~~Confidential~~

Helsinki, 27 June 2022

Addressees
Registrant(s) of JS_801-941-7 as listed in Appendix 3 of this decision

Date of submission of the dossier subject to this decision
20/10/2017

Registered substance subject to this decision ("the Substance")
Substance name: Benzene, 1-(decyloxy)-2-(1-methylpropyl)-4-(triphenylmethyl)-
EC number: 801-941-7

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 ***2 July 2025***.

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

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)
2. Long-term toxicity testing on aquatic invertebrates (triggered by Annex VII, Section 9.1.1., column 2; test method: EU C.20./OECD TG 211)

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

3. Long-term toxicity testing on fish (triggered by Annex VIII, Section 9.1.3., column 2; test method: EU C.47./OECD TG 210)
4. Sediment simulation testing (triggered by Annex VIII, Section 9.2.; 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. Soil simulation testing (triggered by Annex VIII, Section 9.2.; 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.
6. Identification of degradation products (triggered by Annex VIII, Section 9.2; test method: using an appropriate test method or test method: EU C.24./OECD TG 308 or EU C.23./OECD TG 307)
7. Bioaccumulation in aquatic species (triggered by Annex I, sections 0.6.1. and 4.; Annex XIII, Section 2.1.; test method: EU C.13./OECD TG 305, aqueous exposure/dietary exposure)

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 addressees of the decision and their corresponding information requirements based on registered tonnage band are listed in Appendix 3.

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

0. Reasons common to several requests

0.1. Triggering of long-term toxicity testing on aquatic invertebrates and fish

1 This section concerns the assessment of information provided for long-term aquatic toxicity at Annexes VII and VIII.

2 Long-term toxicity testing on aquatic invertebrates and fish must be considered (Annex VII, Section 9.1.1., Column 2, and Annex VIII, Section 9.1.3., Column 2) if the substance is poorly water soluble.

3 Poorly water soluble substances require longer time frames to reach steady-state conditions. As a result, short-term tests do not give a true measure of toxicity for these type of substances and the long-term tests are required. A substance is regarded as poorly water soluble if, for instance, it has a water solubility below 1 mg/L or below the detection limit of the analytical method of the test material (Guidance on IRs and CSA, Section R.7.8.5).

4 In the provided OECD TG 105 (2013), the saturation concentration of the Substance in water was determined to be <=0.0087 mg/L.

5 Therefore, the Substance is poorly water soluble and information on long-term toxicity on aquatic invertebrates and fish must be provided at Annexes VII and VIII.

0.2. Rejection of adaptation according to Column 2 for algal toxicity

6 This section concerns the assessment of information provided for algal toxicity for which you have provided a Column 2 adaptation.

7 Under Annex VII section 9.1.2, Column 2, first indents, to REACH, the study may be omitted if aquatic toxicity is unlikely, for instance if the Substance is highly insoluble in water or the substance is unlikely to cross biological membranes. Guidance on IRs and CSA, Section R.7.8.5 explains that there is no scientific basis to define a cut off limit for solubility below which toxicity is unlikely. Therefore, the justification must demonstrate very low water solubility and low likelihood to cross biological membranes. For the latter, the same Guidance 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 (Guidance on IRs and CSA, 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).

8 Unless it can reliably be demonstrated that aquatic toxicity is unlikely to occur, the Substance must be considered as poorly water soluble.

9 Your registration dossier provides:

- information on the solubility of the Substance in water <=0.0087 mg/L based on OECD TG 105;

- a conclusion of low likelihood to cross biological membranes based on hindered uptake of the Substance substantiated with the following physico-chemical indicators: water solubility <=0.0087 mg/L, molecular weight 532.8, large molecular size (unspecified by you). Furthermore, a log Kow of >6.5 (OECD TG 117) provided by you;
- no experimental chronic toxicity studies in mammals or birds or experimental chronic ecotoxicity studies and no experimental mammalian toxicokinetic studies.

10 Even though the water solubility of the Substance is low, the following does not support your justification:

- molecular weight is <1100 and the information cannot exclude that the log Kow is above 10 or molecular size is above specific thresholds listed in ECHA Guidance; and
- there is no supporting experimental evidence of hindered uptake.

11 Therefore, you have not demonstrated that toxicity is unlikely to occur and your adaptation is rejected and the Substance must be considered as poorly water soluble. Hence, your adaptation is rejected.

0.3. Rejection of adaptation according to Annex XI, Section 2

12 This section concerns assessment of information provided for long-term aquatix toxicity and algal toxicity for which you have provided an adaptation under Annex XI, Section 2.

13 According to Annex XI section 2, 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. 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. OECD TG 210 and OECD TG 211 specify that, for difficult to test substances (including for substances poorly soluble in water), you must consider the approaches described in OECD GD 23 or other approaches, if more appropriate for your substance.

14 In all circumstances where proposals for adaptation of the standard testing regime are based on such grounds, a detailed justification must be provided in writing (ECHA Guidance on IR & CSA, Chapter R.5., section R.5.2.2).

15 The Substance is poorly water soluble (<=0.0087 mg/L) and thus difficult to test.

16 You have not provided a detailed justification explaining what methods and approaches have been considered and applied by you for aquatic toxicity testing of the Substance and why those were technically not possible.

17 Therefore, you have not demonstrated that aquatic toxicity testing is technically not possible and your adaptation is rejected.

0.4. Rejection of adaptation according to Annex XI, Section 3

18 This section concerns assessment of information provided for long-term aquatix toxicity and algal toxicity for which you have provided an adaptation under Annex XI, Section 3.

0.4.1. Assessment of adaptation for the algal toxicity

19 Under Annex XI Section 3.1, only the information required in Sections 8.6 and 8.7 of Annex VIII and in accordance with Annex IX and Annex X may be omitted based on the exposure scenario(s) developed in the Chemical Safety Report. Growth inhibition study on aquatic plants is an information requirement under Annex VII to REACH (Section 9.1.2.).

20 Thus, Annex XI, Section 3 is not applicable to the information requirement under Annex VII, Sections 9.1.2. and your adaptation is therefore rejected.

0.4.2. Assessment of adaptation for the long-term aquatic toxicity

21 Long-term toxicity testing on aquatic invertebrates and fish must be considered (Sections 9.1.1 and 9.1.3, Column 2 of Annexes VII and VIII respectively) if the substance is poorly water soluble.

22 Under Annex XI, Section 3, 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 any one of the following criteria:

(a) It can be demonstrated that all the following conditions are met:
   i. the absence or no significant exposure in all scenarios of the manufacture and all identified uses referred to in Annex VI, Section 3.5., and
   ii. a PNEC can be derived from available data, which:
      - must be relevant and appropriate both to the information requirement to be omitted and for risk assessment purposes and therefore must be based on reliable information on the hazardous properties of the substance on at least three trophic levels;
      - must take into account the increased uncertainty resulting from the omission of the information requirement, in this case by selecting an appropriate assessment factor (AF) as described in Guidance on IRs and CSA, Section R.10.3.
      - the ratio between the results of the exposure assessment (PECs) and the PNEC are always well below 1.

(b) 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;

(c) For substances incorporated in articles with no intended releases, the following conditions are met:
   i. the substance is not released during its life cycle and,
   ii. the likelihood that workers and the general public are exposed to the substance under normal or reasonable foreseeable conditions is negligible, and,
   iii. the substance is handled according to the conditions as set out in Article 18(4)(a) to (f) during all manufacturing and production stages including the waste management of the substance during these stages.

0.4.2.1. Assessment against conditions of Annex XI, Sections 3.2(b-c)

23 As explained in the section 5.2 below, conditions described in Annex XI, section 3.2 (c) are not relevant for the uses of the Substance and conditions of section 3.2 (b) are not justified by you.

0.4.2.2. Assessment against conditions of Annex XI, Sections 3.2(a)

24 Reliable PNECs are to be derived under Annex XI section 3.2(a)(ii).

25 For the reasons explained under requests No 1, 2 and 3, your dossier does not include reliable information on the hazardous properties of the substance on at least three trophic levels of aquatic organisms. Therefore, you have not demonstrated that an appropriate PNEC can be derived and the condition of Annex XI, Section 3.2(a)(ii) is not met.

26 Moreover, for substances satisfying the PBT and vPvB criteria of Annex XIII long-term effects and the estimation of the long-term exposure cannot be carried out with sufficient reliability (Annex I, Section 4.0.1). As a result, for such substances, PNECs and PECs cannot be derived with sufficient reliability to demonstrate that the ratio between PECs and the PNEC are always well below 1. As explained in section 4 below, the information from your dossier currently does not allow excluding that the Substance may be PBT/vPvB. Therefore, the conditions set out under Annex XI, Section 3.2(a) are not met.

27 Therefore, your adaptation is rejected.

Reasons related to the information under Annex VII of REACH

1. Growth inhibition study aquatic plants

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

1.1. Information provided

29 You have provided adaptation which ECHA understands refers to Annex VII, Section 9.1.2., Column 2 as well as to Annex XI, section 3 of REACH:

30 "In accordance with column 2 of REACH annex VII, the study does not need to be conducted if there are mitigating factors indicating that aquatic toxicity is unlikely to occur, for instance, if the substance is highly insoluble in water or the substance is unlikely to cross biological membranes. As the substance is both highly insoluble in water (WS <8 ug/l) and has a high molecular weight and size making availability very unlikely, aquatic toxicity is unlikely and this endpoint is waived. Additionally, as the use is in fuels, resulting in combustion, no relevant exposure of the aquatic compartment is expected."

1.2. Assessment of the information provided

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

32 As explained under section 0.2. above your adaptations are rejected.

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

1.3. Study design and test specifications

34 The Substance is difficult to test due to the low water solubility (<=0.0087 mg/L, OECD TG 105) and adsorptive properties (log Kow >6.5, OECD TG 117). 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.

2. Long-term toxicity testing on aquatic invertebrates

35 Short-term toxicity testing on aquatic invertebrates is an information requirement under Column 1 of Annex VII to REACH (Section 9.1.1.). However, long-term toxicity testing on aquatic invertebrates must be considered (Section 9.1.1., Column 2) if the substance is poorly water soluble.

36 As explained under section 0.1 above, the Substance is poorly water soluble and information on long-term toxicity on aquatic invertebrates must be provided.

2.1. Information provided

37 In respect of short-term toxicity testing on aquatic organisms you have provided an adaptation which ECHA understands refers to Annex VII, Section 9.1.1., Column 2 as well as to Annex XI, section 3 of REACH. Furthermore, in respect of long-term toxicity on aquatic invertebrates you have provided an adaptation which ECHA understands refers to to Annex XI, sections 2 and 3 of REACH:

38 "*Benzene,1-(decyloxy)-2-(1-methylpropyl)-4-(triphenylmethyl)- is highly insoluble in water (WS <8 ug/l) and has a high molecular weight and size making availability to aquatic organisms very unlikely. Thus, aquatic toxicity is unlikely and the conduct of the study is also not technically feasible. Additionally, as this substance is used is in fuels, resulting in combustion, no relevant exposure of the aquatic compartment is expected.*"

2.2. Assessment of the information provided

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

40 As explained under section 0.2. above your adaptations for the long-term toxicity on aquatic invertebrates are rejected.

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

2.3. Study design and test specifications

42 OECD TG 211 specifies that, for difficult to test substances, OECD GD 23 must be followed. As already explained above, the Substance is difficult to test. Therefore, you must fulfil the requirements described in 'Study design' under the section 1.3 above.

Reasons related to the information under Annex VIII of REACH

3. Long-term toxicity testing on fish

43 Short-term toxicity testing on fish is an information requirement under Column 1 of Annex VIII to REACH (Section 9.1.3.). However, long-term toxicity testing on fish must be considered (Section 9.1.3., Column 2) if the substance is poorly water soluble. As explained under section 0.1 above, the Substance is poorly water soluble and information on long-term toxicity on fish must be provided.

3.1. Information provided

44 In respect of short-term toxicity testing on fish you have provided an adaptation which ECHA understands refers to Annex VIII, Section 9.1.3., Column 2 as well as to Annex XI, section 3 of REACH. Furthermore, in respect of long-term toxicity on fish you have provided an adaptation which ECHA understands refers to Annex XI, sections 2 and 3 of REACH:

45 "Benzene,1-(decyloxy)-2-(1-methylpropyl)-4-(triphenylmethyl)- is highly insoluble in water (WS <8 ug/l) and has a high molecular weight and size making availability to aquatic organisms very unlikely. Thus, aquatic toxicity is unlikely and the conduct of the study is also not technically feasible. Additionally, as this substance is used is in fuels, resulting in combustion, no relevant exposure of the aquatic compartment is expected."

3.2. Assessment of the information provided

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

47 As explained under section 0 above your adaptations for the long-term toxicity on fish are rejected.

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

3.3. Study design and test specifications

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

50 OECD TG 210 specifies that, for difficult to test substances, OECD GD 23 must be followed. As already explained above, the Substance is difficult to test. Therefore, you must fulfil the requirements described in 'Study design' under the section 1.3 above.

4. Sediment simulation testing

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

4.1. Trigger

52 This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (Guidance on IRs and CSA, Section R.11.4.). This is the case if the Substance itself or any of its constituent

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

- it is potentially persistent or very persistent (P/vP) as:
  - it is not readily biodegradable (*i.e.* <60/70% degradation in an OECD 301F)
- it is potentially bioaccumulative or very bioaccumulative (B/vB) as:
  - it has a high potential to partition to lipid storage (*e.g.* log K_{ow} > 4.5);

53 Your registration dossier provides the following:

- The Substance is not readily biodegradable less than 0% degradation after 28 days in OECD TG 301F
- The Substance has a high potential to partition to lipid storage (Log K_{ow} of > 6.5 based on OECD TG 117)

54 Furthermore, the information in your dossier is currently incompliant and therefore:

- it is not possible to conclude on the bioaccumulation potential of the Substance (see section 4.2.1 below of this decision), and
- it is not possible to conclude on the toxicity of the Substance (see Requests for long-term fish, invertebrate, and algal data of this decision).

55 Under section 2.3 of your IUCLID dossier and section 8 of your CSR ('PBT assessment'), you conclude that the Substance is not B/vB. In support of your conclusion you provide the following additional information: "Due to a very high predicted log Kow value (EPISUITE log Kow estimate = 13.48), Benzene, 1-(decyloxy)-2-(1-methylpropyl)-4-(triphenylmethyl)- is not expected to be bioavailable. The bioaccumulation potential of Benzene, 1-(decyloxy)-2-(1-methylpropyl)-4-(triphenylmethyl)-was assessed via an EPISUITE QSAR, and the predicted log BCF and (BCFBAF V3.01 in EPISUITE) for the substance is 0.946 L/kg wet weight. This indicates a low probability to bioconcentrate. The predicted EPI Suite QSAR predictions of BCF for several of the impurities present in Benzene, 1-(decyloxy)-2-(1-methylpropyl)-4-(triphenylmethyl)- indicate that both the test substance and associated impurities are not expected to be bioaccumulative (B)". The similar justification in respect of bioaccumulation potential is provided in the section 5.3.1 of the registration dossier.

56 Furthermore, in respect of sediment simulation testing you provide following information in the section 5.2.2 of the registration dossier: "the study does not need to be conducted because the substance is highly insoluble in water".

4.1.1. Assessment of supporting information provided on bioaccumulation

4.1.1.1. Rejection of information based on low bioavailability

57 Under section 0.2 above it is explained what indicators used for low likelihood of a high bioaccumulation potential (Guidance on IRs and CSA, Figure R.11-4) must be considered.

58 Furthermore, under the same section above it is explained that neither physico-chemical indicators nor lack of supporting experimental evidence allow to demonstrate low potential to cross biological membranes, i.e. low potential of bioaccumulation. Thus, you have not demonstrated that the Substance has low bioaccumulation due to the low bioavailability.

4.1.1.2. Rejection of QSAR predictions

59 Under Appendix C of the OECD Guidance document on the validation of (Q)SAR models (ENV/JM/MONO(2007)2) and ECHA Guidance R.6.1.6.3., adequate and reliable documentation must include a (Q)SAR Model Reporting Format document (QMRF) and a (Q)SAR Prediction Reporting Format document (QPRF).

60 You have not provided information about the model or the prediction.

61 In absence of such information, ECHA cannot establish that the model can be used to predict the endpoint/property and the prediction is reliable.

62 Therefore, the additional information on bioaccumulation is not adequate to conclude that the Substance is not a potential B/vB substance.

63 Based on the above, the available information on the Substance indicates that it is a potential PBT/vPvB substance. Further, the additional information from your PBT assessment is not adequate to conclude on the PBT/vPvB properties of the Substance.

4.1.2. Assessment of information provided on sediment simulation testing

64 You stated that "the study does not need to be conducted because the substance is highly insoluble in water".

65 However, this does not mean that the Substance is not P/vP and this claim, in any case, is unsubstantiated as discussed below.

66 Therefore, you have not demonstrated that sediment simulation testing is technically not possible.

67 Furthermore, the Substance has low water solubility (< 0.0087 mg/L), a high partition coefficient (log Kow > 6.5) and high adsorption coefficient (log $K_{oc,soil}$ of > 5.63, OECD TG 121), indicating high potential to adsorb to sediment.

68 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation. Based on the adsorptive properties of the Substance, sediment represents a relevant environmental compartment.

4.2. Information provided

69 ECHA understands that you provided an adaptation that the testing is not technically feasible under Annex XI, Section 2 : "the study does not need to be conducted because the substance is highly insoluble in water".

4.3. Assessment of the information provided

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

71 Under section 0.3 above it is explained that a detailed justification as to why testing is not technically possible should be provided.

72 You have not provided a detailed justification explaining what methods and approaches have been considered and applied by you for the sediment simulation testing of the Substance and why those were technically not possible.

73 Therefore, you have not demonstrated that sediment simulation testing is technically not possible and your adaptation is rejected.

4.4. Study design and test specifications

74 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.

75 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.

76 The required test temperature is 12°C, which corresponds to the average environmental temperature for the EU (Guidance on IRs and CSA, Table R.16-8) and is in line with the applicable test conditions of the OECD TG 308.

77 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.

78 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.).

5. Soil simulation testing

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

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

81 As already explained in section 4 above, the Substance is a potential PBT/vPvB substance.

82 Further, the Substance has low water solubility (< 0.1 mg/L), high partition coefficient (log Kow > 6.5) and high adsorption coefficient (log $K_{oc,soil}$ of > 5.63, OECD TG 121), indicating high potential to adsorb to soil.

83 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation. Based on the adsorptive properties of the Substance, soil represents a relevant environmental compartment.

5.1. Information provided

84 ECHA understands that you provided an adaptation under Annex XI, Section 3 of REACH, using the following information in the section 5.2.3 of the registration dossier: "low exposure to the terrestrial environment is expected based on the use pattern, which is in fuels that undergo combustion."

5.2. Assessment of the information provided

85 As explained, in the Annex XIII, Section 2.1., where the process and use conditions of the substance meet the conditions as specified only in Section 3.2(b) or (c) of Annex XI the additional information may be omitted, and subsequently the substance is considered as if it is a PBT or vPvB in the registration dossier. Therefore, Section 3.2(a) of Annex XI is not relevant; that Section is indeed not relevant since, in such a case, hazard assessment, including derivation of a reliable PNEC, cannot be assessed with sufficient reliability (Annex I, Section 4.0.1).

86 In the registration dossier you identify that the Substance is formulated and used in fuels at industrial, professional settings and by the consumers. Thus, the Substance is not incorporated in articles and only the conditions described in Annex XI, section 3.2 (b) are relevant and assessed below.

87 In the chemical safety report you provide 4 Exposure Scenarios (ESs) with generic description of uses. For the consumer uses you indicate in the respective ES that "[redacted]"

5.2.1. Assessment of conditions for identified use

88 Articles 18(4) lists following cumulative strictly controlled conditions:

- the substance is rigorously contained by technical means during its whole lifecycle including manufacture, purification, cleaning and maintenance of equipment, sampling, analysis, loading and unloading of equipment or vessels, waste disposal or purification and storage;
- procedural and control technologies shall be used that minimise emission and any resulting exposure;
- only properly trained and authorised personnel handle the substance;
- in the case of cleaning and maintenance works, special procedures such as purging and washing are applied before the system is opened and entered;
- in cases of accident and where waste is generated, procedural and/or control technologies are used to minimise emissions and the resulting exposure during purification or cleaning and maintenance procedures;
- substance-handling procedures are well documented and strictly supervised by the site operator.

89 You have not provided any information to assess these conditions.

90 Thus, without this information you have not demonstrated that strictly controlled conditions as set out in Article 18(4)(a) to (f) apply throughout the life cycle of the Substance, i.e. it is not demonstrated that the Substance is used as if it is PBT or vPvB.

91 Therefore, your adaptation is rejected.

5.3. Study design and test specifications

92 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.

93 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).

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

95 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.

96 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.).

6. Identification of degradation products

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

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

99 As already explained in Request in section 4 above, the Substance is a potential PBT/vPvB substance.

100 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation.

101 You have not provided information on biodegradation products in the registration dossier.

6.1. Study design and test specifications

102 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 studies requested in Requests under sections 4 and 5 above 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.

103 To determine the degradation rate of the Substance, the requested studies according to OECD TG 308/307 (Requests under sections 4 and 5 above) 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).

104 You may also use other appropriate and suitable test method(s) to provide information on the identity of the transformation/degradation products, for example an enhanced screening level degradation test or modelling tools. You will need to provide a scientifically valid justification for the chosen method. The provided information should include, identification, stability, behaviour, molar quantity of transformation/degradation products relative to the parent compound. In addition, degradation half-life, log K_{ow} and potential toxicity of the transformation/degradation may need to be investigated.

7. Bioaccumulation in aquatic species

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

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

107 As already explained in Request in section 4 above, the Substance is a potential PBT/vPvB substance.

108 Therefore, the chemical safety assessment (CSA) indicates the need for further investigation on bioaccumulation in aquatic species.

7.1. Information provided

109 ECHA understands that you applied a QSAR adaptation under Annex XI, Section 1.3, by using the following information in the section 5.3.1 of the registration dossier: "the study does not need to be conducted because the substance has a low potential to cross biological membranes. Quantitative Structure Activity Relationship (QSAR) data show that due to the high Kow of the substance (log Kow = 13.5) and the relatively high molecular weight (i.e. 532.8), this substance is not expected to appreciable bioaccumulate due to low bioavailability (QSAR results = log BCF = 0.946; log BAF = 1.906)."

7.2. Assessment of the information provided

110 Under Annex XI, Section 1.3., the following conditions must be fulfilled whenever a (Q)SAR approach is used:

- the prediction needs to be derived from a scientifically valid model,
- the substance must fall within the applicability domain of the model,
- results need to be adequate for the purpose of risk assessment or classification and labelling, and
- adequate and reliable documentation of the method must be provided.

111 With regard to these conditions, we have identified the following issue(s):

112 For the reasons provided under section 4.2.1 above, your registration dossier does not provide adequate and reliable documentation.

113 Therefore, your adaptation is rejected.

7.3. Study design and test specification

114 Bioaccumulation in fish: aqueous and dietary exposure (Method EU C.13 / OECD TG 305) is the preferred test to investigate bioaccumulation (Guidance on IRs and CSA, Section 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 material 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.

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

116 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).

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.5 Adaptation of information requirements; 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).

All Guidance on REACH is 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

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 8 July 2021.

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

ECHA did not receive any comments within the commenting period.

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: Addressees 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 Annex VII to REACH, for registration at 1-10 tonnes per year (tpa), or as a transported isolated intermediate in quantity above 1000 tpa;
- the information specified in Annexes VII and VIII to REACH, for registration at 10-100 tpa;
- the information specified in Annexes VII, VIII and IX to REACH, for registration at 100-1000 tpa;
- 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]

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].

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 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

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.