EUROPEAN CHEMICALS AGENCY

~~Confidential~~

Helsinki, 03 June 2021

Addressees
Registrant of BUNFS CAS91078-64-7EC293-346-9 as listed in the last Appendix of this decision

Date of submission of the dossier subject to this decision
23/08/2016

Registered substance subject to this decision ("the Substance")
Substance name: Naphthalenesulfonic acids, branched and linear Bu derivs., sodium salts
EC number: 293-346-9
CAS number: 91078-64-7

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 ***11 September 2023***.

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. 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 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. Non-extractable residues (NER) must be quantified and a scientific justification of the selected extraction procedures and solvents must be provided.

5. Identification of degradation products (Annex IX, 9.2.3.; test method: using an appropriate test method)

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

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) of REACH:

- 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.

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

- Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.)
- Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)
- Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.)

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 (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].

I. Predictions for (eco) toxicological properties

You read-across between the structurally similar substances, Sodium diisopropylnaphthalenesulphonate, EC No. 215-343-3 (CAS No. 1322-93-6), hereafter referred as "source substance [1]" and the Substance as target substance.

In addition, you have provided information on the test material Sodium diisobutylnaphthalenesulphonate, EC No. 248-326-4 (CAS No. 27213-90-7) and Sodium 2,3-dibutylnaphthalene-1-sulfonate, EC No. 246-960-6 (CAS No. 25417-20-3). While you have not identified this information as an analogue approach, the test material used and reported in the technical dossier corresponds to information obtained from a different substance than the substance subject to this decision. Therefore, the provided studies conducted with EC No. 248-326-4 and EC No. 246-960-6 (hereafter referred to as the "source substance [2] and "source substance [3]", respectively") will be evaluated as a read-across adaptation under Annex XI, Section 1.5 of REACH.

You have not provided a read-across justification documentation under the relevant endpoints sections in the dossier. For this reason, we rejected your read-across approach in the draft decision sent to you.

[2] ECHA Guidance R.6: QSARs and grouping of Chemicals.
[3] Read-Across Assessment Framework (RAAF).
[4] Read-across assessment framework (RAAF) - considerations on multi-constituent substances and UVCBs.

In your comments to the draft decision you have provided a Read across justification document in Annex I and a document [redacted] in Annex II.

In your comments you explain that "the Read Across document was attached in section 1.1 of IUCLID" instead of in section 13.

ECHA points out that a registrant who submits an adaptation must set out clearly, in the relevant part of its registration dossier the grounds for the adaptation, and the scientific information which substantiates those grounds (*See paragraph 35 of the Board of Appeal decision of 4.05.2020, in Case A-011-2018*). There was no reference in the dossier indicating that the read-across justification document was located in the section 1.1 of IUCLID, which refers to substance identification. Therefore, ECHA was initially not in a position to evaluate the justification and has only evaluated it following your reference to the location in the comments on the draft decision.

We have evaluated the read-across justification you refer to in your comments to the draft decision.

You have provided the following reasoning for the predictions of (eco)toxicological properties in your justification document (Annex I): "*Considering the high structural similarity, the similar physiochemical profile and the comparable composition, the three substances are expected to have a comparable toxicokinetic profile and comparable toxicological properties. [...] This is also confirmed by the QSAR predictions as attached in Annex II of the present document*". Further (in Annex II) you have indicated: "*In more details it was proved that their evident structural similarity is also supported by a high similarity in terms of foreseen mechanisms of actions relevant for the end points to be read-across*"

Based on the above, ECHA understands that you used the information on these analogues to 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(s).

With regards to prediction(s) of ecotoxicological properties ECHA identified issues that are common to ecotoxicological and environmental fate information requirements under consideration (Growth inhibition study aquatic plants, Simulation testing on ultimate degradation in surface water) and also shortcoming(s) that are specific for these information requirements individually. Altogether they result in a failure to meet the requirement of an adaptation according to Annex XI, 1.5. The common issues are set out here, while the specific issues are set out under the information requirement concerned in the Appendices below.

Supporting information for 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*"[5]. 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).

[5] ECHA Guidance R.6: Section R.6.2.2.1.f

Supporting information must include information to confirm that the Substance and the source substances have similar (eco)toxicological properties and that the structural differences would not affect the predicted properties of the substances.

You have provided the following information to support your hypothesis:

- Alert profiles using the QSAR Toolbox

In your Annex II document, you have provided profilers that you have considered as relevant to support the predictions of environmental effects (acute aquatic toxicity MOA by OASIS, aquatic toxicity classification by ECOSAR, acute aquatic toxicity classification by Verhaar) and fate (Biodegradation probability from 1 to 7 (BIOWIN) and Biodegradation fragments BIOWIN).
You conclude that the information from the profilers indicates mechanistic similarity among the predicted structures for the aquatic toxicity and biodegradability and therefore the read-across approach could be applied for both endpoints.

- Physicochemical properties

You claim that for aquatic toxicity, similar logKow and aqueous solubility values between the source and target chemicals are to be used to support the read-across, because logKow is known to be a determinant of the toxicity in aquatic organisms when the effect is mediated by mechanisms of narcosis. You also compare the hydrophobicity, expressed as octanol/water partition coefficient, to support your prediction on biodegradation.

- Data matrix

In the read-across justification you provide a data matrix where you compare the environmental effects and fate properties and argue that the target and source substances have similar ecotoxicity properties. You have referred to the following experimental data in the justification document for aquatic toxicity and the biodegradation on the Substance and the analogue substances which are also provided in the registration dossier:

i. Acute toxicity to aquatic Algae, Daphnia and fish, conducted with the source substance [2] (EC No. 248-326-4).
ii. Simulation test in sewage treatment activated sludge (OECD TG 303A, [redacted] 1984) conducted with source substance [2],
iii. Ready biodegradation study (OECD TG 301B) and inherent biodegradability experimental study (OECD TG 302B) conducted with the source substance [1] (EC No. 215-343-3).

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

- Regarding the alerts obtained from the QSAR toolbox

There are structural differences between the target and source substances (for instance with regard to the position variation of the alkyl chain and the sulfonate group or in the composition of the Substance and the source substance [1]). While the similarity in presence or absence of structural alerts may indicate that the differences do not influence the reactivity of the substance e.g. on the protein or DNA, this information does not confirm, on its own, that the Substance and the source substances have similar (quantitative) ecotoxicological properties, in particular aquatic toxicity.

- Regarding the physicochemical properties

While the physicochemical and degradation properties might be relevant to support similarity in toxicokinetic/partitioning behaviour in aquatic compartment or in sewage treatment plant, this information does not confirm, on its own, that the Substance and the source substances have similar (quantitative) ecotoxicological and environmental fate properties.

- Regarding the data matrix

ECHA has identified shortcomings with the information provided in the data matrix to support your predictions :

i. Regarding the aquatic toxicity to algae, *Daphnia* and fish, data is provided for source substance [2] only. In the absence of any aquatic toxicity data for the Substance, the properties of the substances cannot be compared.
ii. Regarding the Biodegradation, data is provided for source substance [1] only. In the absence of any degradation data for the Substance, the properties of the substances cannot be compared.

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.

II. Conclusions on the read-across approach

As explained above with regard to the ecotoxicological and environmental fate properties, 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.

2. Assessment of your Qualitative or quantitative structure-activity relationship ((Q)SAR) adaptation under Annex XI, Section 1.3

In your dossier you seek to adapt the following standard information requirements by applying Qualitative or quantitative structure-activity relationship ((Q)SAR) approaches in accordance with Annex XI, Section 1.3:

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

In your comments to the draft decision, you state that the QSAR prediction under Annex XI, Section 1.3. on the Substance for toxicity to aquatic plants is no longer included.

ECHA has considered the scientific and regulatory validity of your ((Q)SAR) approaches in general before assessing the specific standard information requirements in the following appendices.

According to Annex XI, Section 1.3., four conditions shall be necessarily fulfilled to use QSAR results instead of testing. Firstly, the prediction needs to be derived from a scientifically valid model. Secondly, the prediction must fall within the applicability domain of the model. Thirdly, results need to be adequate for the purpose of risk assessment or classification and labelling. Finally, adequate and reliable documentation about the applied method must be provided.

The documentation is considered adequate when it includes the information specified in or equivalent to the QSAR Model Reporting Format (QMRF) and QSAR prediction reporting format

(QPRF) templates. The QMRF contains information on the source, type, development, validation, and possible applications of the model. In the QPRF, the prediction outcome is presented with some reasoning. The reliability of the prediction should also be assessed and provided.[6]

In your dossier you have provided a generic description of the models in the QSAR endpoint study records in the dossier, and reported the generic outcome of the prediction. However, no QMRF and QPRF specific information was provided about the predictions.

In your comments to the draft decisison you have provided a document (i.e. *In silico* predictions in Annex II) describing the results obtained from the QSAR prediction. However no QMRF and QPRF specific information was provided.

In absence of specific information about the models and the prediction (i.e. QMRF and QPRF), ECHA cannot assess whether the substance falls within the applicability domain of the model and if the prediction is adequate for the purpose of risk assessment and/or classification and labelling.

However, you have indicated in the document attached to you comments on the draft decisions that for aquatic toxicity the information predicted are not reliable.

[6] ECHA Guidance R.6: QSARs and grouping of chemicals.

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

1. 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 a Grouping of substances and read-across approach under Annex XI, Section 1.5. You have provided following information in your dossier:

i. Toxicity to aquatic algae ([redacted] 1999) conducted with the source substance [2] Sodium 2,3-diisobutylnaphthalene-1-sulfonate (EC No. 248-326-4).

In addition, you have adapted this information requirement by using a Qualitative and quantitative structure activity relationship ((Q)SAR) under Annex XI, Section 1.3. You have provided the following information in your dossier:

ii. *In silico* prediction for the Substance on toxicity to aquatic algae (S-IN soluzioni informatiche, 2013)

iii. *In silico* prediction for the source substance [3] Sodium 2,3-dibutylnaphthalene-1-sulfonate (EC No. 246-960-6) on toxicity to aquatic algae (S-IN soluzioni informatiche, 2013)

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

As explained in the Appendix on Reasons common to several requests, your adaptations in accordance with Annex XI, Section 1.5. and Annex XI, Section 1.3. are rejected. On this basis, the information requirement is not fulfilled.

In your comments to the draft decision you agree to perform the requested test with the Substance.

Appendix B: 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 in Annex IX to REACH.

You have provided following key study conducted with the Substance in your dossier:

i. Short-term oral repeated dose toxicity (non-guideline; [redacted], 1984) conducted with the Substance.

In addition you have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. You have provided the following information:

ii. Short-term repeated dose toxicity: inhalation (OECD TG 412; BASF, 1990) conducted with source substance [2] sodium diisobutylnaphthalenesulphonate (EC No. 248-326-4).

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

Information provided with the Substance

A. To be considered compliant and enable concluding whether the Substance has dangerous properties and supports the determination of the No-Observed Adverse Effect Level (NOAEL), a study has to meet the requirements of OECD TG 408. The key parameter of this test guideline include, among others that
   - Dosing of the Substance daily for a period of 90 days until the scheduled termination of the study

   The short-term toxicity study conducted with the Substance (i) does not have the required exposure duration of 90 days, but only 28 days.

Information from analogue substance(s)

B. According to Annex XI, Section 1.5., if the grouping concept is applied then in all cases the results to be read across should:
   - cover an exposure duration comparable to or longer than the corresponding test method;
   - have adequate and reliable coverage of the key parameters foreseen to be investigated in the corresponding test methods referred to in Article 13(3).

   According to the provisions of Annex IX, Section 8.6.2., information on sub-chronic toxicity study (90-day), as specified in the OECD TG 408/413 shall be provided. The key parameters foreseen to be investigated in a sub-chronic toxicity study (90-day) include but are not limited to
   - dosing of the Substance daily for a period of 90 days until the scheduled termination of the study; and
   - at least 10 female and 10 male animals should be used at each dose level (including control group)

   The short-term toxicity study (ii) does not have the required exposure duration of 90, but only 28 days. It was also conducted with less than 10 animals per test dose group (5/sex/group), and therefore, does does not meet the key parameters of the sub-chronic toxicity study (90-day).

Consequently, the source study (ii) does not meet the conditions as required by Annex XI, Section 1.5.

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

In your comments to the draft decision you agree with the deficiencies of the source studies identified by ECHA and you agree to perform the requested test.

Study design

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.Based on the information you provided in the dossier and the chemical safety report regarding the properties of the Substance (powder with median particle size above 170 µm) and its uses (non-industrial spraying), indicate that human exposure to the Substance by the inhalation route is likely. However, according to the Chemical Safety Report, the risk management measures are in place to prevent exposure of humans via inhalation. Hence, the test shall be performed by the oral route.

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

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.).

In your dossier you have provided the following information:

- A justification to omit the study. In support of your adaptation, you provided the following justification: "*The information regarding invertebrates toxicity is sufficient to assess the risk related to the substance*".

In your comment to the draft decision you reiterate that no further long-term testing is needed on aquatic organisms since the chemical safety assessment according to Annex I does not indicate the need to investigate further the effects on aquatic organisms (PEC/PNEC < 1).

We have assessed this information and identified the following issue:

In general, a registrant may adapt the standard testing regime in accordance with the specific rules set out in column 2 of Annexes VII to X (if applicable) or the general rules set out in Annex XI. For the present information requirement, column 2 of Annex IX, Section 9.1, does not allow omitting the need to submit information on long-term toxicity to aquatic invertebrates under Column 1 (Decision of the Board of Appeal in case A-011-2018).

Your adaptation does not refer to any of the general adaptation possibilities under Annex XI. It is therefore unclear what adaptation possibility you refer to under Annex XI.

Your adaptation is therefore rejected.

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 provided the following information:

- A justification to omit the study. In support of your adaptation, you provided the following justification: "*The information regarding fish toxicity is sufficient to assess the risk related to the substance".*

In your comment to the draft decision you reiterate that no further long-term testing is needed on aquatic organisms since the chemical safety assessment according to Annex I does not indicate the need to investigate further the effects on aquatic organisms (PEC/PNEC < 1)

We have assessed this information and identified the following issue:

In general, a registrant may adapt the standard testing regime in accordance with the specific rules set out in column 2 of Annexes VII to X (if applicable) or the general rules set out in Annex XI. For the present information requirement, column 2 of Annex IX, Section 9.1, does not allow omitting the need to submit information on long-term toxicity to fish under Column 1 (Decision of the Board of Appeal in case A-011-2018).
Your adaptation does not refer to any of the general adaptation possibilities under Annex XI. It is therefore unclear what adaptation possibility you refer to under Annex XI.

Your adaptation is therefore rejected.

On this basis, the information requirement is not fulfilled.

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 by using a Grouping of substances and read-across approach under Annex XI, Section 1.5. You have provided the following information as a key study:

i. Simulation test in sewage treatment activated sludge (OECD TG 303A, [redacted] 1984) conducted with source substance [2] sodium diisobutylnaphthalenesulphonate (EC No. 248-326-4).

We have assessed this information and identified the following issues:

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

B. 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

   To fulfil the information requirement and to allow concluding on the P/vP criteria, ultimate biodegradation simulation tests must simulate degradation under relevant environmental conditions, such as those found in surface water, freshwater sediment or soil (Annex VIII, Section 9.2. and Annex XIII to REACH; ECHA Guidance R.11.4.).

   Your registration dossier provides an OECD TG 303A study. On that basis, you conclude that the Substance does meet the P criteria but not the vP criteria.

ECHA Guidance R.11.4.1.1. clarifies that, because it does not simulate degradation under relevant environmental conditions, the SCAS test (*i.e.* OECD TG 303A) cannot be used to conclude that a substance does or does not fulfil the criteria for P or vP.

Therefore, the source study is not adequate.

Consequently, the source study does not meet the conditions as required by Annex XI, Section 1.5.

In you comment to the draft decision you disagree to perform the requested study, and provide the following arguments:

1- While you acknowledge that the Substance is not readily biodegradable, you have however considered it as inherently biodegradable based on the results provided in the dossier from the OECD 302B study performed on the source substance (EC 215-343-3);

2- You consider that simulation study in surface water is not needed since the exposure in water compartment is limited.

3- You consider that the results from the soil study provided in the dossier on the Substance can be extrapolated to the water compartment;

4- You mentioned further under the Bioaccumulation justification that you intend to clarify the vP properties of the Substance by performing an enhanced biodegradability test.

We have assessed the comments above and identified the following issues:

A. To adapt this information requirement, the conditions set-out in either Annex IX, Section 9.2.1.2, Column 2 or the general adaptations set in Annex XI have to be fulfilled. For the present information requirement, Column 2 stipulates that the study does not need to be conducted if the substance is highly insoluble or is readily biodegrdable.

   You acknowledge that the Substance is not readily biodegradable and state that the Substance would be inherently biodegradable based on OECD 302B study performed on the source substance (EC 215-343-3).

   Firstly, the inherent ready biodegradability that you are referring to does not fulfil any conditions set in those provisions in column 2 of Annex IX Section 9.2. Secondly, for the same reasons explained under the Appendix on Reasons common to several requests, Section 1, the read-across approach is rejected. Thirdly, the results provided in your dossier (i.e. degradation rate of 27% after 8 days) did not meet the criteria specified in ECHA Guidance R.11.4., therefore the Substance cannot be considered as inherently biodegradable. Therefore your argument does not constitute a valid adaptation.

B. Under Annex XI, Section 3.2(b) (Substance-tailored exposure-driven testing), this information may be omitted based on the exposure scenario(s) developed in the Chemical Safety Report. The justification must be based on a rigorous exposure assessment in accordance with Annex I, Section 5 and must meet the following criteria:
   - For substances that are not included in articles, it must be demonstrated for all relevant scenarios that strictly controlled conditions as set out in Article 18(4)(a)

to (f) apply throughout the life cycle;
- In all cases, adequate justification and documentation must be provided when testing is omitted;
- The justification based on Annex XI section 3.2 (b) must include a qualitative assessment including three elements: the description of operational conditions and risk management measures in all related exposure scenarios; the quantification of the resulting release/exposure for all routes; and a qualitative statement why the release is low enough (ECHA Guidance R.5.1.3).

In your comments on the draft decision, you state that the risk to water compartment is limited due to existing of risk management measures on the site, and also due to the fact that the Substance is regulated under plant protection products under Regulation (1107/2009). However you have not provided any justification or documentation demonstrating that the criteria set out in Section 3.2. of Annex XI are met.

Therefore, you have not documented that strictly controlled conditions throughout the life-cycle including waste stage of the Substance apply.

In conclusion, your adaptation is rejected.

C. If a conclusion on the persistency is reached for one compartment, no further testing or assessment of persistence of other environmental compartments is normally necessary (ECHA Guidance R.11.4.1.1.).
Furthermore, simulation studies should be conducted at environmentally relevant temperatures, by default at 12 °C. If information on degradation half-life is already available from existing simulation degradation tests performed at a higher temperature, they should be normalised to a half-life corresponding to 12 °C by using the Arrhenius equation (ECHA Guidance R.7.9.).

You have provided a soil simulation study that was conducted on the Substance at a temperature of 20 °C. A DT-50 (half-life) value of 137 days was determined. Based on that the Substance was concluded as persistent (P).

D. We acknowledge that you have already provided data that may allow to reach a conclusion on the P/vP properties of the Substance. However the study was conducted at 20 °C, and you have not normalised the temperature to environmentally relevant temperature (i.e. 12 °C), using the Arrhenius equation. This may influence the interpretation of the soil simulation study and the conclusions drawn for P or vP assessment. The PBT/vPvB assessment of UVCB substance needs to cover the whole Substance including its constituents, impurities and additives present in concentration above 0.1% (ECHA guidance R.11.4.1.). Ready biodegradability tests are intended for pure substances and are generally not applicable for complex compositions containing different types of constituents, like UVCB. For an UVCB substance, observed biodegradation may indeed represent the biodegradation of only some constituents (ECHA Guidance R.7.9.4.1.).

The Substance is a UVCB and you propose to perform a prolonged ready biodegradation study on the Substance to conclude that that the Substance is not P/vP.

Based on the enhanced biodegradation test it cannot be excluded that some constituents or relevant transformation/degradation product may be P/vP, even if the study would show that the Substance mineralizes more than 60%. Therefore, on its own this information is not adequate to conclude on the PBT/vPvB properties of the

Substance.

Based on the above, ECHA disagrees with your proposal to perform an enhanced biodegradability test to decide if further testing is needed.

On this basis, the information requirement is currently not fulfilled.

Study design

Simulation degradation studies must include two types of investigations (ECHA Guidance R.7.9.4.1.):

1. a degradation pathway study where transformation/degradation products are quantified and, if relevant, are identified, and
2. a kinetic study where the degradation rate constants (and degradation half-lives) of the parent substance and of relevant transformation/degradation products are experimentally determined.

You must perform the 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.11.4.1.1.3.).

The required test temperature is 12°C, which corresponds to the average environmental temperature for the EU (ECHA Guidance R.16, Table R.16-8) and is in line with the applicable test conditions of the OECD TG 309.

As specified in ECHA Guidance R.7.9.4.1., the organic carbon (OC) concentration in surface water simulation tests is typically 2 to 3 orders of magnitude higher than the test substance concentration and the formation of non-extractable residues (NERs) may be significant in surface water tests. Therefore, non-extractable residues (NER) must be quantified. 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.11.4.1.1.3.). Further recommendations may be found in the background note on options to address non-extractable residues in regulatory persistence assessment available on the ECHA website.

Relevant transformation/degradation products are at least those detected at ≥ 10% of the applied dose at any sampling time or those that are continuously increasing during the study even if their concentrations do not exceed 10% of the applied dose, as this may indicate persistence (OECD TG 309; ECHA Guidance R.11.4.1.).

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 provided no information on the identity of transformation/degradation products for the Substance.

This information is required for the purpose of the PBT/vPvB assessment (Annex I, Section 4) and the risk assessment (Annex I, Section 6) of the Substance.

In you comments to the draft decision you disagree to identify the degradation products and you have provided the same justification as for the endpoint of Section 4. Above of this Appendix.

To adapt this information requirement, the conditions set-out in Annex IX, Section 9.2.3., Column 2 or the general adaptations has to be fulfilled.

As explained above, the information presented in your comments on the draft decision does not allow to adapt this information requirement.

Therefore, this information requirement is not met.

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 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 (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.).

You have provided the following information:

i. an adaptation under Annex IX, Section 9.3.2., Column 2 with the following justification: "the Substance has low potential for bioaccumulation".

We have assessed this information and identified the following issue:

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 of 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).

Your registration dossier provides an adaptation stating that the log Kow is < 3 and the Substance is not bioaccumulative.

The Substance is a surfactant (surface tension 0.0311 N/m (OECD TG 115)) and thus, based on high surface activity, it may react with cell membranes. Therefore, log Kow is not a valid descriptor of the bioaccumulation potential of the Subtance and your adaptation is rejected.

In your comments to the draft decision you acknowledge that the LogKow is not considered a valid descriptor of the bioaccumulation potential but disagree to perform the requested study, and provide the following arguments:

1- You consider that as the Substance is ionisable and it thus does not readily diffuse across biological membranes and the relatively high molecular weight could normally be considered too large to cross biological membranes;
2- While you acknowledge that the Substance is not readily biodegradable, you have however considered it as inherently biodegradable based on the results provided in the dossier from the OECD 302B study performed on the source substance (EC 215-343-3). Further you state that as the Substance does not meet the P and T criteria, on this basis the Substance cannot be considered as PBT. You intend to perform an enhanced ready biodegradability study with an incubation period extended to 60 days to substantiate this claim and only if the Substance does not reach the pass level of 60 % or 70 % (in the enhanced screening test), the evaluation of bioaccumulation will be considered as necessary in order to conclude on the vPvB classification.

3- In case a bioaccumulation study is required, you intend to provide the following to adapt this information requirement:
   a. A freshwater amphipod Hyalella Azteca study
   b. An OECD test guideline 319 study, the metabolization will be used to parameter an in silico prediction models for rainbow trout BCF calculation
   c. the determination of an experimental membrane water partitioning coefficient

We have assessed your comments and identified the following issues:

1- Under Section 9.3.2., Column 2, first indent, Annex IX to REACH, the study may be omitted if the Substance is unlikely to cross biological membranes. ECHA Guidance R.7.8.5. explains that there is no scientific basis to define molecular characteristics that would render a substance unlikely to cross biological membranes. In this context, the indicators used for low likelihood of a high bioaccumulation potential (ECHA Guidance R.11, Figure R.11-4) must be considered, including:

   - physico-chemical indicators of hindered uptake due to large molecular size (*e.g.* D_{max} > 17.4 Å and MW > 1100 or MML > 4.3 nm) or high octanol-water partition coefficient (log K_{ow} > 10) or low potential for mass storage (octanol solubility (mg/L) < 0.002 x MW), and
   - supporting experimental evidence of hindered uptake (no chronic toxicity for mammals and birds, no chronic ecotoxicity, no uptake in mammalian toxicokinetic studies, very low uptake after chronic exposure).

   In your comments on the draft decision, you state that the Substance has a low potential to cross the biological membranes. However you have not provided any of the justification listed above.

Therefore there is no information available on the Substance to support that the Substance is unlikely to cross biological membranes.

Therefore your adaptation is rejected.

2- To adapt this information requirement, the conditions set-out in Annex IX, Section 9.3.2, Column 2 or the general adaptations set in Annex XI have to be fulfilled. For this information requirement, Column 2 stipulates that the study need not be conducted if the substance has a low potential for bioaccumulation (for instance a log Kow ≤ 3) and/or a low potential to cross biological membranes, or direct and indirect exposure of the aquatic compartment is unlikely.

Neither the inherent ready biodegradability nor the PBT argument that you are referring to fulfil any conditions set in those provisions to adapt this information requirement.

Therefore you argument does not constitute a valid adaptation.

Furthermore, as explained above under Section 4. of this Appendix, the ready biodegradation test is not considered appropriate to conclude on the persistency of the UVCB Substance and according to the existing results of the soil simulation study the Substance does meet the P/vP criteria (DT-50 =137 days, according to OECD 307). Any further ready biodegradation test does not overrule the results of the simulation test in soil to conclude that the Substance is either P or vP.

In addition of that as explainded under Section 2. and 3. of this Appendix, and under Section 2. of Appendix B, the information requirements are not fulfilled and therefore there are currently no data available to conclude on the T properties of the Substance. Therefore you have not clarified the PBT potential of the Substance.

3- With regards to the bioaccumulation testing plan, in the absence of the above information ECHA cannot currently take a position of the validity of the proposed approach. However, ECHA emphasizes that, as specified under Annex IX, Section 9.3.2, Column 1 and in conjunction with Article 13(3), bioaccumulation in fish is the preferred test to investigate the bioaccumulation properties of a substance. ECHA will assess the compliance of your approach in the follow-up to the dossier evaluation.

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.

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

1. Test methods, GLP requirements and reporting

A. 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.

B. 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.

C. 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[7].

2. Test material

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

   The Test Material used to generate the new data must be selected taking into account the following:

   1. the boundary composition(s) of the Substance,
   2. 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*

   1. 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.
   2. 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.

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

Appendix D: Technical instructions on how to report the above is available in the manual on How to prepare registration and PPORD dossiers[8].General recommendations when conducting and reporting new tests for REACH purposes

- **Strategy for the PBT/vPvB assessment**

  Under Annex XIII, the information must be based on data obtained under conditions relevant for the PBT/vPvB assessment. You must assess the PBT properties of each relevant constituent of the Substance present in concentrations at or above 0.1% (w/w) and of all relevant transformation/degradation products. Alternatively, you would have to justify why you consider these not relevant 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.

- **Environmental testing for substances containing multiple constituents**

  Your Substance contains multiple constituents 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:

  A. the "known constituents approach" (by assessing specific constituents), or
  B. the "fraction/block approach, (performed on the basis of fractions/blocks of constituents), or
  C. the "whole substance approach", or
  D. 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 synthesize its relevant constituents and/or fractions.

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

Appendix E: 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 17 December 2019.

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 amended the requests, however did not amend the deadline.

> In the draft decision communicated to you, the time indicated to provide the requested information was 27 months from the date of adoption of the decision. In your comments on the draft decision, you requested ECHA to extend the standard granted time to a total of 36 months to allow time to perform the bioaccumulation test, using an alternative method (i.e. *Hyalella azteca* Bioconcentration test, HYBIT) as a part of Weight of Evidence instead of the OECD TG 305 requested in the draft decision. You considered that the extension of 36 months is needed because the test guideline is supposed to be released only in Q1 2022 (According to the Work Plan for the Test Guidelines Programme provided as a reference in you comment).
>
> ECHA sets deadlines to provide the studies requested in a decision. You have not provided any justification that would explain why the deadline set in this decision would not allow you to perform the requested bioaccumulation study. Therefore ECHA considers that the deadline set allows you to perform the requested studies to meet the information requirements addressed in this decision.
>
> On this basis, ECHA has not modified the deadline to provide the information.

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: List of references - ECHA Guidance[9] 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)[10]

RAAF - considerations on multiconstituent substances and UVCBs (RAAF UVCB, March 2017)[10]

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.

[9] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
[10] https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across

OECD Guidance documents[11]
Guidance Document on aqueous-phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD 23.

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.

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

Appendix G: 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]

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.