~~Confidential~~

Helsinki, 22 February 2024

Addressee(s)
Registrants of 25103-58-6_JS as listed in Appendix 3 of this decision

Date of submission of the dossier subject to this decision
18 May 2022

Registered substance subject to this decision ("the Substance")
Substance name: tert-dodecanethiol
EC/List number: 246-619-1

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

DECISION ON TESTING PROPOSAL(S)

Under Article 40 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below by ***31 May 2027***.

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

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

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

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

2. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.; test method: EU C.47./OECD TG 210)

3. Soil simulation testing (Annex IX, Section 9.2.1.3.; test method: EU C.23./OECD TG 307) 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 OECD TG 307 and OECD TG 308)

The reasons for the decision(s) are explained in Appendix 1.

Information required depends on your tonnage band

You must provide the information listed above for all REACH Annexes applicable to you in accordance with Articles 10(a) and 12(1) of REACH. The addressee(s) of the decision and their corresponding information requirements based on registered tonnage band are listed in Appendix 3.

In the requests above, the same study has been requested under different Annexes. This is because some information requirements may be triggered at lower tonnage band(s). In such cases, only the reasons why the information requirement is triggered are provided for the lower tonnage band(s). For the highest tonnage band, the reasons why the standard information requirement is not met and the specification of the study design are provided. Only one study is to be conducted; all registrants concerned must make every effort to reach an agreement as to who is to carry out the study on behalf of the others under Article 53 of REACH.

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 requirements for testing and reporting new tests under REACH, see Appendix 4. In addition, 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 this Appendix.

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 Mike Rasenberg, Director of Hazard Assessment

Appendix 1: Reasons for the decision
Appendix 2: Procedure
Appendix 3: Addressees of the decision and their individual information requirements
Appendix 4: Conducting and reporting new tests under REACH

[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 1: Reasons for the decision

Contents

Reasons for the decision(s) related to the information under Annex VIII of REACH

1. Long-term toxicity testing on fish

1 Short-term toxicity testing on fish is an information requirement under Annex VIII, Column 1, Section 9.1.3. However, long-term toxicity testing on fish may be required by the Agency (Section 9.1.3., Column 2) if the substance is poorly water soluble, i.e. solubility below 1 mg/L.

1.1. Triggering of the information requirement

2 Poorly water-soluble substances require longer time to reach steady-state conditions. As a result, the short-term tests do not give a true measure of toxicity for this type of substances and the long-term test is required.

3 Under Section 4.8 of your technical dossier, you have provided an OECD TG 105 study (modified slow stir method) and a QSAR based on the EPIWEB v4.0 model. The saturation concentration of the Substance in water was determined to be 3.93 µg/L in the OECD TG 105 and predicted to be 0.28 mg/L based on EPIWEB 4.0 model.

4 Therefore, the Substance is poorly water soluble and information on long-term toxicity on fish must be provided.

5 The examination of the information provided, your considerations of alternative methods, of third party comments (if applicable), as well as the selection of the requested test and the test design are addressed under request 2.

Reasons for the decision(s) related to the information under Annex IX of REACH

2. Long-term toxicity testing on fish

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

2.1. Information provided to fulfil the information requirement

7 You have submitted a testing proposal for a Fish, Early-Life Stage Toxicity Test (test method: OECD TG 210).

8 Your registration dossier does not include any information on long-term toxicity on fish.

9 ECHA requested your considerations for alternative methods to fulfil the information requirement for long-term toxicity on fish. You provided your considerations concluding that there were no alternative methods which could be used to adapt the information requirement(s) for which testing is proposed. ECHA has taken these considerations into account.

10 ECHA agrees that an appropriate study on long-term toxicity on fish is needed.

2.2. Test selection and study specifications

11 The proposed Fish, Early-Life Stage Toxicity Test (test method: OECD TG 210) is appropriate to cover the information requirement for long-term toxicity on fish (Guidance on IRs and CSA, Section R.7.8.4.1.).

12 The Substance is difficult to test due to the low water solubility (0.00393 mg/L in an OECD TG 105) and adsorptive properties (log kow > 6.2 in an OECD TG 117). OECD TG 210 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 210. 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 solutions.

13 For multi-constituents/UVCBs, the analytical method must be adequate to monitor qualitative and quantitative changes in exposure to the dissolved fraction of the test material during the test (e.g. by comparing mass spectral full-scan GC or HPLC chromatogram peak areas or by using targeted measures of key components).

14 If you decide to use the Water Accommodated Fraction (WAF) approach, in addition to the above, you must:

- use loading rates that are sufficiently low to be in the solubility range of most constituents (or that are consistent with the PEC value). This condition is mandatory to provide relevant information for the hazard and risk assessment (Guidance on IRs and CSA, Appendix R.7.8.1-1, Table R.7.8-3);
- provide a full description of the method used to prepare the WAF (including, among others, loading rates, details on the mixing procedure, method to separate any remaining non-dissolved test material including a justification for the

separation technique);
- prepare WAFs separately for each dose level (i.e. loading rate) and in a consistent manner.

2.3. Outcome

15 Your testing proposal is accepted under Article 40(3)(a) and you are requested to conduct the test, as specified above.

16 In the comments to the draft decision, you agree to perform the requested study.

3. Soil simulation testing

17 Soil simulation testing is an information requirement under Annex IX to REACH (Section 9.2.1.3.) for substances with a high potential for adsorption to soil.

18 Substances with a log K_{oc} > 4 are considered to have a high potential for adsorption to soil (Guidance on IRs and CSA, Section R.7.9.4.3.).

19 The Substance has a low water solubility (3.93 µg/L), high partition coefficient (log K_{ow} > 6.2) and high adsorption coefficient (log K_{oc} 3.6) and therefore has high potential for adsorption to soil.

3.1. Information provided to fulfil the information requirement

20 In the registration dossier, you have submitted a testing proposal for an Aerobic and Anaerobic Transformation in soil test (test method: EU C.23/OECD TG 307).

21 Your registration dossier does not include any information on aerobic and anaerobic transformation in soil.

22 ECHA agrees that an appropriate degradation simulation study in soil is needed.

23 In the comments to the draft decision, you indicate your intention to adapt this information requirement. You provide the following information:

i. You claim that testing is technically not possible due to the low water solubility of the Substance.

ii. You provide a justification to omit the study which to ECHA's understanding you consider to be based on Annex IX, Section 9.2., Column 2. In support of your adaptation, you explain that $PNEC_{soil}$ is not calculated because you expect the Substance to rapidly volatilise from soil to the air compartment due to its physico-chemical properties (water solubility at 20°C: 3.9 µg/L; vapour pressure at 25°C: 20 Pa) and because you claim that the Substance is not discharged from wastewater treatment plants or mixed with soils. Further, you claim that because of the lack of $PNEC_{soil}$ value, it is not possible to indicate if CSA trigger a need for further investigation of biotic degradation.

iii. You reference the conclusion of the PBT/vPvB assessment submitted by the United Kingdom in 2014 (that the Substance is not B/vB) and discussed in the PBT Expert Group Meeting (2013). Further, you reference Section 2.1 of Annex XIII, and claim that the BCF value of the Substance is below 2000 L/kg and conclude that the Substance is not B/vB and because of this, no additional information needs to be generated.

iv. You consider the Substance to be persistent. On this basis, you argue that there would be no added value in conducting soil simulation testing on the Substance, except to obtain information on its degradation products. In your comments, you present QSAR data for identifying the potential degradation products and screening them for PBT/vPvB properties. You propose to submit this data as part of your dossier update.

24 ECHA understands that in your comment under points i. and iv., you intend to adapt the standard information requirement under Annex XI, Section 2, and under Annex XI, Section 1.3, respectively.

25 We have assessed this information and identified the following issues:

3.2. Assessment of the information provided

3.2.1. Your claim that testing is not possible is rejected

26 Annex XI, Section 2 specifies that testing for a specific endpoint may be omitted, if it is technically not possible to conduct the study as a consequence of the properties of the substance: e.g. very volatile, highly reactive or unstable substances cannot be used, mixing of the substance with water may cause danger of fire or explosion or the radio-labelling of the substance required in certain studies may not be possible. The guidance given in the test methods referred to in Article 13(3), more specifically on the technical limitations of a specific method, shall always be respected.

27 According to paragraph 5 of OECD TG 307, the test method is applicable to all chemical substances (non-labelled or radiolabelled) for which an analytical method with sufficient accuracy and sensitivity is available, including water-soluble and water-insoluble substances.

28 ECHA notes that you have not provided any information about the potential shortcomings of the available analytical methods (e.g. issues related to repeatability and sensitivity of the analytical method; recovery rates, limit of detection and quantification, etc.). Therefore, you have not demonstrated that no analytical method for the OECD TG 307 test is available for the Substance.

29 Because of this, your claim that the testing is technically not feasible is not supported by specific scientific information.

30 Therefore, your adaptation is rejected.

3.2.2. Annex IX, Section 9.2., Column 2 is not a valid basis to omit the study

31 Annex IX, Section 9.2., Column 2 provides that "further" biodegradation testing must be proposed if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. That provision allows a registrant to propose, or ECHA to require, biotic degradation testing not covered by the information on degradation listed under Annex IX, section 9.2., Column 1. Therefore, this provision cannot be used as a justification for omitting the submission of information on soil simulation testing required under Annex IX, Section 9.2.1.3, Column 1.

32 Therefore, your adaption is rejected.

3.2.3. Your justification to omit the study has no legal basis

33 A registrant may only adapt this information requirement based on the general rules set out in Annex XI or the specific rules set out in Annex IX, Section 9.2.1.3., Column 2.

34 Your justification to omit this information based on the conclusion of a previous PBT/vPvB assessment of the Substance submitted by the United Kingdom and based on the available BCF value of the Substance does not refer to any legal ground for adaptation under Annex XI to REACH or Annex IX, Section 9.2.1.3., Column 2.

35 Therefore, you have not demonstrated that this information can be omitted.

36 Furthermore, ECHA notes that the PBT Expert Group provides non-binding scientific advice on matters related to the identification of persistent, bioaccumulative and toxic (PBT) and very persistent, very bioaccumulative (vPvB) properties of chemicals. The advice does not anticipate or interfere with the regulatory decision-making of the present decision.

3.2.4. The QSAR result is not equivalent to results obtained from the required experimental test

37 Results from (Q)SAR models are adequate for risk assessment or classification and labelling when they are equivalent to results obtained from the required experimental test. The corresponding study that must normally be performed for this particular information requirement is test method OECD TG 307, which measures the following key parameters:

- the rate of aerobic and anaerobic transformation of the test material in four soil types, and
- the identity and rates of formation and decline of transformation products in at least one soil type.

38 You have provided the prediction from a (Q)SAR model EAWAG Biocatalysis / Biodegradation Database Pathway Prediction System (EAWAG-BBD Pathway Prediction System), which provides qualitative data on the identities of potential degradation products by predicting plausible pathways for microbial degradation of chemical compounds. The model uses biotransformation rules, which are based on reactions found in the EAWAG-BBD database or in the scientific literature.

39 The model predicts the identity of the potential biodegradation products but does not predict the rate of aerobic and anaerobic transformation of the test material in different soil types and the rates of formation and decline of transformation products. Therefore, the prediction is not adequate to meet the information requirement for soil simulation testing for the purpose of classification and labelling and/or risk assessment.

40 Therefore, the information requirement is not fulfilled.

3.3. Test selection and study specifications

41 The proposed Aerobic and Anaerobic Transformation in soil test (test method: EU C.23/OECD TG 307) is appropriate to cover the information requirement for degradation/biodegradation (Guidance on IRs and CSA, Section R.7.9.4.1).

42 Simulation degradation studies must include two types of investigations (Guidance on IRs and CSA, Section 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.

43 In accordance with the specifications of OECD TG 307, you must perform the test using at least four soils representing a range of relevant soils (i.e. varying in their organic content, pH, clay content and microbial biomass).

44 The required test temperature is 12°C, which corresponds to the average environmental temperature for the EU (Guidance on IRs and CSA, Section R.16, Table R.16-8) and is in line with the applicable test conditions of the OECD TG 307.

45 In accordance with the specifications of OECD TG 307, non-extractable residues (NER) must be quantified. The reporting of results must include a scientific justification of the used extraction procedures and solvents (Guidance on IRs and CSA, Section 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) (Guidance on IRs and CSA, Section 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.

46 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 307; Guidance on IRs and CSA, Section R.11.4.1.).

3.4. Outcome

47 Your testing proposal is accepted under Article 40(3)(a) and you are requested to conduct the test, as specified above.

4. Sediment simulation testing

48 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.

49 Substances with a log Koc > 4 are considered to have a high potential for adsorption to sediment (Guidance on IRs and CSA, Section R.7.9.4.3.).

50 The Substance has a low water solubility (3.93 µg/L), high partition coefficient (log K_{ow} > 6.2) and high adsorption coefficient (log K_{oc} 3.6) and therefore has high potential for adsorption to sediment.

51 Therefore, the Substance is considered to have a high potential for adsorption to sediment and information on Sediment simulation testing must be provided.

4.1. Information provided to fulfil the information requirement

52 In the registration dossier, you have submitted a testing proposal for an Aerobic and Anaerobic Transformation in Aquatic Sediment Systems (test method: EU C.24/OECD TG 308).

53 Your registration dossier does not include any information on aerobic and anaerobic transformation in aquatic sediment systems.

54 ECHA agrees that an appropriate degradation simulation study in sediment is needed.

55 In the comments to the draft decision, you indicate your intention to adapt this information requirement. You provide the following information:

i. You provide a justification to omit the study which to ECHA's understanding you consider to be based on Annex IX, Section 9.2., Column 2. In support of your adaptation, you state that the results from the CSA do not trigger a

need for further investigation of biotic degradation as risk for the sediment compartment are acceptable in every scenario (RCR < 1).

ii. You reference the conclusion of the PBT/vPvB assessment submitted by the United Kingdom in 2014 (that the Substance is not B/vB) and discussed in the PBT Expert Group Meeting (2013). Further, you reference Section 2.1 of Annex XIII, and claim that the BCF value of the Substance is below 2000 L/kg and conclude that the Substance is not B/vB and because of this, no additional information needs to be generated.

iii. You consider the substance to be persistent. On this basis, you argue that there would be no added value in conducting sediment simulation testing on the Substance, except to obtain information on its degradation products. In your comments, you present QSAR data for identifying the potential degradation products and screening them for PBT/vPvB properties. You propose to submit this data as part of your dossier update.

56 ECHA understands that in your comment under point iii. you intend to adapt the standard information requirement under Annex XI, Section 1.3.

57 We have assessed this information and identified the following issues:

4.2. Assessment of the information provided

4.2.1. Annex IX, Section 9.2., Column 2 is not a valid basis to omit the study

58 Annex IX, Section 9.2., Column 2 provides that "further" biodegradation testing must be proposed if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. That provision allows a registrant to propose, or ECHA to require, biotic degradation testing not covered by the information on degradation listed under Annex IX, section 9.2., Column 1. Therefore, this provision cannot be used as a justification for omitting the submission of information on sediment simulation testing required under Annex IX, Section 9.2.1.4, Column 1.

59 Therefore, your adaption is rejected.

4.2.2. Your justification to omit the study has no legal basis

60 A registrant may only adapt this information requirement based on the general rules set out in Annex XI or the specific rules set out in Annex IX, Section 9.2.1.4., Column 2.

61 As explained above in request 3, your justification to omit this information based on the conclusion of a previous PBT/vPvB assessment of the Substance submitted by the United Kingdom and based on the available BCF value of the Substance does not refer to any legal ground for adaptation under Annex XI to REACH or Annex IX, Section 9.2.1.4., Column 2.

62 Therefore, you have not demonstrated that this information can be omitted.

4.2.3. The QSAR result is not equivalent to results obtained from the required experimental test

63 Results from (Q)SAR models are adequate for risk assessment or classification and labelling when they are equivalent to results obtained from the required experimental test. The corresponding study that must normally be performed for this particular information requirement is test method OECD TG 308, which measures the following key parameters:

- the rate of aerobic and/or anaerobic transformation of the test material on

at least two sediments, and
- the identity and rates of formation and decline of transformation products.

64 You have provided the prediction from a (Q)SAR model EAWAG-BBD Pathway Prediction System, which provides qualitative data on the identities of potential degradation products by predicting plausible pathways for microbial degradation of chemical compounds. The model uses biotransformation rules, which are based on reactions found in the EAWAG-BBD database or in the scientific literature.

65 The model predicts the identity of the potential biodegradation products but does not predict the rate of aerobic and anaerobic transformation of the test material in different sediment types and the rates of formation and decline of transformation products. Therefore, the prediction is not adequate to meet the information requirement for sediment simulation testing for the purpose of classification and labelling and/or risk assessment.

66 Therefore, the information requirement is not fulfilled.

4.3. Test selection and study specifications

67 The proposed Aerobic and Anaerobic Transformation in Aquatic Sediment Systems test (test method: EU C.24/OECD TG 308) is appropriate to cover the information requirement for degradation/biodegradation (Guidance on IRs and CSA, Section R.7.9.4.1).

68 Simulation degradation studies must include two types of investigations (Guidance on IRs and CSA, Section 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.

69 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.

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

71 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 (Guidance on IRs and CSA, Section 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) (Guidance on IRs and CSA, Section 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.

72 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; Guidance on IRs and CSA, Section R.11.4.1.).

4.4. Outcome

73 Your testing proposal is accepted under Article 40(3)(a) and you are requested to conduct the test, as specified above.

5. Identification of degradation products

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

5.1. Information provided to fulfil the information requirement

75 In the registration dossier, you have provided no information on the identity of transformation/degradation products for the Substance.

76 In the comments to the draft decision, you have provided the following QSAR adaptation:

- Data generated with EAWAG-BBD Pathway Prediction System, for identifying the potential degradation products of the Substance;
- Data generated with EPI Suite models, for screening the PBT/vPvB properties of the potential degradation products that were predicted by the EAWAG-BBD Pathway Prediction System.

77 Based on the above screening information, you conclude that none of the potential degradation products of the Substance have PBT/vPvB properties.

78 Further, you indicate your intention to provide the above screening information in a future update of your registration dossier.

79 ECHA acknowledges the screening information you have submitted in the comments to the draft decision.

80 We have assessed this information and identified the following issue.

5.2. The QSAR result is not adequate for the purpose of classification and labelling and/or risk assessment

81 The third indent of Annex XI, Section 1.3 specifies that results of (Q)SARs may be used instead of testing when they are adequate for the purpose of classification and labelling and/or risk assessment.

82 Further, Section R.7.9.3.1 of ECHA Guidance on IRs and CSA, Chapter R.7b explains that the suitability of qualitative data on biodegradation pathways may only contribute to the hazard, persistence, and risk assessments as part of a Weight of Evidence approach, if other data are available.

83 In addition to the above, for the PBT assessment of substances containing multiple constituents, impurities and/or additives, Section R.11.4.2.2.3 of ECHA Guidance on IRs and CSA, Chapter R.11 explains that results from QSARs-profiling can be used for justifying the test material selection (i.e. for identifying the worst case constituents which can be targeted for further assessment and testing).

84 In the comments to the draft decision, you have provided screening information on the identity of the potential degradation products from the predicted degradation pathways of the Substance, using EAWAG – Biocatalysis / Biodegradation Database Pathway Prediction System (EAWAG-BBD Pathway Prediction System).

85 Furthermore, you have screened the PBT/vPvB properties of the potential degradation products that were predicted by the EAWAG-BBD Pathway Prediction System. For this screening, you have used EPI Suite.

86 Predictions generated with EAWAG-BBD Pathway Prediction System are identifying potential degradation products on the basis of a library of plausible microbial degradation reactions. As this library collates known biodegradation pathways that have been published in the open literature and were observed under a range of different experimental conditions (including tests using pure cultures of microorganisms, tests using pre-adapted inocula, etc.), it cannot be excluded that the system identifies a different (e.g., more diverse) set of degradation products compared to the set of degradation products that can, in practice, be experimentally identified under the defined test conditions of simulation tests.

87 Because of this, information on the identity of the potential degradation products, generated with EAWAG-BBD Pathway Prediction System / OASIS Catalogic normally represents an overly conservative prediction result. In the absence of further justification or other type of available data, you have not demonstrated that the set of potential degradation products predicted by EAWAG-BBD Pathway Prediction System represents a prediction result that is potentially obtained from the simulation test (e.g. not overly conservative) for the hazard, persistence, and risk assessments as the only piece of the information available. On this basis, in itself, your prediction is not sufficiently adequate, for the purposes of classification and labelling and/or risk assessment, or for the purposes of further regulatory risk management (e.g. SVHC identification in cases where PBT/vPvB and/or PMT/vPvM degradation products are identified).

88 Further, the data generated with EPI Suite models is not adequate, because you used the set of potential degradation products predicted by the EAWAG-BBD Pathway Prediction System, which have the potential deficiency explained above, as an input.

89 Therefore, the information requirement is not fulfilled, and an identification of degradation products is needed.

5.3. Test selection and study specifications

90 To determine the degradation rate of the Substance, the requested studies according to OECD TG 308 and 307 (requests 3 and 4) must be conducted at 12°C and at test material application rates 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).

91 With regard to the screening information you provided on the PBT/vPvB properties of the potential degradation products of the Substance, ECHA notes the following. The predicted degradation products of the constituents of the Substance should be screened for P/vP, B/vB, and M/vM properties, on the basis of available relevant experimental data (if any), and predictions for ready biodegradability, log Kow, and log Koc values. In case the screening results for some of the predicted degradation products of specific constituents are indicating a potential PBT/vPvB and/or PMT/vPvM hazard, this should be considered when selecting a test material for the study.

5.4. Outcome

92 Under Article 40(3)(c) of REACH, ECHA may require a registrant to carry out one or more additional tests in case of non-compliance of the testing proposal with Annexes IX, X or XI of the REACH Regulation. The information requirement on Degradation (Section 9.2.) at Annex IX covers Biotic degradation (Section 9.2.1.) and Identification of degradation products (Section 9.2.3.) for the Substance. However, you have submitted testing proposals for soil and sediment simulation testing only. As explained above, the information requirement for Identification of degradation products is not fulfilled. Therefore, under Article 40(3)(c), you are requested to conduct the additional test, as specified above.

References

The following documents may have been cited in the decision.

Guidance on information requirements and chemical safety assessment (Guidance on IRs & CSA)

Chapter R.4 Evaluation of available information; ECHA (2011).
Chapter R.6 QSARs, read-across and grouping; ECHA (2008).
Appendix to Chapter R.6 for nanoforms; ECHA (2019).
Chapter R.7a Endpoint specific guidance, Sections R.7.1 – R.7.7; ECHA (2017).
Appendix to Chapter R.7a for nanomaterials; ECHA (2017).
Chapter R.7b Endpoint specific guidance, Sections R.7.8 – R.7.9; ECHA (2017).
Appendix to Chapter R.7b for nanomaterials; ECHA (2017).
Chapter R.7c Endpoint specific guidance, Sections R.7.10 – R.7.13; ECHA (2017).
Appendix to Chapter R.7a for nanomaterials; ECHA (2017).
Appendix R.7.13-2 Environmental risk assessment for metals and metal compounds; ECHA (2008).
Chapter R.11 PBT/vPvB assessment; ECHA (2017).
Chapter R.16 Environmental exposure assessment; ECHA (2016).

Guidance on data-sharing; ECHA (2017).
Guidance for monomers and polymers; ECHA (2012).
Guidance on intermediates; ECHA (2010).

All guidance documents are available online: https://echa.europa.eu/guidance-documents/guidance-on-reach

Read-across assessment framework (RAAF)

RAAF, 2017 Read-across assessment framework (RAAF); ECHA (2017)
RAAF UVCB, 2017 Read-across assessment framework (RAAF) – considerations on multi- constituent substances and UVCBs); ECHA (2017).

The RAAF and related documents are available online:
https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across

***OECD Guidance documents* (OECD GDs)**

OECD GD 23 Guidance document on aquatic toxicity testing of difficult substances and mixtures; No. 23 in the OECD series on testing and assessment, OECD (2019).
OECD GD 29 Guidance document on transformation/dissolution of metals and metal compounds in aqueous media; No. 29 in the OECD series on testing and assessment, OECD (2002).
OECD GD 150 Revised guidance document 150 on standardised test guidelines for evaluating chemicals for endocrine disruption; No. 150 in the OECD series on testing and assessment, OECD (2018).
OECD GD 151 Guidance document supporting OECD test guideline 443 on the extended one-generation reproductive toxicity test; No. 151 in the OECD series on testing and assessment, OECD (2013).

Appendix 2: Procedure

ECHA started the testing proposal evaluation in accordance with Article 40(1) on 20 April 2022.

ECHA held a third-party consultation for the testing proposal(s) from 16 June 2022 until 1 August 2022. ECHA did not receive information from third parties.

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

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.

The deadline of the decision is set based on standard practice for carrying out OECD TG tests. It has been exceptionally extended by 12 months from the standard deadline granted by ECHA to take into account currently longer lead times in contract research organisations.

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 3: Addressee(s) of this decision and their corresponding information requirements

In accordance with Articles 10(a) and 12(1) of REACH, the information requirements for individual registrations are defined as follows:

- the information specified in Annexes VII and VIII to REACH, for registration at 10-100 tpa;
- the information specified in Annexes VII to X to REACH, for registration at more than 1000 tpa.

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

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.

Appendix 4: Conducting and reporting new tests for REACH purposes

1. Requirements when conducting and reporting new tests for REACH purposes

1.1. 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].

(4) Under the introductory part of Annexes VII/VIII/IX/X to REACH, where a test method offers flexibility in the study design, for example in relation to the choice of dose levels or concentrations, the chosen study design must ensure that the data generated are adequate for hazard identification and risk assessment.

1.2. 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 the careful identification and description of the characteristics of the Tests Materials in accordance with OECD GLP

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

(ENV/MC/CHEM(98)16) and EU Test Methods Regulation (EU) 440/2008 (Note, Annex), namely all the constituents must be identified as far as possible as well as their concentration. Also any constituents that have harmonised classification and labelling according to the CLP Regulation must be identified and quantified using the appropriate analytical methods,

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

Technical instructions on how to report the above is available in the manual on How to prepare registration and PPORD dossiers (https://echa.europa.eu/manuals).

2. General recommendations for conducting and reporting new tests

2.1. 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 Guidance on IRs & CSA, Sections R.7.9, 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.

2.2. Environmental testing for substances containing multiple constituents

Your Substance contains multiple constituents and, as indicated in Guidance on IRs & CSA, Section R.11.4.2.2, you are advised to consider the following approaches for persistency, bioaccumulation and aquatic toxicity testing:

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

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

References to Guidance on REACH and other supporting documents can be found in Appendix 1.