table 4. All these constituents also possessed a high PROMETHEUS score (see section 5.1.2.2 below for explanation), giving a first indication of the validity of this PBT screening model.

Table 4: Identified constituents present on REACH Annex XIV list for PBT properties

CAS number	Name	Constituent Group	Carbon nr	PROMETHEUS score
191-24-2	Fluoranthene	Polyaromatic	16	0.834
129-00-0	Pyrene	Polyaromatic	14	0.741
206-44-0	Benzo[k]fluoranthene	Polyaromatic	20	0.723
50-32-8	Anthracene	Polyaromatic	14	0.706
218-01-9	Benz[a]phenanthracene	Polyaromatic	16	0.702
85-01-8	Phenanthrene	Triaromatic	22	0.663
207-08-9	Benzo[a]pyrenebenzo [def]chrysene	Polyaromatic	20	0.648
56-55-3	Benz[a]anthracene	Polyaromatic	18	0.643
120-12-7	Chrysene	Triaromatic	18	0.639

5.1.2.2 PROMETHEUS

Running QSARs “blindly” can lead to a lot of wrong (false positive/false negative) results. Several studies show that depending on the chemical of interest one predictive model may be appropriate but changing the target chemical a different model may be more appropriate. This is a well-known issue, related to the so-called applicability domain of the model. PROMETHEUS is using a multiple criteria decision making (MCDM) method model for the PBT/vPvB parameters, ensuring that the applicability domain is respected (UBA, Benfenati et al., 2016).

Table 5 gives an overview of the reported parameters and the QSARs/datasets used for prediction via the MCDM method.

Table 5: Overview of datasets and QSARs as used by PROMETHEUS

Criterion	Datasets (used for defining applicability domain of QSARs)	QSARs
P	Literature, ANTARES EC project*, OECD QSAR toolbox database	SARpy****, IstChemFeat**

Criterion	Datasets (used for defining applicability domain of QSARs)	QSARs
Log Kow	Experimental data from REACH dossiers (CALEIDOS project)***, VEGA databases****	ALog P1.0.0, VlogP1.0.0; VEGA KOWWIN****, EPA KOWWIN, EpiSuite******
B	ANTARES project*	
T	ANTARES*, MED-Duluth (available at EPA)*****, ECHA CHEM database (CALEIDOS, OECD QSAR Toolbox)	ECOSAR*****, T.E.S.T., VEGA v 1.0.8 – Fathead minnow LC50 96 hr (EPA) v 1.0.6, VEGA v 1.0.8 – Fish LC50 classification v 1.0.1, Fish Toxicity k-NN/Read-Across model (In-house/VEGA)****

*(ANTARES EC, 2011), ** (Kode Chemo Informatics, 2015), *** (CALEIDOS EC, 2015), **** (VEGA, 2013), ***** (US EPA, 2012)

Based on a workflow approach, constituents are scored and normalised with a value from 0 (low) to 1 (high) for the P, B, T criterion separately and for the combined PBT/vPvB screening. In this scoring, the reliability of the result has also been taken into account. With a low reliability (and thus with high uncertainty) all values tend towards the 0.5 value, while with higher reliability, constituents can be better distinguished on the basis of the property value.

All 574 constituents have been evaluated by PROMETHEUS (see Annex 6, Prometheus results). Hereby, the identified SMILES notation has been used as input. In total, 352 constituents were scored with >=0.5. These results are summarised in Figure 3.

Besides the notable difference amongst the constituent groups (Polyaromatic group scoring the highest, n-Paraffins scoring low), another general trend can also be observed. The PROMETHEUS score increases as the carbon number increases until C16-20 after which it decreases again for the longer constituents.

Figure 3: PROMETHEUS maximum score per constituent group/ carbon number

Constituent Group	Branched	Carbon nr																													
		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	#N/A	MAX
polyaromatic	NO												0.66	0.83	0.72	0.65	0.56	0.72		0.69		0.57										0.83
triaromatic	YES									0.50		0.61	0.72	0.66		0.58	0.57	0.62	0.55	0.60	0.57	0.55	0.61	0.63	0.60	0.60	0.60	0.60	0.41			0.72
triaromatic	NO										0.65	0.74		0.66																		0.74
diaromatic	YES					0.50		0.55	0.58	0.55	0.62	0.63	0.57	0.80	0.76	0.61	0.63	0.63	0.63	0.56	0.63	0.63	0.41	0.63								0.80
mono-aromatic	YES				0.31	0.31	0.52	0.54	0.57	0.59	0.63	0.65	0.69	0.66	0.60																	0.69
naphthenic aromatics	YES						0.48	0.52	0.56	0.60	0.61	0.66	0.64	0.60	0.65	0.64	0.67	0.62	0.56	0.54		0.49	0.50	0.58	0.57	0.47	0.57	0.57			0.67
naphthenic aromatics	NO									0.64	0.60	0.62	0.63	0.64	0.63	0.60	0.57															0.64
naphthenics (non aromatics)	YES				0.27	0.46	0.42	0.45	0.48	0.50	0.51	0.50	0.65	0.52	0.60	0.67	0.69	0.61	0.67	0.61	0.50	0.49	0.48	0.41	0.41	0.40	0.39	0.40	0.39	0.39		0.69
SPAC	NO				0.23	0.20	0.50	0.26			0.64	0.38		0.63	0.61																0.36	0.64
heavily branched paraffin	YES		0.53			0.56	0.61	0.63	0.66	0.69	0.67	0.70	0.64	0.54	0.54	0.52		0.50				0.47	0.46	0.46	0.45	0.45	0.45	0.45				0.70
iso-Paraffins	YES	0.39	0.57	0.55	0.55	0.58	0.65	0.64	0.66	0.67	0.64	0.69	0.63	0.56			0.51		0.50	0.49	0.48	0.47		0.46	0.45	0.45	0.45	0.45				0.69
n-Paraffins	NO	0.38	0.37	0.36	0.40	0.44	0.44	0.44	0.41	0.46	0.41	0.47	0.38	0.70	0.38	0.37	0.36	0.36	0.35	0.34	0.34	0.33	0.33	0.32	0.32	0.32	0.32	0.32				0.70
olefins		0.33	0.41	0.55	0.54		0.63	0.55		0.65																						0.65
steranes																															0.54	0.54
hopanes																															0.60	0.60
MAX		0.39	0.57	0.55	0.55	0.58	0.65	0.64	0.66	0.69	0.67	0.74	0.72	0.83	0.76	0.67	0.69	0.72	0.67	0.69	0.63	0.63	0.61	0.63	0.60	0.60	0.60	0.60	0.41	0.39	0.60	0.83

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

5.1.2.3 PETRORISK library derived PBT screening

PETRORISK is a spreadsheet-based tool developed for performing environmental risk assessment for petroleum substances using principles provided by ECHA for fulfilling stakeholder obligations under EU REACH (Redman et al., 2014). It is designed to evaluate environmental exposure and ecological risks at both local and regional scales for a wide

range of petroleum products from naphtha (gasoline), kerosene, gas oils, to heavy fuel, lubricant oils, etc.

Physical-chemical properties for the various hydrocarbon blocks (high or low resolution) are derived from a library of chemical properties for individual representative structures that are derived from basic structure types typically found in petroleum. All the chemical properties except for sub-cooled liquid solubility, but including Henry's Law Constant (HLC), log Kow, molecular volume, boiling point, chemical class and molecular weight have been estimated using EPIWIN/HCBIOWIN (US EPA, 2012). The subcooled liquid solubility is estimated from SPARC v4.2 (May 2008), an on-line program that computes physical-chemical properties from chemical structure (Karickhoff et al., 1991). This library from PETRORISK has been used to perform PBT screening for the selected petroleum constituents using the PBT criteria as described in the ECHA Guidance R.11.

Overall, a relatively high degree of similarity between PROMETHEUS and PETRORISK library derived PBT screening was observed.

Only for the iso paraffins, PETRORISK clearly shows lower PBT screening compared to PROMETHEUS. See comparison in Figure 4 for 21 isomers of a C14 alkane.

As expected, the tetramethyl (4 branches) isomers score the highest with PROMETHEUS and actually mainly indicate the vPvB criterion. EPIWIN/HCBIOWIN does not indicate P for those isomers.

The isomers with one methyl or one 1 ethyl branch also have a high (almost similar) score with PROMETHEUS, here because of indications of the PBT criterion. EPIWIN/HCBIOWIN does not indicate P for those isomers.

Given that PROMETHEUS takes into account the applicability range and reliability of several underlying QSARS via a workflow approach, the PROMETHEUS results and screening have remained as final conclusion for the scope of this project. It has indeed already been confirmed by Rorije et al. (2012) that EPIWIN/HCBIOWIN typically underestimates half-lives for branched petroleum constituents. A comparison of PBT screenings in PROMETHEUS and HCBIOWIN is provided in Figure 4.

Figure 4: Comparison of PBT screening PROMETHEUS versus HCBIOWIN (as in PETRORISK)

P	B	T
P/vP	B	T
not P	vB	potentially T

Prometheus								HCBIOWIN v4.00 sediment HL	
SMILES	branches	LogKow	P	B (log BCF)	T	score PBT	score vPvB	h	P
CCCCCC(C)C(C)C(C)C(C)C	4	6.43	P/vP	3.69	0.03	0.704	0.743	2091	not P
CCC(C)CC(C)CC(C)CC(C)C	4	6.43	P/vP	3.67	0.03	0.702	0.74	2091	not P
CCCCCCCCCC(CC)CC	1	6.85	P/vP	3.46	0.009	0.694	0.705	1369	not P
CCCCCCCCCCC(C)CC	1	6.85	P/vP	3.46	0.009	0.694	0.705	1369	not P
CCCCCCCCCCC(C)CC	1	6.85	P/vP	3.46	0.009	0.694	0.705	1369	not P
CCCCCCCCCCCC(C)C	1	6.85	P/vP	3.46	0.009	0.694	0.705	1369	not P
CCCCC(CCC)CC(C)CCC	2	6.71	P/vP	3.28	0.035	0.644	0.667	1576	not P
CCCCCCC(CC)CC(C)CC	2	6.71	P/vP	3.26	0.035	0.642	0.664	1576	not P
CCCCC(CC)CCCC(C)CC	2	6.71	P/vP	3.25	0.035	0.64	0.661	1576	not P
CCCCCCCC(C)CCC(C)C	2	6.71	P/vP	3.25	0.035	0.639	0.66	1576	not P
CCCCCCC(C)CCCC(C)C	2	6.71	P/vP	3.25	0.035	0.639	0.66	1576	not P
CCCC(C)CCCC(CC)CCC	2	6.71	P/vP	3.25	0.035	0.639	0.66	1576	not P
CCCCCCCCCC(C)C(C)C	2	6.71	P/vP	3.24	0.035	0.638	0.658	1576	not P
CCCCCCCCC(C)CC(C)C	2	6.71	P/vP	3.24	0.035	0.638	0.659	1576	not P
CCCCCC(CC)CC(C)C(C)C	3	6.57	P/vP	3.15	0.039	0.62	0.637	1815	not P
CCCCCC(C)CC(C)CC(C)C	3	6.57	P/vP	3.14	0.039	0.617	0.634	1815	not P
CCCCCCCC(C)C(C)C(C)C	3	6.57	P/vP	3.14	0.039	0.616	0.633	1815	not P
CCCCCCC(C)CC(C)C(C)C	3	6.57	P/vP	3.14	0.039	0.616	0.633	1815	not P
CCCC(C)CCCC(C)CC(C)C	3	6.57	P/vP	3.12	0.039	0.614	0.629	1815	not P
CC(C)CCCC(C)CCCC(C)C	3	6.57	P/vP	3.13	0.039	0.614	0.63	1815	not P
CC(C)CCCCCC(C)CC(C)C	3	6.57	P/vP	3.12	0.039	0.613	0.628	1815	not P

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

Please note that only a lower tier[9] PBT screening was carried out when using the PETRORISK library data. Within the current lower tier PBT screening, compartment specific half-life information is used to decide whether or not the "P" criteria is fulfilled, independently of the compartment in which the chemical predominantly resides. In doing so, "P" decisions may be conservative and potentially inappropriate. According to ECHA guidance R11, fate information can be used, in a higher tier, to identify specific environmental compartment(s) of concern, and as such, may be used as supporting information as weight of evidence (WoE) under the PBT assessment (see scheme Figure R.11-3 in ECHA R11 Guidance).

5.1.3 CMR screening

5.1.3.1 CMR classification screening

The ECHA C&L Inventory has been screened for applicable CMR classifications of the constituents. When available, harmonized classifications are reported, else the classifications based on joint entries or the highest number of notifiers are indicated.

Herewith the H-phrases given in Table 6 have been used as indicator for CMR.

Table 6 CMR indication CLP H-phrases

H-phrase	Description
H340	May cause genetic defects

[9] For more information on a tiered PBT approach, please see ECHA R.11 guidance.

H-phrase	Description
H341	Suspected of causing genetic defects
H350	May cause cancer
H351	Suspected of causing cancer
H360	May damage fertility or the unborn child
H361	Suspected of damaging fertility or the unborn child
H361d	Suspected of damaging the unborn child

The complete constituent classification, including the CMR classification, has been collected for the constituents for which a CAS number was identified (310 constituents). This is included in Annex 7 (ED CMR classification screening). Some substances are not classified, some are classified but not for CMR properties while others are also classified for CMR.

5.1.3.2 OECD QSAR Toolbox screening

The complete constituent library has been screened for CMR properties by using the freely available OECD QSAR toolbox (v4.3.1) (OECD, 2015). In addition, 25 selected constituents (covering all constituent groups) were further evaluated by performing chemical profiling. A chemical category is a group of chemicals whose, in this case, carcinogenic, mutagenic and/or reprotoxic properties are likely to be similar or follow a regular pattern, usually as a result of structural similarity. The following grouping and profiling methods (see Table 7 below) in the OECD QSAR Toolbox have been used to rank the substances.

Table 7 Summary of the Grouping Methods in the OECD QSAR Toolbox

Summary of the Grouping Methods in the OECD QSAR Toolbox	
Grouping Method	**Description**
DNA Binding by OECD	This grouping method contains categories or chemical methods of DNA binding. The profiler was created following the mapping of existing structural alerts for mutagenicity and carcinogenicity.
DNA Binding by OASIS	This grouping method contains categories or chemical methods of DNA binding. This method is particularly relevant for genotoxicity endpoints.
in vitro mutagenicity (Ames test) developed by ISS (Istituto Superiore di Sanita)	This profiler is based on the Mutagenicity/Carcinogenicity module of the software Toxtree. It works as a decision tree for estimating in vitro (Ames test) mutagenicity, based on a list of 30 structural alerts (SAs). The SAs for mutagenicity are molecular functional groups or substructures known to be linked to the mutagenic activity of chemicals.
Oncologic Primary Classification	This grouping method is based on structural criteria of chemical classes of potential carcinogens.
Carcinogenicity (genotox and non-genotox) alerts by ISS	This profiler is an expanded and updated version of the correspondent module of the software Toxtree. It works as a decision tree for estimating carcinogenicity, based on a list of 55 structural alerts (SAs)
in vivo mutagenicity (Micronucleus) alerts by ISS	These structural alerts are molecular functional groups or substructures that are known to be linked to the induction of effects in the in vivo micronucleus assay.

These profiles have been selected based on their potential to differentiate between the different chemicals and obtain different results.

Following the chemical profiling, the OECD QSAR toolbox provides one of the following results for each chemical profile (see Table 8 below).

Table 8: Potential chemical profiling results available from the OECD QSAR toolbox

Grouping Method	Potential result 1	Potential result 2	Potential result 3
DNA Binding by OECD	SN1 >> Carbenium Ion Formation >> Polycyclic (PAHs) and heterocyclic (HACs) aromatic hydrocarbons-SN1	Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes	No alert
DNA Binding by OASIS	SN2 >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polycyclic Aromatic Hydrocarbon	SN1 >> Alkylation after metabolically formed carbenium ion species >> Polycyclic Aromatic Hydrocarbon and Naphthalenediimide Derivatives;	Non-covalent interaction >> DNA intercalation >> Polycyclic Aromatic Hydrocarbon
in vitro mutagenicity (Ames test) alerts by ISS	Polycyclic Aromatic Hydrocarbons	Heterocyclic Polycyclic Aromatic Hydrocarbons	No alert
Oncologic Primary Classification	Polycyclic Aromatic Hydrocarbons – Homocyclic	No alert	/
Carcinogenicity (genotox and nongenotox) alerts by ISS	Polycyclic Aromatic Hydrocarbons (Genotox);	Heterocyclic Polycyclic Aromatic Hydrocarbons (Genotox);	No alert
in vivo mutagenicity (Micronucleus) alerts by ISS	Polycyclic Aromatic Hydrocarbons	Heterocyclic Polycyclic Aromatic Hydrocarbons	No alert

As a conclusion following chemical structures are highlighted for potential CMR properties:

- the presence of Aromatic rings (alert) or the absence of these (no alert).
- The presence of Heterocyclic Aromatic Hydrocarbons (i.e. SPAC constituent group) or the absence of these (no alert).

5.1.3.3 Summary – CMR Screening of the Constituent Library

A scoring mechanism has been applied to summarise the CMR screening as follows:

- In case CMR classification is applicable to a specific constituent a score of 1 is given to the respective constituent group/carbon number combination
- In case the constituent group has been identified by chemical profiling in the OECD QSAR Toolbox a score of 0.5 has been given to the respective group. If the constituent

group/carbon number combination already was indicated by CMR classification, the score of 1 is remained.

The maximum CMR score per constituent group/carbon number is indicated in the last column in Figure 5 below.

Figure 5 Maximum CMR score per constituent group/carbon number

Constituent Group	Branched	Carbon nr																													
		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	#N/A	MAX
polyaromatic	NO											0.5	0.5	0.5	0.5	1.0		1.0		1.0		1.0										1.0
triaromatic	YES									0.5		0.5	1.0	0.5		0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5			1.0
triaromatic	NO										0.5	0.5		0.5																		0.5
diaromatic	NO					0.5		0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5								0.5
mono-aromatic	YES			1.0	1.0	1.0	1.0	0.5	1.0	0.5	0.5	0.5	0.5	0.5	0.5																	1.0
naphthenic aromatics	YES						0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5		0.5	0.5	0.5	0.5	0.5	0.5	0.5				0.5
naphthenic aromatics	NO									0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5															
naphthenics (non aromatics)	YES			1.0																												1.0
SPAC	NO				0.5	0.5	0.5	1.0			1.0	0.5		0.5	0.5																		1.0
heavily branched paraffin	YES																															
iso-Paraffins	YES	1.0																														1.0
n-Paraffins	NO	1.0		1.0																												1.0
olefins		1.0	1.0																													1.0
steranes																																
hopanes																																
MAX		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	1.0	0.5	1.0	0.5	0.5	1.0	0.5	1.0	0.5	1.0	0.5	1.0	0.5	0.5	0.5	0.5	0.5	0.5	0.5			1.0

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

5.1.4 ED screening

The constituent library has been automatically screened using the ED screener tool (ARCHE and Chemycal, 2020) for presence in several existing EU programs and endocrine disruptor properties related databases (Candidate list of SVHCs, EU priority list of potential EDs, other international review programs, CLP classification of Repr Tox or STOT-RE). For this screening, only constituents for which a CAS number is available (310 constituents) could be screened, as this is required minimum input for using the tool. This screening approach is based upon the stepwise approach for a targeted determination of ED indications of co-formulants in biocidal products, as developed by the respective competent authorities (EC Biocides Coordination Group, 2019).

Based on this screening, none of the constituents have been highlighted as having known ED properties, although several are classified as toxic to reproduction (see Annex 7). Consequently, no further activities specifically for ED have been performed, as this seems not to be a deciding parameter in the final selection and CMR classification is already covered.

6 Step 4: Prioritisation of constituent groups/marker constituents for detailed analysis

A scoring methodology has been applied to perform the screening for the selection of priority constituent groups and their representing marker constituents.

- The PROMETHEUS PBT score has been used as a first decisive parameter. In case of similar PBT score, preference has been given for
  - constituents that were included lately on the ANNEX XIV list in case of similar PBT score.
  - inclusion of larger polyaromatic constituents in order to enable differentiation versus triaromatics in the behavior and fate modelling
  - inclusion of alkylated (branched and heavily branched) constituents in case of similar PBT score.
- The suspected presence of the constituent in the substance has been used as a next decisive parameter (see Annex 5). Due to the overlapping nature of the iso-paraffins group (all heavily branched paraffins are iso-paraffins), both iso-paraffins and heavily branched paraffins haven been combined into one group.
- After evaluation of the two parameters above a further refinement has been performed by using the CMR score as explained above. In case of similar PBT score and presence, preference has been given to constituents with highest CMR score.

The details of the actual selection, including the PBT score, presence identification and CMR score can be found in Annex 8 (SVHC screening). Figure 6 presents the final priority list of constituent groups and their represented marker constituent (Final short list provided in Annex 9).

Figure 6 Priority constituent group and representing marker constituents

Selected Constituent groups			Marker					
Constituent group	Branched	Carbon range	Marker CAS	Marker Name	PBT score	Presence	CMR score	Prometheus
polyaromatic	NO	18-20	207-08-9	benzo[k]fluoranthene	1	1	0.5	0.723
triaromatic	NO	14-16	120-12-7	anthracene	1	1	0.5	0.706
triaromatic	YES	15-16	832-69-9	1-methylphenanthrene	1	1	1	0.673
biphenyls	YES	16-18	28575-17-9	diethylbiphenyl	1	1	0.5	0.795
mono-aromatic	YES	14-16	15181-14-3	1,3,5-tripropylbenzene	1	1	1	0.686
naphthenic aromatics	YES	14-17	1430-97-3	2-methylfluorene	1	1	0.5	0.66
naphthenic aromatics	NO	13-17	86-73-7	Fluorene	1	1	0.5	0.656
naphthenics (non aromatics)	YES	18-21	N/A	2,4-dimethylheptyldecahydronaphthalene	1	1		0.69
Heavily branched Paraffins / Iso-Paraffins	YES	12-14	N/A	2,3,4,5-Tetramethyldecane	1	1		0.704
SPAC	NO	13-16	132-64-9	dibenzofuran	1	1	0.5	0.642

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

Back-up markers have been identified for some of the groups, which can be used in the behavior and fate assessment when no data can be generated for the primary markers. These are given in Figure 7.

Figure 7 Priority constituent group and back-up marker constituents

Selected Constituent groups			Back-up Marker (1)			Back-up Marker (2)		
Constituent group	Branched	Carbon range	Marker CAS	Marker Name	Prometheus	Marker CAS	Marker Name	Prometheus
polyaromatic	NO	18-20	56-55-3	benz[a]anthracene	0.603	206-44-0	Fluoranthene	0.834
triaromatic	NO	14-16	85-01-8	phenantrene	0.741			
triaromatic	YES	15-16	832-64-4	4-methylphenanthrene	0.654			
biphenyls	YES	16-18	7116-96-3	4-pentylbiphenyl	0.758			
mono-aromatic	YES	14-16						
naphthenic aromatics	YES	14-17						
naphthenic aromatics	NO	13-17						
naphthenics (non aromatics)	YES	18-21						
Heavily branched Paraffins / Iso-Paraffins	YES	12-14	6418-41-3	3-methyltridecane	0.694			
SPAC	NO	13-16						

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

In addition, a narrow carbon number range has been identified for each constituent. As explained above, the PBT score for each constituent group increases with carbon number until a "plateau" is reached and then decreases again with higher carbon number. The indicated range represents the 'plateau' for each constituent group.

The final shortlist of constituents for more detailed analysis in this study is presented below. In addition to the ten marker constituents in Figure 6, four further constituents (italicised and marked with an asterisk) which were originally selected as back-up marker constituents in Figure 7 were also included in the core analysis. A further constituent (italicised and marked with two asterisks) was selected in Figure 7 as a back-up in case insufficient data were available for the first back-up. Given that feedback was provided through consultation for this study for most of these back-up constituents, a total of 15 constituents were included in the main analysis.

Table 9: Shortlisted constituent groups and marker constituents

Constituent groups			Marker constituents	
Group	**Branched?**	**Carbon range**	**Name**	**CAS No.**
Polyaromatic	No	18-20	benzo[k]fluoranthene	207-08-9
			*benz[a]anthracene**	*56-55-3*
			*fluoranthene***	*206-44-0*
Triaromatic	No	14-16	anthracene	120-12-7
			*phenanthrene**	*85-01-8*
	Yes	15-16	1-methylphenanthrene	832-69-9
Biphenyls	Yes	16-18	diethylbiphenyl	28575-17-9
			*4-pentylbiphenyl**	*7116-96-3*
Mono-aromatic	Yes	14-16	1,3,5-tripropylbenzene	15181-14-3
Naphthenic aromatics	Yes	14-17	2-methylfluorene	1430-97-3
	No	13-17	fluorene	86-73-7

Constituent groups			**Marker constituents**	
Naphthenics (non aromatics)	Yes	18-21	2,4-dimethylheptyldecahydronaphthalene	N/A
Heavily branched Paraffins / Iso-Paraffins	Yes	12-14	2,3,4,5-Tetramethyldecane	N/A
			*3-methyltridecane**	*6418-41-3*
SPAC	No	13-16	dibenzofuran	132-64-9

7 Step 5: Final shortlist of the relevant substance-constituent-process-product combinations

7.1 Introduction

The lists of the relevant uses/processes/products and constituents relevant to each of the 53 substances were revised taking into account the information received during the consultation. The revised lists are presented below. The final shortlist is also provided in Annex 9.

7.2 Revised list of substance-constituent combinations

Some of the consultees provided comments on the presence of the 15 prioritised constituents in the 53 substances within the scope of this study. The revised list is presented below where substance/constituent pairings that have been confirmed as not relevant are indicated by NR (not relevant) in the conclusion column. Constituents whose presence has been confirmed are indicated by PC (presence confirmed) in the conclusion column. The constituents for which the conclusions remain to be primarily based on literature review suggests are marked as LR (Literature review) in the conclusion column and applies to all constituents in that cell. Where some constituents within a cell are highlighted in **bold** in a PC cell, it means that they were not confirmed by stakeholder consultation (and thus remain LR).

Table 10: The presence of the 15 prioritised constituents in the 53 PetCo substances

Category	Substance	Conclusion	Constituents
Naphtha	Naphtha (petroleum), full-range straight run	LR	Monoaromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3)
Naphtha	Naphtha (petroleum), heavy catalytic cracked	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Naphtha	Naphtha (petroleum), light catalytic cracked	LR	Mono- and Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3) (1,3,5-tripropylbenzene, CAS No 15181-14-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Naphtha	Naphtha (petroleum), full-range alkylate, butane-contg.	LR	Naphthenics (2,4-dimethylheptyldecahydronaphthalene)

Category	Substance	Conclusion	Constituents
Naphtha	Naphtha (petroleum), unsweetened	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9)
Naphtha	Naphtha (petroleum), catalytic reformed	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Naphtha	Naphtha (petroleum), hydrotreated heavy	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Naphtha	Naphtha (petroleum), full-range alkylate	LR	Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3) Iso-paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Naphtha	Naphtha (petroleum), isomerization	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Iso-paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Naphtha	Naphtha (petroleum), light hydrocracked	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9)

Category	Substance	Conclusion	Constituents
			Iso-paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)
Bitumen	Residues (petroleum), vacuum	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9)
Heavy fuel oil components (HFO)	Gas oils (petroleum), heavy vacuum	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil components (HFO)	Clarified oils (petroleum), catalytic cracked	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil components (HFO)	Residues (petroleum), hydrocracked	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil components (HFO)	Residues (petroleum), atmospheric	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil components (HFO)	Residues (petroleum), catalytic cracking	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil components (HFO)	Fuel oil, residual	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Heavy fuel oil components (HFO)	Residues (petroleum), atm. tower	LR	Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil	Distillates (petroleum), vacuum	LR	Polyaromatic (benzo[k]fluoranthene: CAS No 207-08-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)

Category	Substance	Conclusion	Constituents
components (HFO)			Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Heavy fuel oil components (HFO)	Distillates (petroleum), petroleum residues vacuum	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9)
Vacuum Gas Oils, Hydrocracked Gas Oils & Distillate Fuels (VHGO)	Gas oils (petroleum), light vacuum	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Cracked Gas Oils (Cracked GO)	Distillates (petroleum), light catalytic cracked	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Cracked Gas Oils (Cracked GO)	Distillates (petroleum), light thermal cracked	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Straight-run Gas Oils (SRGO)	Distillates (petroleum), full-range straight-run middle	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9;

Category	Substance	Conclusion	Constituents
			Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Other Gas Oils (Other GO)	Distillates (petroleum), hydrodesulfurized middle	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Other Lubricant Base Oils (LBO)	Distillates (petroleum), heavy hydrocracked	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
Other Lubricant Base Oils (LBO)	Residual oils (petroleum), solvent deasphalted	LR	Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
Straight-run Gas Oils (SRGO)	Gas oils (petroleum), straight-run	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9)
Kerosene	Kerosene (petroleum)	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)

Category	Substance	Conclusion	Constituents
Kerosene	Kerosine (petroleum), hydrodesulfurized	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
Unrefined / Acid Treated Oils (UATO)	Distillates (petroleum), light paraffinic	LR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene) Aromatic naphthenics (2-methylfluorene, CAS No 1430-97-3; Fluorene, CAS No 86-73-7)
LOA Category G - Fuel Oils	Residues (petroleum), steam cracked	PC	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
LOA Category G - Fuel Oils	Benzene, ethylenated, residues	PC or LR (in bold)	Aromatics **(1,3,5-tripropylbenzene, CAS No 15181-14-3**; Diethylbiphenyl, CAS No 28575-17-9; **4-pentylbiphenyl, CAS No 7116-96-3**; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) **Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)** **Naphthenics (2,4-dimethylheptyldecahydronaphthalene)**
LOA Category G - Fuel Oils	Distillates (petroleum), light steam-cracked naphtha	PC or LR (in bold)	Aromatics (**1,3,5-tripropylbenzene, CAS No 15181-14-3**; Diethylbiphenyl, CAS No 28575-17-9; **4-pentylbiphenyl, CAS No 7116-96-3**; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) **Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)**

Category	Substance	Conclusion	Constituents
			Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
LOA Category G - Fuel Oils	Aromatic hydrocarbons, distn. residues, naphthalene-rich	PC or LR (in bold)	Aromatics (**1,3,5-tripropylbenzene, CAS No 15181-14-3**; Diethylbiphenyl, CAS No 28575-17-9; 4-**pentylbiphenyl, CAS No 7116-96-3**; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) **Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)** **Naphthenics (2,4-dimethylheptyldecahydronaphthalene)**
LOA Category G - Fuel Oils	Residues (petroleum), steam-cracked light, arom.	PC or LR (in bold)	Aromatics (**1,3,5-tripropylbenzene, CAS No 15181-14-3**; Diethylbiphenyl, CAS No 28575-17-9; **4-pentylbiphenyl, CAS No 7116-96-3**; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) **Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)** **Naphthenics (2,4-dimethylheptyldecahydronaphthalene)**
LOA Category G - Fuel Oils	Distillates (petroleum), naphtha steam cracking-derived, hydrotreated light arom.	PC	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) **Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)** **Naphthenics (2,4-dimethylheptyldecahydronaphthalene)**
LOA Category H - High Benzene Naphthas	Gasoline, pyrolysis, debutanizer bottoms	NR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
LOA Category H - High Benzene Naphthas	Aromatic hydrocarbons, C7-8, ethylene-manuf.-by-product	NR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9;

Category	Substance	Conclusion	Constituents
			Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)
LOA Category L - Resin Oils & Cyclic Dienes	Distillates (petroleum), steam-cracked, C8-12 fraction	NR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
LOA Category L - Resin Oils & Cyclic Dienes	Naphtha (petroleum), light steam-cracked, debenzenized, C8-16-cycloalkadiene conc	NR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3)
LOA Category J - Low Benzene Naphthas	Extracts (petroleum), heavy naphtha solvent	NR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
LOA Category J - Low Benzene Naphthas	Solvent naphtha (petroleum), heavy arom.	NR	Aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3; Diethylbiphenyl, CAS No 28575-17-9; 4-pentylbiphenyl, CAS No 7116-96-3; Anthracene, CAS No 120-12-7; Phenanthrene, CAS No 85-07-8; 1-methylphenanthrene, CAS No 832-69-9; Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3; Dibenzofuran, CAS No 132-64-9) Branched paraffins (2,3,4,5-tetramethyldecane, CAS No N/A; 3-methyltridecane, CAS No 6481-41-3) Naphthenics (2,4-dimethylheptyldecahydronaphthalene)
	Pitch, coal tar, high-temp.	PC	Mono-aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3) Di-aromatics (Diethylbiphenyl, CAS No 28575-17-3; 4-Pentylbiphenyl, CAS No 7116-96-3) Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)

Category	Substance	Conclusion	Constituents
	Tar, coal, high-temp.	PC	Mono-aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3) Di-aromatics (Diethylbiphenyl, CAS No 28575-17-3; 4-Pentylbiphenyl, CAS No 7116-96-3) Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Distillates (coal tar)	LR	Di-aromatics (Diethylbiphenyl, CAS No 28575-17-3; 4-Pentylbiphenyl, CAS No 7116-96-3) Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Distillates (coal tar), light oils	LR	Mono-aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3) Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Distillates (coal tar), heavy oils	PC	Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Extract residues (coal tar), high-temperature, naphthalene oil alkaline, distn. overheads	LR	Mono-aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3) Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Anthracene oil, anthracene-low	LR	Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Anthracene oil, anthracene paste	LR	Mono-aromatics (1,3,5-tripropylbenzene, CAS No 15181-14-3) Polyaromatics (Fluoranthene, CAS No 206-44-0; Benzo[k]fluoranthene, CAS No 207-08-9; Benz[a]anthracene, CAS No 56-55-3)
	Anthracene oil	PC	Benzo[k]fluoranthene Benz[a]anthracene Fluoranthene Phenanthrene 1-methylphenanthrene Fluorene Dibenzofuran

Substance/constituent pairings that have been confirmed as not relevant are indicated by NR (not relevant) in the conclusion column. Constituents whose presence has been confirmed are indicated by PC (presence confirmed) in the conclusion column. The constituents for which the conclusions remain to be primarily based on literature review suggests are marked as LR (Literature review) in the conclusion column and applies to all constituents in that cell. Where some constituents within a cell are highlighted in **bold**, the conclusion of LR applies.

Most notably, one of the REACH registration consortia disagreed with the possibility that the relevant marker constituents are potentially present in the substances belonging to categories H (high benzene naphthas), J (low benzene naphthas), and L (resin oils and cyclic dienes). The listing of the potentially relevant constituents against these substances in the

questionnaire for this study was made for reasons of erring on the side of caution and only on the basis of the presence of the relevant high-level constituent group – no definitive evidence was identified under Step 1 that the 15 marker constituents are present in the relevant LOA substances belonging to categories H, J, and L. In addition, the information provided by LOA arguing that there is a limited potential for constituents with PBT properties (which is the key criterion for constituent prioritisation under Steps 3 and 4) is reproduced below. For these reasons, these substance-constituent combinations relevant to categories H, J and L LOA substances were removed from further assessment under this study.

Table 11: The presence of the 15 prioritised constituents in the 53 PetCo substances

Category	Details	Persistence and Bioaccumulation (PB) evaluation
Category H – High Benzene Naphthas	Category members are usually produced by the distillation of products from a steam cracking process or by pyrolysis. The category contains predominantly hydrocarbons greater than C6. The high benzene naphthas category contains hydrocarbons (aliphatic, aromatic and olefinic) with carbon numbers predominantly in the C5-C10 range and boiling from approximately 30°C to 300°C. Members of this category contain >0.1% benzene and contain varying amounts of toluene, xylenes and n-hexane. Some category members contain naphthalenes, isoprene and 1,3-butadiene and this has been quantified where possible. All the streams in this category are complex UVCBs containing ≤ 50% paraffins, ≤ 60% isoparaffins, ≤ 90% olefins, ≤ 90% naphthenics, ≤100% aromatics, and above 0.1% benzene.	The screening of the category was conducted using the constituent-based approach. This approach was appropriate as the analytical data indicated that the category is well characterised. Of the 272 constituents included in the category only 2 were identified as Potentially vP and 4 as Potentially P and none as Potentially B/vB. None of the constituents were identified as both Potentially P or vP and Potentially B/vB. Therefore, the screening assessment indicates that the category is Not PB and hence cannot be considered to meet the screening PBT/vPvB criteria. The following conclusion applies to the category. ***Conclusion (i): The substance does not fulfil the PBT and vPvB criteria. For screening assessment: there is no indication of P or B properties.***
Category J – Low Benzene Naphthas (<0.1%)	All streams are predominantly produced by the distillation of products from a steam cracking process or by pyrolysis. The following high-level process description has been derived from proprietary data submitted by registrants; however, the data was anonymised to ensure that confidentiality is maintained. The Low Benzene Naphthas category contains hydrocarbons (aliphatic, aromatic and olefinic) with carbon numbers predominantly in the C7-C13 range and boiling from approximately 80 °C to 300 °C. Members of this category contain <0.1% benzene and contain varying amounts of toluene, xylenes and ethylbenzene. Category members are typically produced by the	The screening of the category was conducted using the constituent-based approach. This approach was appropriate as the analytical data indicated that the category is well characterised. Of the 62 constituents included in the category eight were identified as Potentially P and none were identified as Potentially vP. The bioaccumulation evaluation indicates that two of the constituents were Potentially B. Finally, none of the constituents were identified as both Potentially P or vP and Potentially B/vB. Therefore, the screening assessment indicates that the category is Not PB and hence cannot be considered to meet the screening PBT/vPvB criteria. The following conclusion applies to the category.

Category	Details	Persistence and Bioaccumulation (PB) evaluation
	distillation of products from a steam cracking process or by pyrolysis	***Conclusion (i): The substance does not fulfil the PBT and vPvB criteria. For screening assessment: there is no indication of P or B properties.***
Category L – Resin Oils and Cyclic Dienes	All streams are predominantly produced by a steam-cracking process. The following high-level process description has been derived from proprietary data submitted by registrants; however, no confidential information has been alluded to: A pyrolysis gas or naphtha starting material is steam-cracked at high heat (800 – 1000°C) and then distilled or filtered progressively at lower temperatures (approx. >200°C) to remove low carbon-number fractions (typically below C9). Further treatments, such as hydrogenation, may also be applied to streams to produce the final product, which is rich in DCPD and mono-aromatic compounds. The category applies to streams with predominantly the following PIONA (paraffins, isoparaffins, olefins, naphthenics and aromatics) analysis: olefins and aromatics up to 100%, isoparaffins at ≤ 25%, naphthenics at ≤ 10%, paraffins at ≤ 1%, and a carbon number range of predominantly C5-C15. The category is characterised by high concentrations of DCPD, as well as other similar cyclic olefins, such as DCPD-isomers and derivatives, indane and indene. Aromatic compounds are also observed, particularly aromatics between C8 – C11. Naphthalenes are reported, but Category L streams do not contain any other poly-aromatic hydrocarbon molecules.	Of the 145 constituents included in the category None of the category constituents met both the P and B criteria, or the vP and vB criteria, or any combination of these criteria. Six constituents were identified as being 'Potentially P' and seven as 'Potentially P / vP'. Only two constituents were identified as being 'Potentially B'. There were no constituents classified as PB. Four constituents could not be evaluated using BioHCwin as they fall out of the QSAR domain. These constituents are temporarily assigned the 'Not P?' classification. However, for the same constituents a 'Not B' classification was awarded and therefore these constituents are unlikely to be PB. Therefore, the screening assessment indicates that the streams in this category are Not PB and hence cannot be considered to meet the screening PBT / vPvB criteria. The following conclusion applies to the category. ***Conclusion (i): The substance does not fulfil the PBT and vPvB criteria. For screening assessment: there is no indication of P or B properties.***

Source: Consultation input from LOA provided for this study (October 2020)

In addition, it was noted by the LOA that the 12 LOA substances (including Category G substances) considered in this study full REACH >1,000 tonne registrations. One of the exposure scenarios included in the CSRs is use as an intermediate. Although the substances are used as intermediates, they have a full REACH Annexes VII-X dataset including an exposure assessment and risk characterisation.

7.3 Revised list of use/process-product combinations

Taking into account stakeholder input into the consultation exercise for this study, the lists of the relevant uses, processes and products for each substance were revised by screening out non-intermediate uses and processes/products not currently used. The revised lists are presented below. Please note that the table below lists all confirmed intermediate uses including those for which subsequent analysis concludes that the relevant constituent is likely to be converted or destroyed and thus not present in the product/output (e.g. the

conclusion for metal ore reduction is that the relevant constituents tend to be destroyed but metal from metal ore reduction is still included in the table below). In addition, in some instances the constituent (even though not destroyed) may not be contained in the product listed in the table below but may become part of the waste created in the relevant process.

Table 12: Confirmed intermediate uses, processes and products/sectors in which outputs are used

Substance(s)	REACH registration consortium	Process(es)	Product(s)/ sector(s) in which products are used
Anthracene oil Distillates (coal tar) heavy oils Distillates (coal tar), heavy athracene oils Distillates (coal tar), naphthalene oils Pitch, coal tar, high-temp. Tar, coal, high-temp.	R4CC	Carbonisation/ pyrolisis	Carbon black and/or coke
Anthracene oil Distillates (coal tar) heavy oils Distillates (coal tar), heavy Distillates (coal tar), heavy athracene oils Tar, coal, high-temp.	R4CC	Distillation	Coal tar fractions
Anthracene oil Distillates (coal tar), heavy Tar, coal, high-temp.	R4CC	Metal ore reduction	Metal
Distillates (coal tar), naphthalene oils	R4CC	Crystallisation	Napthtalene
Pitch, coal tar, high-temp.	R4CC	Carbonisation/ pyrolisis	Metals & Minerals Production/coke/carbon black
Tar, coal, high-temp.	R4CC	Pyrolysis	Substances
Distillates (petroleum), full-range straight-run middle	Concawe	Treating and blending	N/A
Distillates (petroleum), heavy hydrocracked	Concawe	Fluid catalytic cracking	Adhesives & Sealants Polishes & Waxes Coating Anti-freeze Metal Working Fluids Heat Transfer Fluids Hydraulic Fluids Plant Protection Products Substances Agriculture, Forestry & Fishing Printing & Recorded Media Reproduction

Substance(s)	REACH registration consortium	Process(es)	Product(s)/ sector(s) in which products are used
			Rubber Production & Processing Lubricants & Greases
Gas oils (petroleum), heavy vacuum	Concawe	Fluid catalytic cracking	Fuels
Kerosine (petroleum)	Concawe	Catalytic Hydrotreatment	Lubricants & Greases Adhesives & Sealants Polishes & Waxes Anti-freeze Coating Fuels Substances
Kerosine (petroleum), hydrodesulfurized	Concawe	Blending	Lubricants & Greases Adhesives & Sealants Polishes & Waxes Anti-freeze Coating Fuels Substances
Naphtha (petroleum), heavy catalytic cracked	Concawe	Blending	Fuels
Residues (petroleum), atm. Tower	Concawe	Deasphalting	Fuels
Distillates (petroleum), light steam-cracked naphtha Residues (petroleum), steam cracked	LOA	Blending	Fuels

Sources: Consultation responses for this study (R4CC, Eurofer, Concawe, LOA).

The questionnaire response from Concawe did not provide any additional use/process/product information other than the Concawe analytical reports that had already been used for the development of the first list under this study. The analytical information Concawe has at its disposal does not distinguish separately for intermediates. Only one questionnaire response from an individual Concawe member company was received – this response, however, confirms at least some intermediate use for over 80% of the Concawe substances. This appears to confirm that the 'intermediate uses' in REACH registrations are a reality and it can thus be expected that many Concawe substances have at least one intermediate use. In conclusion, although the publicly available REACH data does not allow the determination of specific processes that can be considered intermediate use, they appear to provide a good indication of the fact that the relevant substances have intermediate uses.

For LOA substances, these are clearly underestimated since it is indicated in the LOA consultation input for this study that all of their substances have one scenario for use as intermediate included in the registration CSR.

8 Step 6: Analysis of the fate of prioritised constituents (groups and markers) in the relevant processes (Approaches 0, 1 and 2)

8.1 Introduction

This section of the report sets out the key features of the overall assessment framework, introduces three of the five approaches used for the assessment of the fate of the relevant constituent groups and marker constituents (Approaches 0, 1, and 2) and summarises their results. The remaining two approaches (both of which consider interactions in the supply chain) are presented in Section 8.

A high-level assessment of the fate of **the relevant constituent groups** is hereby carried out:

- **Approach 0 (downstream – literature review, constituent groups only):** considers (for the relevant chemical processes) whether a constituent belonging to a specific constituent group is likely to pass through in the value chain until final inclusion into an end-product (based on temperature, pressure, kinetic reactivity only).

Four analytical approaches (three downstream and one upstream approach) are subsequently used to assess the fate of the relevant **marker constituents.** Two of the four approaches are presented in this section – these take a downstream perspective and focus on the fate in individual uses/processes and do not consider the potential for the constituents to be destroyed further downstream:

- **Approach 1 (downstream – literature review):** this approach includes the study team's assessment of the likelihood of these constituents being converted in the relevant process based on thermodynamic (temperature, pressure) and other factors (such as the presence of catalysts).
- **Approach 2 (downstream – literature review & consultation):** Approach 2 is a further development of the results of Approach 1 and complements the literature review with the information collected through consultation for this study (questionnaire responses and interviews).

Each of these approaches has its advantages and disadvantages (see the table below) and, for this reason, the results of all five approaches are presented in this report and should be taken into account when drawing conclusions about the fate of the relevant constituents.

Table 13: Pros and cons of Approaches 0, 1, and 2

Approach	Advantages	Disadvantages
Approach 0 (downstream – literature review, constituent groups)	1. Does not focus on specific marker constituents (these may or may not be a good predictor for the whole constituent group) 2. Considers the potential for formation, not just pass-through	1. High level assessment only 2. Only considers temperature, pressure, kinetic reactivity, no consideration of catalysts (e.g. in fluid catalytic cracking) 3. Only pass-through in the reaction unit considered

Approach	Advantages	Disadvantages
Approach 1 (downstream – literature review)	1. Comprehensive approach based on a consistent method for all substances/constituents 2. Not based on individual stakeholder input which may reflect their individual experiences	1. Non-intermediate uses are not screened out 2. Includes substance-use/process/product combinations that stakeholders see as irrelevant 3. Includes constituent-substance combinations with which stakeholders disagree 4. Uses/processes considered in isolation, some products may be converted in the next or previous stage in the supply chain 5. A consultee disagrees with logic framework for Concawe substances
Approach 2 (downstream – literature review & consultation)	1. Greater use of stakeholder information: revision on the basis of stakeholder input after literature review and preference given to stakeholder input 2. Non-intermediate uses screened out 3. Greater confidence in the 'positive identification' of a constituent as likely being present since it is based on industry information	1. Stakeholder evidence (or at least absence of evidence to the contrary) required for a conclusion that a constituent is likely to remain – the conclusions may thus reflect the knowledge of specific stakeholders 2. Not a full reflection of the links between the different processes in the supply chain

This section of the report first sets out the logical framework that underpins the assessment of the fate of the constituent groups and marker constituents in the relevant processes, Approaches 0, 1, and 2 are then introduced and their results are presented.

8.2 Summary of the logic for the assessment of the fate in individual processes

8.2.1 The core framework

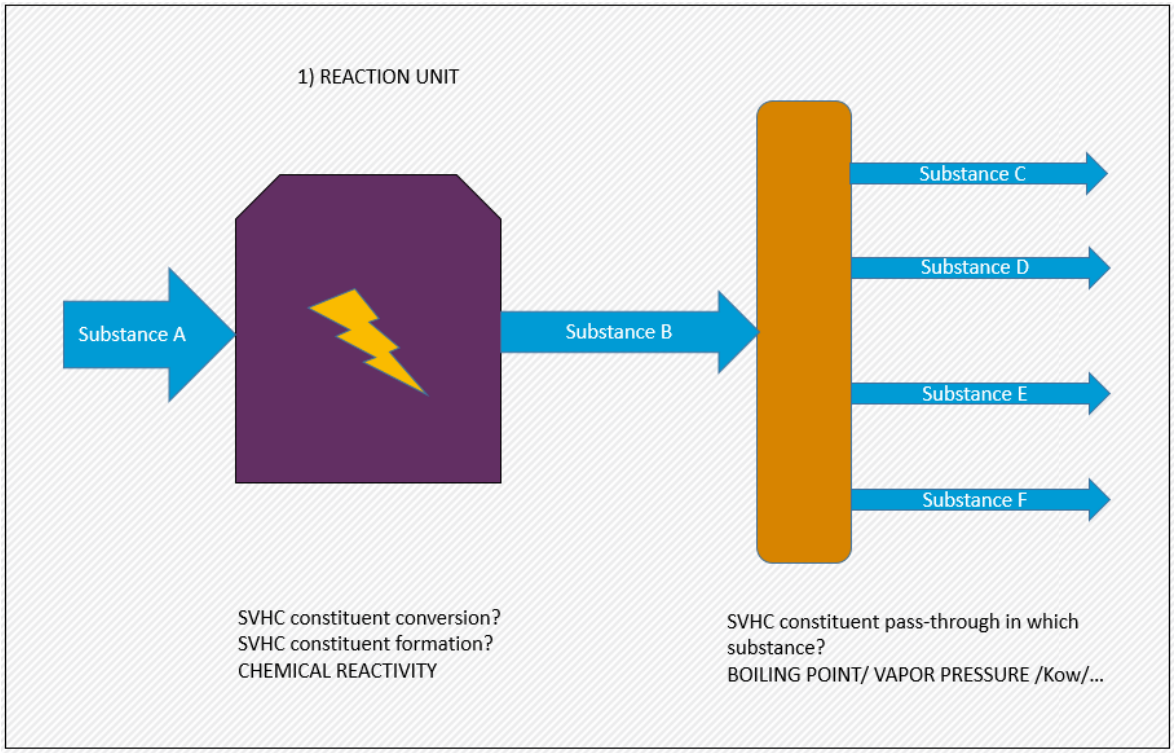
8.2.1.1 Chemical processes in petrochemical plants

Petrochemical plants, typically consist of 2 major processing units:

- the reaction unit, where the intended chemical process takes place
- the purification unit. As the conversions and yields for the above reactions are typically considerably lower than 100% and the starting materials are typically UVCB substances, further purification is needed to create the final substance(s).

The constituents are thus likely to undergo these two main steps. It should therefore be determined whether constituents of concern are converted (or formed) in the reaction unit and in which resulting substance they will pass-through. This is summarised in Figure 8.

Figure 8 Schematic representation of chemical process plants and impact on behavior and fate of the relevant constituents



Source: own illustration, ARCHE Consulting, Gent, Belgium

In the reaction unit, conversion or formation will depend largely on the **chemical stability** of a constituent. Chemical stability or reactivity depends on two factors:

- thermodynamic factors: i.e., whether or not a substance reacts, driven by temperature and/or pressure
- kinetic factors: how fast it reacts (can be facilitated by catalysts)

In the purification unit, physicochemical properties and partitioning coefficients of the constituents will determine to which substance the constituent will pass through.

8.2.1.2 Thermodynamical chemical reactivity assessment

Thermodynamically, a chemical reaction occurs because the products (taken as a group) are at a lower free energy than the reactants; the lower energy state is referred to as the 'more stable state'. The free energy or Gibbs energy (ΔG) is defined according to the following fundamental thermodynamic law:

$$\Delta G = \Delta H - T\,\Delta S$$

Where ΔH represents enthalpy, ΔS entropy and T temperature.

The most important term in this equation is the enthalpy (ΔH)

- ΔH > 0: energy (heat) is required because strong bonds are broken and weak bonds are formed. This is an **endothermic reaction**

- ΔH < 0: energy (heat) is emitted because weak bonds are broken and strong bonds are formed. This is an **exothermic reaction**

Most of the identified priority constituent groups require endothermic reactions in order to react. It is clear that aromatic constituents have achieved a very stable state. By the presence of a cyclic π-electron system the C atoms are at a very low Gibbs energy level. As such, a very elevated endothermic reaction is required to break aromatic bonds thermodynamically. In fact, this will typically only happen at combustion.

Branched/alkylated, SPAC and naphthenic constituents require less energy and could as such be converted in chemical processes only using heat/pressure.

8.2.1.3 Kinetic chemical reactivity assessment

Whether a chemical reaction will occur (by support of catalysts or not) is also dependent on the kinetic reactivity (how fast). Kinetic reactivity for cracking, isomerization, hydrogenation and dehydrogenation related chemical processes proceeds typically through free radical mechanisms.

Three important free radical reaction families can be distinguished (Rice et al. 1931, 1934, 1943): bond scissions, hydrogen abstraction and radical addition reactions.

- Carbon-carbon and carbon-hydrogen bond scissions of molecules and the reverse radical recombinations:

$$R_1 - R_2 \rightleftharpoons R_1^{\bullet} + R_2^{\bullet}$$

For the following sequence of the product radicals, the scission rate increases from left to right (Chen et al., 1988):

vinyl and phenyl (lowest scission rate) < hydrogen < methyl < primary < secondary < tertiary < allyl (highest scission rate)

This means that bonds in aromatic rings (i.e. phenyl) will be the most difficult to break, while alkyl and olefinic (i.e. allyl) branches will be the easiest to break.

- Hydrogen abstraction reactions, both intra- and intermolecular:

$$R_1 - H + R_2^{\bullet} \rightleftharpoons R_1^{\bullet} + R_2 - H$$

Those reactions form the basis for isomerization reactions. In a hydrogen abstraction reaction, a hydrogen atom is transferred from a molecule to a radical. This produces a new radical and a new molecule. The reaction rate coefficient of a hydrogen abstraction is determined by two factors, the nature of the abstracting radical (methyl, ethyl, etc) and the nature of the cracked C-H bond.
It is well known that vinyl type and phenyl type radicals are the most active radicals while

allylic type of radicals are the most inactive. The activity sequence of the hydrocarbon radicals is in decreasing order (Chen, 1988):

vinyl > phenyl > hydrogen > methyl > primary > secondary > tertiary > allyl

This means that if any aromatic (phenyl) radical would be formed, it will quickly be hydrogenated back to its stable from.
The strength of the C-H bond is characterized by its bond dissociation energy. In paraffins a distinction is made between primary, secondary and tertiary carbon atoms. The C-H bond strength decreases from primary to tertiary (Chen, 1988). Hence, the energy necessary to abstract a hydrogen atom from a molecule decreases from primary to tertiary. This means that heavily branched / alkylated constituents will react faster than non-branched constituents.

- Radical addition to olefins/aromatics and the reverse scission of radicals, both intra- and intermolecular:

$$R_1^{\bullet} + R_2 = R_3 \rightleftharpoons R_1 - R_2 - R_3^{\bullet}$$

The reverse reaction of a scission reaction of a radical is a radical addition reaction to an olefin/aromatic. Radical addition reactions are important reactions because they are responsible for the production of heavier constituents that can ultimately lead to the formation of larger (poly)aromatics; This happens via the so-called cycloaddition reaction, where two molecules combine to form a ring. These reactions will occur as of certain temperature/pressure conditions as the thermodynamically more stable aromatic structure can as such be formed.

This means that in certain processes, the creation of (poly)aromatic constituents will occur. This has for example been described for the steam cracking process (Bolado et al., 2003).

8.2.1.4 Summary of the core framework

Taking the above into account, the logic framework for estimating whether a constituent of concern is likely to be present in the product at the end of a process is summarised below.

Table 14: The logic framework for assessing pass through of the relevant constituents

Factor	Reaction unit	Purification unit	Notes
Possible constituent behaviour	Conversion, formation, extraction	Pass-through into a specific substance Transfer to waste water, air or solid waste	

Factor	Reaction unit	Purification unit	Notes
Key question	Likely to convert? Potential to be formed? Extraction intended?	Into which substance or medium will it pass? Is this substance in the product or is it recycled back into the reactor unit or another reactor at the same site?	
Sub-questions	What is the chemical stability/reactivity? Are any potential catalysts present?	Which process? • Distillation / fractionating or extraction processes	Distillation/fractionating processes – constituent will flow into distilled product (depending on boiling point/vapour pressure)
Criteria	• Thermodynamic factors - whether or not it reacts - temperature - pressure • Kinetic factors – how fast it reacts - kinetic reactivity presence of catalysts	• Distillation/fractionating processes, physicochemical properties: - Boiling point - Vapour pressure • Extraction processes: Partitioning coefficients (Kow)	Temperature: most identified priority constituents require an endothermic reaction Aromatic constituents – require an elevated endothermic reaction Branched/alkylated, SPAC and napthenic constituents require less energy

This logic framework has been applied in the following ways:

- Approach 0: fate in the relevant chemical process to assess whether the constituent group passes through in the value chain until final inclusion into an end product (based on temperature, pressure, kinetic reactivity only); and
- Approach 1: fate in the relevant chemical process to assess whether a specific marker constituent passes through into the end product (based on temperature, pressure and the presence of catalysts).
- Approaches 2 and 3 build on the analysis carried out under Approach 1.

8.2.2 Comments on the core framework received during consultation

The different stakeholders are in different situations and it is clear that the framework is more applicable to some than others. For example, R4CC agreed with the use of this framework but Concawe commented that, with regard to their members, the above framework does not offer a sequential method to track constituents and proposed that it may be more useful to follow a refinery process in the logic. More specifically, it was noted that in addition to the intermediate use scenario of reaction and purification units, the logic should include blending to produce fuel substances e.g. gasoline/diesel/fuel oil.

A questionnaire response from a member company of Concawe also did not fully support the core framework and mentioned that the polycyclic aromatic constituents occur to some extent naturally in crude oil and are therefore present in streams produced only by physical

separation processes, according to their distribution behaviour. In fractional distillation, they distribute according to their boiling point, while in solvent extraction they distribute according to their polarity. It further noted that these constituents are also generated in cracking processes, primarily in steam and catalytic cracking, and to a lesser extent in thermal cracking. Meanwhile they are removed by hydrotreatment or solvent extraction from streams destined for applications where they are undesirable such as lubricant base oils. It was further noted that, alongside reaction and purification units, blending operations must also be considered especially for those substances produced by blending multiple individual streams to a specification.

Although blending/finishing is not included in the logic presented in this section, it is expected that the blending stage is unlikely to significantly change the conclusions presented in this study. The blending stage is likely to merge the individual streams into one and thus increase the concentration of the relevant constituents or reduce their concentrations by means of dilution. However, since most of the assessment in this report is not quantitative in the sense that constituent concentrations are considered, it is not expected that the blending stage would change the conclusions presented in this study. It is, however, recognised that dilution might be important for classification & labelling or SVHC status. The concentrations in the relevant products are considered under Approach 4 (where such data are available) and in this way the different blending/finishing/other processes are indirectly taken into account.

8.3 Approach 0: Likelihood of pass-through for prioritised constituent groups (temperature, pressure, kinetic reactivity)

8.3.1 Pass-through in the reaction unit

The table below provides conclusions on chemical reactivity of the constituent groups in the reaction unit of a generic chemical process. This assessment is carried out for the constituent groups defined in Figures 6 and 7 – these were defined under Steps 1, 4 and 5 based on literature review. There was no need to refine these based on the information received through consultation for this study.

Please note that this is based on thermo-dynamic and kinetic parameters only and does not take into account other factors such as specific catalytic interactions in certain processes (e.g. Fluid Catalytic Cracking).

Table 15: Behaviour of the different groups in the reaction unit (thermodynamic and kinetic factors only)

Constituent group	Thermodynamic reactivity (only temperature/pressure driven)	Kinetic reactivity (including cracking, isomerisation, hydrogenation and dehydrogenation)	Behaviour conclusion
Polyaromatic	Likely Low	Likely Low conversion, potential of formation	No conversion likely, potential of formation
Triaromatic branched	Likely Low	Likely Medium conversion (to non-branched form), potential of formation	Conversion to non-branched form possible,

Constituent group	Thermodynamic reactivity (only temperature/pressure driven)	Kinetic reactivity (including cracking, isomerisation, hydrogenation and dehydrogenation)	Behaviour conclusion
			potential of formation
Triaromatic	Likely Low	Likely Low conversion, potential of formation	No conversion likely, potential of formation
Diaromatics branched	Likely Low	Likely Low conversion, potential of formation	Conversion to non-branched form possible, potential of formation
Mono-aromatic	Likely Medium	Likely Medium conversion (to non-branched form), potential of formation	Conversion possible, potential of formation
Naphthenic aromatics, non-branched	Likely Low to Medium	Likely Low to Medium conversion	Possible conversion
Naphthenic aromatics, branched	Likely Low to Medium	Likely Medium conversion (to non-branched form)	Conversion to non-branched form possible
Naphthenics (non aromatics)	Likely Medium	Likely Medium conversion (to non-branched form)	Possible conversion
Heavily branched Paraffins/Iso-Paraffins	Likely high	Likely high conversion	Conversion very likely
SPAC	Likely Medium		Possible Conversion

8.3.2 Pass through assessment in purification unit

Two major processes are typically applied in the purification unit of petrochemical sites:

- Distillation/fractionating processes. Any constituent of concern present will just flow to the distilled product (depending on its including boiling point/vapor pressure). As such, these two parameters will be determining the fate of the constituent.
- Extraction processes. Partitioning coefficients such as K_{ow} will be the determining parameter for estimating whether the constituent is extracted or not.

This means that even if a constituent of concern is not converted in the reactor unit and is still present in the feed of the purification unit (Substance B in figure 8), it still does not necessarily result in presence in all the produced substances (substances C, D, E and F of figure 8). In addition, some of these produced substances might be recycled back to the reactor unit (or at another point in the same chemical production site) and will have no further downstream intermediate or end-use. As such, further analyses on boiling point

ranges and partitioning coefficients of the produced substances would be required to assess the final fate in the supply chain. This analysis was not carried out for the constituent groups in this study although all these factors are likely to have been considered (where relevant) in the stakeholder input that underpins Approaches 2 and 3 and in the product composition data that informs Approach 4.

8.4 Approach 1: Downstream — literature review — pass-through of marker constituents

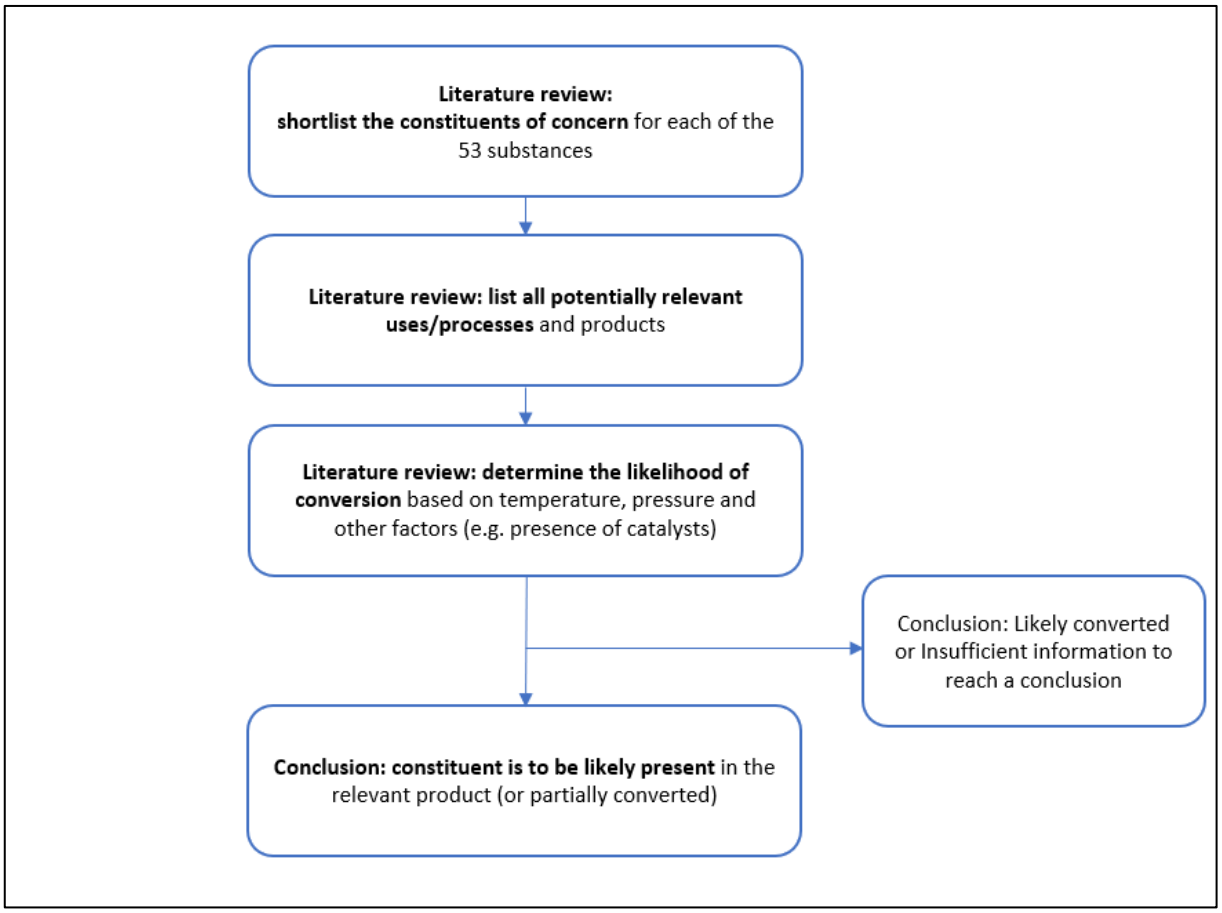
For each relevant substance-marker constituent-process-product combination, the following factors have been considered:

- Temperature (°C) of the process
- Pressure in the process
- Melting point and boiling point of each constituent
- Presence of catalysts
- Other conditions

On the basis of the above information, a conclusion on the likely presence in products is reached. The full analysis is provided in Annex 10 (Detailed assessment for prioritised constituents).

Under Approach 1, the likelihood of the constituents of potential concern being converted in the relevant process is assessed by comparing the characteristics of the constituents with the thermodynamic characteristics of the relevant process (temperature, pressure), as well as other factors such as the presence of catalysts.

Figure 9 Approach 1: Literature review (direction: downstream)



The figure describes, in five boxes, the approach taken in the study for the literature review. It starts by shortlisting the constituents of concern, followed by a literature review step for all potentially relevant uses/processes. The next step is a literature review to determine the likelihood of conversion based certain factors, which is then followed by a conclusion step, if the constituent is likely to be present, is converted or if there is insufficient information to reach a conclusion.

Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

Table 16 shows that of the 689 combinations of substances/processes/products, under Approach 1, one of the 15 constituents is likely not to be converted in over 50% (370) of the substance-constituent-process-product combinations. These combinations relate to 30 substances, all 15 constituents and a wide range of processes and products. However, the results obtained under Approach 1 include processes that cannot be considered intermediate uses and/or are no longer in use – there is insufficient information in the literature to assess these two factors.

Table 16: Results of Approach 1

Approach	Substance-constituent-process combinations	Of which confirmed intermediate use	Likely present	Likely converted	Likely partially converted	No conclusion
Approach 1	689	Not tested	370	113	1	205

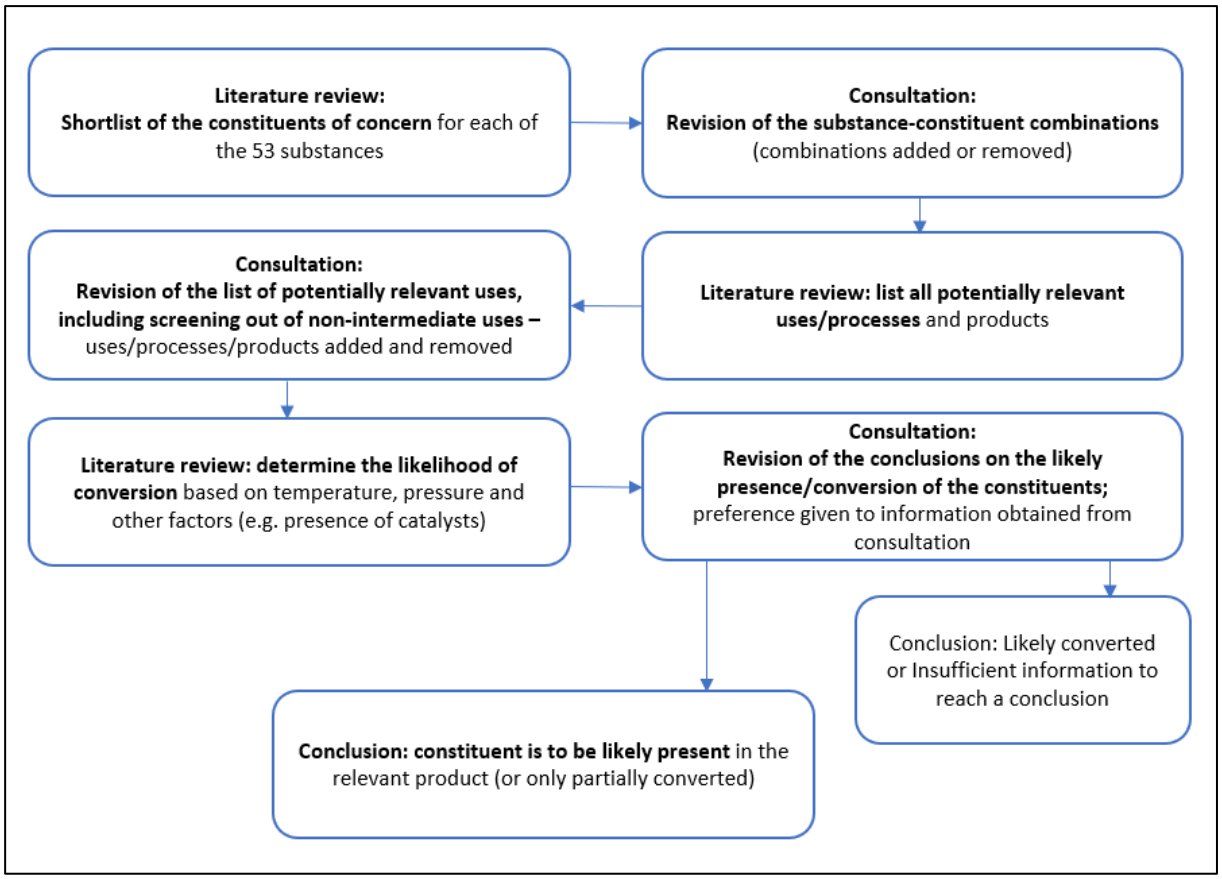
Due to the large number of substance-constituent-process-product combinations in which the relevant constituent is predicted to be passed through, the full results of Approach 1 are not reproduced in the main body of this report; see Annex 11 for the full results.

8.5 Approach 2: Downstream — literature review & consultation — pass-through of marker constituents

Under Approach 2, the results of Approach 1 are revised based on the information collected through consultation. First, uses not identified as intermediate uses by stakeholders and processes indicated as 'not currently in use' are screened out. Second, conclusions made on the basis of literature review under Approach 1 are revised based on stakeholder input.

Stakeholder input was collected through questionnaires[10] and telephone interviews[11].

Figure 10 Approach 2: Literature review & consultation (direction: downstream)



Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

[10] Six completed questionnaires were received: Concawe, Lower Olefins and Aromatics REACH Consortium (LOA), R4CC, Eurofer and an individual petroleum company (and from the Hydrocarbon Solvents REACH Consortium). Please note that, for confidentiality reasons, Annex 10 excludes an extensive questionnaire response provided by this company – however, the input by this company has been taken into account in the tables in this report. The questionnaires can be accessed via the RPA webpage: https://rpaltd.co.uk/petcosubstances

[11] Seven interviews were held with the relevant REACH registration consortia, downstream user associations and an individual company.

The table below provides a comparison of the results of Approach 1 and 2.

Table 17: Comparison of the results of Approaches 1 and 2

Approach	Substance-constituent-process combinations	Of which confirmed intermediate use	Likely present	Likely converted	Likely partially converted	No conclusion
Approach 1	689	Not tested	370	113	1	205
Approach 2	689 (same as above)	280*	134**	144	0	2

Notes:
*Intermediate uses that have not been confirmed include stakeholder responses such as 'process not in use', 'no', 'no information provided'. Where contradictory information was provided by different stakeholders, a positive was recorded if at least one stakeholder indicated that the process should be considered intermediate use.
** Where stakeholder input suggested a different conclusion to Approach 1, stakeholder input was prioritised. At least one stakeholder responding that a constituent is likely to be present was sufficient to record a conclusion of 'likely presence' even where others disagreed.

The results of Approach 2 suggest that of the 689 substance-constituent-process-product combinations, around 40% appear to relate to intermediate uses – of these, the constituent in question may be retained in over half of the cases. These are likely to underestimate the 'real' proportion of cases since positive stakeholder identification or absence of contradiction was required for each 'confirmed' case.[12] On the other hand, Approaches 1 and 2 consider the likelihood of these constituents being retained or converted in specific processes/products but do not consider interrelationships between these processes/products or the potential for the constituents to be converted further down the supply chain.

The results of Approach 2 are summarised in the table below.

Table 18: Results of Approach 2 (constituents likely to be present in a product)

Substance	Constituent	Process	Product/output
Anthracene oil	Benzo[k]fluoranthene Benz[a]anthracene	Pyrolysis	Carbon black, coke
	Dibenzofuran	Distillation	Coal tar fractions
		Metal ore reduction	Metal
		Pyrolysis	Carbon black
Distillates (coal tar) heavy oils	Phenanthrene	Distillation	Coal tar fractions
Distillates (coal tar), heavy	Benz[a]anthracene Fluoranthene Anthracene	Distillation	Coal tar fractions

[12] It should be noted that the study team had to make a judgement call in some instances in terms of the use of some of the information collected. For example, a response from an individual company was sufficient to conclude that a constituent is converted but it was not sufficient to exclude a process-product combination as 'not in use' in case other companies rely on such a process. However, a response from a REACH registration consortium was sufficient to exclude a process-product combination.

Substance	Constituent	Process	Product/output
	1-methylphenanthrene 2-methylfluorene Fluorene		
Distillates (coal tar), heavy athracene oils	Benzo[k]fluoranthene	Distillation	Coal tar fractions
Distillates (petroleum), heavy hydrocracked	Anthracene 1,3,5-tripropylbenzene Fluorene 2,4-dimethylheptyldecahydronaphthalene	Fluid catalytic cracking	Anti-freeze
	Anthracene Phenanthrene 1,3,5-tripropylbenzene Fluorene 2,4-dimethylheptyldecahydronaphthalene		Metal Working Fluids Heat Transfer Fluids Hydraulic Fluids Plant Protection Products Substances Agriculture, Forestry & Fishing Printing & Recorded Media Reproduction Rubber Production & Processing
	Phenanthrene 1,3,5-tripropylbenzene Fluorene 2,4-dimethylheptyldecahydronaphthalene		Adhesives & Sealants Polishes & Waxes Coatings
	1,3,5-tripropylbenzene Fluorene 2,4-dimethylheptyldecahydronaphthalene		Lubricants & Greases
Distillates (petroleum), light steam-cracked naphtha	Benzo[k]fluoranthene Phenanthrene Diethylbiphenyl	Blending	Fuels
Gas oils (petroleum), heavy vacuum	Benzo[k]fluoranthene Anthracene Fluorene	Fluid catalytic cracking	Fuels
Kerosine (petroleum)	Fluoranthene Anthracene 1,3,5-tripropylbenzene Fluorene 2,3,4,5-Tetramethyldecane 3-methyltridecane	Catalytic Hydrotreatment	Fuels

Substance	Constituent	Process	Product/output
	1,3,5-tripropylbenzene Fluorene		Lubricants & Greases
	2,3,4,5-Tetramethyldecane 3-methyltridecane		Adhesives & Sealants Polishes & Waxes Anti-freeze Coating
	Fluorene		Substances
Kerosine (petroleum), hydrodesulfurized	Fluorene 2,3,4,5-Tetramethyldecane 3-methyltridecane	Blending	Lubricants & Greases Fuels Substances
	2,3,4,5-Tetramethyldecane 3-methyltridecane		Adhesives & Sealants Polishes & Waxes Anti-freeze Coating
Naphtha (petroleum), heavy catalytic cracked	Fluorene	Blending	Fuels
Pitch, coal tar, high-temp.	Fluoranthene	Carbonisation/ pyrolisis	Coke/carbon black
	2-methylfluorene	Carbonisation	Metals & Minerals Production
Residues (petroleum), atm. Tower	Anthracene Benzo[k]fluoranthene Fluoranthene Phenanthrene Fluorene	Deasphalting	Fuels
Residues (petroleum), steam cracked	Benzo[k]fluoranthene Benz[a]anthracene Fluoranthene Phenanthrene Diethylbiphenyl	Blending	Fuels
Tar, coal, high-temp.	Benzo[k]fluoranthene Benz[a]anthracene Fluoranthene Anthracene Phenanthrene 1-methylphenanthrene 2-methylfluorene Fluorene	Distillation	Coal tar fractions
	Dibenzofuran	Pyrolysis	Substances

Note: It is possible that some of the 'products' in this table may be full or partial duplicates– for example, there may be some overlap between metals and minerals production and coke. Similarly, where the category 'substances' is not defined, it may overlap with other products/outputs.

9 Step 7: Supply chain analysis and upstream analysis (Approaches 3 and 4)

9.1 Introduction

Potential for pass through the processes does not necessarily mean that the constituent will result in risk to the environment or human health. For example, one of the consultees, indicated that LOA Category G substances are usually the end product of extractions and distillations to obtain other substances. The substances in this category are used primarily as fuels which are burned in closed systems. Thus, for the use as fuels, the constituents would be expected to incinerate at the high temperatures during burning.

Two analytical approaches are used in this study assess the fate of the relevant **marker constituents whilst considering supply chain interactions**:

- **Approach 3 (downstream - literature review & consultation & consideration of supply chain interactions**): Approach 3 further develops Approach 2 by screening the products which are subject to high-temperature processes further downstream (and which have the potential for the relevant constituents to be destroyed).
- **Approach 4 (upstream – literature review):** Approach 4 takes an upstream perspective and reviews the available literature on the presence of some of the relevant constituents in the relevant products, thus providing a back-to-front analysis of the potential uses/processes in which the shortlisted constituents may not be converted.

The advantages and disadvantages of these approaches are summarised below.

Table 19: Pros and cons of the two approaches that consider supply chain interactions

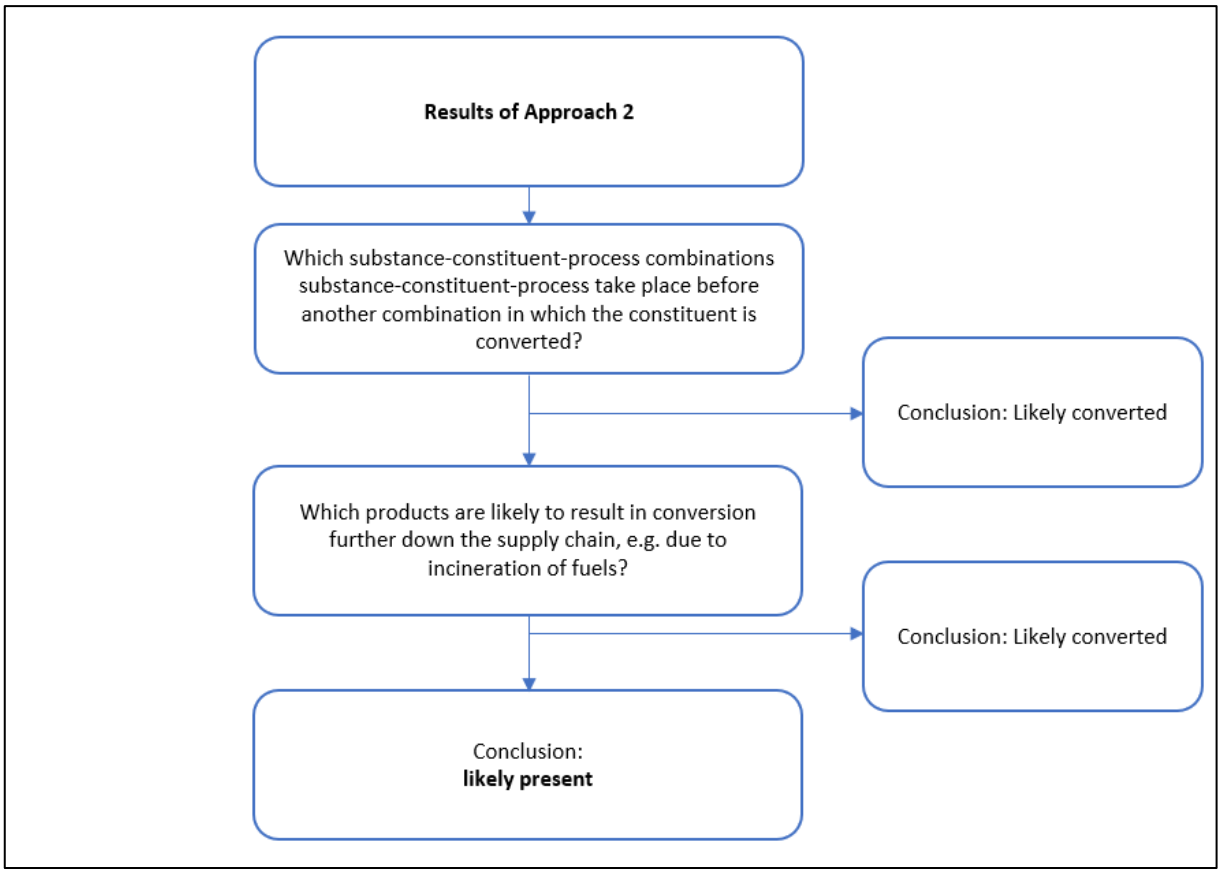
Approach	Advantages	Disadvantages
Approach 3 (downstream – literature review & consultation & supply chain)	Extensive use of stakeholder information Robust conclusions based on 'positive' identification Constituents likely to be converted further downstream screened out	Reliance on 'positive' identification means that this approach is highly likely to exclude situations in which these constituents remain The potential for such exclusion is greater than under Approach 2 due to the exclusion of 'combustive' processes further downstream
Approach 4 (upstream – literature review)	Upstream approach with most reliable conclusions about the presence of the constituents of concern in products Not based on experiences of individual stakeholders Concentration data available for some constituents-products and blending/finishing/other processes are thus indirectly taken into account	There are limited current data relevant to the EU, data used may not be representative of the current situation in the EU Does not differentiate between intermediate and non-intermediate uses Data on product composition are likely to be available only for products that have been highlighted as being of concern The focus is on the final part of the supply chain and it does not provide

Approach	Advantages	Disadvantages
		an indication of the potential for environmental releases in earlier stages

9.2 Approach 3: Downstream - literature review & consultation, incl. supply chain considerations - pass-through of marker constituents

Approach 3 is a further development of Approach 2 additionally screening out the products which are likely to be further processed by high-temperature processes such as combustion further downstream (fuels, coke, metals and minerals production). Approach 3 is shown graphically in Figure 11.

Figure 11 Approach 3: Literature review & consultation incl. consideration of the structure of the supply chain (direction: downstream)



Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

The table below provides a comparison of the results of Approaches 2 and 3.

Table 20: Comparison of the results of Approaches 2 and 3

Approach	Substance-constituent-process combinations	Of which confirmed intermediate use	Likely present	Likely converted (at any stage in the supply chain)
Approach 2	689	280 (same as above)	134	144
Approach 3	689 (same as above)	280 (same as above)	102*	175

Note: * As Table 18 but with fuels, coke, metals and minerals production screened out.

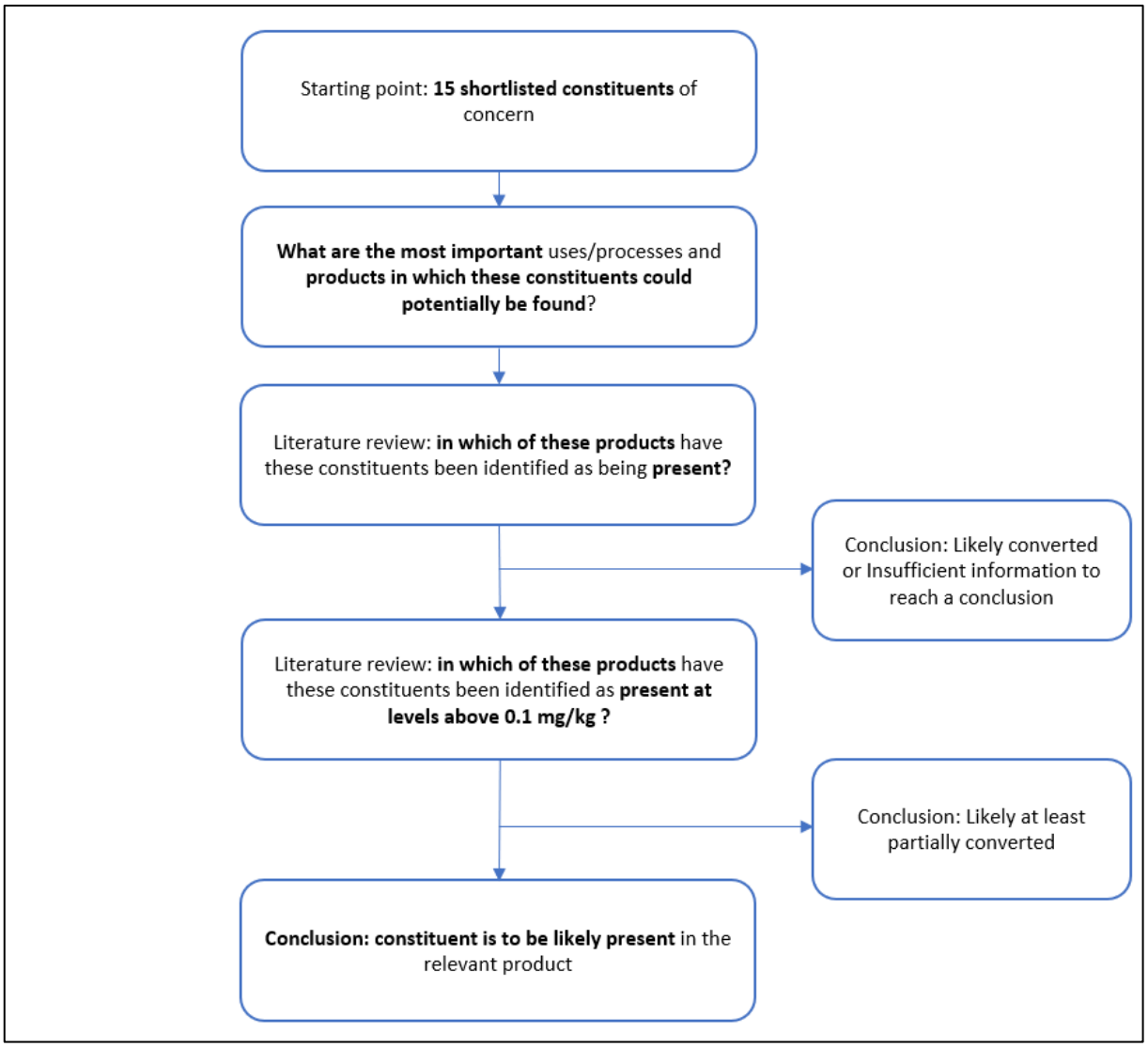
Whilst the robustness of 'positive identification' is even greater under Approach 3 than under Approach 2, Approach 3 also has several disadvantages: some products of the relevant processes are defined in a way that does not facilitate the screening of the subsequent processes, e.g. a product of distillation of coal tar is defined as 'coal tar fractions' which include both coal tar pitch high temperature (CTPHT) which is further processed by pyrolysis/carbonisation (i.e. high temperature processes which have a high likelihood of conversion of the relevant constituents) and other fractions for which more limited information was collected by this study.

It should also be noted that processing further downstream by high-temperature processes such as combustion (fuels, coke, metals and minerals production) has been indicated in stakeholder input as likely destroying the relevant constituents of concern but it is possible that these processes do not result in perfect destruction. For this reason, Approach 4 has been developed which relies on an upstream assessment involving a literature review of the presence of the fifteen constituents of concern in key products.

9.3 Approach 4: Upstream — literature review — pass-through of marker constituents

Approach 4 is summarised in the figure below.

Figure 12 Approach 4: Literature review incl. the supply chain (direction: upstream)



Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

Table 21 summarises the results of Approach 4. Cells marked with a ✘ show product-constituent combinations for which the reviewed literature does not identify the presence of the relevant constituent, cells marked with ✓✓ mark constituent/product combinations in which a level above 0.1 mg/kg is observed, those with a ✓ are ones where literature identifies the presence of a substance but does not specify a concentration value.

Table 21: Results of Approach 4

	benzo[k]fluoranthene	benz[a]anthracene	Fluoranthene	Anthracene	Phenanthrene	1-methylphenanthrene	4-pentylbiphenyl	1,3,5-tripropylbenzene	2-methylfluorene	Fluorene	Dibenzofuran
Fuels	✓	✓	✓	✓	✓	✓✓	✘	✓	✓	✓	✓✓
Perfumes, fragrances,	✓✓	✓✓	✓✓	✘	✓✓	✘	✘	✘	✘	✘	✘

	benzo[k]fluoranthene	benz[a]anthracene	Fluoranthene	Anthracene	Phenanthrene	1-methylphenanthrene	4-pentylbiphenyl	1,3,5-tripropylbenzene	2-methylfluorene	Fluorene	Dibenzofuran
cosmetics & personal care products											
Lubricants & Greases	✓	✓✓	✓	✓	✓	✗	✗	✗	✗	✓	✓✓
Adhesives & Sealants	✓	✓✓	✓	✓	✓	✗	✗	✗	✗	✓	✗
Polishes & Waxes	✗	✗	✗	✗	✓	✗	✗	✗	✗	✗	✗
Coatings	✓	✓	✓	✓	✓	✗	✗	✗	✗	✓	✗
Rubber Production & Processing	✓	✓	✓	✓	✓	✗	✗	✗	✗	✓	✗
Plant Protection Products	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓
Agriculture, Forestry & Fishing	✓	✓	✓	✓	✓	✓	✗	✗	✗	✓✓	✓
Coal tar fractions	✓	✓	✓	✓	✓	✗	✗	✗	✓	✓	✓
Carbon black	✓✓	✓✓	✓	✓✓	✓	✗	✗	✗	✗	✓	✗
Coke	✗	✗	✗	✗	✓	✗	✗	✗	✗	✗	✗
Graphite	✗	✗	✗	✓✓	✗	✗	✓✓	✗	✗	✓✓	✗
Inks & Toners	✓✓	✓✓	✓✓	✓✓	✓	✗	✗	✗	✗	✓✓	✗

Table 22 provides a comparison of the results of Approaches 3 and 4.

Table 22: Results of Approaches 3 and 4

Approach	Combinations examined	Of which confirmed intermediate use	Likely present	Likely converted (at any stage in the supply chain)
Approach 3	689 (substance-constituent-process-product combinations)	280 (40%)	Excl. fuels and coke 102 (15%)	175 (25%)
Approach 4	315 (potential constituent-product combinations)	Unknown	Excl. fuels and coke:	242 (80%)

Approach	Combinations examined	Of which confirmed intermediate use	Likely present	Likely converted (at any stage in the supply chain)
			19 (present> 0.1 mg/kg) (5%) 43 (present) (15%) Incl. fuels and coke: 21 (present> 0.1 mg/kg) (5%) 52 (present) (15%)	

The results of Approaches 3 and 4 are not directly comparable since, for example, Approach 4 does not differentiate between intermediate and non-intermediate uses of the relevant substances and since there is no certainty that the presence of the relevant constituents can be traced back to one of the 53 substances, and also because Approach 3 considers substance-constituent-process-product combinations whilst Approach 4 considers constituent-product combinations. Also, Approach 4 does not consider some of the products considered under Approach 3. However, Table 22 shows that, under both approaches, the constituents of concern are likely to be present in a number of products.

Although the study team focused on recent articles (post-2005), recent regulatory developments mean that some of the data may no longer be fully representative of the present day situation. For example, placing on the market for supply to the general public of articles containing polycyclic aromatic hydrocarbons (PAHs) is restricted by entry 50[13] of Annex XVII to REACH Regulation if any of their rubber or plastic components that come into direct as well as prolonged contact or short-term repetitive contact with human skin or the oral cavity contain more than 1 mg/kg (0,0001% by weight of this component) of any of the 8 PAHs listed in the restriction. In addition, some of the identified studies provide data for non-EU jurisdictions with different regulatory regimes for chemicals.

Table 23 provides a comparison of the products in which constituents of concern were identified as potentially present under either Approach 3 or 4. Cells marked with ✓✓ show instances in which both Approaches 3 and 4 identified the potential presence of the constituent. Where only one approach identified the potential presence of the constituent, this is shown with a '✓2', '✓3' or '✓4' for the relevant approach – please note that all combinations identified under Approach 3 were also identified under Approach 2. Where neither approach identified the presence of a constituent, this is shown with a ✘. Please note that only product categories considered under Approach 4 are included in Table 21 and some additional product categories were considered under Approach 3 (e.g. anti-freeze, metal working fluids, heat transfer fluids, hydraulic fluids, substances, etc.).

A full summary of the results of Approaches 1-4 is provided in Annex 12.

[13] https://echa.europa.eu/documents/10162/4f099937-658f-8b86-2f62-5e767fab4d6e

Table 23: Results of Approaches 2, 3 and 4

	benzo[k]fluoranthene	benz[a]anthracene	Fluoranthene	Anthracene	Phenanthrene	1-methylphenanthrene	4-pentylbiphenyl	1,3,5-tripropylbenzene	2-methylfluorene	Fluorene	Dibenzofuran	2,4-dimethylheltyld	Diethylbiphenyl	2,3,4,5-tetramethyldec	3-methyldecane
Fuels	✓✓	✓✓	✓✓	✓✓	✓✓	✓4	✗	✓✓	✓4	✓✓	✓4	✗	✓ 2	✗	✗
Perfumes, fragrances, cosmetics & personal care products	✓4	✓4	✓4	✗	✓4	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Lubricants & Greases	✓4	✓4	✓4	✓4	✓4	✗	✗	✓ 3	✗	✓✓	✓4	✓ 3	✗	✓ 3	✓ 3
Adhesives & Sealants	✓4	✓4	✓4	✓4	✓✓	✗	✗	✗	✗	✓✓	✗	✓ 3	✗	✓ 3	✓ 3
Polishes & Waxes	✗	✗	✗	✗	✓✓	✗	✗	✗	✗	✓ 3	✗	✓ 3	✗	✓ 3	✓ 3
Coatings	✓4	✓4	✓4	✓4	✓✓	✗	✗	✗	✗	✓✓	✗	✓ 3	✗	✓ 3	✓ 3
Rubber Production & Processing	✓4	✓4	✓4	✓✓	✓✓	✗	✗	✓ 3	✗	✓✓	✗	✓ 3	✗	✗	✗
Plant Protection Products	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓4	✓ 3	✗	✗	✗
Agriculture, Forestry & Fishing	✓4	✓4	✓4	✓✓	✓✓	✓4	✗	✓ 3	✗	✓✓	✓4	✓ 3	✗	✗	✗
Coal tar fractions	✓✓	✓✓	✓✓	✓✓	✓✓	✓ 3	✗	✗	✓✓	✓✓	✓✓	✗	✗	✗	✗
Carbon black	✓✓	✓✓	✓4	✓4	✓4	✗	✗	✗	✗	✓4	✓ 3	✗	✗	✗	✗
Coke	✗	✗	✗	✗	✓4	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Graphite	✗	✗	✗	✓4	✗	✗	✓4	✗	✗	✓4	✗	✗	✗	✗	✗
Inks & Toners	✓4	✓4	✓4	✓✓	✓✓	✗	✗	✓ 3	✗	✓✓	✗	✓ 3	✗	✗	✗

There is a large degree of agreement between the different approaches for some product categories such as fuels, rubber, agriculture, forestry and fishing, coal tar fractions, carbon black and inks and toners. As regards specific constituents, the results of the approaches agree to the greatest degree for phenanthrene, fluorene, anthracene, benzo[k]fluoranthene and benz[a]anthracene. Interestingly, some of the information in the literature contradicts the outcome of Approaches 1-3 (e.g. for inks and toners, graphite, carbon black) including for products which are derived using high temperature processes. The fate of the the shortlisted marker constitents, as a summary of appoaches 1-4, is provided as Annex 12.

10 Step 8: Overview of the potential for process releases/environmental releases

10.1 Introduction

Emissions into the environment can potentially occur through a variety of pathways, both during the uses considered in this study (where a constituent is not reacted) as well as during downstream use, the useful life and end-of-life disposal of the relevant end-products.

The term 'release' is used in this study in the sense of process releases (before end-of-pipe mitigation measures) (see Figure 13) and the term 'emission' is used more in the context of finally ending up in the relevant environmental compartment. In many cases, it should be noted that the terms "release" and "emission" are often used interchangeably in the literature. However, this study differentiates between them whenever possible.

Table 24: Potential emission routes

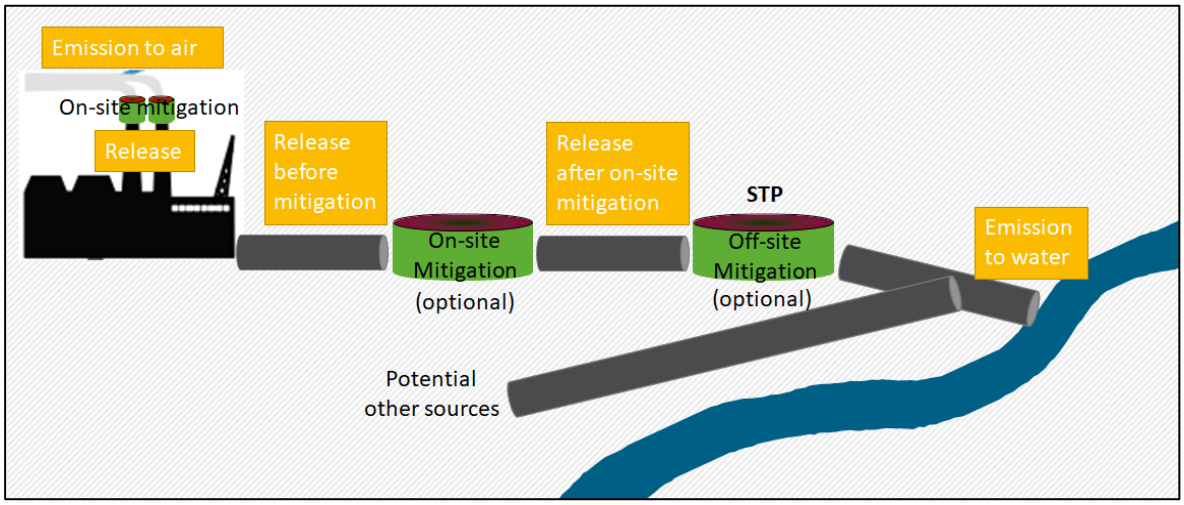
Stage	Air	Water	Soil	Waste
Intermediate use	Direct emissions Indirect: waste incineration	Direct emissions	Direct emissions Indirect: sewage sludge	Waste incineration: air, soil Wastewater treatment: water, soil
Downstream uses/end-product use and disposal	Direct emissions from use Direct emissions from further processing Indirect: waste incineration	Direct emissions from use Direct emissions from further processing Indirect: wastewater disposal	Direct emissions from use Direct emissions from further processing Indirect: sewage sludge	Waste incineration: air, soil Wastewater treatment: water, soil Landfilling: water, soil

As can be seen from Table 24, there is a potential for emissions to occur at both the intermediate use stage as well as further downstream, including during the use and disposal of the relevant end-products. These two value chain stages are dealt with in the subsequent sections.

10.2 Intermediate use stage

In the upstream stages of the value chain, this study focuses on the potential for environmental emissions which arise from both direct emissions to air, water and soil, as well as indirect emissions via waste. The potential for direct emissions is shown schematically in Figure 13, differentiating between releases and emissions.

Figure 13 Releases and emissions from industrial plant and potential associated risk mitigation measures



Source: own illustration, ARCHE Consulting, Gent, Belgium

The potential of emissions to air and wastewater are, under REACH, conservatively described by the so-called ERC (Environmental Release Categories) or, more specifically for the petroleum and solvent sector by the SPERCs (Sector Specific Environmental Release Categories) developed by ESIG (European Solvents Industry Group). These SPERCs are based on a variety of sources including former A-tables (from the New & Existing Substance Directive), OECD emission scenario documents, US EPA documents and CONCAWE emission inventories. Several SPERCs have release fractions that are dependent on the water solubility (for release to water) and vapor pressure (for release to air). The general assumption in ESIG/ESVOC SPERCs and PETRORISK is that increasing vapor pressure leads to increasing release to air and increasing water solubility leads to increasing release to water. It is, however, possible that constituents with low solubility and vapour pressure may also be emitted into the environment where sewage sludge is used in agriculture or where they are not fully destroyed during waste incineration.

The SPERCs published by ESIG for petroleum substances and petrochemicals include ESVOC SPERC 6.1a.v2 which is applicable to use as a chemical intermediate:

> *Use of the substance as an intermediate (not related to Strictly Controlled Conditions). Includes recycling/ recovery, material transfers, storage, sampling, associated laboratory activities, maintenance and loading (including marine vessel/barge, road/rail car and bulk container).*

It is of note that some of the intermediate uses of PetCo substances considered in this study are on-site isolated intermediates (Article 17 of REACH), some are transported isolated intermediates where the subsequent synthesis of (an)other substance(s) from that intermediate takes place under strictly controlled conditions (Article 18(4) of REACH). For approximately one half of confirmed intermediate uses of PetCo substances, the precise nature of intermediate use was not identified by this study.

The SPERC for intermediate use encompasses a number of sub-SPERCs which are defined by the vapour pressure and water solubility of the relevant substance/constituent.

This section provides the following information:

- an overview of the chemical characteristics of the relevant constituents (vapour pressure and water solubility);
- a summary of the release rates in the intermediate use SPERC for the relevant constituents, i.e. those that under Approach 2 are expected not to be converted and for which it is therefore expected that there may be some potential for their release. This is complemented with a summary of the information collected for this study; and
- model fate in wastewater treatment plants (WWTPs) to assess the potential emissions to the different environmental compartments from WWTPs (not modelled in SPERCs and considered separately).

10.2.1 Characteristics of the relevant constituents

Table 25 and 26 present the data for water solubility and vapour pressure for the marker constituents for which under Approach 2 it was concluded that it is likely that they are not converted in the relevant processes. These can be treated as a crude proxy for their release potential to wastewater and air respectively, leading to the following conclusions.

- SPAC, naphthenic aromatics and triaromatics show the highest release potential to wastewater
- Iso/heavily branched paraffins, mono aromatics and naphthenic non aromatics show the highest release potential to air.

Table 25 Water solubility

Name	Constituent group	Solubility (mg/l)
1,3,5-tripropylbenzene	mono-aromatics	0.0996
1-methylphenanthrene	triaromatics, branched	0.263
2,3,4,5-Tetramethyldecane	heavily branched paraffins/iso-paraffins	0.0159
2,4-dimethylheptyldecahydronaphthalene	naphthenics (non aromatics), branched	0.000385
2-methylfluorene	naphthenic aromatics, branched	0.541
3-methyltridecane	heavily branched paraffins/iso-paraffins	0.01028
4-pentylbiphenyl	diaromatics	0.1446
Anthracene	triaromatics, non branched	0.691
Benz[a]anthracene	polyaromatics	0.02907

Name	Constituent group	Solubility (mg/l)
Benzo[k]fluoranthene	polyaromatics	0.0108
Dibenzofuran	SPAC	1.48
Diethylbiphenyl	diaromatics	0.403
Fluoranthene	polyaromatics	0.1297
Fluorene	naphthenic aromatics, non branched	1.34
Phenanthrene	triaromatics, non branched	0.677

Table 26 Vapour pressure

Name	Constituent group	Vapor pressure (Pa)
1,3,5-tripropylbenzene	mono-aromatics	0.476
1-methylphenanthrene	triaromatics, branched	0.0438
2,3,4,5-Tetramethyldecane	heavily branched paraffins/iso-paraffins	77.4
2,4-dimethylheptyldecahydronaphthalene	naphthenics (non aromatics), branched	0.252
2-methylfluorene	naphthenic aromatics, branched	0.19
3-methyltridecane	heavily branched paraffins/iso-paraffins	0.000142134
4-pentylbiphenyl	diaromatics	0.0000002792
Anthracene	triaromatics, non branched	0.000998
Benz[a]anthracene	polyaromatics	0.000000004646
Benzo[k]fluoranthene	polyaromatics	0.00000292
Dibenzofuran	SPAC	0.133
Diethylbiphenyl	diaromatics	0.0163
Fluoranthene	polyaromatics	0.000000037
Fluorene	naphthenic aromatics, non branched	0.109

Name	Constituent group	Vapor pressure (Pa)
Phenanthrene	triaromatics, non branched	0.0000001961838

10.3 Release rates in the intermediate use SPERC

The intermediate use SPERC contains a number of sub-SPERCs for substances with different water solubility (WS) and vapour pressure (VP). The estimated release rates are thus dependent on WS and VP and do not differentiate between the different intermediate uses. The release rates for the constituents that are expected not to be converted (under Approach 2) are summarised below.

Table 27 Intermediate use SPERC – emission or release factors for the relevant constituents

Name	Constituent group	Air (1)	Water (2)	Soil (3)	Waste (4)
1,3,5-tripropylbenzene	mono-aromatics	0%	0.001%	0.1%	5%
1-methylphenanthrene	triaromatics, branched	0%	0.001%	0.1%	5%
2,3,4,5-Tetramethyldecane	heavily branched paraffins/iso-paraffins	0%	0.003%	0.1%	5%
2,4-dimethylheptyldecahydronaphthalene	naphthenics (non aromatics), branched	0%	0.001%	0.1%	5%
2-methylfluorene	naphthenic aromatics, branched	0%	0.001%	0.1%	5%
3-methyltridecane	heavily branched paraffins/iso-paraffins	0%	0.001%	0.1%	5%
4-pentylbiphenyl	diaromatics	0%	0.001%	0.1%	5%
Anthracene	triaromatics, non branched	0%	0.001%	0.1%	5%
Benz[a]anthracene	polyaromatics	0%	0.001%	0.1%	5%
Benzo[k]fluoranthene	polyaromatics	0%	0.003%	0.1%	5%
Dibenzofuran	SPAC	0%	0.003%	0.1%	5%
Diethylbiphenyl	diaromatics	0%	0.003%	0.1%	5%
Fluoranthene	polyaromatics	0%	0.003%	0.1%	5%
Fluorene	naphthenic aromatics, non branched	0%	0.003%	0.1%	5%
Phenanthrene	triaromatics, non branched	0%	0.001%	0.1%	5%

Name	Constituent group	Air (1)	Water (2)	Soil (3)	Waste (4)

Notes:
Not adjusted for use of RMMs (Risk Management Measures).
Wastewater RMM removal efficiencies are typically substance- and site-specific, and therefore are not explicitly assumed in the SPERC, i.e. this is a release factor. See the section for WWTP modelling for more detail on the fate in waste-water.
RMMs are not assumed in the SPERC.
Refers to solid waste. Subsequent treatment methods are not known.

The table above suggests that the release factor for substances with the characteristics of the relevant constituents are 0% for air emissions and 0.001% and 0.003% of the use amounts for water. Emissions into the soil are estimated to be 0.1%. The greatest potential for emissions is expected to be via waste (the category 'waste' in the table above refers to solid waste). However, as noted by one of the consultees, principal hydrocarbon streams are not typically treated as waste which would be impractical due to their volume. Waste streams containing the constituents relevant to this questionnaire are primarily emissions to air and water. Minor amounts may also be extracted during cleaning and maintenance including shutdowns.

In general, limited data for environmental emissions is available. A comment provided by one consultee was that for environmental exposures 'All legally required compliance checks are conducted' and that 'companies are legally obliged to monitor the emissions from their plants and to keep records of such monitoring in accordance to EU and National requirements.' However, this is unlikely to involve the monitoring of the specific constituents of potential concern considered in this study. In addition, such monitoring does not cover the potential for environmental emissions from products further downstream.

Potential for environmental release during intermediate application was reported by one consultee as off-gas treatment and that mitigation measures in place were technical measures (e.g. exhaust ventilation, incineration) and personal protection equipment (PPE). Another general comment was that emissions are not distinguished per process but instead total emissions are monitored per site.

R4CC explained that the raw material for coal chemicals is Tar, coal, high-temp. [EC# 266-024-0# (COT). COT is consumed in a dedicated refinery at the end of its life cycle, and is separated by distillation according to the volatility of constituents, to be collected in separate tanks. The residue and distillation cuts may be further processed by re-distillation, extraction or formulation to obtain UVCB substances with specific properties. These processes take place in closed systems. Tank sludge is formed over the years, requiring discharge for waste incineration. Process water is treated and finally forwarded to an authorised sewage treatment unit. Off-gases are condensed and recycled or incinerated.

The refinery depends on a 100 % consumption of the raw material. Therefore, all fractions are sold for specific uses or used as fuel. R4CC claim that there is no real waste from the production of these products, and that any by-products are recycled after purification.

The plants using coal chemicals fall under the national implementation of Directive 2010/75/EU and are under a regime of permit requirements and inspections by authorities. Permits are based on BAT conclusions as issued by the EU Commission. Most plants are classified SEVESO plants, and therefore operate under an extended safety regime to prevent hazardous related major incidents.

It was pointed out by R4CC that the environmental release from COT conversion into new UVCB substance cannot be assigned to single substances. Usually, the total emissions of a refinery are reported as more substances are manufactured at the same production step to avoid multiple counting of emissions when evaluating the environmental release of the manufacturing process. This evaluation occurs on a substance-by-substance basis, and is not performed in parallel. Therefore, the same emission can be accounted for several times, resulting in an overestimation in some cases for single products.

R4CC commented that minimising harmful releases to air, water and soil in typical operations is a continuous improvement process, as is the prevention of incidents that may lead to releases.

10.4 WWTP emission modelling

10.4.1 SimpleTreat

The fate of the different compounds in wastewater treatment plants has been modelled using the SimpleTreat assessment tool. This tool considers the most relevant processes such as adsorption, degradation, mixing and volatilization in a biological treatment design (with aeration tanks and primary/secondary clarifiers). A possible input parameter is half-life in wastewater treatment plant. However, as the selected constituents are suspected to be persistent or very persistent it was decided to model the WWTP emissions without degradation in order to consider the worst case scenario. SimpleTreat is also embedded in EUSES, the regulatory environmental exposure assessment tool under REACH and BPR EU legislations. There are currently two available versions of SimpleTreat: v3.1 and the updated v4.0. Both of them has been tested and compared, with almost identical results. Therefore, it was chosen to proceed with the newer version v4.0 (Struijs J, 2014).

The following input parameters were specified for each constituent:

- Henry coefficient
- Molecular weight
- Organic carbon partition coefficient
- Octanol-water partition coefficient
- Solubility
- Vapor pressure

The physical and chemical properties of the majority of the constituents have been retrieved from the PETRORISK library. Values for the other constituents were calculated with EPISuite (US EPA, 2012) via the OECD QSAR toolbox (OECD, 2015).

Besides the selected markers and back-up markers, some supplementary constituents were also modelled to cover the full carbon range of the selected constituent groups.

10.4.2 Summary WWTP emission assessment

The outcome of the assessment is represented in Table 28. For comparison, the results are represented per constituent group/branched indication/carbon number. The relevant marker constituents are indicated in bold.

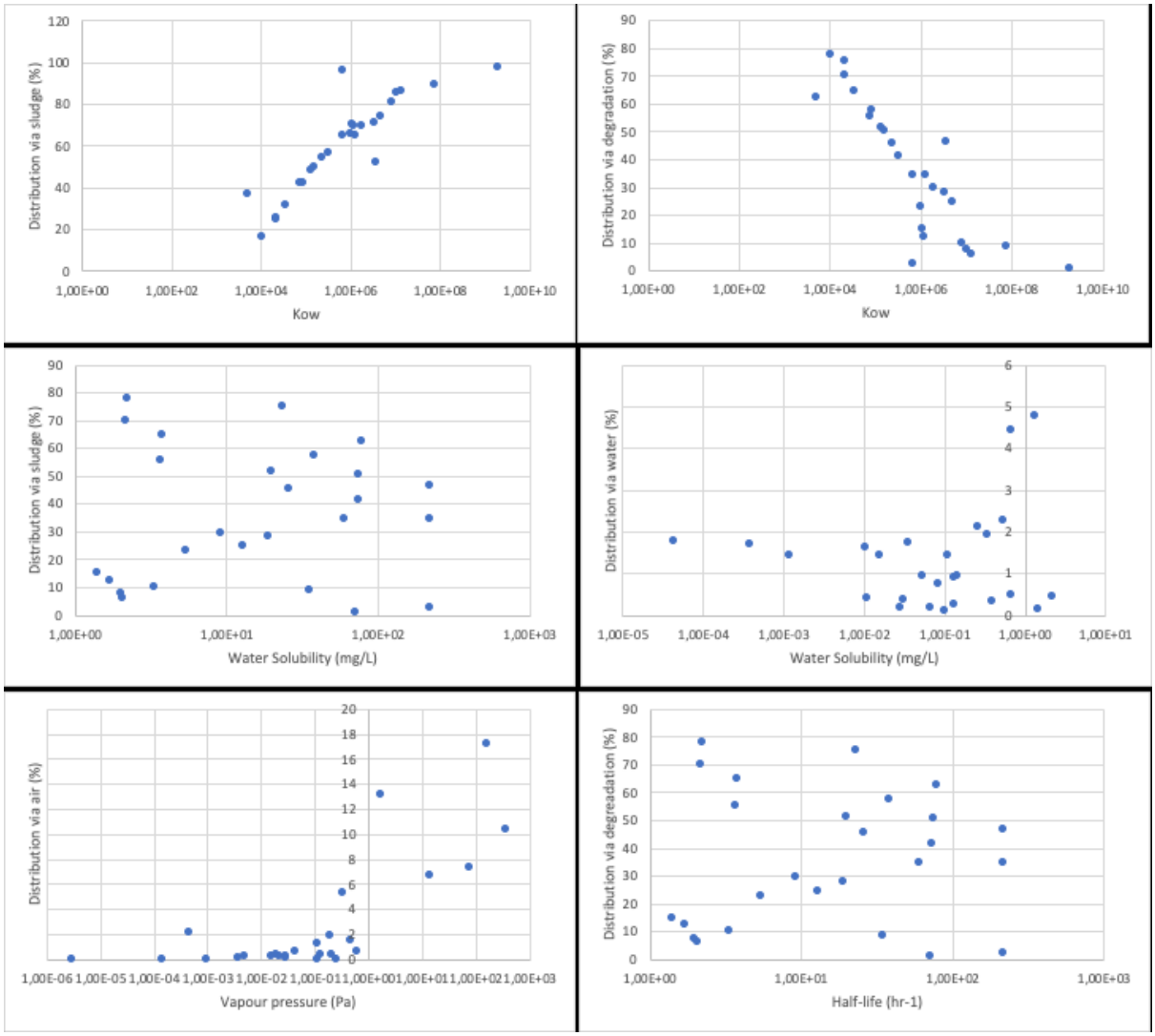
It can be seen that for all constituents, the majority of the content was eliminated via sludge (although a large proportion of sludge is used in agriculture, it is expected that sludge from wastewater from intermediate use of PetCo chemicals is not used in agriculture; the intermediate use Specific Environmental Release Category (SPERC) presumes that a site-specific waste water treatment plant (WWTP) is in place rather than a standard municipal WWTP). For larger molecules, small release to air can be observed, which can be explained by their corresponding higher boiling points and vapor pressure. It can be also noted for all constituents that the higher the number of branches the smaller the release to water.

Regarding the specific constituent groups, some further observations can be made.

- Non-aromatic containing constituent group: iso-/heavily branched paraffins and naphthenic non aromatics show for higher emission to water for larger constituents
- Aromatic containing constituent groups: “jumps” in the behavior can be recognized per extra ring
  - For mono aromatics and Tri-aromatic constituents, smaller constituents are corresponding to more emission to water
  - For Diaromatics (biphenyls) and Poly-aromatics (containing 4 rings), larger constituents are corresponding to more emission to water

When looking at the physicochemical properties of the constituents, similar observations can be made. Higher molecules are linked to higher molecular weight, higher Kow and Koc values while they also relate to lower solubility. The vapour pressure is an important predictor for the distribution to air (see Figure 14). The octanol water partition coefficient K_{ow} is an important predictor for the distribution to sludge, the higher it is the more adsorption onto sludge can be observed. It is more difficult to relate physico-chemical properties to distribution to water.

Figure 14 Impact of physicochemical properties on fate in wastewater treatment plants for selected constituents



Source: own illustration, Risk & Policy Analysts Ltd, Norwich, United Kingdom

Table 28 SimpleTreat modelling output, results of the exposure assessment in waste water treatment plant (constituents in bold are those selected for a detailed assessment in this study)

Details on constituents (bold constituents are those selected for a detailed assessment in this study)				Distribution (%)		
Name	**Constituent group**	**Branched**	**carbon number**	**to air**	**to water**	**via sludge**
diethylbiphenyl	**diaromatics**	**yes**	**16**	**6.69**	**5.64**	**87.67**
4-pentylbiphenyl	diaromatics	yes	17	1.00	5.71	93.29
4-iso-Hexylbiphenyl	diaromatics	yes	18	0.94	3.59	95.47
2,6-Diethyloctane	iso-paraffins	yes	12	26.18	2.04	71.78
3-methyltridecane	iso-Paraffins	yes	14	8.92	1.91	89.18
3,3,6,6-Tetramethyloctane	heavily branched paraffins/iso-paraffins	yes	12	27.69	2.06	70.26
2,3,4,5-Tetramethyldecane	**heavily branched paraffins/iso-paraffins**	**yes**	**14**	**11.90**	**1.93**	**86.17**
1,3-Dibutylbenzene	mono-aromatics	yes	14	22.19	3.12	74.69
1,3,5-tripropylbenzene	**mono-aromatics**	**yes**	**15**	**42.26**	**2.61**	**55.14**
1,3-Dipentylbenzene	mono-aromatics	yes	16	7.50	2.18	90.32
Fluorene	**naphthenic aromatics**	**no**	**13**	**8.37**	**68.38**	**23.25**
Tetrahydro-phenanthrene	naphthenic aromatics	no	14	3.25	26.85	69.89
Benzo(a)fluorene	naphthenic aromatics	no	17	0.03	26.70	73.27
2-methylfluorene	**naphthenic aromatics, branched**	**yes**	**14**	**14.78**	**41.74**	**43.47**

Details on constituents (bold constituents are those selected for a detailed assessment in this study)				Distribution (%)		
n-Propyl-tetrahydro-phenanthrene	naphthenic aromatics, branched	yes	17	0.74	4.26	95.00
2,6 dimethyl heptyl hexahydroindane	naphthenics (non aromatics)	yes	18	2.69	1.85	95.47
2,4-dimethylheptyldecahydronaphthalene	**naphthenics (non aromatics)**	**yes**	**19**	**0.47**	**1.83**	**97.71**
2,4,6 trimethyloctyl-2-decalin	naphthenics (non aromatics)	yes	21	0.21	1.82	97.96
benz[a]anthracene	polyaromatics	no	18	37.64	2.27	60.09
benzo[k]fluoranthene	**polyaromatics**	**no**	**20**	**0.00**	**7.35**	**92.65**
dibenzofuran	**SPAC**	**no**	**13**	**4.65**	**40.63**	**54.73**
anthracene	**triaromatics, non branched**	**no**	**14**	**0.11**	**63.13**	**36.76**
phenantrene	triaromatics, non branched	no	14	2.20	61.30	36.50
Fluoranthene	triaromatics, non branched	no	16	0.56	36.59	62.85
1-methylphenanthrene	**triaromatics, branched**	**yes**	**15**	**4.92**	**35.15**	**59.93**
2-Ethyl anthracene	triaromatics, branched	yes	16	2.16	19.46	78.37

10.5 Downstream use and end-product useful life and end-of-life

The potential for environmental emissions further downstream is significant. For example, as noted in Table 23 in Section 8 (comparison of the results of Approaches 2, 3, and 4), there is a potential for lubricants & greases to contain some of the constituents considered in this study. In this regard, the following sectors are hereby listed as downstream users of lubricants & greases:

- Automotive manufacturing
- Aerospace
- Machinery
- Metals
- Mining
- Wind
- Chemicals
- Engineered wood
- Food and beverage
- Metal goods
- Power generation
- Pulp and paper
- Sugar

Due to the large number of downstream sectors where the relevant products may be used and due to the limited quantitative data for constituent concentrations in products, a comprehensive overview of the potential for environmental emissions from downstream/product use is not provided in this study.

However, some insights can be gleaned from the relevant SPERCs. The scope of the SPERCs for the constituents (and processes) for which it was concluded in Section 8 that are unlikely to be converted is summarised below.

Table 29 Potentially relevant SPERCs

Product	SPERC (s)	Scope
Lubricants & Greases	SPERC 08: Lubricants, industrial	Covers the use of formulated lubricants in closed and open systems including transfer operations, operation of machinery/engines and similar articles, reworking on reject articles, equipment maintenance and disposal of wastes.
Lubricants & Greases	SPERC 08: Lubricants, professional (high release)	Covers the use of formulated lubricants in closed and open systems including transfer operations, operation of engines and similar articles,

Product	SPERC (s)	Scope
		reworking on reject articles, equipment maintenance and disposal of waste oil.
Lubricants & Greases	SPERC 08: Lubricants, professional - low exposure	As above
Lubricants & Greases	SPERC 08: Consumer - high release	Covers the consumer use of formulated lubricants in closed and open systems including transfer operations, application, operation of engines and similar articles, equipment maintenance and disposal of waste oil.
Lubricants & Greases	SPERC 08: Consumer - low release	As above
Coating	SPERC 03: Uses in coatings - industrial	Covers the use in coatings (paints, inks, adhesives, etc) including exposures during use (including materials receipt, storage, preparation and transfer from bulk and semi-bulk, application by spray, roller, spreader, dip, flow, fluidised bed on production lines and film formation) and equipment cleaning, maintenance and associated laboratory activities.
Coating	SPERC 03: Uses in coatings - professional	Covers the use in coatings (paints, inks, adhesives, etc) including exposures during use (including materials receipt, storage, preparation and transfer from bulk and semi-bulk, application by spray, roller, brush, spreader by hand or similar methods, and film formation), and equipment cleaning, maintenance and associated laboratory activities.
Coating	SPERC 03: Uses in coatings - consumer	Covers the use in coatings (paints, inks, adhesives, etc) including exposures during use (including product transfer and preparation, application by brush, spray by hand or similar methods) and equipment cleaning.
Polishes & Waxes	SPERC 06: Cleaning agents, industrial	Covers the use as a component of cleaning products including transfer from storage, pouring/unloading from drums or containers. Exposures during mixing/diluting in the preparatory phase and cleaning activities (including spraying, brushing, dipping, wiping, automated and by hand), related equipment cleaning and maintenance.
Polishes & Waxes	SPERC 06: Cleaning agents, professional	Covers the use as a component of cleaning products including pouring/unloading from drums or containers; and exposures during mixing/diluting in the preparatory phase and cleaning activities (including spraying, brushing, dipping, wiping automated and by hand).
Polishes & Waxes	SPERC 06: Cleaning agents, consumer	Covers general exposures to consumers arising from the use of household products sold as washing and cleaning products, aerosols, coatings, de-icers, lubricants and air care products.
Rubber Production & Processing	SPERC 19: Rubber production and processing	Manufacture of tyres and general rubber articles, including processing of raw (uncured) rubber, handling and mixing of rubber additives, vulcanising, cooling and finishing.

Product	SPERC (s)	Scope
Anti-freeze	SPERC 15: De-icing - professional	Ice prevention and de-icing of vehicles, aircraft and other equipment by spraying
Anti-freeze	SPERC 15: De-icing - consumer	De-icing of vehicles and similar equipment by spraying
Metal Working Fluids	SPERC 9: Metal working fluids - industrial	Covers the use in formulated MWFs/rolling oils including transfer operations, rolling and annealing activities, cutting/machining activities, automated and manual application of corrosion protections (including brushing, dipping and spraying), equipment maintenance, draining and disposal of waste oils.
Metal Working Fluids	SPERC 9: Metal working fluids - professional	Covers the use in formulated MWFs including transfer operations, open and contained cutting/machining activities, automated and manual application of corrosion protections, draining and working on contaminated/ reject articles, and disposal of waste oils.
Hydraulic fluids & heat transfer fluids	SPERC 14: Functional fluids - industrial	Use as functional fluids e.g. cable oils, transfer oils, coolants, insulators, refrigerants, hydraulic fluids in industrial equipment including maintenance and related material transfers
Hydraulic fluids & heat transfer fluids	SPERC 14: Functional fluids - consumer	Use of sealed items containing functional fluids e.g. transfer oils, hydraulic fluids, refrigerants
Agriculture, Forestry & Fishing	SPERC 12: Agrochemical uses (biocidal product) - professional - biocidal product	Use as an agrochemical excipient for application by manual or machine spraying, smokes and fogging; including equipment clean-downs and disposal.
Agriculture, Forestry & Fishing	SPERC 12: Agrochemical uses (biocidal products) - consumer	Covers the consumer use in agrochemicals in liquid and solid forms.
Fuels	SPERC 13: Use as fuel - industrial	Covers the use as a fuel (or fuel additive) and includes activities associated with its transfer, use, equipment maintenance and handling of waste.
Fuels	SPERC 13: Use as fuel - professional	Covers the use as a fuel (or fuel additive) and includes activities associated with its transfer, use, equipment maintenance and handling of waste.
Fuels	SPERC 13: Use as fuel - consumer	Covers consumer uses in liquid fuels

The relevant data from the SPERCs for the constituents and processes identified where it was concluded in Section 8 that these constituents are unlikely to be converted is summarised below.

Table 30 Potentially relevant SPERCs other than the intermediate use SPERC – release factors for the relevant constituents

Product/output of intermediate use	SPERC	Constituent(s)	Air	Water	Soil	Waste
Lubricants & Greases	SPERC 08: Lubricants, industrial	1,3,5-tripropylbenzene, 2,4-dimethylheptyldecahydronaphthalene, 3-methyltridecane	0.01%	0.0001 %	0.1%	1%
Lubricants & Greases	SPERC 08: Lubricants, industrial	Fluorene	0.05%	0.0001 %	0.1%	1%
Lubricants & Greases	SPERC 08: Lubricants, industrial	2,3,4,5-Tetramethyldecane	0.1%	0.0001 %	0.1%	1%
Lubricants & Greases	SPERC 08: Lubricants, professional (high release)	1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene, 3-methyltridecane	0.5%	5%	5%	35%
Lubricants & Greases	SPERC 08: Lubricants, professional (high release)	2,3,4,5-Tetramethyldecane	1.5%	5%	5%	35%
Lubricants & Greases	SPERC 08: Lubricants, professional - low exposure	1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	**5%**	1%	1%	35%
Lubricants & Greases	SPERC 08: Consumer - high release	1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene, 3-methyltridecane	0.5%	5%	5%	35%
Lubricants & Greases	SPERC 08: Consumer - high release	2,3,4,5-Tetramethyldecane	1.5%	5%	5%	35%
Lubricants & Greases	SPERC 08: Consumer - low release	1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	**5%**	1%	1%	15%

Product/output of intermediate use	SPERC	Constituent(s)	Air	Water	Soil	Waste
Coating	SPERC 03: Uses in coatings - industrial	Phenanthrene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	98%	0.002 %	0%	5%
Coating	SPERC 03: Uses in coatings - professional	Phenanthrene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	98%	1%	1%	2%
Coating	SPERC 03: Uses in coatings - consumer	Phenanthrene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	98.5%	1%	0.5%	7%
Polishes & Waxes	SPERC 6: Cleaning agents, industrial	2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	98%	0.0000 1%	0%	4%
Polishes & Waxes	SPERC 6: Cleaning agents, professional	2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	4%	0.0001 %	0.0000 2%	4%
Polishes & Waxes	SPERC 6: Cleaning agents, consumer	2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	95%	2.5%	2.5%	4%
Rubber Production & Processing	SPERC 19: Rubber production and processing	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene, 2,4-dimethylheptyldecahydronaphthalene	1%	0.001 %	0.01%	4%
Rubber Production & Processing	SPERC 19: Rubber production and processing	Fluorene	1%	0.003 %	0.01%	4%

Product/output of intermediate use	SPERC	Constituent(s)	Air	Water	Soil	Waste
Anti-freeze	SPERC 15: De-icing - professional	Anthracene, Phenanthrene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	95%	1%	4%	10%
Anti-freeze	SPERC 15: De-icing - consumer	Anthracene, Phenanthrene, 2,4-dimethylheptyldecahydronaphthalene, 2,3,4,5-Tetramethyldecane, 3-methyltridecane	95%	1%	4%	10%
Metal Working Fluids	SPERC 9: Metal working fluids - industrial	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene, 2,4-dimethylheptyldecahydronaphthalene	5%	0.0001 %	0%	10%
Metal Working Fluids	SPERC 9: Metal working fluids - industrial	Fluorene	5%	0.0003 %	0%	10%
Metal Working Fluids	SPERC 9: Metal working fluids - professional	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene	0.5%	5%	0%	20%
Hydraulic fluids & heat transfer fluids	SPERC 14: Functional fluids - industrial	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene, 2,4-dimethylheptyldecahydronaphthalene	0.001 %	0.0001 %	0.1%	1%
Hydraulic fluids & heat transfer fluids	SPERC 14: Functional fluids - industrial	Fluorene	0.01%	0.0003 %	0.1%	1%
Hydraulic fluids & heat transfer fluids	SPERC 14: Functional fluids - consumer	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene	5%	5%	5%	15%
Agriculture, Forestry & Fishing	SPERC 12: Agrochemical uses (biocidal product) -	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene,	90%	1%	9%	5%

Product/output of intermediate use	SPERC	Constituent(s)	Air	Water	Soil	Waste
	professional - biocidal product	Fluorene, 2,4-dimethylheptyldecahydronaphthalene				
Agriculture, Forestry & Fishing	SPERC 12: Agrochemical uses (biocidal products) - consumer	Anthracene, Phenanthrene, 1,3,5-tripropylbenzene, Fluorene, 2,4-dimethylheptyldecahydronaphthalene	90%	1%	9%	15%
Fuels	SPERC 13: Use as fuel - industrial	Benzo[k]fluoranthene, Anthracene, Fluoranthene, Benz[a]anthracene, Fluorene, Phenanthrene, Diethylbiphenyl, 1,3,5-tripropylbenzene	0.6%	0.001 %	0%	2%
Fuels	SPERC 13: Use as fuel - professional	Benzo[k]fluoranthene, Anthracene, Fluoranthene, Benz[a]anthracene, Fluorene, Phenanthrene, Diethylbiphenyl, 1,3,5-tripropylbenzene	0.5%	0.0001 %	0.025 %	2%
Fuels	SPERC 13: Use as fuel - consumer	Benzo[k]fluoranthene, Anthracene, Fluoranthene, Benz[a]anthracene, Fluorene, Phenanthrene, Diethylbiphenyl, 1,3,5-tripropylbenzene	0.01%	0.00002%	0.005 %	2%

The table above shows that the release factors estimated in the SPERCs for some of the relevant products/downstream activities vary a lot but some can be significant. A summary of the relevant SPERCs are provided in Annex 13.

Quantification of the amounts of the relevant constituents released is not possible. Even if the tonnages used in intermediate uses were known, there are insufficient data to quantify the presence of the relevant constituents in the relevant products (in fact, this is challenging since the starting substances are UVCBs).

11 Conclusion

A number of constituents of PetCo substances have properties of potential concern. In this study, 15 such constituents are shortlisted for a more detailed assessment based on a screening of CMR (carcinogenic, mutagenic, reprotoxic), PBT (persistent, bioaccumulative and toxic) and ED (endocrine disrupting) properties.

Given the limitations in the data used for each of the approaches to the assessment of the fate of the shortlisted marker constituents, all assessment approaches developed for this study need to be considered together when drawing conclusions about the likely presence of the constituent of concern in the relevant products and the potential for their emissions into the environment.

Some degree of agreement exists between the different approaches for some product categories: for example, fuels, coal tar fractions, agriculture, forestry and fishing, inks and toners, etc. It should be noted that fuels and coal tar fractions are subject to high-temperature processing further downstream.

With regard to specific constituents, the greatest degree of agreement on the likelihood of pass-through is established for: phenanthrene, fluorene, anthracene, benzo[k]fluoranthene and benz[a]anthracene.

Interestingly, some of the information in the literature used under Approach 4 (upstream perspective literature review) is not consistent with the outcome of Approaches 1-3, including products derived using high temperature processes. However, it should be noted that due to data limitations, older and non-EU studies were used as well for the literature review under Approach 4. Also, Approach 4 does not differentiate between products derived as a result of intermediate and non-intermediate use.

Quantification of the amounts of the relevant constituents released is not possible due to multiple reasons, e.g. insufficient data to quantify the presence of the relevant constituents in the relevant products (this is challenging since the starting substances are UVCBs).

This study is expected to highlight issues (i.e. filling in the recognised knowledge gaps or potential follow-up on a regulatory level) and trigger further discussion and subsequent research, which may address some of the data limitations that affect the robustness of the conclusions under Approaches 0-4.

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13 List of Annexes

The annexes to the report are provided as separate Excel files:

- Annex 1: List of 53 substances
- Annex 2: Constituents of the 53 substances
- Annex 3: Uses, products and processes
- Annex 4: Constituent library
- Annex 5: Suspected presence of constituents
- Annex 6: Prometheus results
- Annex 7: ED_CMR classification screening
- Annex 8: SVHC screening
- Annex 9: Final shortlist
- Annex 10: Fate of the shortlisted marker constituents (Approach 1)
- Annex 11: Fate of the shortlisted marker constituents (Approach 2)
- Annex 12: Fate of the shortlisted marker constituents (Summary of approaches 1-4)
- Annex 13: Summary of the relevant SPERCs