EUROPEAN CHEMICALS AGENCY

Helsinki, 26 January 2021

Addressees
Registrant(s) of ethoxylated [redacted] as listed in the last Appendix of this decision

Date of submission of the dossier subject to this decision
23/09/2019

Registered substance subject to this decision ("the Substance")
Substance name: 2,4,7,9-Tetramethyldec-5-yne-4,7-diol, ethoxylated
EC number: 500-022-5
CAS number: 9014-85-1

Decision number: Please refer to the REACH-IT message which delivered this communication (in format CCH-D-XXXXXXXXXX-XX-XX/F)

DECISION ON A COMPLIANCE CHECK

Under Article 41 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below, by the deadline of ***31 October 2022***for the requests A.1-3, B.1-3 and C.1; and the information listed in B.8-9 and C.4-5 by the deadline of ***3 May 2023***; and by the deadline of ***31 October 2024*** for all the remaining requests.

Requested information must be generated using the Substance unless otherwise specified.

A. Information required from all the Registrants subject to Annex VII of REACH

1. In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.; test method: EU B.13/14. / OECD TG 471)

2. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.; test method: EU C.2./OECD TG 202)

3. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.; test method: EU C.3./OECD TG 201)

B. Information required from all the Registrants subject to Annex VIII of REACH

1. In vitro cytogenicity study in mammalian cells (Annex VIII, Section 8.4.2.; test method: OECD TG 473) or In vitro micronucleus study (Annex VIII, Section 8.4.2.; test method: OECD TG 487)

2. If negative results are obtained in tests performed for the information requirement of Annex VII, Section 8.4.1. and Annex VIII, Section 8.4.2. then: In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.; test method: OECD TG 476 or TG 490)

3. Screening for reproductive/developmental toxicity (Annex VIII, Section 8.7.1.; test method: EU B.63/OECD TG 421 or EU B.64/OECD TG 422) by oral route, in rats

4. Adsorption/ desorption screening (Annex VIII, Section 9.3.1.; test method: OECD TG 106)

5. Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.; test method: OECD TG 203)

6. Long-term toxicity testing on aquatic invertebrates also requested below (triggered by Annex VIII, Section 9.1.3., column 2)

7. Long-term toxicity testing on fish also requested below (triggered by Annex VIII, Section 9.1.3., column 2)

8. Simulation testing on ultimate degradation in surface water also requested below (triggered by Annex VIII, Section 9.2.)

9. Identification of degradation products also requested below (triggered by Annex VIII, Section 9.2.)

10. Bioaccumulation in aquatic species also requested below (triggered by Annex I, Sections 0.6.1. and 4; Annex XIII, Section 2.1.)

C. Information required from all the Registrants subject to Annex IX of REACH

1. Sub-chronic toxicity study (90-day) (Annex IX, Section 8.6.2.; test method: OECD TG 408) by oral route, in rats,

2. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.; test method: EU C.20./OECD TG 211)

3. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.; test method: OECD TG 210)

4. Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.; test method: EU C.25./OECD TG 309) at a temperature of 12 °C

5. Identification of degradation products (Annex IX, 9.2.3.; test method: EU C.25./OECD TG 309)

6. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2; test method: OECD TG 305)

7. Long-term toxicity testing on terrestrial invertebrates (triggered by Annex IX, Section 9.4., column 2; test method: OECD TG 222 or 220 or 232)

8. Effects on soil micro-organisms (Annex IX, Section 9.4.2.; test method: EU C.21./OECD TG 216 and test method: EU C.22./ OECD TG 217)

9. Long-term toxicity to terrestrial plants (triggered by Annex IX, Section 9.4., column 2; test method: OECD TG 208 with at least six species or ISO 22030)

Reasons for the request(s) are explained in the following appendices:

- Appendix entitled "Reasons common to several requests";
- Appendices entitled "Reasons to request information required under Annexes VII to IX of REACH", respectively.

Information required depends on your tonnage band

You must provide the information listed above for all REACH Annexes applicable to you, and in accordance with Articles 10(a) and 12(1) REACH:

- the information specified in Annex VII to REACH, for registration at 1-10 tpa;
- the information specified in Annexes VII and VIII to REACH, for registration at 10-100 tpa;
- the information specified in Annexes VII, VIII and IX to REACH, for registration at 100-1000 tpa;

You are only required to share the costs of information that you must submit to fulfil your information requirements.

For certain endpoints, ECHA requests the same study from registrants at different tonnages. In such cases, only the reasoning why the information is required at lower tonnages is provided in the corresponding Appendices. For the tonnage where the study is a standard information requirement, the full reasoning for the request including study design is given. Only one study is to be conducted; the registrants concerned must make every effort to reach an agreement as to who is to carry out the study on behalf of the other registrants under Article 53 of REACH.

How to comply with your information requirements

To comply with your information requirements you must submit the information requested by this decision in an updated registration dossier by the deadline indicated above. You must also update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information.

You must follow the general testing and reporting requirements provided under the Appendix entitled "Requirements to fulfil when conducting and reporting new tests for REACH purposes". In addition, you should follow the general recommendations provided under the Appendix entitled "General recommendations when conducting and reporting new tests for REACH purposes". For references used in this decision, please consult the Appendix entitled "List of references".

The studies relating to biodegradation and bioaccumulation are necessary for the PBT assessment. However, to determine the testing needed to reach the conclusion on the persistency and bioaccumulation of the Substance you should consider the sequence in which these tests are performed and other conditions described in Appendix entitled "Requirements to fulfil when conducting and reporting new tests for REACH purposes".

Appeal

This decision, when adopted under Article 51 of REACH, may be appealed to the Board of Appeal of ECHA within three months of its notification to you. Please refer to http://echa.europa.eu/regulations/appeals for further information.

Failure to comply

If you do not comply with the information required by this decision by the deadline indicated above, ECHA will notify the enforcement authorities of your Member State.

Authorised[1] under the authority of Christel Schilliger-Musset, Director of Hazard Assessment

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

Appendix on Reasons common to several requests

1. Assessment of your read-across approach under Annex XI, Section 1.5.

You seek to adapt the information requirements for the following standard information requirements by grouping substances and applying a read-across approach in accordance with Annex XI, Section 1.5:

- In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.)
- In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)
- In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)
- Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.)
- Adsorption/desorption screening (Annex VIII, Section 9.3.1.)
- Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.)
- Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
- Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)
- Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)

You have provided the following two read-across adaptations:

1) a read-across adaptation based on a category "Acetylenic geminalic diols"
2) a read-across based on an analogue approach

ECHA has considered the scientific and regulatory validity of your grouping and read-across approach in general before assessing the specific standard information requirements in the following appendices.

Grouping of substances and read-across approach

Annex XI, Section 1.5. specifies two conditions which must be fulfilled whenever a read-across approach is used. Firstly, there needs to be structural similarity between substances which results in a likelihood that the substances have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category (addressed under 'Scope of the grouping'). Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group (addressed under 'Assessment of prediction(s)').

Additional information on what is necessary when justifying a read-across approach can be found in the ECHA Guidance[2] and related documents[3, 4].

ECHA has evaluated the category approach under section I below and the analogue approach under section II. The arguments presented for the prediction of properties are similar between the two approaches and, therefore, only addressed under section II.

I. Assessment of the Grouping of substances and read-across approach under Annex XI, Section 1.5. (category)

[2] Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals. 2008 (May) ECHA, Helsinki. 134. pp. Available online: https://echa.europa.eu/documents/10162/13632/information_requirements_r6_en.pdf/77f49f81-b76d-40ab-8513-4f3a533b6ac9

[3] Read-Across Assessment Framework (RAAF). 2017 (March) ECHA, Helsinki. 60 pp. Available online: Read-Across Assessment Framework (https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across)

[4] Read-across assessment framework (RAAF) - considerations on multi-constituent substances and UVCBs. 2017 (March) ECHA, Helsinki. 40 pp. Available online: https://doi.org/10.2823/794394

A. Scope of the grouping

i. Description of the grouping

In your registration dossier you have formed a group (category) of 'Acetylenic geminalic diols'. You have provided a read-across justification document in IUCLID Section 0.

For the purpose of this decision, the following abbreviations are used for the group members:
[1] Surfynol 104 2,4,7,9-tetramethyldec-5-yne-4,7-diol (EC No. 204-809-1);
[2] Surfynol 124 2,5,8,11-tetramethyldodec-6-yne-5,8-diol (EC No. 269-348-0);
[3] Surfynol 440 ethoxylated 2,4,7,9-tetramethyldec-5-yne-4,7-diol (EC No. 500-022-5);
[4] Surfynol 2502 ethoxylated propoxylated 2,4,7,9-tetramethyldec-5-yne-4,7-diol (EC No. 638-783-1);
[5] Envirogem AD01 2,4,7, 9-tetramethyl-4,7-dodecanediol (EC No. 451-160-7).

The Substance is not listed in this justification document.

You provide the following reasoning for the grouping the substances: *"Acetylenic geminalic diols are considered a chemical category based on structural similarity and similar properties in environmental and biological systems."*

You define the structural basis for the grouping as *"members of the category begin with an acetylene group as their core structure; in one member, this acetylene group has been fully hydrogenated. [...] Alpha to the acetylene are the geminal hydroxyl groups, which can be derivatized with ethoxylates and propoxylates in order to achieve desired functionalities of surfactants. Distal to the geminal hydroxyl groups is either an isobutyl group (methyl isopropyl) or an isopentyl group (ethyl isopropyl). These are short chain alkyls displaying an incremental increase in carbon chain length. All substances have two stereogenic centers (chiral carbons) in alpha-position to the carbon triple bond."* ECHA understands that this is the applicability domain of the grouping and will assess your predictions on this basis.

ii. Assessment of the grouping

ECHA notes the following shortcomings with regards to your grouping approach.

Characterisation of the group members

Annex XI, Section 1.5 of the REACH Regulation provides that *"substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of chemical similarity may be considered as group."*

According to the ECHA Guidance, *"in identifying a category, it is important that all potential category members are described as comprehensively as possible"*, because the purity profile and composition can influence the overall toxicity/properties of the potential category members.[5] Therefore, qualitative and quantitative information on the compositions of the category members should be provided to confirm the category membership.

Furthermore, the provided information for categories consisting of UVCB (Unknown or Variable composition, Complex reaction products or of Biological materials) substances needs to include qualitative compositional information of the individual constituents of the category members; as well as quantitative characterisation in the form of information on the

[5] Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals, Section R.6.2.4.1

concentration of the individual constituents of these substances; to the extent that this is measurable.[6]

You have defined the applicability domain of the category as explained above. Your read-across justification document contains compositional information for the members of your category. Several category members (Surfynol 440, Surfynol 2502) are UVCBs including ethoxylated and propoxylated diols of various carbon chain lengths. The degree of ethoxylation or propoxylation is not provided for these category members. The same applies to the Substance, which is not included as category member.

Without consideration of the distribution of the ethoxylation and propoxylation amongst constituents with different carbon chain lengths, and information on the composition of test materials, no qualitative or quantitative comparative assessment of the different category members can be completed. Therefore, the category membership cannot be confirmed.

B. Predictions for properties

You have presented a hypothesis and arguments similar to those for a separate analogue approach and only read-across applied for the Bioaccumulation in aquatic species is addressed by you solely in category approach justifying document. They are rejected for the same reasons described below (see section **II** below).

C. Conclusion on the read-across category approach

As explained above, you have not demonstrated that the established category can be used as a basis to to predict properties of the Substance from data on the analogue substances. Therefore, your adaptation does not comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and your grouping and read-across approach is rejected.

II. Assessment of the Grouping of substances and read-across approach under Annex XI, Section 1.5. (analogue approach)

A. Predictions for properties

You have provided a justification document in IUCLID Section 13.

You read-across between the structurally similar substances, Surfynol 104 (2,4,7,9-tetramethyldec-5-yne-4,7-diol), EC No. 204-809-1 (CAS No. 126-86-3), and Surfynol 440 (2,4,7,9-Tetramethyl-5-decyne-4,7-diol, ethoxylated (3.8)), EC No. 500-022-5 (CAS No. 9014-85-1) as source substances and the Substance Surfynol 420 (2,4,7,9-Tetramethyldec-5-yne-4,7-diol, ethoxylated (1.3)), EC No. 500-022-5 (CAS No. 9014-85-1) as target substance.

You have provided the following reasoning for the prediction of (eco-)toxicological properties: "*This read-across is based on the hypothesis that source and target substances have similar toxicological and ecotoxicological properties. [...] For most endpoints, data are available for the source substances 2,4,7,9-Tetramethyl-5-decyne-4,7-diol, ethoxylated (3.8) and 2,4,7,9-Tetramethyl-5-decyne-4,7-diol. The results are interpolated to the target substance, where appropriate, or the worst-case result is used for chemical safety assessment.*".

ECHA understands that you predict the properties of the Substance using a read-across hypothesis which assumes that different compounds have the same type of effects. The

[6] Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals, Section R.6.2.5.5

properties of your Substance are predicted to be quantitatively equal to those of the source substance, or, for selected endpoints, based on a worst-case approach.

You intend to predict the properties of the Substance from information obtained from the following source substances:

In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.)
- Surfynol 104 (OECD TG 471, 1999)
- Envirogem AD01 (OECD TG 471, 2003)

In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)
- Surfynol 104 (OECD TG 473, 1999)
- Envirogem AD01 (OECD TG 473, 2003)

In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)
- Surfynol 104 (OECD TG 476, 2010)

Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.)
- Surfynol 104 (non-guideline 91-Day feeding study in rats, 1979; non-guideline 91-Day feeding study in dogs, 1979)
- Surfynol 440 (non-guideline 91-Day feeding study in rats, 1977; non-guideline 91-Day feeding study in dogs, 1979)

Adsorption/desorption screening (Annex VIII, Section 9.3.1.)
- Surfynol 440 (OECD TG 121, 2001)

Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.)
- Surfynol 104 (OECD TG 202, 1999)
- Surfynol 104 (OECD TG 202, 1991)
- Surfynol 440 (ISO/CD 14669 "Determination of Acute Lethal Toxicity to Marine Copepods", 2002)

Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
- Surfynol 104 (OECD TG 201, 2000)

Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)
- Surfynol 104 (OECD TG 203, 2000)
- Surfynol 104 (OECD TG 203, 1991)
- Surfynol 440 (OECD TG 203, 2002)

Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)
- Surfynol 124 (non-guideline study - Bioconcentration test of chemical substances in fish and shellfish, 2010)

ECHA notes the following shortcoming(s) with regards to prediction(s) of (eco-)toxicological properties.

1. Supporting information

Annex XI, Section 1.5 of the REACH Regulation states that *"physicochemical properties, human health effects and environmental effects or environmental fate may be predicted from data for reference substance(s)"*. For this purpose *"it is important to provide supporting*

information to strengthen the rationale for the read-across"[7]. The set of supporting information should allow to verify the crucial aspects of the read-across hypothesis and establish that the properties of the Substance can be predicted from the data on the source substance(s).

Supporting information must include bridging studies to compare properties of the Substance and the source substances.

a. *Missing supporting information to compare properties between analogue substances*

As indicated above, your read-across hypothesis is based on the assumption that the structurally similar substances cause the same type of effect(s). In this context, relevant, reliable and adequate information allowing to compare the properties of the Substance and the source substance is necessary to confirm that both substances cause the same type of effects. Such information can be obtained, for example, from bridging studies of comparable design and duration for the category members.

In your read-across hypothesis, there are no experimental studies conducted with the Substance, which could serve as bridging studies to compare (eco-)toxicological profiles between source substances and the Substance (e.g. OECD TG 422 or aquatic toxicity data for the same species). The data set reported in the technical dossier does not include relevant, reliable and adequate information for the target substance in order to compare to the source substances to support your read-across hypothesis.

In the absence of such information, you have not established that the Substance and the source substance(s) are likely to have similar properties. Therefore you have not provided sufficient supporting information to strengthen the rationale for the read-across.

b. *Missing supporting information to substantiate worst-case*

As indicated above, your read-across hypothesis is in some cases based on the assumption that the source substance constitutes a worst-case for the prediction of the property under consideration of the Substance. In this context, relevant, reliable and adequate information allowing to compare the properties of the Substance and of the source substance(s) is necessary to confirm a conservative prediction of the properties of the Substance from the data on the source substance(s). Such information can be obtained, for example, from bridging studies of comparable design and duration for the Substance and of the source substance(s).

In your read-across hypothesis, you indicate that "*The only difference between the target substance and the source substances is the degree of Ethoxylation. [...] Ethoxylation seems to lead to lower toxicity as demonstrated by higher effect levels in the subchronic toxicity studies as well as in the QSAR calculations performed for short-term toxicity to fish, Daphnia, and algae. Thus, using the toxicity and ecotoxicity results obtained with the non-ethoxylated source substance* [Surfynol 104] *is a sufficiently conservative approach to fill the data gaps of the target substance.*" Furthermore, the following is noted for the Bioaccumulation in aquatic species in the category approach justifying document: "*Surfynol®124, with the highest octanol/water partition coefficient, was selected to be tested in a bioaccumulation assay in fish, and found to have a low propensity for bioconcentration (BCF < 24). Category members with lower log Kow values would be expected to have lower BCF values. Therefore, these substances can be considered "not bioaccumulative".*"

[7] Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of Chemicals, Section R.6.2.2.1.f

However, in your read-across hypothesis, you have not considered the impact of the ethoxylation status and the degree of ethoxylation on the bioavailability of the Substance and source substances:

- the Substance is more polar than the source substance Surfynol 104 due to ethoxylation, and
- the Substance has a lower molecular weight than the source substance Surfynol 440 due to a higher proportion of constituents with short ethoxylated chains (i.e. with 1-2 ethoxylate units).

You did not provide any toxicokinetic data for the Substance and source substances to compare their bioavailability. You also did not provide comparable toxicological studies, which could establish a worst-case on the basis of toxicological properties.

There are multiple factors potentially determining toxicological properties, such as bioavailability. In this case, (1) you have not addressed how the ethoxylation status, degree of ethoxylation, polarity and molecular weight (i.e. proportion of constituents with short ethoxylated chains) may impact bioavailability. Furthermore (2) you have not demonstrated lower toxicity of the source substance Surfynol 104 (see section a. above).

Furthermore, as noted in the section above, there are no aquatic toxicity data for the same species available to confirm the hypothesis that "*Ethoxylation seems to lead to lower toxicity*". Moreover, in both read-across justification documents you note that source and target substances are surfactants and as explained in the section on assessment of (quantitative) structure-activity relationships (QSAR) estimations based on octanol-water partitioning coefficient (Kow), such estimations and prediction of properties based on Kow are not reliable for the surfactants. Thus, information used by you to support your hypothesis that target substances are worst-case for the prediction of aquatic toxicity and bioaccumulation of the Substance is not reliable.

In the absence of such supporting information, you have not established that the source substances Surfynol 104 and Surfynol 124 constitutes a worst-case for the prediction of the property under consideration of the Substance. Therefore you have not provided sufficient supporting information to strengthen the rationale for the read-across.

2. *Quality of aquatic toxicity source studies*

According to Annex XI, Section 1.5., if the grouping concept is applied then in all cases the results to be read across should:

- be adequate for the purpose of classification and labelling and/or risk assessment.

With the aquatic source studies with Surfynol 440 that you have used in your read-across approach, i.e. ISO/CD 14669 "Determination of Acute Lethal Toxicity to Marine Copepods", 2002 and OECD TG 203, 2002, you address standard requirement of Annex VII, Section 9.1.1. and Annex VIII, Section 9.1.3. respectively.

According to the provisions of Annex VII, Section 9.1.1. and Annex VIII, Section 9.1.3. information on Short-term toxicity testing on aquatic invertebrates and Short-term toxicity testing on fish as specified in the OECD TG 202 and OECD TG 203 respectively shall be provided. To comply with OECD TG 202 and OECD TG 203 requirements the following requirements must be met:

- the analytical measurement of test concentrations are conducted;

- adequate information on the analytical method (including performance parameters of the method) and on the results of the analytical determination of exposure concentrations are provided;
- the test procedure, conditions and design is reported (*e.g.* composition of the test medium, number of replicates and test animal per replicate).

In the dossier there is no information provided on analytical measurements of test concentrations and its results, on the test procedure, conditions and design (except number of test concentrations used in both studies, and number of organisms per test vessel and test temperature for OECD TG 203, 2002) for the reported aquatic toxicity studies with Surfynol 440.

Based on the above, you have not demonstrated compliance with the above requirements and the reporting of the study is not sufficient to conduct an independent assessment of its reliability. Therefore, the results of these studies are not adequate for the purpose of classification and labelling and/or risk assessment and cannot be used to support your read-across.

B. Conclusions on the read-across analogue approach

As explained above, you have not established that relevant properties of the Substance can be predicted from data on the analogue substances. Therefore, your adaptation does not comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and your grouping and read-across approach is rejected.

2. Assessment of (quantitative) structure-activity relationships estimations based on octanol-water partitioning

You have provided information based on QSAR application to support your read-across adaptation according to Annex XI, Section 1.5 for the following standard information requirements:

1. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.)
2. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
3. Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)
4. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)

Information generated by application of various QSARs applied by you raises the same deficiencies irrespective of the information requirement for which it is invoked. Accordingly, ECHA addressed these deficiencies in the present Appendix, before assessing the specific standard information requirements in the following appendices.

Annex XI, Section 1.3. states that results obtained from valid QSAR models may be used instead of testing when several cumulative conditions are met, and in particular the following:

- the results are adequate for classification and labelling and/or risk assessment.

In the registration dossier you have provided estimation of aquatic toxicity effect concentrations (by ECOSAR v1.11 model) and of bioaccumulation potential (bioconcentration factors (BCFs) by BCFBAF v3.01 model) for the nine constituents of the Substance. For the aquatic toxicity estimations you note that "*The QSARs in ECOSAR for both neutral organics and classes with excess toxicity are based on a linear mathematical relationship between the measured log Kow values and the corresponding log of the measured toxicity values (mmol/L) for a suite of training set chemicals within each class of interest.*" and for the estimation of BCFs you note that equations based on Kow are used.

In regard of Kow for surfactants following is noted in various parts of ECHA Guidance documents:

- R.7a (p. 78-79): None of the experimental methods is very well suited for determining the Kow of surface active substances. A working approach for surfactants might be the comparison of measured solubilities in octanol and water. However, it would then be prudent to take the critical micelle concentration in water (CMC) as a solubility limit, in order to avoid the artefact of unrealistically low Kow values.
- R.7b (p. 83) for aquatic toxicity: QSAR modelling is potentially very difficult since the Kow cannot usually be measured.
- R.7c, Appendix R.7.10-3: A log Kow may be used to support assessment of potential for bioaccumulation if the partitioning to lipids is the sole mechanism driving the bioaccumulation potential of a substance. For some groups of substances (e.g. organometals, ionisable substances, surfactants) other partitioning mechanisms may drive bioaccumulation (e.g. binding to protein/cell membranes). For this reason log Kow is not considered a valid descriptor of the bioaccumulation potential for such substances.

In both read-across justification documents provided in the dossier you note that source and target substances are surfactants. There is no evidence provided in the dossier that CMC was used for estimation of Kow for constituents of the Substance or of any other source substances as well as there is no evidence provided that the partitioning to lipids is the sole mechanism driving the bioaccumulation potential of these substances (constituents).

Therefore, QSAR estimations of aquatic toxicity effect concentrations and of BCFs based on Kow are not reliable for the constituents of the Substance. Consequently, the results of such QSAR estimations are not adequate for classification and labelling and/or risk assessment and cannot be used to support your read-across adaptation according to Annex XI, Section 1.5.

3. Assessment of your adaptation for effects on terrestrial organisms

You have provided the same Annex IX, Section 9.4., Column 2 adaptation for the following standard information requirements:

1. Long-term toxicity testing on terrestrial invertebrates (triggered by Annex IX, Section 9.4., column 2)
2. Effects on soil micro-organisms (Annex IX, Section 9.4.2)
3. Long-term toxicity to terrestrial plants (triggered by Annex IX, Section 9.4., column 2)

You have provided the following justification for the adaptation: "*The substance is water soluble (2.3 g/L), has as an assumed worst-case log Kow of 2.5 and a bioaccumulation factor of clearly below 2000, based on supporting data. Furthermore the Koc value based on calculation is well below 1000. This is demonstrating a negligible potential to adsorb to soil and for accumulation in the aqueous and terrestrial compartments. It shall be also noted that in the environmental exposure assessments the local and regional RCRs are resulting below 1, which is indicating a low risk to organisms in the different environmental compartments. Hence according to Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, 9.4 Effects on terrestrial organisms, COLUMN 2, of REGULATION (EC) No 1907/2006, studies on the effects on terrestrial organisms do not need to be conducted.*"

We have assessed this information and identified the following issue(s):

According to Annex IX, Section 9.4., Column 2 soil toxicity testing does not need to be conducted if direct and indirect exposure of the soil compartment is unlikely.

In the absence of toxicity data for soil organisms, the equilibrium partitioning method (EPM) may be applied to assess the hazard to soil organisms. According to ECHA Guidance R.7c, Section R.7.11.6, where there is adequate data available to derive a PNEC for aquatic organisms, this PNEC can be used in a screening assessment of risks for soil through the use of the EPM approach.

Regarding direct and indirect exposure of the soil compartment: In the CSR you report a number of various industrial, professional and consumer uses of the substance including agricultural application of the Substance by professional users (outdoor), consumers application of sprays with the Substance (outdoor) etc where direct and indirect exposure of the soil is identified in the respective exposure scenarios (ESs) by the release factor to the soil and/or estimated predicted environmental concentration (PEC) in soil being not equal to zero.

Regarding EPM: In the CSR, predicted no-effect concentration (PNEC) for soil was derived by you by using EPM from the PNEC for aquatic organisms.

Regarding direct and indirect exposure of the soil compartment: As noted above, the CSR indicates a number of identified uses which lead to the direct and indirect exposure of soil. Therefore, your consideration that exposure of soil, i.e. in your words "*accumulation in the aqueous and terrestrial compartments*", is unlikely, i.e. "negligible" in your words, is not supported by the evidence provided in the dossier, including the CSR. Thus, this argument based on exposure considerations for omitting toxicity testing with soil organisms is not acceptable.

Regarding EPM: For the reasons explained under requests in the Appendix A, Sections on short-term toxicity testing on aquatic invertebrates and growth inhibition study aquatic plants, in the Appendix B, Section on short-term toxicity testing on fish and Appendix C, Sections on long-term toxicity testing on aquatic invertebrates and fish, your dossier does not include reliable hazard information for the Substance on aquatic organisms from at least three trophic levels. Therefore, a reliable PNECs cannot be derived and risk characterisation for aquatic compartment cannot be performed. Therefore, accurate allocation of an appropriate soil hazard category according to table R7.11-2 (ECHA Guidance R.7c) is not possible at this time. Consequently, it is not possible to omit the standard information requirements for the terrestrial compartment through an initial screening assessment based upon the EPM, mentioned in Annex IX, Section 9.4, Column 2.

Thus, your adaptation is rejected.

Appendix A: Reasons to request information required under Annex VII of REACH

1. In vitro gene mutation study in bacteria

In vitro gene mutation study in bacteria is a standard information requirement under Annex VII to REACH (Section 8.4.1.).

You have adapted this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5.

In support of your adaptation you have provided two key studies for this endpoint in your dossier:

i. OECD TG 471 study with the analogue substance Surfynol 104 (1999)
ii. OECD TG 471 study with the analogue substance Envirogem AD01 (2003).

As explained in the Appendix on Reasons common to several requests, section 1 (Assessment of your read-across approach under Annex XI, Section 1.5.), your adaptation under Annex XI, Section 1.5 is rejected.

Accordingly, it is not possible to conclude whether your Substance has or has not the particular dangerous property foreseen to be investigated in an OECD TG 471 study.

In your comments to the draft decision, you agree to carry out an in vitro gene mutation study in bacteria (OECD 471).

Based on the above, the information you provided does not fulfil the information requirement.

Study design

To fulfil the information requirement for the Substance, the *in vitro* gene mutation study in bacteria (OECD TG 471) is considered suitable.

2. Short-term toxicity testing on aquatic invertebrates

Short-term toxicity testing on aquatic invertebrates is an information requirement under Annex VII to REACH (Section 9.1.1.).

You have adapted this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5.

In support of your adaptation you have provided following information for this endpoint in your dossier:

- Key study with the analogue substance Surfynol 104 (OECD TG 202, 1999)
- Key study with the analogue substance Surfynol 104 (OECD TG 202, 1991)
- Key study with the analogue substance Surfynol 440 (ISO/CD 14669 "Determination of Acute Lethal Toxicity to Marine Copepods", 2002)
- Supporting information: QSAR estimation of short-term aquatic invertebrates toxicity effect concentrations (by ECOSAR v1.11 model) for the nine constituents of the Substance.

We have assessed this information and identified the following issues:

As explained in the Appendix on Reasons common to several requests:

- section 1: your adaptations under Annex XI, Section 1.5 is rejected; and

- section 2: QSAR estimations of aquatic toxicity effect concentrations based on Kow are not reliable for the constituents of the Substance.

In your comments to the draft decision, you note that you will first revise the robust study summaries (RSSs) of the existing studies for the analogue substances and check, whether this studies fulfil the information requirement. Additionally, you will strengthen the read-across approach for this information requirement. Furthermore, you agree to perform short-term toxicity study with aquatic invertebrates, if the existing data do not fulfil the information requirement.

It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

On this basis, the information requirement is not fulfilled.

3. Growth inhibition study aquatic plants

Growth inhibition study aquatic plants is an information requirement under Annex VII to REACH (Section 9.1.2).

You have adapted this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5.

In support of your adaptation you have provided following information for this endpoint in your dossier:

- Key study with the analogue substance Surfynol 104 (OECD TG 201, 2000)
- Supporting information: QSAR estimation of algae toxicity effect concentrations (by ECOSAR v1.11 model) for nine constituents of the Substance.

We have assessed this information and identified the following issues:

As explained in the Appendix on Reasons common to several requests:
- section 1: your adaptation under Annex XI, Section 1.5 is rejected; and
- section 2: QSAR estimations of aquatic toxicity effect concentrations based on Kow are not reliable for the constituents of the Substance.

In your comments to the draft decision, you note that you will first revise RSSs of the existing studies for the analogue substances and check, whether this studies fulfil the information requirement. Additionally, you will strengthen the read-across approach for this information requirement. Furthermore, you agree to perform growth inhibition study in aquatic plants, if the existing data do not fulfil the information requirement.

It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

On this basis, the information requirement is not fulfilled.

Appendix B: Reasons to request information required under Annex VIII of REACH

1. In vitro cytogenicity study in mammalian cells or In vitro micronucleus study

In vitro cytogenicity study in mammalian cells is a standard information requirement in Annex VIII to REACH (Section 8.4.2.).

You have adapted this information requirement by using a Grouping of substances and read-across approaches under Annex XI, Section 1.5.

In support of your adaptation, you have provided the following sources of information:
i. OECD TG 473 study with the analogue substance Surfynol 104 (1999)
ii. OECD TG 473 study with the analogue substance Envirogem AD01 (2003).

As explained in the Appendix on Reasons common to several requests your adaptation according to Annex XI, Section 1.5. is rejected.

In your comments to the draft decision, you agree to provide further data on this endpoint. You further stated that you will strengthen the read across approach for this endpoint. It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

Based on the above, the information you provided does not fulfil the information requirement.

To fulfil the information requirement for the Substance, both *in vitro* cytogenicity study in mammalian cells (Annex VIII, Section 8.4.2., test method OECD TG 473) and *in vitro* micronucleus study (Annex VIII, Section 8.4.2., test method OECD TG 487) are considered suitable.

2. In vitro gene mutation study in mammalian cells

An *in vitro* gene mutation study in mammalian cells is a standard information requirement in Annex VIII to REACH (Section 8.4.3.) in case of a negative result in the *in vitro* gene mutation test in bacteria and the *in vitro* cytogenicity test.

You have adapted this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5.

You have provided one key study for this endpoint in your dossier:
i. OECD TG 476 study with the analogue substance Surfynol 104 (2010)

As explained in the Appendix on Reasons common to several requests, section 1, your adaptation according to Annex XI, Section 1.5. is rejected.

In your comments to the draft decision, you agree to provide further data on this endpoint. You further stated that you will strengthen the read across approach for this endpoint. It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

Therefore, the information requirement is not fulfilled.

Consequently, you are required to provide information for this endpoint, if the *in vitro* gene mutation study in bacteria and the *in vitro* cytogenicity study in mammalian cells or an *in vitro* micronucleus study provide a negative result.

To fulfil the information requirement for the Substance, both the *in vitro* mammalian cell gene mutation tests using the hprt and xprt genes (OECD TG 476) and the thymidine kinase gene (OECD TG 490) are considered suitable.

3. Screening for reproductive/developmental toxicity

A Screening for reproductive/developmental toxicity study (test method: EU B.63/OECD TG 421 or EU B.64/OECD TG 422) is a standard information requirement under Annex VIII to REACH, if there is no evidence from analogue substances, QSAR or *in vitro* methods that the Substance may be a developmental toxicant. There is no information available in your dossier indicating that your Substance may be a developmental toxicant.

You have adapted this information requirement by using read-across approach under Annex XI, Section 1.5.

You have provided one key study for this endpoint in your dossier:

i) Single Generation Reproduction Study in the Rat ([redacted], 1979) with the analogue substance Surfynol 104.

As explained in the Appendix on Reasons common to several requests, section 1, your adaptation according to Annex XI, Section 1.5. is rejected.

In your comments to the draft decision, you agree to carry out a Screening study for reproductive/developmental toxicity (OECD 422 or OECD 421). You indicated a preference to perform an OECD 422 study.

Based on the above, the information you provided do not fulfil the information requirement.

A study according to the test method EU B.63/OECD TG 421 or EU B.64/OECD TG 422 must be performed in rats with oral[8] administration of the Substance.

4. Adsorption/ desorption screening

Adsorption/desorption screening is a standard information requirement under Annex VIII to REACH (Section 9.3.1.).

You have adapted this information requirement by using:

- An adaptation in accordance with Annex VIII, Section 9.3.1., column 2;
- An OECD TG 121 study with an analogue substance, Surfynol 440 in accordance with Annex XI, Section 1.5 (key study, 2012);
- Data derived from Qualitative or quantitative structure-activity relationship (QSAR) in accordance with Annex XI, Section 1.3 and Annex XI, Section 1.5 for an analogue Substance, Surfynol 440 (key study);
- Data derived from Qualitative or quantitative structure-activity relationship (QSAR) in accordance with Annex XI, Section 1.3 for the Substance (supporting study).

We have assessed this information and identified the following issues:

[8] ECHA Guidance R.7a, Section R.7.6.2.3.2.

A: Column 2 adaptation

Annex VIII, Section 9.3.1., column 2 states that the study does not need to be conducted if based on the physicochemical properties the substance can be expected to have a low potential for adsorption (e.g. the substance has a low octanol water partition coefficient).

However, as explained in ECHA Guidance on information requirements and chemical safety assessment (version 6.0., July 2017), Chapter R.7a, Section R.7.1.15.3.: '*...measured values will normally be needed for surface active substances (e.g. surfactants), because Kow values (predicted or measured) are likely to be poor predictors of adsorption for these types of substance.*'

You state that '*the study does not need to be conducted because the substance has a low octanol water partition coefficient and the adsorption potential of this substance is related to this parameter*'.

However, based on the information in your dossier, you report that the surface tension of the Substance is 33.2 mN/m. Under section 3 of your technical dossier you report that the Substance is used with a technical function as a surface active agent.

The information included in your dossier thus indicates that the Substance has surface active properties and measured values are needed.

Therefore, your adaptation of the information requirement cannot be accepted.

B: OECD TG 121 study with an analogue substance, Surfynol 440.

Your adaptation is rejected already for the reasons explained in the Appendix on Reasons common to several requests.

In addition, we have identified the following deficiency with this source study:

ECHA Guidance R.7a, Section R.7.1.15.3 specifies that the OECD TG 121/EU C.19 method is not suitable for some classes of chemical, for instance surface active substances.

The study you have provided to cover this information requirement was conducted according to OECD TG 121/EU C.19.

Based on the information in your dossier, you report that the surface tension of the analogue substance Surfynol 440 is 33.2 mN/m.

The information included in your dossier indicates that the source substance has surface active properties. Therefore the results of the study conducted according to OECD TG 121/EU C.19 are not considered reliable.

Therefore, your adaptation of the information requirement cannot be accepted.

C: QSAR

You have adapted this information requirement by using a QSAR approach under Annex XI, Section 1.3 of the REACH Regulation and you have provided:

(i) a key study to estimate the Log Koc of the analogue Substance, Surfynol 440 by calculation (KOCWIN Program (v2.00), Estimation Programs Interface Suite™ United States Environmental Protection Agency, Washington, DC, USA. version 4.00)

(ii) supporting study to estimate the Log Koc of the Substance by calculation (KOCWIN Program (v2.00), Estimation Programs Interface Suite™ United States Environmental Protection Agency, Washington, DC, USA. version 4.00)

We have assessed this information and identified the following issues:

Annex XI, Section 1.3. states that results obtained from valid QSAR models may be used instead of testing when the following cumulative conditions are met:

1. results are derived from a QSAR model whose scientific validity has been established;
2. the substance falls within the applicability domain of the QSAR model;
3. adequate and reliable documentation of the applied method is provided; and the results are adequate for classification and labelling and/or risk assessment.

According to ECHA's Practical guide "How to use and report (Q)SARs", section 3.4, a QSAR Model Reporting Format (QMRF) and a QSAR Prediction Reporting Format (QPRF) are required to establish the scientific validity of the model, to verify that the Substance falls within the applicability domain of the model, and to assess the adequacy of the prediction for the purposes of classification and labelling.

You have provided an estimated Log Koc (0.8882-1.8535) for the different constituents of the Substance based on KOCWIN Program (V2.00) and a QMRF describing the KOCWIN methodology of the KOCWIN program.

Based on the information in your dossier both the Substance and the source substance are surface active (33.2 mN/m).

Your adaptation does not meet the general rule for adaptation of Annex XI, Section 1.3. because:

- You have not established the scientific validity of the selected QSAR approach, in particular considering that the Substance and the source substance are surface active. There is uncertainty due to the presence of very few similar compounds with comparable surface tension in the training set of the model. Indeed, as indicated in ECHA Guidance Chapter R.7a, Section R.7.1.15.3.: *'...measured values will normally be needed for surface active substances (e.g. surfactants)'.*
- You did also not demonstrate that the selected chemical structure falls within the applicability domain of the selected QSAR. The Fragment correction applied [redacted] has two instances in the major constituent of the Substance, while in the training set there are only examples with one instance in the same molecule.

Therefore, your adaptation of the information requirement cannot be accepted.

In your comments to the draft decision, you agree to carry out a study on adsorption/desorption using a batch equilibrium method.

Therefore in summary the information provided does not fulfil the information requirement.

Study design

Batch equilibrium method (OECD 106) is to be used for surface active substances, as indicated in the ECHA Guidance on information requirements and chemical safety assessment (version 6.0., July 2017), Chapter R.7a, Section R.7.1.15.3.

5. Short-term toxicity testing on fish

Short-term toxicity testing on fish is an information requirement under Annex VIII to REACH (Section 9.1.3.).

You have adapted this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5.

In support of your adaptation you have provided following information for this endpoint in your dossier:

- Key study with the analogue substance Surfynol 104 (OECD TG 203, 2000)
- Key study with the analogue substance Surfynol 104 (OECD TG 203, 1991)
- Key study with the analogue substance Surfynol 440 (OECD TG 203, 2002)
- Supporting information: QSAR estimation of short-term fish toxicity effect concentrations (by ECOSAR v1.11 model) for the nine constituents of the Substance.

We have assessed this information and identified the following issues:

As explained in the Appendix on Reasons common to several requests
- section 1: your adaptations under Annex XI, Section 1.5 are rejected; and
- section 2: QSAR estimations of aquatic toxicity effect concentrations based on Kow are not reliable for the constituents of the Substance.

In your comments to the draft decision, you note that you will first revise the RSSs of the existing studies for the analogue substances and check, whether these studies fulfil the information requirement. Additionally, you will strengthen the read-across approach for this information requirement. Furthermore, you agree to perform short-term toxicity study with fish, if the existing data do not fulfil the information requirement.

It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

On this basis, the information requirement is not fulfilled.

6. Long-term toxicity testing on aquatic invertebrates

Long-term aquatic toxicity testing as described in Annex IX shall be considered if the chemical safety assessment according to Annex I indicates the need to investigate further effects on aquatic organisms (Annex VIII, Section 9.1.3., column 2).

You have provided the following information in the dossier on long-term aquatic invertebrates toxicity: *"The chemical safety assessment does not indicate the need to investigate further the effects on aquatic organisms, since the risk characterisation ratio is below 1 for the aquatic compartment. (Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, COLUMN 2, of REGULATION (EC) No 1907/2006)."*

This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further investigation on long-term aquatic toxicity (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT substance (ECHA Guidance R.11.4). This is the case if the Substance itself or any of its constituent or impurity

present in concentration ≥ 0.1% (w/w) or relevant transformation/degradation product meets the following criteria:

- it is potentially persistent or very persistent (P/vP) as:
  - it is not readily biodegradable (*i.e.* <60/70% degradation in ready biodegradability tests, e.g. an OECD 301), and
- it is potentially bioaccumulative or very bioaccumulative (B/vB) as:
  - for some groups of substances (e.g. organometals, ionisable substances, surfactants) other partitioning mechanisms may drive bioaccumulation (e.g. binding to protein/cell membranes) and high potential for bioaccumulation cannot be excluded solely based on its potential to partition to lipid.

Your registration dossier provides the following:
- the Substance is not readily biodegradable, as concluded by you in the registration dossier;
- the Substance is a surfactant and therefore high potential for bioaccumulation cannot be excluded based on water-octanol partitioning coefficient.

Furthermore, the information in your dossier is currently incomplete and therefore:
- it is not possible to conclude on the persistence of the Substance (see Appendix C, Section 4. of this decision), and
- there is no adequate data to conclude on bioaccumulation potential of the Substance (see Appendix C, Section 6 of this decision).

The information above indicates that the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for long-term aquatic toxicity investigation.

For ECHA's response, to your comments to the draft decision regarding this request, see request C.2. below.

The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Appendix C, Section 2.

7. Long-term toxicity testing on fish

Long-term aquatic toxicity testing as described in Annex IX shall be considered if the chemical safety assessment according to Annex I indicates the need to investigate further effects on aquatic organisms (Annex VIII, Section 9.1.3., column 2).

You have provided the following information in the dossier on long-term fish toxicity: "*The chemical safety assessment does not indicate the need to investigate further the effects on aquatic organisms, since the risk characterisation ratio is below 1 for the aquatic compartment. (Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, COLUMN 2, of REGULATION (EC) No 1907/2006).*"

This information requirement is triggered in case the CSA indicates the need for further investigation on long-term aquatic toxicity (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT substance (ECHA Guidance R.11.4).

As already explained in the Appendix B, Section on long-term toxicity testing on aquatic invertebrates above, the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for long-term aquatic toxicity investigation.

In your comments to the draft decision, you agree to carry out a study on long-term toxicity testing on fish only, if this is triggered, i.e. in case the CSA (including PBT/vPvB assessment

and risk characterisation) indicates the need to investigate further effects on aquatic organisms.

The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Appendix C, Section 3.

8. Simulation testing on ultimate degradation in surface water (triggered by Annex VIII, Section 9.2.)

Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., Column 2).

You have provided the following information in the dossier on the degradation simulation in water: *"According to REACh regulation, Annex IX, 9.2, further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The exposure assessment demonstrated, that the risk for environment is controlled and thus, there is no need for further testing of biodegradation."*

This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (ECHA Guidance R.11.4).

As already explained in the Appendix B, Section 6., the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for further degradation investigation.

For ECHA's response, to your comments to the draft decision regarding this request, see request C.4. below.

The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Appendix C, Section 4.

9. Identification of degradation products

Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., Column 2).

You have provided the following information in the dossier on the degradation products: *"According to REACh regulation, Annex IX, 9.2, further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The exposure assessment demonstrated, that the risk for environment is controlled and thus, there is no need for further testing of biodegradation."*

This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance (itself or any of its constituent or impurity present in concentration ≥ 0.1% (w/w) or relevant transformation/degradation product) is a potential PBT/vPvB substance (ECHA Guidance R.11.4).

As already explained in the Appendix B, Section 6. above, the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for further degradation investigation including identification of degradation products.

For ECHA's response, to your comments to the draft decision regarding this request, see request C.5. below.

The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Appendix C, Section 5.

10. Bioaccumulation in aquatic species (triggered by Annex I, Sections 0.6.1. and 4; Annex XIII, Section 2.1.)

Bioaccumulation in aquatic species is required for the purpose of PBT/vPvB assessment (Annex I, Sections 0.6.1 and 4 to REACH).

You have provided the following information in the dossier on bioaccumulation:

- Key study with the analogue substance Surfynol 124 (non-guideline study - Bioconcentration test of chemical substances in fish and shellfish, 2010);and
- Supporting information: QSAR estimation of bioconcentration factors (by BCFBAF v3.01 model) for the nine constituents of the Substance; and
- Justification for data waiving: "the study does not need to be conducted because the substance has a low potential for bioaccumulation based on log Kow <=3".

This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further investigation on bioaccumulation in aquatic species (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (ECHA Guidance R.11.4).

As already explained in the Appendix B, Section 6., the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for bioaccumulation investigation.

For ECHA's response, to your comments to the draft decision regarding this request, see request C.6. below.

The examination of the available information or adaptations, as well as the selection of the requested test and the test design are addressed in Appendix C Section 6.

Appendix C: Reasons to request information required under Annex IX of REACH

1. Sub-chronic toxicity study (90-day)

A Sub-chronic toxicity study (90 day) is a standard information requirement under Annex IX to REACH (Section 8.6.2.).

You have adapted this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5.

In support of your adaptations, you have provided the following sources of information:

i. Two combined subchronic + one-generation oral studies (1979) in rats with the analogue substances (Surfynol 104 and Surfynol 440).
ii. Two subchronic oral studies (1979) in dogs with the analogue substances (Surfynol 104 and Surfynol 440).

We have assessed this information and identified the following issue(s):

Adaptations according to Annex XI

As explained in the Appendix on Reasons common to several requests your adaptation according to Annex XI, Section 1.5. is rejected.

Based on the above, the information you provided does not fulfil the information requirement.

Information on the design of the study to be performed

Referring to the criteria provided in Annex IX, Section 8.6.2, Column 2, the oral route is the most appropriate route of administration to investigate repeated dose toxicity, because the substance is a waxy solid.

In your comments to the draft decision, you agree to provide further data on this endpoint and to perform a sub-chronic toxicity study (90-day), if the existing data do not fulfill the data requirements to investigate possible sub-chronic toxic effects on mammalians. You state that you will first, revise the RSS of the existing study on the read across substance EC 204-809-1 of this category and check, whether this study fulfills the data requirements. Additionally, you will strengthen the read across approach for this endpoint using data from data request B.3 (study for reproductive/developmental toxicity (OECD 422), if it turns out to show similar toxic behavior between both substances.

It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

Therefore the sub-chronic toxicity study must be performed according to the OECD TG 408, in rats and with oral administration of the Substance.

2. Long-term toxicity testing on aquatic invertebrates

Long-term toxicity testing on aquatic invertebrates is an information requirement under Annex IX to REACH (Section 9.1.5.).

You have adapted this information requirement according to Annex IX, Section 9.1, Column

2 with the following justification: "*The chemical safety assessment does not indicate the need to investigate further the effects on aquatic organisms, since the risk characterisation ratio is below 1 for the aquatic compartment. (Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, COLUMN 2, of REGULATION (EC) No 1907/2006).*"

We have assessed this information and identified the following issues:

Under Section 9.1., Column 2, Annex IX to REACH, the study may be omitted if the CSA does not indicate the need for further aquatic toxicity testing. The justification for this adaptation must be documented in the Chemical Safety Report (CSR) and include all the following elements:

- the predicted no effect concentrations (PNEC) for the aquatic compartment which must be based on:
  - reliable information on the hazardous properties of the Substance on at least three trophic levels,
  - an appropriate assessment factor (AF) (ECHA Guidance R.10, Section R.10.3),
- a quantitative exposure assessment which leads to derivation of predicted environmental concentrations (PECs),
- the outcome of the risk characterisation ratio (RCR) which demonstrates that the risks are adequately controlled (*i.e.* PEC < PNEC);
- adequate evidence demonstrating that the substance is not potential PBT substance.

For the reasons explained in Appendix A, Sections on short-term toxicity testing on aquatic invertebrates and growth inhibition study aquatic plants, in Appendix B, Section on short-term toxicity testing on fish and Appendix C, Section on long-term toxicity testing on fish, your dossier does not include reliable hazard information for the Substance on at least three trophic levels. Therefore, a reliable PNECs cannot be derived and risk characterisation for aquatic compartment cannot be performed. Therefore, your adaptation is not acceptable.

Furthermore, as already explained in the Appendix B, Section 6. above, the Substance is a potential PBT. Therefore, the CSA indicates the need for long-term aquatic toxicity investigation.

Therefore, you have not demonstrated that the CSA does not indicate the need for further long-term aquatic toxicity testing and your adaption is rejected.

In your comments to the draft decision, you agree to carry out a study on long-term toxicity testing on aquatic invertebrates to investigate further effects on aquatic organisms.

On this basis, the information requirement is not fulfilled.

3. Long-term toxicity testing on fish

Long-term toxicity testing on fish is an information requirement under Annex IX to REACH (Section 9.1.6.).

You have adapted this information requirement according to Annex IX, Section 9.1, Column 2 with the following justification: "*The chemical safety assessment does not indicate the need to investigate further the effects on aquatic organisms, since the risk characterisation ratio is below 1 for the aquatic compartment. (Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, COLUMN 2, of REGULATION (EC) No 1907/2006).*"

We have assessed this information and identified the following issues:

Under Section 9.1., Column 2, Annex IX to REACH, the study may be omitted if the CSA does not indicate the need for further aquatic toxicity testing. The justification for this adaptation must be documented in the Chemical Safety Report (CSR) and include all the following elements:

- the predicted no effect concentrations (PNEC) for the aquatic compartment which must be based on:
  - reliable information on the hazardous properties of the Substance on at least three trophic levels,
  - an appropriate assessment factor (AF) (ECHA Guidance R.10, Section R.10.3),
- a quantitative exposure assessment which leads to derivation of predicted environmental concentrations (PECs),
- the outcome of the risk characterisation ratio (RCR) which demonstrates that the risks are adequately controlled (*i.e.* PEC < PNEC);
- adequate evidence demonstrating that the substance is not potential PBT substance.

For the reasons explained in Appendix A, Sections on short-term toxicity testing on aquatic invertebrates and growth inhibition study aquatic plants, in Appendix B, Section on short-term toxicity testing on fish and Appendix C, Section on long-term toxicity testing on aquatic invertebrates, your dossier does not include reliable hazard information for the Substance on at least three trophic levels. Therefore, a reliable PNECs cannot be derived and risk characterisation for aquatic compartment cannot be performed. Therefore, your adaptation is not acceptable.

Furthermore, as already explained in the Appendix B, Section 6. above, the Substance is a potential PBT. Therefore, the CSA indicates the need for long-term aquatic toxicity investigation.

Therefore, you have not demonstrated that the CSA does not indicate the need for further long-term aquatic toxicity testing and your adaption is rejected.

In your comments to the draft decision, you agree to carry out a study on long-term toxicity testing on fish only, if this is triggered, i.e. in case the CSA (including PBT/vPvB assessment and risk characterisation) indicates the need to investigate further effects on aquatic organisms.

ECHA notes that following the recent Board of Appeal decision taken for the case (A-011-2018), Annex IX, Section 9.1., Column 2 does not allow omitting the need to submit information on long-term toxicity to fish under Column 1. It must be understood as a trigger for providing further information on long-term toxicity to fish if the chemical safety assessment according to Annex I indicates the need.

On this basis, the information requirement is not fulfilled.

Study design

To fulfil the information requirement for the Substance, the Fish, Early-life Stage Toxicity Test (test method OECD TG 210) is the most appropriate (ECHA Guidance R.7.8.2.).

4. Simulation testing on ultimate degradation in surface water

Simulation testing on ultimate degradation in surface water is an information requirement under Annex IX to REACH (Section 9.2.1.2.).

You have adapted this information requirement according to Annex IX, Section 9.2., Column 2 with the following justification: "*According to REACh regulation, Annex IX, 9.2, further biotic*

degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The exposure assessment demonstrated, that the risk for environment is controlled and thus, there is no need for further testing of biodegradation."

We have assessed this information and identified the following issues:

Under Section 9.2., Column 2 of Annex IX to REACH, the study may be omitted if the chemical safety assessment (CSA) does not indicate the need for further biotic degradation testing. The CSA does indicate such need (Annex I, Section 4; Annex XIII, Section 2.1) if, for instance, the substance is a potential PBT/vPvB substance (ECHA Guidance R.11.4).

As already explained in the Appendix B, Section 6. above, the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for further degradation investigation.

Therefore, you have not demonstrated that the CSA does not indicate the need for further biotic degradation testing and your adaption is rejected.

In your comments to the draft decision, you indicate that the data is requested in order to clarify the potential PBT/vPvB properties of the substance. You propose to employ a stepwise approach, i.e. first clarify the bioaccumulation potential of the substance and based on the outcome of it to conclude, whether further examination on degradation of the substance is needed to clarify whether the substance fulfils the PBT/vPvB criteria. You state that if the substance does not fulfil the B criterion, the PBT/vPvB characteristics do not apply and consequently a generation of further data for the PBT/vPvB assessment are not necessary.

According to the Annex XIII PBT/vPvB assessment shall also take account of the PBT/vPvB properties of relevant constituents of a substance and relevant transformation/degradation products. Therefore, after addressing bioaccumulation potential of only of the major constituent or of some of constituents of the Substance, may not be possible to conclude if the Substance is a potential PBT/vPvB substance and consequently, not possible to justify omission of the simulation degradation testing and identification of degradation products.

On this basis, the information requirement is not fulfilled.

Study design

Under Annex XIII, the information must be based on data obtained under conditions relevant for the PBT/vPvB assessment. Therefore:

- You must perform the OECD TG 309 test, by following the pelagic test option with natural surface water containing approximately 15 mg dw/L of suspended solids (acceptable concentration between 10 and 20 mg dw/L) (ECHA Guidance R.11).

- You must perform the test at the temperature of 12 °C, the average environmental temperature for the EU (ECHA Guidance R.16, Table R.16-8). Performing the test at this temperature is in line with the applicable test conditions of the OECD TG 309.

Non-extractable residues (NER) must be quantified in all simulation studies. The reporting of results must include a scientific justification of the used extraction procedures and solvents. By default, total NER is regarded as non-degraded Substance. However, if reasonably justified and analytically demonstrated a certain part of NER may be differentiated and quantified as irreversibly bound or as degraded to biogenic NER. Such fractions could be regarded as removed when calculating the degradation half-life(s) (ECHA Guidance R.11).

Under Annex XIII, you must assess the PBT/vPvB properties of the relevant constituents of the Substance. Therefore, the persistence of each relevant constituent present in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable must be assessed. Alternatively, you would have to justify why you consider these not relevant for the PBT/vPvB assessment.

5. Identification of degradation products

Identification of degradation products is an information requirement under Annex IX to REACH (Section 9.2.3.).

You have adapted this information requirement according to Annex IX, Section 9.2., Column 2 with the following justification: *"According to REACh regulation, Annex IX, 9.2, further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The exposure assessment demonstrated, that the risk for environment is controlled and thus, there is no need for further testing of biodegradation."*

We have assessed this information and identified the following issues:

Under Section 9.2., Column 2 of Annex IX to REACH, the study may be omitted if the chemical safety assessment (CSA) does not indicate the need for further biotic degradation testing. The CSA does indicate such need (Annex I, Section 4; Annex XIII, Section 2.1) if, for instance, the substance (itself or any of its constituent or impurity present in concentration ≥ 0.1% (w/w) or relevant transformation/degradation product) is a potential PBT/vPvB substance (ECHA Guidance R.11.4).

As already explained in the Appendix B, Section 6., the Substance is a potential PBT/vPvB substance. Therefore, the CSA indicates the need for further degradation investigation including identification of degradation products.

Therefore, you have not demonstrated that the CSA does not indicate the need for further biotic degradation testing including identification of degradation products and your adaption is rejected.

For ECHA's response, to your comments to the draft decision regarding this request, see request C.4. above.

On this basis, the information requirement is not fulfilled.

Study design

Regarding the selection of appropriate and suitable test method(s), the method(s) will have to be substance-specific. Identity, stability, behaviour, and molar quantity of the degradation/transformation products relative to the Substance must be evaluated and reported, when analytically possible. In addition, degradation half-life, log K_{ow} and potential toxicity of the transformation/degradation may need to be investigated. You may obtain this information from the degradation study requested in the Appendix C, Section 4. or by some other measure. If any other method is used for the identification of the transformation/degradation products, you must provide a scientifically valid justification for the chosen method.

To determine the degradation rate of the Substance, the requested study according to OECD TG 309 (Appendix C, Section 4.) must be conducted at 12°C and at a test concentration <

100 µg/L. However, to overcome potential analytical limitations with the identification and quantification of major transformation/degradation products, you may consider running a parallel test at higher temperature (but within the frame provided by the test guideline, *e.g.* 20°C) and at higher application rate (*i.e.* > 100 µg/L).

6. Bioaccumulation in aquatic species

Bioaccumulation in aquatic species is a standard information requirement under Annex IX to REACH (Section 9.3.2.).

In the registration dossier you have provided following information on bioaccumulation:

- Adaptation for this information requirement by using Grouping of substances and read-across approaches under Annex XI, Section 1.5. and in support of your adaptation you have provided following information for this endpoint in your dossier:
    - Key study with the analogue substance Surfynol 124 (non-guideline study - Bioconcentration test of chemical substances in fish and shellfish, 2010);and
    - Supporting information: QSAR estimation of bioconcentration factors (by BCFBAF v3.01 model) for the nine constituents of the Substance; and

- Adaptation for this information requirement under Annex IX, Section 9.3.2., Column 2 with the following justification: "*the study does not need to be conducted because the substance has a low potential for bioaccumulation based on log Kow <=3*".

We have assessed this information and identified the following issues:

a) Rejection of adaptation under Annex XI, Section 1.5

As explained in the Appendix on Reasons common to several requests:
- section 1: your adaptations under Annex XI, Section 1.5 is rejected; and
- section 2: QSAR estimations of aquatic toxicity effect concentrations based on Kow are not reliable for the constituents of the Substance.

b) Quality of the source study

According to Annex XI, Section 1.5., if the grouping concept is applied then in all cases the results to be read across should:
- be adequate for the purpose of classification and labelling and/or risk assessment; and
- have adequate and reliable coverage of the key parameters addressed in the corresponding test method referred to in Article 13(3).

According to the provisions of Annex IX, Section 9.3.2. information on bioaccumulation in aquatic species as specified in the OECD TG 305 shall be provided. In the dossier you indicated that the route of exposure is 'feed', so ECHA understands that the test with dietary exposure of fish was performed. To comply with OECD TG 305 requirements the following requirements must be met:

- Coverage of the key parameter which is the bioaccumulation potential of the test substance in whole fish, which must be determined based on the following parameters:
    1) the uptake rate constant (k_1) and loss rate constants including the depuration rate constant (k_2), and/or
    2) the kinetic bioconcentration factor (BCF_K), and/or
    3) the dietary biomagnification factor (BMF).

- For a test to be valid the following conditions apply:

1) the concentration of the test substance in fish food before and at the end of the uptake phase is within a range of ± 20% (based on at least three samples at both time points);
2) a high degree of homogeneity of substance in the spiked food is demonstrated (i.e. less than ± 15% from the mean in at least three sample);
3) concentrations of test substance is below detection level, or only at typical trace levels, in un-spiked food or control fish tissues;
4) Mortality or other adverse effects/disease in both control and test group fish should be ≤10% at the end of the test.

- a study can be terminated at the end of the uptake period (or with the second depuration sample) only if:
  1) all validity criteria are fulfilled, and
  2) the lack of uptake is not due to some other shortcoming of the test, and
  3) appropriate justification is provided (*e.g.* analysis of faeces for undigested test substance as part of a "mass balance" approach);
- the analytical method used for the quantification of the test material in the feed and in fish tissues is described;
- the BCF/BMF is based on the total concentration in the fish (*i.e.* per total wet weight of the fish);
- tabulated test material concentration data in fish, mean measured concentration at end of uptake, the derived (overall) depuration rate constant and concentration in fish at start of depuration phase are provided;
- the results of the determination of the test substance in test and control diets at least in triplicate are reported;
- method of estimation of the corresponding BCF value from the dietary test is reported.

However, you have provided a study record without information on the above key parameters and validity criteria.

Without this information, you have not demonstrated that the study fulfils the OECD TG 305's key parameters and validity criteria and therefore it is rejected and cannot be used to support your read-across.

c) Rejection of adaptation under Annex IX, Section 9.3.2., Column 2

Under Section 9.3.2., Column 2, first indent of Annex IX to REACH, the study may be omitted if the substance has a low potential for bioaccumulation and/or a low potential to cross biological membranes. A low log Kow (*i.e.* log Kow < 3) may be used to support low potential for bioaccumulation if the partitioning to lipids is the sole mechanism driving the bioaccumulation potential of a substance. For some groups of substances (e.g. organometals, ionisable substances, surfactants) other partitioning mechanisms may drive bioaccumulation (e.g. binding to protein/cell membranes). For this reason log Kow is not considered a valid descriptor of the bioaccumulation potential for such substances (ECHA Guidance R.7c, Appendix R.7.10-3).

In the registration dossier you note that the Substance is surfactant which is supported by the provided evidence on surface tension equal to 33 mN/m at 20 °C and 100 mg/l concentration on the basis of read-across from Surfynol 104 and Surfynol 440. Therefore, log Kow is not a valid descriptor of the bioaccumulation potential of the Substance and your adaptation is rejected.

In your comments to the draft decision, you note that will first revise RSS of the existing study for the analogue substance and check, whether this study fulfils the information requirement. Additionally, you state you will strengthen the read-across approach for this

information requirement. Furthermore, you agree to perform bioaccumulation in aquatic species study, if the existing data do not fulfil the information requirement.

It is in your discretion to generate and provide the necessary supporting information in order to justify your read-across adaptation. If you do so, you are responsible for demonstrating the fulfilment of the requirements of Section 1.5 of Annex XI to REACH. If it fails and the resulting data does not support, or even contradict, your read-across hypothesis, you remain responsible for complying with this decision by the set deadline.

On this basis, the information requirement is not fulfilled.

Study design

Bioaccumulation in fish: aqueous and dietary exposure (Method EU C.13 / OECD TG 305) is the preferred test to investigate bioaccumulation (ECHA Guidance R.7.10.3.1.). Exposure via the aqueous route (OECD TG 305-I) must be conducted unless it can be demonstrated that:

- a stable and fully dissolved concentration of the test substance in water cannot be maintained within ± 20% of the mean measured value, and/or
- the highest achievable concentration is less than an order of magnitude above the limit of quantification (LoQ) of a sensitive analytical method.

This test set-up is preferred as it allows for a direct comparison with the B and vB criteria of Annex XIII of REACH.

You may only conduct the study using the dietary exposure route (OECD 305-III) if you justify and document that testing through aquatic exposure is not technically possible as indicated above. You must then estimate the corresponding BCF value from the dietary test data according to Annex 8 of the OECD 305 TG and OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation (ENV/JM/MONO(2017)16).

Under Annex XIII, you must assess the PBT/vPvB properties of the relevant constituents of the Substance. Therefore, the bioaccumulation of each relevant constituent present in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable must be assessed. Alternatively, you would have to justify why you consider these not relevant for the PBT/vPvB assessment.

7. Long-term toxicity on terrestial invertebrates

Short-term toxicity testing on invertebrates is an information requirement under Annex IX to REACH (Section 9.4.1.). Long-term toxicity testing on invertebrates must be considered (Annex IX, Section 9.4., Column 2) if the substance has a high potential to adsorb to soil or is very persistent.

You have adapted this information requirement according to Annex IX, Section 9.4., Column 2 with the following justification: "*The substance is water soluble (2.3 g/L), has as an assumed worst-case log Kow of 2.5 and a bioaccumulation factor of clearly below 2000, based on supporting data. Furthermore the Koc value based on calculation is well below 1000. This is demonstrating a negligible potential to adsorb to soil and for accumulation in the aqueous and terrestrial compartments. It shall be also noted that in the environmental exposure assessments the local and regional RCRs are resulting below 1, which is indicating a low risk to organisms in the different environmental compartments. Hence according to Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, 9.4 Effects on terrestrial organisms, COLUMN 2, of REGULATION (EC) No 1907/2006, studies on the effects on terrestrial organisms do not need to be conducted.*"

We have assessed this information and identified the following issues:

a) Triggering of the long-term toxicity testing

According to ECHA Guidance R.7c, Section R.7.11.6.3. substances that are ionisable or have a log K_{ow}/K_{oc} >5 are considered highly adsorptive, whereas substances with a half-life >180 days (default setting, unless classified as readily biodegradable) are considered very persistent in soil.

Based on the information provided in the registration dossier and as explained in Appendix B, Section 6. the Substance is not readily biodegradable and there is no half-life of the Substance in soil available, therefore the Substance is considered to be very persistent (ECHA Guidance R.7c).

Thus, the long-term toxicity testing on terrestrial organisms is required.

b) Rejection of adaptation

As explained in the Appendix on Reasons common to several requests, Section 3, your adaptation according to Annex IX, Section 9.4., Column 2 is rejected.

In your comments to the draft decision, you agreed to carry out a study on long-term toxicity to terrestrial invertebrates in order to evaluate the risk for this compartment.

On this basis, the information requirement is not fulfilled.

Study design

The earthworm reproduction test (OECD TG 222), Enchytraeid reproduction test (OECD TG 220), and Collembolan reproduction test (OECD TG 232) are each considered capable of generating information appropriate for the fulfilment of the information requirement for long-term toxicity testing on terrestrial invertebrates.

ECHA notes that when log Kow >5 or log Koc >4, the test OECD 232 is not appropriate as the dominant route of exposure for Collembolans is via pore water.ECHA is not in a position to determine the most appropriate test protocol, since such determination is dependent upon species sensitivity and substance properties.

8. Effects on soil micro-organisms

Effects on soil micro-organisms is an information requirement under Annex IX to REACH (Section 9.4.2.).

You have adapted this information requirement according to Annex IX, Section 9.4., Column 2 with the following justification: "*The substance is water soluble (2.3 g/L), has as an assumed worst-case log Kow of 2.5 and a bioaccumulation factor of clearly below 2000, based on supporting data. Furthermore the Koc value based on calculation is well below 1000. This is demonstrating a negligible potential to adsorb to soil and for accumulation in the aqueous and terrestrial compartments. It shall be also noted that in the environmental exposure assessments the local and regional RCRs are resulting below 1, which is indicating a low risk to organisms in the different environmental compartments. Hence according to Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, 9.4 Effects on terrestrial organisms, COLUMN 2, of REGULATION (EC) No 1907/2006, studies on the effects on terrestrial organisms do not need to be conducted.*"

We have assessed this information and identified the following issue:

As explained in the Appendix on Reasons common to several requests, Section 3 your adaptation according to Annex IX, Section 9.4., Column 2 is rejected.

In your comments to the draft decision, you propose to employ a stepwise approach. In the first step you propose to perform the study on terrestrial species (invertebrates or plants) and based on the outcome of this study, risk assessment for the soil compartment has to be evaluated. You claim only if a risk for the soil is indicated, the soil micro-organisms study would be conducted.

As outlined in Appendix E below, EPM extrapolation is not applicable for this information requirement as the intrinsic properties of soil microorganism communities are not addressed through this method.

On this basis, the information requirement is not fulfilled.

Study design

According to ECHA Guidance R.7c, Section R.7.11.3.1., the nitrogen transformation test is considered sufficient for most non-agrochemicals. However, as the substance has identified agrochemical uses, ECHA considers that both the nitrogen (EU C.21./OECD TG 216) and carbon transformation (EU C.22./OECD TG 217) tests should be performed simultaneously.

9. Long-term toxicity on terrestial plants

Short-term toxicity to plants is an information requirement under Annex IX to REACH (Section 9.4.3.). Long-term toxicity testing on plants must be considered (Section 9.4., Column 2) if the substance has a high potential to adsorb to soil or is very persistent.

You have adapted this information requirement according to Annex IX, Section 9.4., Column 2 with the following justification: "*The substance is water soluble (2.3 g/L), has as an assumed worst-case log Kow of 2.5 and a bioaccumulation factor of clearly below 2000, based on supporting data. Furthermore the Koc value based on calculation is well below 1000. This is demonstrating a negligible potential to adsorb to soil and for accumulation in the aqueous and terrestrial compartments. It shall be also noted that in the environmental exposure assessments the local and regional RCRs are resulting below 1, which is indicating a low risk to organisms in the different environmental compartments. Hence according to Annex IX, 9. ECOTOXICOLOGICAL INFORMATION, 9.4 Effects on terrestrial organisms, COLUMN 2, of REGULATION (EC) No 1907/2006, studies on the effects on terrestrial organisms do not need to be conducted.*"

We have assessed this information and identified the following issues:

a) Triggering of the long-term toxicity testing

As explained in the Appendix C, Section on Long-term toxicity on terrestial invertebrates above, the long-term toxicity testing on terrestrial organisms is required.

b) Rejection of adaptation

As explained in the Appendix on Reasons common to several requests, Section 3, your adaptations according to Annex IX, Section 9.4., Column 2 is rejected.

In your comments to the draft decision, you propose to employ a stepwise approach. In the

first step you state that the study on terrestrial species (invertebrates or plants) has to be done and based on the outcome of this study risk assessment for the soil compartment has to be evaluated. You claim that only if a risk for soil would be indicated, the long-term toxicity to terrestrial plants study would be conducted.

As outlined in Appendix E below, if the results of the requested aquatic toxicity testing allow the subsequent derivation of a PNEC for aquatic organisms, you may consider the ITS as recommended in ECHA Guidance R.7c (Section R.7.11.6) and determine the need for further testing on terrestrial organisms via the EPM extrapolation method. If you conclude that no further investigation of long-term toxicity to terrestrial plants is required, you should update your technical dossier by clearly stating the reasons for adapting the information requirement.

On this basis, the information requirement is not fulfilled.

Study design

OECD TG 208 (Terrestrial plants, growth test) considers the need to select the number of test species according to relevant regulatory requirements, and the need for a reasonably broad selection of species to account for interspecies sensitivity distribution. For long-term toxicity testing, ECHA considers six species as the minimum to achieve a reasonably broad selection. Testing shall be conducted with species from different families, as a minimum with two monocotyledonous species and four dicotyledonous species, selected according to the criteria indicated in the OECD TG 208 guideline. You should consider if testing on additional species is required to cover the information requirement.

Terrestrial plants, growth test (OECD TG 208 with at least six species) and Soil Quality – Biological Methods – Chronic toxicity in higher plants (ISO 22030) are each considered capable of generating information appropriate for the fulfilment of the information requirement for long-term toxicity testing on terrestrial plants.

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Appendix D: Requirements to fulfil when conducting and reporting new tests for REACH purposes

A. Test methods, GLP requirements and reporting

1. Under Article 13(3) of REACH, all new data generated as a result of this decision must be conducted according to the test methods laid down in a European Commission Regulation or to international test methods recognised by the Commission or ECHA as being appropriate.

2. Under Article 13(4) of REACH, ecotoxicological and toxicological tests and analyses must be carried out according to the GLP principles (Directive 2004/10/EC) or other international standards recognised by the Commission or ECHA.

3. Under Article 10(a)(vi) and (vii) of REACH, all new data generated as a result of this decision must be reported as study summaries, or as robust study summaries, if required under Annex I of REACH. See ECHA Practical Guide on How to report robust study summaries[9].

B. Test material

Before generating new data, you must agree within the joint submission on the chemical composition of the material to be tested (Test Material) which must be relevant for all the registrants of the Substance.

1. *Selection of the Test material(s)*

   The Test Material used to generate the new data must be selected taking into account the following:
   a) the variation in compositions reported by all members of the joint submission,
   b) the boundary composition(s) of the Substance,
   c) the impact of each constituent/ impurity on the test results for the endpoint to be assessed. For example, if a constituent/ impurity of the Substance is known to have an impact on (eco)toxicity, the selected Test Material must contain that constituent/ impurity.

2. *Information on the Test Material needed in the updated dossier*

   a) You must report the composition of the Test Material selected for each study, under the "Test material information" section, for each respective endpoint study record in IUCLID.
   b) The reported composition must include the careful identification and description of the characteristics of the Tests Materials in accordance with OECD GLP (ENV/MC/CHEM(98)16) and EU Test Methods Regulation (EU) 440/2008 (Note, Annex), namely all the constituents must be identified as far as possible as well as their concentration. Also any constituents that have harmonised classification and labelling according to the CLP Regulation must be identified and quantified using the appropriate analytical methods,

With that detailed information, ECHA can confirm whether the Test Material is relevant for the Substance and whether it is suitable for use by all members of the joint submission.

Technical instructions on how to report the above is available in the manual on How to prepare registration and PPORD dossiers[10].

[9] https://echa.europa.eu/practical-guides
[10] https://echa.europa.eu/manuals

Appendix E: General recommendations when conducting and reporting new tests for REACH purposes

A. Strategy for the PBT/vPvB assessment

You are advised to consult ECHA Guidance R.7b (Section R.7.9.), R.7c (Section R.7.10) and R.11 on PBT assessment to determine the sequence of the tests needed to reach the conclusion on PBT/vPvB. The guidance provides advice on 1) integrated testing strategies (ITS) for the P, B and T assessments and 2) the interpretation of results in concluding whether the Substance fulfils the PBT/vPvB criteria of Annex XIII.

In particular, you are advised to first conclude whether the Substance fulfils the Annex XIII criteria for P and vP, and then continue with the assessment for bioaccumulation. When determining the sequence of simulation degradation testing you are advised to consider the intrinsic properties of the Substance, its identified uses and release patterns as these could significantly influence the environmental fate of the Substance. You must revise your PBT assessment when the new information is available.

B. Testing strategies for terrestrial toxicity testing

If the results of the requested aquatic toxicity tests on fish, aquatic invertebrates and algae allow the subsequent derivation of a PNEC for aquatic organisms, you may consider the Integrated Testing Strategy (ITS) as recommended in ECHA Guidance R.7c (Section R.7.11.6) and determine the need for further testing on terrestrial organisms. If you conclude that no further investigation of effects on terrestrial organisms is required, you should update your technical dossier by clearly stating the reasons for adapting the information requirements of Annex IX, Section 9.4. of the REACH Regulation.

ECHA emphasises that the intrinsic properties of soil microbial communities are not addressed through the EPM extrapolation method and therefore the potential adaptation possibility outlined for the information requirement of Annex IX, Section 9.4. does not apply for the endpoint of Effects on soil micro-organisms.

C. Environmental testing for substances containing multiple constituents

Your Substance contains multiple constituens and, as indicated in ECHA Guidance R.11 (Section R.11.4.2.2), you are advised to consider the following approaches for persistency, bioaccumulation and aquatic toxicity testing:

- the "known constituents approach" (by assessing specific constituents), or
- the "fraction/block approach, (performed on the basis of fractions/blocks of constituents), or
- the "whole substance approach", or
- various combinations of the approaches described above

Selection of the appropriate approach must take into account the possibility to characterise the Substance (i.e. knowledge of its constituents and/or fractions and any differences in their properties) and the possibility to isolate or synthetize its relevant constituents and/or fractions.

Appendix F: Procedure

This decision does not prevent ECHA from initiating further compliance checks at a later stage on the registrations present.

ECHA followed the procedure detailed in Articles 50 and 51 of REACH.

The compliance check was initiated on 5 November 2019.

The decision making followed the procedure of Article 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA took into account your comments and did not amend the request(s) but amended the deadline.

Deadline to submit the requested information in this decision

The timeline indicated in the draft decision to provide the information requested is as follows:

A.1-3, B.1-3, B.8-9, C.1, C.4-5 by the deadline of exact date of 18 months from the date of the decision and all the remaining information listed by the deadline of exact date of 42 months from the date of the decision.

In your comments on the draft decision, you requested an extension of the timeline from 18 months to 30 months for the information requested under B.8-9 and C.4-5. You justified your request on the following grounds:

"The timeline of 18 months for the simulation testing on ultimate degradation in surface waterand identification of degradation products indicated in the draft decision for submitting the update of the registration dossier containing the information required is too short. Please note, that this substance is considered as difficult to analyze due to its surface-active properties. From experience we are aware that we need to develop and validate sophisticated analytical methods, which is time consuming and will extend the timeframe of the study enormously. Further, this requested test is of a complex nature which requires careful planning and selection of a reliable testing facility who is able to carry out such tests. Experience shows that these activities require a considerable period of time. Last not least, if the proposed sequential testing approach is implemented, also the timeline has to be extended accordingly. For these studies, at least 24 months have to be calculated including experimental setup, synthesis of the radiolabeled substance, analytical work and reporting. It is not clear, if experienced laboratories are able to start such type of studies immediately. Additionally there are the same data requests in other draft decisions on compliance checks for the same group of substances, all within the category. These are: EC 204-809-1; EC 500-022-5; EC 451-160-7 and EC 269-348-0 So it would be best to perform this type of study for all of the relevant substances in the same laboratory. Which might be difficult to deal in parallel and needs additional time for the laboratory. Therefore, we ask to prolong the timeline to at least 30 months."

In support of your request you provided document from the test laboratory justifying the extension of the deadline. In the document it is explained that the testing might take between 16-26 months.

It is not clear from the documentation whether longer or shorter testing period would be needed for the Substance. Therefore, in order not to delay the testing, mean duration of 21

month for the testing is granted with additional 3 months to cover necessary administrative steps. In respect of the sequential testing, as noted in the Appendix D above, it is advised to first conclude whether the Substance (including relevant constituents and relevant transformation/degradation products) fulfils the Annex XIII criteria for P and vP, and then continue with the assessment for bioaccumulation.

Therefore, on these grounds, ECHA has partially granted the request and set the deadline to 24 months for the information requested under B.8-9 and C.4-5.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

Appendix G: List of references - ECHA Guidance[11] and other supporting documents

Evaluation of available information
Guidance on information requirements and chemical safety assessment, Chapter R.4 (version 1.1., December 2011), referred to as ECHA Guidance R.4 where relevant.

QSARs, read-across and grouping
Guidance on information requirements and chemical safety assessment, Chapter R.6 (version 1.0, May 2008), referred to as ECHA Guidance R.6 where relevant.

Read-across assessment framework (RAAF, March 2017)[12]

RAAF - considerations on multiconstituent substances and UVCBs (RAAF UVCB, March 2017)

Physical-chemical properties
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Toxicology
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

Environmental toxicology and fate
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7b (version 4.0, June 2017), referred to as ECHA Guidance R.7b in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

PBT assessment
Guidance on information requirements and chemical safety assessment, Chapter R.11 (version 3.0, June 2017), referred to as ECHA Guidance R.11 in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.16 (version 3.0, February 2016), referred to as ECHA Guidance R.16 in this decision.

Data sharing
Guidance on data-sharing (version 3.1, January 2017), referred to as ECHA Guidance on data sharing in this decision.

OECD Guidance documents[13]
Guidance Document on aqueous–phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD 23.

[11] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
[12] https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across
[13] http://www.oecd.org/chemicalsafety/testing/series-testing-assessment-publications-number.htm

Guidance document on transformation/dissolution of metals and metal compounds in aqueous media – No 29, referred to as OECD GD 29.

Guidance Document on Standardised Test Guidelines for Evaluating Chemicals for Endocrine Disruption – No 150, referred to as OECD GD 150.

Guidance Document supporting OECD test guideline 443 on the extended one-generation reproductive toxicity test – No 151, referred to as OECD GD 151.

ECHA
EUROPEAN CHEMICALS AGENCY

Appendix H: Addressees of this decision and the corresponding information requirements applicable to them

You must provide the information requested in this decision for all REACH Annexes applicable to you.

Registrant Name	Registration number	Highest REACH Annex applicable to you
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]

Where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas ECHA will send the decision to the actual registrant.