EUROPEAN CHEMICALS AGENCY

Helsinki, 11 February 2020

Addressees
Registrants of [redacted] listed in the last Appendix of this decision

Date of submission for the jointly submitted dossier subject of this decision
16/02/2018

Registered substance subject to this decision, hereafter 'the Substance'
Substance name: Polysulfides, di-tert-nonyl
EC number: 270-336-2
CAS number: 68425-16-1

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

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (REACH), ECHA requests that you submit the information listed below by the deadlines provided.

A. Requirements applicable to all the Registrants subject to Annex VII of REACH

1. Water solubility (Annex VII, Section 7.7.) with the Substance

2. Skin sensitisation (Annex VII, Section 8.3.):

   - i) *in vitro/in chemico* skin sensitisation information on molecular interactions with skin proteins (OECD TG 442C), inflammatory response in keratinocytes (OECD TG 442D) and activation of dendritic cells (OECD TG 442E) (Annex VII, Section 8.3.1.) with the Substance; and
   - ii) *in vivo* skin sensitisation (Annex VII, Section 8.3.2.; test method: EU B.42./OECD TG 429) with the Substance, in case the *in vitro/in chemico* test methods specified under point i) are not applicable for the Substance or the results obtained are not adequate for classification and risk assessment;

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

B. Requirements applicable to all the Registrants subject to Annex VIII of REACH

1. In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.; test method OECD TG 476 or TG 490) with the Substance

2. Adsorption/desorption screening (Annex VIII, Section 9.3.1.; using an appropriate test method) with the Substance

C. Requirements applicable to all the Registrants subject to Annex IX of REACH

1. Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method OECD TG 414) in a first species (rat or rabbit), oral route with the Substance

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

3. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.; test method OECD TG 210) with the Substance

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

5. Soil simulation testing (Annex IX, Section 9.2.1.3.; test method EU C.23./OECD TG 307) at a temperature of 12 °C with the Substance including degradation of each relevant constituent present in concentration at or above 0.1% (w/w).

6. Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method EU C.24./OECD TG 308) at a temperature of 12 °C with the Substance including degradation of each relevant constituent present in concentration at or above 0.1% (w/w).

7. Identification of degradation products (Annex IX, 9.2.3.) using an appropriate test method, among those requested above C.4, C.5 and C.6., with the Substance

8. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD TG 305, aqueous/dietary exposure with the Substance including each relevant constituent present in concentration at or above 0.1% (w/w) and relevant degradation products.

Conditions to comply with the requested information

You are bound by the requests for information corresponding to the REACH Annexes applicable to your own registered tonnage of the Substance at the time of evaluation. Therefore you have to comply with the requirements of you have to comply with the requirements of Annexes VII, VIII and IX of REACH, if you have registered a substance at 100-1000 tpa.

The Appendix on general considerations addresses common arguments that are applicable throughout the present decision while the other Appendices state the reasons for the requests for information to fulfil the requirements set out in the respective Annexes of REACH.

The Appendix entitled Observations and technical guidance addresses the generic approach for the selection and reporting of the test material used to perform the required studies and provides generic recommendations and references to ECHA guidance and other reference documents.

The studies relating to biodegradation and bioaccumulation (request C.4-C.8) 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 test are performed and other conditions described in Appendix F section 5.

You must submit the information requested in points A.1-2; B.1-2; C.1 above in an updated registration dossier by ***18 February 2021*** and the information requested in points C.2- 8 above by ***18 August 2022***.

You must also update the chemical safety report, where relevant, including any changes to classification and labelling based on the newly generated information. The timeline has been set to allow for sequential testing where relevant.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, has to be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under: http://echa.europa.eu/regulations/appeals.

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 general considerations

(i) Assessment of the Grouping of substances and read-across approach, in light of the requirements of Annex XI, Section 1.5.

You seek to adapt the following standard information requirements by applying (a) read-across approach(es) in accordance with Annex XI, Section 1.5:

- Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.)
- Water solubility (Annex VII, Section 7.7)
- Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
- Adsorption/desorption screening (Annex VIII, Section 9.3.1)
- Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.)
- Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.)
- Sediment simulation testing (Annex IX, Section 9.2.1.4.)
- Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)

ECHA has considered the scientific and regulatory validity of your read-across approach(es) 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. 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.

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].

A. Predictions for toxicological properties, for water solubility and adsorption/desorption

Annex XI, Section 1.5 requires that whenever read-across is used adequate and reliable documentation of the applied method must be provided.

You have provided studies conducted with substances other than your Substance in order to comply with the REACH information requirements. You have not provided documentation as to why this information is relevant for your Substance. In your dossier you have provided a 'Read across justification for polysulfides, di-tert nonyl' document. That document covers only environmental endpoints.

In addition, you have not provided supporting experimental data (e.g. a screening test) with the Substance in support of a read-across adaptation for toxicological endpoints.

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[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

In the absence of such documentation concerning toxicological properties, water solubility and adsorption/desorption, including justification with supporting evidence, ECHA cannot verify that the properties of your Substance can be predicted from the data on the source substance(s).

ECHA notes that in your comments on the initial draft decision you explain that you plan to update your justification and include information on metabolites of source and target/analogue substances, and additional toxicological data on EC 270-335-7 and EC 273-103-3. You also mention "*Consideration of laboratory studies to support predicted metabolites, if necessary*". ECHA will evaluate your updated Annex XI, Section 1.5 adaptation in the follow-up, after the expiry of the deadline for provision of information set in this decision.

B. Predictions for ecotoxicological properties and environmental fate

You have provided a read-across justification document in IUCLID Section 5.3.1, 6.1.2 and 6.1.4.

You read across to your Substance from the structurally similar substance, di-tert-dodecyl Polysulfides, EC No. 270-335-7 (CAS No. 68425-15-0) as source substance and the Substance as target substance.

You have provided the following reasoning for the prediction of aquatic toxicity: "Both substances are structually similar, therefore a similar lack of toxicity is expected for target and source substances in aquatic toxicity studies".

You have provided the following reasoning for the prediction of biodegradation: "Due to the structural similarity the rate and extent of biodegradation will be similar, and degradation products will also be similar".

You have provided the following reasoning for the prediction of bioaccumulation: "For bioaccumulation, both substances are poorly soluble and unlikely to be maintained in the aquatic compartment in order to be taken up and bioaccumularted".

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 properties of your Substance are predicted to be quantitatively equal to those of the source substance.

ECHA notes the following shortcomings with regards to prediction(s) of ecotoxicological properties and environmental fate:

1. *Insufficient read-across hypothesis for ecotoxicological properties and environmental fate*

According to Annex XI, Section 1.5., two conditions shall be necessarily fulfilled. 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. 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 (read-across approach).

A read-across hypothesis needs to be provided, establishing why a prediction for a toxicological or ecotoxicological property is reliable. This hypothesis should be based on

recognition of the structural similarities and differences between the source substance(s) and your Substance[5]. It should explain why the differences in the chemical structures should not influence the ecotoxicological properties or should do so in a regular pattern.

Your read-across hypothesis is that the similarity in chemical structure, for aquatic toxicity and biodegradation, and in some of the physico-chemical properties, for bioaccumulation, between the source substance(s) and your Substance is a sufficient basis for predicting the properties of your Substance for other endpoints.

Aquatic toxicity and biodegradation: You have not provided an explanation of how and to what extent the differences in the chemical structures (i.e. difference in chain length of the alkyl chain) may affect the prediction of the properties of your Substance for the relevant endpoints.

Finally, in the read-across justification document section 2.6 (Bias that influence the prediction), you claim that "the chosen source substance, polysulfides, di-tert-dodecyl, is a closer structural analogue to the target substance (than another structually similar substance, polysulfides, di-tert-butyl), as the alkyl chain length is more similar, therefore this is considered to be a more suitable source substance".

However, the data set reported in the technical dossier does not include any relevant, reliable and adequate information for shorter alkyl chain, polysulfides, di-tert-butyl.

Bioaccumulation: Although you state that both substances are poorly soluble, you have not provided any experimental data or other adequate and reliable information for the aqueous solubility of the Substance.

Similarity in chemical structure or similarity of some of the physico-chemical properties does not necessarily lead to predictable or similar environmental properties in other endpoints. As described above, a well-founded hypothesis is needed to establish a reliable prediction for a ecotoxicological property, based on recognition of the structural similarities and differences between the source substance(s) and your Substance.

In the absence of this information, ECH cannot verify that the properties of the Substance can be predicted from the data on the source substance for the relevant endpoints.

Furtheremore, you have not established that the source substance is indeed more similar to the Substance and thus can be considered to be more suitable source substance than polysulfides, di-tert-butyl for aquatic toxicity and biodegradation. Therefore you have not provided sufficient supporting information to strengthen the rationale for the choice of source substance and the read-across approach (i.e. analogue rather than a category).

2. *Missing supporting information/ bridging study to compare ecotoxicological and environmental fate properties*

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*"[6]. The set of supporting information should allow to verify the crucial aspects of the read-across hypothesis and

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

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

establish that the properties of the Substance can be predicted from the data on the source substance(s).

"Supporting information" must include bioavailability information, information/bridging studies to compare properties of the target and source substances.

As indicated above, your read-across hypothesis on aquatic toxicity and biodegradation is based on the assumption that the structurally similar target and source substances cause the same type of effect(s).

For bioaccumulation, your read-across hypothesis is that the physico-chemical similarity (i.e. solubility in water) between the source substance(s) and your Substance is a sufficient basis for predicting the properties of your Substance.

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 of the source substance is necessary to confirm that both substance cause the same type of effects. Such information can be obtained, for example, from bridging studies of comparable design and duration for the Substance and of the source substance.

(1) Aquatic toxicity

In the technical dossier for the aquatic toxicity, you have submitted two studies only on short-term fish with the Substance (2000 and 2002) performed according to OECD TG 203 and EU C.1. respectively.

For the reasons provided below (section 3. *Adequacy and reliability of source study)* these studies are not adequate to conclude on aquatic toxicity on the Substance.

Consequently currently there are no aquatic toxicity studies on the Substance available which are considered adequate and reliable.

In the absence of any valid aquatic toxicity studies on the Substance, the data set reported in the technical dossier does not include such relevant, reliable and adequate information for the Substances to support your read-across hypothesis.

Furthermore, you have not provided an evidence supporting that the difference in the chemical structures and in aqueous solubility do not affect the bioavailability and the prediction of the properties of your Substance.

(2) Biodegradation

For biodegradation you state that "both substances are likely to degrade at similar rate, follow similar degradation pathways and results in similar degradation pathways and results on similar primary degradation products".

However, you have not provided any experimental data or other adequate and reliable information on neither the aqueous solubility and rate of biodegradation of your Substance, nor degradation products of your Substance and the source substance.

(3) Bioaccumulation

Your read-across hypothesis is that the physico-chemical similarity (i.e. solubility in water) between the source substance(s) and your Substance is a sufficient basis for predicting the properties of your Substance.

In addition to the read-across hypothesis based on the poor solubilities in water, in your read-across justification document you state that "although some differences in bioaccumulation potential are possible between the source and target substance, due to difference in chain length and molecular weight, as the source substance could not be detected in fish following 14 days of exposure, it is considered that even if the target substance is found to be slightly more bioavailable it is still extreamly unlikely to sugnificantly biomagnify or bioaccumulate".

You have not provided any evidence supporting the claim that the difference in chemical structure such as the chain length and molecular weight and aqueous solubility do not affect the bioavailability and the prediction of the properties of your Substance.

In the absence of such information, you have not established that the Substance and of 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.

ECHA notes the following additional shortcoming with regards to prediction(s) of ecotoxicological properties:

3. Adequacy and reliability of 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.

In particular, poorly water soluble substance requires long time to reach steady-state conditions. Hence, the short-term tests may not give true measure of toxicity (irrespective of whether analytical monitoring was performed or not) for this type of the substances and the long-term test would be needed.

You have provided studies for short-term aquatic toxicity to support your read-across approach, OECD TG 203, 2000, EU C.1., 2002, on the Substance and EU C.2., 1998 and OECD TG 203, 2010 on an analogue substance.

You indicated on the Short-term fish endpoint in the supporting study (OECD TG 203, 2000), as well as other information (EU C.1., 2002) that the Substance could not be detected above the limit of detection of the analytical method used (i.e. 0.11 mg/L). No experimental data on water solubility were provided for the Substance.

As discussed below (request A-1), you did not provide reliable information on water solubility of the Substance. However, you indicated on the Short-term fish endpoint in the supporting study (OECD TG 203, 2000), as well as other information (EU C.1., 2002) that the Substance could not be detected above the limit of detection of the analytical method used (i.e. 0.11 mg/L). Although currently there is no water solubility value on the Substance, ECHA considers that the evidence from the short-term fish studies is a sufficient basis to consider the Substance to be poorly water soluble.

Therefore, the short term aquatic toxicity studies are not adequate for the purpose of classification and labelling and/or risk assessment and thus not adequate for the purpose of read-across.

C. Conclusions on the read-across approach

As explained above, you have not established that relevant properties of the Substance can be predicted from data on the analogue substance. 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.

In your comment on the initial draft decision you explain that you are planning to update your dossier with a read-across hypothesis and justification written in line with the RAAF criteria. ECHA will evaluate your updated Annex XI, Section 1.5 adaptation in the follow-up, after the expiry of the deadline for provision of information set in this decision.

(ii) Assessment of the Qualitative or quantitative structure-activity relationships adaptations, in light of the requirements of Annex XI, Section 1.3

You have adapted the following standard information requirements by using data derived from Qualitative or quantitative structure-activity relationship (QSAR) in accordance with Annex XI, Section 1.3:

- Water solubility (Annex VII, Section 7.7.);
- Adsorption/desorption screening (Annex VIII, Section 9.3.1.).

We have assessed this information and identified the following general issue:

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, in particular:

- the substance falls within the applicability domain of the QSAR model;
- adequate and reliable documentation of the applied method is provided

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 not included QMRFs and a QPRFs in your dossier for any of the endpoints listed above. Therefore ECHA cannot verify whether the cumulative conditions of Annex XI, Section 1.3 listed above are met.

In addition, the predictions with the model used (WSKOW) for water solubility of Substance can not be considered reliable because the Substance does not fall within the applicability domain of the model. Indeed, the training set of the model includes disulfides but not higher number of sulfides.

Your adaptations do not comply with the general rules of adaptation as set out in Annex XI, Section 1.3. Therefore, your adaptations are rejected.

Appendix A: Reasons for the requests to comply with Annex VII of REACH

In accordance with Articles 10(a) and 12(1) of REACH, a technical dossier registered at 1 to 10 tonnes or more per year must contain, as a minimum, the information specified in Annex VII to REACH.

1. Water solubility (Annex VII, Section 7.7.)

Water solubility is a standard information requirement in Annex VII to REACH.

You have adapted this information requirement by using

- a Grouping of substances and read-across approach under Annex XI, Section 1.5. based on OECD TG 105 study (2016) with an analogue substance (key study), and
- data derived from Qualitative or quantitative structure-activity relationship (QSAR) in accordance with Annex XI, Section 1.3 with the Substance (supporting study, 2009)

As explained in the Appendix on general considerations sections (i) and (ii) above, your adaptations are rejected.

Therefore the information provided does not fulfil the information requirement and there is a data gap that needs to be filled in.

In your comment on the initial draft decision you indicate that you will perform a study.

2. Skin sensitisation (Annex VII, Section 8.3.);

Skin sensitisation is a standard information requirement under Annex VII. Registrants must submit information allowing a conclusion whether the substance is a skin sensitiser and whether it can be presumed to have the potential to produce significant sensitisation in humans (Cat. 1A), and risk assessment, where required. [7]

You have provided a key study according to OECD TG 406 (Guinea Pig Maximisation Test, 2002) and a supporting study according to OECD TG 406 (Guinea Pig Maximisation Test, 1979).

To fulfil the information requirement, the study has to meet the requirements of OECD TG 406 (1981 and/or 1992). The key parameters of this test guideline include:

a) Positive control to establish the sensitivity and reliability of the experimental technique (OECD TG 406, paragrapgh 11), and
b) Selection of challenge concentration: The concentration used for challenge should be the highest non-irritant concentration (OECD TG 406, paragraph 14).

The reported study does not comply with these key parameters for the following reasons:

a) Information on positive control group to establish the sensitivity and reliability of the study is missing,
b) No information on irritation following induction exposure was provided. Also, no justification for selecting a very low concentration of 1% for a non-irritating substance was provided.

[7] ECHA Guidance R.7a, Section R.7.3.7.2.

Therefore, the information provided does not cover the key parameters required by OECD TG 406. Consequently, the information requirement is not fulfilled, and your conclusion that the Substance does not cause skin sensitisation is rejected.

Further information on the Testing and assessment strategy for skin sensitisationcan be found in ECHA guidance R.7a, Section R.7.3.7.

ECHA notes that in your comments on the initial draft decision you express your intention to improve your dossier by including "*Further information on irritation, positive control group and justification for dose selection for the skin sensitization study*". ECHA will evaluate your updated Annex XI, Section 1.5 adaptation in the follow-up, after the expiry of the deadline for provision of information set in this decision.

3. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.);

Growth inhibition study aquatic plants is a standard information requirement in Annex VII to REACH.

You have provided

- Key study: An OECD TG 201 study (2000) with an analogue substance

We have assessed this information and identified following issues:

A. As explained in the Appendix on general considerations above, your adaptation is rejected.

In addition we have identified the following deficiency with the study (2000).

B. Tests on substances must be conducted in accordance with OECD test guidelines or another recognised international test method (Article 13(3) of REACH).

The OECD TG 201 and the OECD GD 23, require(s) that the following conditions are met (among others):

- analytical monitoring of exposure concentrations.
- if an analytical procedure for determination of the test substance in the concentration range used is available, the test solutions should be analysed to verify the initial concentrations and maintenance of the exposure concentrations during the test (see OECD TG 201, paragraph 36) .
- chemical analysis to demonstrate attainment of equilibrium in WAF preparation and stability during the conduct of the test (see OECD Guidance 23, paragraph 150).
- exposure concentrations should be confirmed and their stability demonstrated by analysis unless the dissolved concentration is less than the limit of quantification of the most sensitive analytical method (see OECD Guidance 23, paragraph 162).
- Effect concentrations based on the measured values rather than nominal values unless the test concentrations are maintained within 20% of the measured initial concentrations throughout testing (see OECD TG 201 paragraph 39 and ECHA Guidance R7B, section R.7.8.4.1) .

As discussed above (Appendix on general consideration, section i.b.), the Substance is considered poorly water soluble.

For the key studies (2000), you have used the WAF preparation for poorly soluble substances under OECD GD 23. In this study, the saturation concentration of the test substance was below the detection limit of the analytical method used (HPLC). Therefore you did not

demonstrate the attainment of equilibrium in WAF preparation, presence of the Substance in the test medium (i.e. initial concentration), compositional stability and maintenance of exposure concentrations. In addition, you have not demonstrated that the method used is the most sensitive method available for the detemination of the Substance in the concentration range used in the test. However, you have demonstrated in long-term studies on the Substance (OECD TG 211 and 210, 2016) that analytical procedure (i.e. UPLC-MS/MS) for determination of the test substance in the concentration range used is available.

The aforementioned conditions are not met, therefore the information provided does not fulfil information requirement. In particular, for the key study (2000), the analytical methods used were not sensitive enough considering the solubility of the Substance, while more sensitive methods exist (i.e. UPLC-MS/MS), as was used for the long term tests on the Substance in the registration dossier (OECD TG 210 and OECD TG 211, 2016).

Therefore, the information provided does not fulfill the information requirement and there is a data gap that needs to be filled in.

In your comment on the initial draft decision you indicate that you will perform a study.

Appendix B: Reasons for the requests to comply with Annex VIII of REACH

In accordance with Articles 10(a) and 12(1) of REACH, a technical dossier registered at 10 to 100 tonnes or more per year must contain, as a minimum, the information specified in Annexes VII and VIII to REACH.

1. In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)

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

Your dossier contains negative results for both Ames and *in vitro* cytogenicity studies. Therefore, the information requirement is triggered.

Your dossier does not contain any study or adaptation in accordance with column 2 of Annex VIII, Section 8.4.3. or with the general rules of Annex XI for this standard information requirement.

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.

2. Adsorption/desorption screening (Annex VIII, Section 9.3.1.)

Adsorption/desorption screening is a standard information requirement in Annex VIII to REACH.

You have adapted this information requirement by using

- An OECD TG 121 study (2010) with an analogue substance (key study), and
- Data derived from Qualitative or quantitative structure-activity relationship (QSAR) in accordance with Annex XI, Section 1.3 with the Substance (supporting study, 2009)

As explained in the Appendix on general considerations sections (i) and (ii) above, your adaptations are rejected.

Therefore the information provided does not fulfil the information requirement and there is a data gap that needs to be filled in.

In your comment on the initial draft decision you indicate that you will perform a study.

Appendix C: Reasons for the requests to comply with Annex IX of REACH

In accordance with Articles 10(a) and 12(1) of REACH, a technical dossier registered at 100 to 1000 tonnes or more per year must contain, as a minimum, the information specified in Annexes VII-IX to REACH.

1. **Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.) in a first species;**

A Pre-natal developmental toxicity (PNDT) study (OECD TG 414) in one species is a standard information requirement in Annex IX to REACH.

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

As explained in the Appendix on general considerations above, your adaptation is rejected.

Therefore, the information requirement is not fulfiled.

A PNDT study according to the test method OECD TG 414 should be performed in rat or rabbit as preferred species with oral[8] administration of the Substance.

2. **Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.);**

Long-term toxicity testing on aquatic invertebrates is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. based on OECD TG 211 study (2016) with an analogue substance.

As explained in the Appendix on general considerations above your adaptation is rejected.

Therefore the study provided does not fulfil the information requirement and there is a data gap that needs to be filled in.

3. **Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.);**

Long-term toxicity testing on fish is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5 based on OECD TG 210 study (2016) with an analogue substance.

As explained in the Appendix on general considerations above your adaptation is rejected.

Therefore the study provided does not fulfil the information requirement and there is a data gap that needs to be filled in.

4. **Simulation testing on ultimate degradation in surface water (Annex IX,**

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

Section 9.2.1.2.)

Simulation testing on ultimate degradation in surface water is a standard information requirement at Annex IX to REACH.

You have sought to adapt this information based on the low solubility and the Log Koc of the Substance as well as based on exposure.

ECHA has assessed this justification and identified the following issue(s):

Simulation testing on ultimate degradation in surface water does not need to be conducted if the substance is highly insoluble in water or is readily biodegradable (Annex IX, Section 9.2.1.2, column 2).

You claim that the substance has a water solubility of <0.154 mg/L but you have not provided any experimental study for the water solubility of the Substance in the technical dossier. Screening information provided in your dossier indicates that the Substance is not readily biodegradable (0 % in 28 days in EU Method C.4-E).

As explained above in the Request A.1 above, there is no valid and reliable water solubility data on the Substance. As discussed above (Appendix on general consideration, section B.3), the Substance is considered poorly water soluble. However, the information available does not allow to conclude that the Substance is highly insoluble in water. Therefore the adaptation is rejected.

Chemical Safety Assessment needs to assess and document that risks arising from the Substance are controlled to demonstrate that there is no need to conduct further testing (Annex 1. Section 0.1; Annex IX, Section 9.2, Column 2).

In particular according to Annex I elements to be taken into account for that demonstration include:

- justification for why there is no need to provide any further information on degradation of the Substance.

To assess the degradation of the Substance, the P/vP assessment must cover all environmental compartments, including surface water unless, based on the fate and release(s) of the substance, it is considered that water compartment is not at all relevant environmental compartment (Annex XIII of REACH and ECHA Guidance R.11, Section R.11.4.1.1). Since by default the surface water compartment receives a significant amount of emission, testing should start with the OECD TG 309 simulation study, as long as it is technically feasible to conduct the simulation surface water study (Explanatory Notes to Figure R.11-3. Point 4. in ECHA Guidance R.11).

In your adaptation you claim that the intrinsic properties of the Substance (log Koc of 8.5 and water solubility) indicates that the Substance will be strongly adsorbed to sediment and therefore water is not the final destination compartment. High logKow of the Substance (reported logKow=5.2) indicates that the Substance may have potential for adsorption.

The Substance is not readily biodegradable (see above) but there is no further biodegradation studies.

However, as explained above and also in request A1 ad B2, your adaptation based on read-across (Section (i)) and QSAR (Section (ii)) are rejected. Therefore, currently there is no information on neither logKoc nor water solubility on the Substance. Therefore your

adaptation based on logKoc and water solubility of the Substance cannot be accepted as a valid waiver. In the absence of reliable information such as logKoc and water solubility, it is not possible to reliably predict the fate of the Substance on the environmental compartments. Therefore, there is no evidence that water compartement is not at all relevant environmental compartment.

Furthermore, even if the Substance has a potential for adsorption, the exposure to water cannot be excluded for the following reasons;.

- Direct and indirect exposure of the water compartment cannot be excluded based on the reported uses of the Substance (e.g. industrial, professional and consumer use as lubricant and greases in open systems, General industrial, professional and consumer use in vehicle or machinery).
  Therefore, adapting the information requirement for this endpoint according to Annex XI, Section 3 of REACH is not applicable.
- The absence of the chemical safety assessment cannot be regarded as an indication that there is no concern for this endpoint.
- The Substance is potentially P or vP based on the screening information (ready biodegradability).
- There is no information in the dossier on the degradation products and their fate.

Therefore, you have not provided sufficient supporting information to strengthen the rationale for the adaptation.

Therefore, your adaptation is rejected.

The information is needed for PBT/vPvB assessment.

Study design
OECD TG 309 is an appropriate method for studying the degradation in surface water. When performing the OECD TG 309 test, 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) must be followed (ECHA Guidance R.11).

Annex XIII indicates that information used for PBT/vPvB assessment must be obtained under relevant conditions. Therefore, simulation tests should be performed 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.

Quantification of non-extractable residues (NER) needs to be carried out 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 Chapter R.11).

The biodegradation of each relevant constituent present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable must be assessed. This can be done simultaneously during the same study. Alternatively, you must provide a justification for why you consider these as not relevant for the PBT/vBvB assessment.If you should encounter technical difficulties to perform the requested OECD TG 309 test, such difficulties and attempted solutions should be clearly demonstrated and documented.

5. Soil simulation testing (Annex IX, Section 9.2.1.3.)

Soil simulation testing is a standard information requirement at Annex IX of REACH for substances with a high potential for adsorption to soil.

You have sought to adapt this information requirement based on Annex IX, Section 9.2.1.3, Column 2. You justified the adaptation by stating that "direct exposure to soil is considered as unlikely and indirect exposure to soil is considered very limited and negligible compared to other routes of emission".

We have assessed this information and identified the following issues:

A. The Substance has a high potential for adsorption to soil (logKow>5.2).

B. Simulation testing on soil does not need to be conducted if direct or indirect exposure of soil is unlikely (Annex IX, Section 9.2.1.3, column 2).

The absence of exposure has not been demonstrated because of the following reasons:
- Based on the uses identified above in request C-4, direct and indirect exposure of the soil compartment cannot be excluded.
- The absence of the chemical safety assessment cannot be regarded as an indication that there is no concern for this endpoint.

Therefore, your adaptation is rejected and simulation test in soil is needed.

The information is needed for PBT/vPvB assessment.

Study design
The requested simulation test must be performed under relevant conditions (12 °C) and non-extractable resdues (NER) must be quantified for the reasons explained above in request C-4. The biodegradation of each 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. This can be done simultaneously during the same study. Alternatively, you must provide a justification for why you consider these as not relevant for the PBT/vBvB assessment.

6. Sediment simulation testing (Annex IX, Section 9.2.1.4.)

Sediment simulation testing is a standard information requirement at Annex IX of REACH for substances with a high potential for adsorption to sediment.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5 based on OECD TG 308 study (2014) with an analogue substance.

We have assessed this information and identified the following issues:

A. The Substance has a high potential for adsorption to sediment [logKow>5.2].

B. As explained in the Appendix on general considerations above your adaptation is rejected.

C. In addition, we have identified following additional issue.

For the same reasons explained in request C-5, the absence of exposure to sediment has not been demonstrated. Therefore simulation test in sediment is needed.

Therefore, the information requirement is not fulfilled.

In your comment on the initial draft decision you indicate that you will perform a study.

Study design
The requested simulation test must be performed under relevant conditions (12 °C) and non-extractable resdues (NER) must be quantified for the reasons explained above in request C-4. The biodegradation of each constituent present in concentrations at or above 0.1% (w/w) or, if not teachnicallyu feasible, in concentrations as low as technically detectable, must be assessed. This can be done simultaneously during the same study, Alternatively, you must provide a justification for why you consider these as not relevant for the PBT/vBvB assessment.

7. Identification of degradation products (Annex IX, 9.2.3.)

Identification of the degradation products is a standard information requirement at Annex IX of REACH.

You have not provided any information on the identification of degradation products, nor an adaptation in accordance with column 2 of Annex IX, Sections 9.2 or 9.2.3. or with the general rules of Annex XI for this standard information requirement.

Identity and relevance and of degradation products must be included in the risk assessment and PBT assessment.

Identification of degradation products does not need to be conducted if the substance is readily biodegradable (Annex IX, Section 9.2.3, column).

You have concluded the Substance as not readily biodegradable.

In addition, you have not provided any justification in your chemical safety assessment (CSA) or in the dossier for why there is no need to provide information on the degradation products further information is needed. Information is needed for the PBT/vPvB assessment and risk assessment.

Therefore, the information provided does not fulfil the information requirement.

Study design
You must obtain this information from the simulation studies also requested in this decision (Appendix C, sections 4-6 above). If any other method is used for identification of the transformation/degradation products, you must provide a scientifically valid justification for the chosen method.

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 Kow and potential toxicity of the metabolite may be investigated

8. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.), aqueous/dietary exposure)

Bioaccumulation in aquatic species, preferably fish is a standard information requirement at Annex IX of REACH.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. based on OECD TG 305 study (2017) with an analogue substance.

As explained in the Appendix on general considerations above your adaptation is rejected.

Therefore, the information requirement is not fulfilled.

Bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to investigate bioaccumulation (ECHA *Guidance, Chapter R.7c, R.7.10.3.1*). Whenever technically feasible, the aqueous route of exposure (OECD TG 305-I) must be used as the results obtained can be used directly for comparison with the B and vB criteria of Annex XIII of REACH. If testing through aquatic exposure is technically not possible, you must provide scientifically valid justification for the infeasibility. In case you conduct the study using the dietary exposure route (OECD 305-III), you must also attempt to 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. In any case you must report all data derived from the dietary test as listed in the OECD TG 305-III.

You must provide information on the bioaccumulation of all relevant constituents present in concentration of ≥ 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable must be assessed. Alternatively, you must provide a justification for why you consider certain constituents present in concentration of ≥ 0.1% (w/w) as not relevant for the PBT/vPvB assessment. This can be done simultaneously during the same study.

Appendix E: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of registration dossiers after the date on which you were notified the draft decision according to Article 50(1) of the REACH Regulation.

The compliance check was initiated on 02 October 2018.

ECHA notified you of the draft decision and invited you to provide comments within 30 days of the notification.

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

Included in your comments, you outlined your current tonnage volumes. As this matter does not affect the decision making process of this decision, ECHA dealt with this matter in a separate communication.

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 F: Observations and technical guidance

1. This compliance check decision does not prevent ECHA from initiating further compliance checks at a later stage on the registrations present.
2. Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of the Member States.
3. Test guidelines, GLP requirements and reporting

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

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

   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: 'How to report robust study summaries[9]'.

4. **Test material**

   While selecting the test material you must take into account 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. Any constituents that have harmonised classification and labelling according to the CLP Regulation (Regulation (EC) No 1272/2008) must be identified and quantified using the appropriate analytical methods.

   The OECD Series on Principles of Good Laboratory Practice and Compliance Monitoring, Number 11 [ENV/MC/CHEM(98)16] requires a careful identification of the test material and description of its characteristics. In addition, the Test Methods Regulation (EU) 440/2008, as amended by Regulation (EU) 2016/266, requires that "*if the test method is used for the testing of a* [...] *UVCB* [...] *sufficient information on its composition should be made available, as far as possible, e.g. by the chemical identity of its constituents, their quantitative occurrence, and relevant properties of the constituents*".

   In order to meet this requirement, all the constituents/group of constituents of the test material used for each test shall be identified as far as possible. For each constituent/group of constituents the concentration value in the test material shall be reported in the Test material section of the endpoint study record.

   Technical Reporting of the test material for UVCB substances

   The composition of the selected test material must be reported in the respective endpoint study record, under the Test material section. The composition must include all constituents/group of constituents of the test material and their concentration values.

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

Without such detailed reporting, ECHA may not be able to confirm that the test material is relevant for the Substance and to all the registrants of the Substance.

Technical instructions are available in the manual "How to prepare registration and PPORD dossiers" on the ECHA website[10].

5. Information required for PBT/vPvB assessment

Before conducting the tests (requests C.3-C.7) 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 and the necessity to conduct all of them. 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. Your assessment shall consider each constituent present in a concentration at or above 0.1% (w/w) and relevant degradation/transformation product or, if not technically feasible, in concentrations as low as technically quantifiable. Alternatively, you shall provide a justification for why you consider these as not relevant for the PBT/vPvB assessment.

You are advised to first conclude whether the Substance may fulfil the Annex XIII criteria of being P or vP, and then continue with the assessment for bioaccumulation. The sequence of the simulation tests also needs to consider the intrinsic properties of the Substance, its identified use and release patterns as these could significantly influence the environmental fate of the Substance. You shall revise the PBT assessment when the new information is available.

6. Environmental testing on UVCB substances

The purpose of the environmental hazard assessment under REACH is to perform the PBT assessment, to determine classification and labelling of the Substance and to perform the risk assessment (e.g. for PNEC derivation).
Your Substance is a complex UVCB and, as indicated in the ECHA Guidance R.11, to fulfil information requirements for persistency, bioaccumulation and aquatic toxicity, you need to consider the following approaches:
- 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.

The selection of the proper approach depends on the purpose of the study and the ability to characterise the Substance i.e. knowledge of constituents and/or fractions of the Substance and differences in the properties amongst them.

Use of Water Accommodated Fraction (WAF) approach for ecotoxicity testing
Before conducting the requested test[s] (x-z) you are advised to consult ECHA Guidance R.11 (Section R.11.4.2.2), R7b (Table R.7.8-3 and Appendix R.7.9-4) and the OECD GD 23 [ENV/JM/MONO(2000)6/REV1] on conducting and reporting the results of ecotoxicity test(s) on difficult to test substances.
If you elect to use the Water Accommodated Fraction (WAF) approach in your ecotoxicity tests, you must conduct chemical analyses of the WAF and the test medium. The following key information must be reported:
- Identity of those constituents to which the test organisms are exposed.

[10] https://echa.europa.eu/manuals

- A demonstration that equilibrium has been obtained in the WAF.
- A demonstration of stability in the exposure concentrations during the conduct of the test.
- Full description of the method used to prepare the WAF.
- Test results expressed in terms of measured concentrations, unless you can demonstrate that exposure concentrations remain within ±20% of the initial loading rate.

In order to be able to provide the above you should:
- Carefully consider and choose the analytical methods relevant for your substance.
- Choose a method for preparing the WAF that is consistent with the conditions applied during the conduct of the test (including e.g. the use of co-solvents or the stirring methods).

If it is not possible to provide the above information when using the WAF approach you should consider the use of newer techniques (e.g. passive dosing) as noted in the revised OECD GD 23 that may be better suited for your Substance.

7. List of references of the ECHA Guidance and other guidance/ reference documents[11]

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 in this decision.

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 in this decision.

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

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

[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

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.

OECD Guidance documents[13]
Guidance Document on aqueous–phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD23.
Guidance Document supporting the OECD TG 443 on the extended one-generation reproductive toxicity test – No 151, referred to as OECD GD151.

[13] http://www.oecd.org/chemicalsafety/testing/series-testing-assessment-publications-number.htm

Appendix G: List of the registrant to which the decision is addressed and the corresponding information requirements applicable

Registrant Name	Registration number	(Highest) Data requirements to be fufilled
[redacted]	[redacted]	[redacted]

Note: where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas the decision is sent to the actual registrant.