~~Confidential~~

Helsinki, 07 September 2021

**Addressees**
Registrants of JS_Di-tert-amyl peroxide as listed in the last Appendix of this decision

**Date of submission of the dossier subject to this decision**
18/11/2020

**Registered substance subject to this decision ("the Substance")**
Substance name: Di-tert-pentyl peroxide
EC number: 234-042-8
CAS number: 10508-09-5

**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 ***12 September 2024***.

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

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

3. 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.

4. Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method: EU C.24./OECD TG 308) 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)

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

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

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

**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 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 provided the following information:

i. OECD TG 201, key study, test substance: di-tert-amyl peroxide (EC 234-042-8, CAS 10508-09-5) [redacted] (2013).

We have assessed this information and identified the following issues:

To fulfil the information requirement, a study must comply with OECD TG 201 and the requirements of OECD GD 23 (ENV/JM/MONO(2000)6/REV1) if the substance is difficult to test (Article 13(3) of REACH). Therefore, the following specifications must be met:

- exponential growth in the control cultures is observed over the entire duration of the test;
- the mean coefficient of variation for section-by-section specific growth rates (days 0-1, 1-2 and 2-3, for 72-hour tests) in the control cultures is ≤ 35%;
- the coefficient of variation of average specific growth rates during the whole test period in replicate control cultures is ≤ 7% in tests with *Pseudokirchneriella subcapitata*. For other less frequently tested species, the value is ≤ 10%;
- one of the two alternative growth medium (*i.e.* the OECD or the AAP medium) is used. Any deviations from recommended test media must be described and justified;

- the test media prepared specifically for analysis of exposure concentrations during the test is treated identically to those used for testing (*i.e.* inoculated with algae and incubated under identical conditions);
- the results can be based on nominal or measured initial concentration only if the concentration of the test material has been maintained within 20 % of the nominal or measured initial concentration throughout the test;
- if the concentration of the test material has not been maintained within 20 % of the nominal or measured initial concentration throughout the test, results must be based on the geometric mean of measured concentrations during exposure or on a model describing the decline of the concentration of the test material.

However, your registration dossier provides an OECD TG 201 showing the following:

- section-by-section growth rates in the control cultures, i.e. 0-24h, 24-48h and 48-72h were not provided;
- the mean coefficient of variation for section-by-section specific growth was not provided;
- the coefficient of variation of average specific growth rates during the whole test period in replicate control cultures was not provided;
- the study corresponds to a limit test and the number of replicates was 3;
- the test medium is not described;
- the test media prepared specifically for analysis of exposure concentrations was not inoculated with algae;
- the concentration of the test material was determined at various time points (0, 24, 48 and 72h) during the test. However, the measured concentration was 8 mg/L at the beginning of the test (0h) or below the detection (0.0048 mg/L) and quantification (0.016 mg/L) limits after 24, 48 and 72 hours. In spite of this the nominal concentration (200 mg/L) was applied in the results;

- the test media prepared specifically for analysis of exposure concentrations was not inoculated with algae;

Based on the above, the validity criteria of OECD TG 201 are not met since the exponential growth is not shown for section-by-section during the study period and also the extent of variability (i.e. coefficient of variation) for growth rates in section-by-section growth rates and during the whole test period are not reported. As the variability of growth in controls is not shown to be within acceptable limits of the test, the results cannot be considered to be reliable. In addition, there are critical methodological deficiencies resulting in the rejection of the study results. More specifically, the number of replicates in the limit test was only three, whereas according to the TG 201 six replicates should be used in the test. Also the composition of the test medium is not described and since its description is always required, an independent assessment of its suitability for the test is not possible. Furthermore, the test media prepared specifically for analysis of exposure concentrations was not inoculated with algae and the measured concentration of the test material deviated more than 20% from the nominal concentration. As the test media was not inoculated with algae and the geometric mean or a model describing the decline was not applied, the actual concentration of the test material in the test is not known. Based on this, it is not known if the measured test material concentration (8 mg/L) in the media at the beginning of the test reflects the actual test material concentration in the test media with algae.

Therefore, the requirements of OECD TG 201 are not met.

In your comments on the draft decision, you submitted clarifications and additional information to the identified incompliances. ECHA has assessed the information against the requirement in OECD TG 201. The information you have provided in your comments addresses the incompliances identified in this decision for this information requirement. However, as the information is currently not available in your registration dossier, the data gap remains. You should therefore submit this information in an updated registration dossier by the deadline set out in the decision.

On this basis, the information requirement is not fulfilled.

*Study design*

The Substance is difficult to test due to the low water solubility (13.83 mg/L) and adsorptive properties: log Kow 4.7 and logKoc 3.11. OECD TG 201 specifies that, for difficult to test substances, you must consider the approach described in OECD GD 23 or other approaches, if more appropriate for your substance. In all cases, the approach selected must be justified and documented. Due to the properties of Substance, it may be difficult to achieve and maintain the desired exposure concentrations. Therefore, you must monitor the test concentration(s) of the Substance throughout the exposure duration and report the results. If it is not possible to demonstrate the stability of exposure concentrations (i.e. measured concentration(s) not within 80-120% of the nominal concentration(s)), you must express the effect concentration based on measured values as described in OECD TG 201. In case a dose-response relationship cannot be established (no observed effects), you must demonstrate that the approach used to prepare test solutions was adequate to maximise the concentration of the Substance in the test solution.

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

### 1. 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 omitted this information and you provided the following justification:

*"According to ECHA guidance on information requirements and chemical safety assessment (v1.2, November 2012), Chapter r7b and to the integrated testing strategy, the chronic Daphnia study was conducted first. Based on the results of the chronic Daphnia test and the application of a relevant assessment factor no risks are observed (PEC/PNEC<1), no long term fish test may be conducted. A chronic Daphnia test result is available, and the results of the chemical risk assessment indicate no risk to the environment, thus the long term fish test is waived."*

We have assessed this information and identified the following issue:

> A registrant may only adapt this information requirement based on the general rules set out in Annex XI. It is noted that 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 justification to omit this information does not refer to any legal ground for adaptation under Annex XI to REACH.
>
> Therefore, you have not demonstrated that this information can be omitted.

On this basis, the information requirement is not fulfilled.

*Study design*

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

As already explained above, the Substance is difficult to test. Therefore, you must fulfil the requirements described in 'Study design' under Appendix A.1.

### 2. Bioaccumulation in aquatic species

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

You have adapted this standard information requirement according to Annex XI, Section 1.2. of REACH (weight of evidence). In support of your adaptation, you have provided the following sources of information:

i. (Q)SAR prediction of bioaccumulation based on BCFBAF model v3.01 from EPI Suite v4.1;
ii. (Q)SAR prediction of bioaccumulation based on CAESAR Hybrid Model to predict bioconcentration factors (BCF).

Annex XI, Section 1.2 states that there may be sufficient weight of evidence from several independent sources of information leading to assumption/conclusion that a substance has or

has not a particular dangerous (hazardous) property, while information from a single source alone is insufficient to support this notion.

According to ECHA Guidance R.4.4, a weight of evidence adaptation involves an assessment of the relative values/weights of different sources of information submitted. The weight given is based on the reliability of the data, consistency of results/data, nature and severity of effects, and relevance of the information for the given regulatory information requirement. Subsequently, relevance, reliability, consistency and results of these sources of information must be balanced in order to decide whether they together provide sufficient weight to conclude that the Substance has or has not the dangerous property investigated by the required study.

Annex XI, section 1.2 also requires that adequate and reliable documentation is provided to describe your weight of evidence approach.

However, for each relevant information requirement, you have not submitted any explanation why the sources of information provide sufficient weight of evidence leading to the conclusion/assumption that the Substance has or has not a particular dangerous property.

In spite of this critical deficiency, ECHA has nevertheless assessed the validity of your adaptation and identified the following issues.

To fulfil the information requirement, normally a study performed according to OECD TG 305 must be provided. OECD TG 305 requires the study to investigate the following key investigations:

1. the uptake rate constant (k1) and loss rate constants including the depuration rate constant (k2), and/or
2. the steady-state bioconcentration factor ($BCF_{SS}$), and/or
3. the kinetic bioconcentration factor ($BCF_K$), and/or
4. The biomagnification factor (BMF).

1. *Concerning key parameter (1) the uptake rate constant (k1) and loss rate constants including the depuration rate constant (k2) and* (4) *the biomagnification factor (BMF)*

None of the sources of information provided information on these key investigations. Therefore, they do not provide information that would contribute to the conclusion on the key investigations 1. and 4.

2. *Concerning key investigations (2) the steady-state bioconcentration factor ($BCF_{SS}$) and (3) the kinetic bioconcentration factor ($BCF_K$)*

The sources of information (i) and (ii) may provide relevant information on bioconcentration factor of the Substance in fish (i.e. the key investigations 2. and 3.).

However, the reliability of these sources of information is significantly affected by the following deficiencies:

*Selection of the representative structure(s)*

Under ECHA Guidance R.6.1.7.3. a prediction is adequate for the purpose of classification and labelling and/or risk assessment if representative structure(s) for the assessment are selected.

Your registration dossier provides for source of information i. and ii. the following:

- In Section 1.1 of your technical dossier, you define the Substance as di-tert-pentyl peroxide (EC 234-042-8, CAS 10508-09-5);
- In Section 1.2, you indicate the following impurities in the composition of your Substance:

[redacted]

- For the assessment, you provided predictions for the following structure for the *source of information i and ii*: di-tert-pentyl peroxide.

You have considered di-tert-pentyl peroxide as the representative structure. You failed to justify your selection.

ECHA disagrees with the representative structure you selected because especially impurity [redacted], typical concentration ca. [redacted] % (w/w), concentration range [redacted] (w/w).) with a predicted logKow (5.9) is likely to be above the 4.5 logKow threshold value and could meet the screening criterion for B assessment and needs also to be followed up.

Therefore, you have not demonstrated that the prediction is adequate for the purpose of classification and labelling and/or risk assessment.

*A. The prediction is not adequate due to low reliability*

Under ECHA Guidance R.6.1.3.4 a prediction is adequate for the purpose of classification and labelling and/or risk assessment when the model is applicable to the chemical of interest with the necessary level of reliability. ECHA Guidance R.6.1.5.3. specifies that, among others, the following cumulative conditions must be met:

- the model predicts well substances that are similar to the substance of interest, and
- reliable input parameters are used, and
- the prediction is consistent with information available for other related endpoint(s).

Your registration dossier provides the following information:

- *source of information i:* No information about similar substances is given.
- *source of information ii:* In the endpoint summary it is indicated that the performances of the BCFBAF model were better than those from the CAESAR model for the test substance. In the QPRF, similar substances are not further discussed.

The predictions for the Substance used as input are not reliable because

- *Source of information i:*
  - there are only two peroxide substances found in the training set;
  - the Meylan model is based on no close analogues in the training set to support the prediction and significant variation of BCF values for a logKow of 4.7, we assess that the prediction is accompanied with considerable uncertainty;
  - the Arnot-Gobas model: The QPRF addresses the applicability of the model for the registered substance, but the result does not seem to be further used in the safety assessment. The number of fragments calculated by the model are

covered by the training set. There is, however, no fragment for the peroxide reported. The predicted bioaccumulation potential with the Arnot-Gobas model is below the the threshold for B, but taking into account the uncertainty, it cannot be excluded that the substance has a BCF above 2000.

- *Source information ii:*
  - the CAESAR model run in the VEGA software (version 1.1.5 ) indicates low reliability of the BCF predictions because of insufficient number of similar substances and insufficient coverage of the peroxide fragment.

Therefore, you have not demonstrated that the prediction for the Substance is adequate for the purpose of classification and labelling and/or risk assessment.

B. *The substance is outside the applicability domain of the model*

Under ECHA Guidance R.6.1.5.3., a substance must fall within the applicability domain specified by the model developer.

- *Source of information i.*

No information about analogues is given. For the Arnot-Gobas model, the peroxide fragment is missing.

There are only two peroxide substances found in the training set. The Meylan model is based on no close analogues in the training set to support the prediction and significant variation of BCF values for a logKow of 4.7. We assess that the prediction is accompanied with considerable uncertainty. The VEGA model (version 1.1.5) run for kM/Half-Life model (Arnot/EpiSuite) and BCF model (Meylan) correspond to the BCFBAF models and confirm the above assessment, that there is considerabe uncertainty in the prediction.

The Arnot-Gobas model: The QPRF addresses the applicability of the model for the registered substance, but the result does not seem to be further used in the safety assessment. The number of fragments calculated by the model are covered by the training set. There is however no fragment for the peroxide reported. The predicted bioaccumulation potential with the Arnot-Gobas model is below the the threshold for B, but taking into account the uncertainty, it cannot be excluded that the substance has a BCF above 2000.

- *Source of information ii:*

The QPRF states that the BCF of the test substance was 64 L/Kg whole body weight, corresponding to a log BCF = 1.80, but that there is the presence of chemical features in the compound (peroxide) that might be associated with a lower reliability of the predicted value.

We used VEGA version 1.1.5 to assess the substance with the BCF model CAESAR 2.1.14. The CAESAR model prediction is 1.8 log(L/kg), but the result may be not reliable. A check of the information should be done, paying particular attention to the following issues:

- only moderately similar compounds with known experimental value in the training set have been found;
- accuracy of prediction for similar molecules found in the training set is not optimal;
- similar molecules found in the training set have experimental values that

disagree with the predicted value;
- the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability;
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found)
- warning: the prediction may be not fully reliable due to the presence of one or more fragments related to model outliers;
- the following relevant fragments have been found: Peroxide (SO 08).

The automated applicability domain check within the model assesses the prediction as not reliable. Furthermore, the CAESAR model in VEGA indicate shortcomings in the prediction, basically based on the lack of a sufficient number of similar structures and the limited presence of the peroxide fragment.

Therefore, you have not demonstrated that the Substance falls within the applicability domain of the models.

In conclusion, the reported information is considered insufficient to estimate bioaccumulation potential of the Substance due to several shortcomings and uncertainties in the applied models. First, the selected model structure does not cover all the relevant impurities of the Substance. Second, the applied models do not provide reliable bioaccumulation estimate for the Substance due to e.g. lack of information on similar/analogue substances. Third, the substance is outside the applicability domain of the applied models and therefore the predicted BCF estimates are not reliable and high bioaccumulation potential cannot be excluded.

As a result of these, it is not possible to conclude, based on any source of information alone or considered together, whether your Substance has or has not bioaccumulation potential foreseen to be investigated in an OECD TG 305 study. Therefore, your adaptation is rejected and the information requirement is not fulfilled.

In your comments on the draft decision you have agreed to perform this study *"following the results of the P assessment as explained in the Appendix D section A of this draft decision and in line with the integrated testing strategy developed in the ECHA Guidance R11."*

*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).

### 3. 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 provided an adaptation under Annex IX, Section 9.2., Column 2 with the following justification:

> *"Further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The choice of the appropriate test(s) depends on the results of the chemical safety assessment and may include simulation testing in appropriate media (e.g. water, sediment or soil). The study of the "ready" aerobic biodegradability of DI-TERT-AMYL PEROXIDE using the OECD method 301 D shows that this item reached a maximum biodegradation level of 7 % in 28 days and 10 % in 56 days. As a consequence, DI-TERT-AMYL PEROXIDE is not readily biodegradable. The PEC/PNEC ratio for water obtained in the exposure assessment was below 1. Based on the exposure assessment, the conduct of a simulation test of the degradation in water (OECD 309) is waived in accordance with column 2 of Annex IX chapter 9.2 of Regulation EC 1907/2006."*

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

- it is potentially persistent or very persistent (P/vP) as:
  - it is not readily biodegradable (*i.e.* <60% degradation in an OECD 301D);
- it is potentially bioaccumulative or very bioaccumulative (B/vB) as:
  - it has a high potential to partition to lipid storage (e.g. log Kow > 4.5);
- it meets the T criteria set in Annex XIII: NOEC or $EC_{10}$ < 0.01 mg/L or classification as carc. 1A or 1B, muta. 1A or 1B, repro. 1A, 1B or 2, or STOT RE 1 or 2.

However, your registration dossier provides the following:

- The Substance is not readily biodegradable (7% degradation after 28 days in OECD TG 301D);
- The Substance has a high potential to partition to lipid storage (Log $K_{ow}$ of 4.7 based on OECD TG 123);

Furthermore, the information in your dossier is currently incomplete and therefore:
- it is not possible to conclude on the bioaccumulation potential of the Substance (see Appendix C.3 of this decision), and
- it is not possible to conclude on the toxicity of the Substance see Appendices A1 and B.1 of this decision).

The information above indicates that the Substance is a potential PBT/vPvB substance.

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

In your comments on the draft decision you state that according to "*the Integrated Testing Strategy provided in the ECHA Guidance R11, it is advisable in the figure R.11-3 to first check the technical feasibility of an OECD 309. If this study is technically feasible then the full study should be performed. But in case this study is not technically feasible then consider whether the compartment specific concern is for sediment or soil and then launch a study OECD 308 or OECD 307. So, before launching a full OECD 309 as requested in the ECHA draft decision, a study on technical feasible will have to be performed especially due to the low water solubility of the substance.*"

We have assessed this comment and agree that technical feasibility can be clarified before performing a full study. However, currently available information on the Substance does indicate that the OECD TG 309 is feasible, since the water solubility of Substance, the main factor limiting feasibility of the test, is 13.83 mg/L. This is well above the recommended test concentration in the TG 309, i.e. less than 1 to 100 µg/L.

On this basis, the information requirement is 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.).

## 4. Sediment simulation testing

Sediment simulation testing is an information requirement under Annex IX to REACH (Section 9.2.1.4.) for substances with a high potential for adsorption to sediment.

You have provided an adaptation under Annex IX, Section 9.2., Column 2 as explained in section B.3 above.

The Substance has a low water solubility (13.83 mg/L), high partition coefficient (log $K_{ow}$ 4.7) and high adsorption coefficient (log $K_{oc}$ 3.11) and therefore has high potential for adsorption to sediment.

As explained in section B.3 above, the information in your dossier indicates that the Substance is a potential PBT/vPvB substance.

In your comments on the draft decision you state that "*the standard fugacity model indicates the soil as a compartment of concern and not water or sediment"* and *"Therefore, the Registrant are of the opinion that in case an additional testing should have been performed in addition to the OECD 309, a soil simulation testing following the OECD 307 guideline is more relevant than an OECD 308."*

We have assessed this comment and note that soil and sediment simulation tests are separate standard information requirements in Annex IX of REACH. Further, Annex IX specifies two conditions when the studies need not to be conducted: 1) if the substance is readily biodegradable or 2) if direct and indirect exposure of sediment is unlikely. Since the substance is not readily biodegradable and the Chemical Safety Report indicates that there is exposure to soil and sediment, both simulation tests must be provided to fulfill information requirements in your dossier.

Therefore, you have not demonstrated that the CSA does not indicate the need for further sediment simulation testing.

*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.

In accordance with the specifications of OECD TG 308, you must perform the test using two sediments. One sediment should have a high organic carbon content (2.5-7.5%) and a fine texture, the other sediment should have a low organic carbon content (0.5-2.5%) and a coarse texture. If the Substance may also reach marine waters, at least one of the water-sediment systems should be of marine origin.

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 308.

In accordance with the specifications of OECD TG 308, non-extractable residues (NER) must be quantified. The reporting of results must include a scientific justification of the used extraction procedures and solvents (ECHA Guidance R.7.9.4.1.). 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 308; ECHA Guidance R.11.4.1.).

## 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.
>
> Therefore, this information requirement is not met.
>
> 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.

On this basis, the information requirement is not fulfilled.

*Study design*

To determine the degradation rate of the Substance, the requested study according to OECD TG 309 (Appendix C.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).

To determine the degradation rate of the Substance, the requested study according to OECD TG 308 (Appendix C.5) must be conducted at 12°C and at a test material application rate reflecting realistic assumptions. 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) and at higher application rate (*e.g.* 10 times).

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

### A. Test methods, GLP requirements and reporting

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

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

3. Under Article 10(a)(vi) and (vii) of REACH, all new data generated as a result of this decision must be reported as study summaries, or as robust study summaries, if required under Annex I of REACH. See ECHA Practical Guide on How to report robust study summaries[2].

### B. Test material

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

1. Selection of the Test material(s)

   The Test Material used to generate the new data must be selected taking into account the following:
   - the variation in compositions reported by all members of the joint submission,
   - the boundary composition(s) of the Substance,
   - 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
   - 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.
   - The reported composition must include all constituents of each Test Material and their concentration values and other parameters relevant for the property to be tested.

This information is needed to assess whether the Test Material is relevant for the Substance and whether it is suitable for use by all members of the joint submission.

Technical instructions on how to report the above is available in the manual on How to prepare registration and PPORD dossiers[3].

[2] https://echa.europa.eu/practical-guides
[3] https://echa.europa.eu/manuals

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

### A. 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.

**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 01 April 2020.

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

ECHA took into account your comments and did not amend the requests.

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[4] 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)[5]

RAAF - considerations on multiconstituent substances and UVCBs (RAAF UVCB, March 2017)[5]

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

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

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

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

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

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

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

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

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

OECD Guidance documents[6]
Guidance Document on aqueous–phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD 23.

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

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

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

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

## Appendix G: Addressees of this decision and their corresponding information requirements

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

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

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.